IIT Bombay

APT-2026



Advances In Proteomics Technologies (APT) - 2026

International Conference and workshops

June 27-29, 2026

APT-2026

Advances in Proteomics Technologies

International Conference & Workshop

ADVANCING PROTEOMICS, MULTI-OMICS AND PRECISION MEDICINE

PROCEEDINGS

Advancing Proteomics, Multi-Omics and Precision Medicine

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PROCEEDINGS

Foreword

It is an absolute privilege and honour to welcome you to the official proceedings of the Advances in Proteomics Technologies, International Conference and Workshop (APT-2026), held from June 27 to June 29, 2026, at the Indian Institute of Technology Bombay (IIT Bombay), Mumbai, India.

Proteomics has evolved from a foundational tool for protein identification into a dynamic, multi-dimensional pillar of modern medicine and systems biology. Today, the discipline stands at a critical crossroads where technological maturity meets clinical application. As precision healthcare increasingly relies on rapid, high-throughput, and highly reproducible molecular profiling, the need for robust, standardised workflows has never been more urgent. APT-2026 was conceived to address this exact imperative, serving as a premier global forum to bridge the gap between benchtop mass spectrometry innovations and bedside clinical translations.

This compilation of proceedings reflects the incredible depth and multifaceted nature of the three-day scientific program. The peer-reviewed abstracts and technical papers contained within this volume span the entire spectrum of modern omics research. From high-impact plenary insights into clinical and cancer proteomics to technical deep dives into 4-D Omics, data-independent acquisition (DIA-PASEF), and single-cell proteomics, these pages capture the breakthroughs redefining our understanding of complex biological systems.

Beyond the core scientific sessions, a defining feature of APT-2026 is its unique integration of theory, practice, and community mentorship. These proceedings document not only the traditional academic tracks but also the structures of eight intensive, hands-on workshops (W1–W8) that provided practical training in state-of-the-art laboratory sample preparation, live instrument runs, and cloud-based bioinformatics platforms. Furthermore, this volume highlights our commitment to cultivating the future scientific ecosystem through a dedicated School Outreach Program and dynamic panel discussions mapping out the opportunities and challenges facing the next generation of investigators.

The success of a conference of this magnitude is the result of an immense collaborative effort. We extend our deepest gratitude to the members of the Organising Committee, the Scientific Advisory Board, and our international reviewers for their tireless dedication to maintaining the highest standards of academic rigour. We are profoundly grateful to our global speakers, industry partners, and session chairs who brought their visionary expertise to Hall A, the Convocation Hall, and our advanced laboratory wings. Most importantly, we thank the contributing authors and young researchers whose breakthrough insights fill these pages.

We trust that you will find these proceedings to be a valuable, high-impact reference text—one that not only captures the milestones achieved at APT-2026 but also serves as an inspiring catalyst for future discoveries, international collaborations, and the continued advancement of global clinical workflows.

Welcome to the proceedings of APT-2026.

Editorial Board

Advances in Proteomics Technologies (APT-2026)

Proteomics Lab, IIT Bombay, Mumbai, India



MESSAGE FROM CONVENOR

Welcome Message from Convenor



It is a distinct privilege to welcome you to the Advances in Proteomics Technology (APT) 2026 at IIT Bombay, a premier forum designed to bridge the gap between fundamental research and clinical implementation. As biomedical science moves toward a data-driven future, our mission is to provide a strategic ecosystem where academia, clinicians, and industry converge to translate high-dimensional omics discoveries into impactful healthcare solutions. By fostering a progressive vision of proteomics, we aim to lead the transition from reactive treatments toward a new era of predictive, preventive, and personalised medicine.

The central theme of APT 2026 emphasises the critical integration of multi-omics technologies to decode the most direct functional readouts of biological systems. We are witnessing a profound paradigm shift where high-resolution mass spectrometry and advanced analytical workflows are no longer confined to discovery research but are actively informing clinical decision-making and biomarker development. This multidisciplinary synergy allows us to explore the clinical relevance of multi-omics for early diagnosis, patient stratification, and the advancement of targeted therapeutic strategies globally.

To ensure a lasting impact on the next generation of researchers, we have created a comprehensive program featuring a five-day pre-conference internship, a two-day scientific exchange, and a dedicated hands-on workshop. This immersive experience is designed to provide in-depth training in the latest analytical platforms, equipping participants with the insights needed to redefine the future of translational research over the coming decade.

I warmly invite you to join us at IIT Bombay as we collectively harness the power of integrated omics to transform the landscape of modern healthcare.

Professor Sanjeeva Srivastava
Convenor, APT-2026
IIT Bombay



ABOUT THE CONFERENCE

About APT-2026

The Advances in Proteomics Technologies, International Conference and Workshop (APT-2026) is a premier global forum dedicated to showcasing cutting-edge milestones and next-generation breakthroughs in translational proteomics and clinical mass spectrometry. Scheduled for June 27 to June 29, 2026, at the prestigious Indian Institute of Technology Bombay (IIT Bombay) in Mumbai, India, this highly anticipated three-day event brings together world-renowned scientists, clinical researchers, bioinformaticians, and industry leaders to chart the future of multi-omics research.

Conference Vision & Scope

The fundamental objective of APT-2026 is to bridge the gap between benchtop mass spectrometry developments and bedside clinical care. As precision medicine increasingly relies on high-throughput, reproducible data, the conference spotlights key areas of innovation, including:

- **Clinical & Cancer Proteomics:** Unveiling breakthrough protein biomarker panels, targeted discovery strategies, and translational pipelines for complex human diseases.
- **Advanced Mass Spectrometry Workflows:** Exploring high-resolution hardware and method designs such as data-independent acquisition (DIA-PASEF), parallel reaction monitoring (PRM), 4-D Omics, and single-cell proteomics.
- **Bioinformatics & Computational Systems:** Addressing automated data parsing, predictive artificial intelligence, machine learning-based feature identification, and massive multi-group pathway network interpretations.

A Dynamic Three-Day Structure

APT-2026 is uniquely structured to offer a balance of scientific dissemination, interactive lab work, and community engagement:

- **Core Scientific Tracks:** Features comprehensive plenary sessions, expert-led panel discussions touching upon decades of historical progress within the field, and insights regarding opportunities or challenges for young investigators.
- **The Academia-Industry Interface:** Acts as a specialized crossroads where top industrial technology providers directly engage with academic institutions to shape future collaborative omics ecosystems.
- **Hands-On Technical Workshops (W1–W8):** Offers intensive parallel tracks focusing on real-world sample preparation, live instrumentation data acquisition runs, and computational biology platforms (ranging from R-based microarrays to automated cloud software like Galaxy and FragPipe).
- **Inspirational Educational Outreach:** Promotes a dedicated School Outreach Program running concurrently alongside deep-tech sessions, targeted at nurturing and mentoring the next generation of scientific minds in health technology, AI, and big data applications.

By integrating rigorous scientific exchange with concrete, state-of-the-art laboratory training, APT-2026 serves as a key catalyst driving innovation, standardizing global clinical workflows, and empowering the international proteomics community to unlock profound biological insights.



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The Advances in Proteomics Technologies 2026 (APT-2026) conference and workshops are made possible through the generous support of a distinguished group of funding agencies, industry sponsors, technology partners, and scientific collaborators who share a common vision of advancing proteomics, multi-omics, precision medicine, and translational research.

APT-2026 is supported by premier national funding and research organizations, including the Anusandhan National Research Foundation (ANRF), IIT Bombay Institution of Eminence (IoE), SPARC, and the Indian Council of Medical Research (ICMR). Their support underscores the importance of fostering cutting-edge scientific research, capacity building, and international collaboration in the life sciences.

The conference is further strengthened by leading global technology and life science companies, including Bruker, Thermo Fisher Scientific, and Merck, whose innovative platforms continue to drive advances in mass spectrometry, proteomics, metabolomics, and biomedical research. Additional support from organizations such as MMI and DSS reflects the growing interdisciplinary ecosystem that connects research, technology, and healthcare innovation.

APT-2026 also benefits from partnerships with several academic, media, outreach, and technology organizations, including eRentals, Techloris IT Services, NexGen Media, VOH (Voice of Healthcare), Proteomica International Private Limited, Nrityanjali, JS-Radiance AI, and Identica Brains. These partners contribute to conference operations, scientific communication, outreach activities, digital engagement, and technology dissemination.

Together, these sponsors and partners play a pivotal role in creating a vibrant platform for knowledge exchange, innovation, training, and collaboration. Their collective support enables APT-2026 to bring together leading scientists, clinicians, industry experts, educators, and young investigators from around the world to explore emerging frontiers in proteomics and multi-omics research, ultimately advancing precision healthcare and biomedical discovery.

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Bruker is enabling scientists to make breakthrough discoveries and develop new applications that improve the quality of human life. Bruker's high-performance scientific instruments and high-value analytical and diagnostic solutions enable scientists to explore life and materials at molecular, cellular and microscopic levels. In close cooperation with our customers, Bruker is enabling innovation, improved productivity and customer success in life science molecular research, in applied and pharma applications, in microscopy and nanoanalysis, and in industrial applications, as well as in cell biology, preclinical imaging, clinical phenomics and proteomics research and clinical microbiology.

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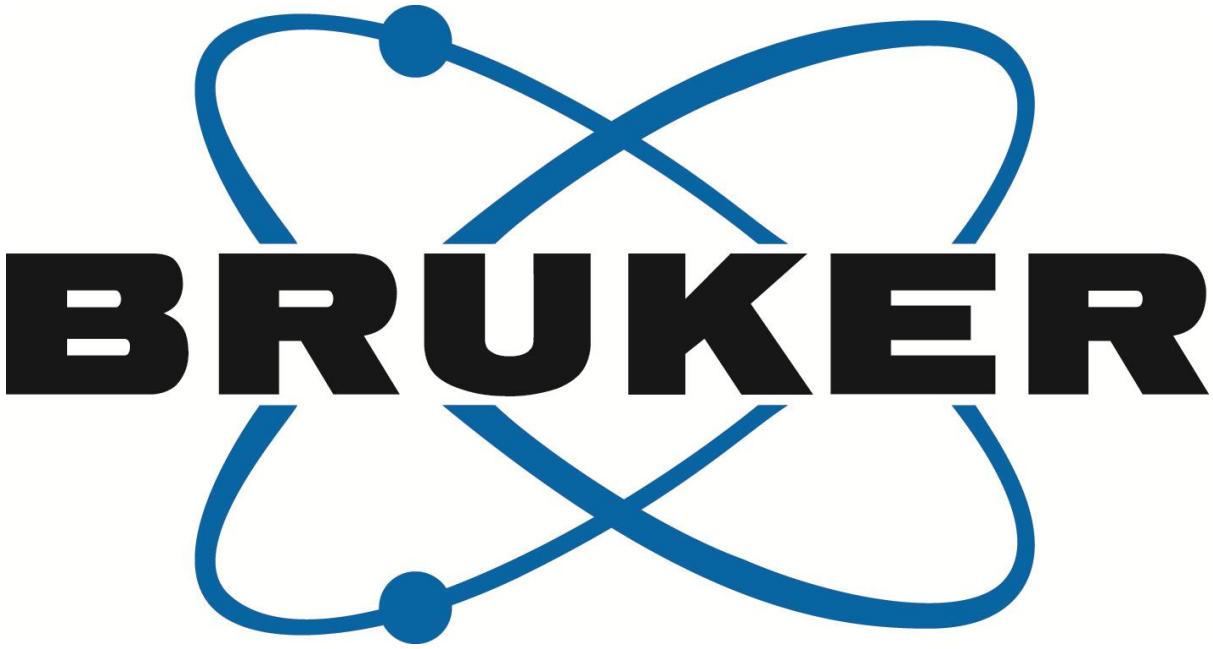
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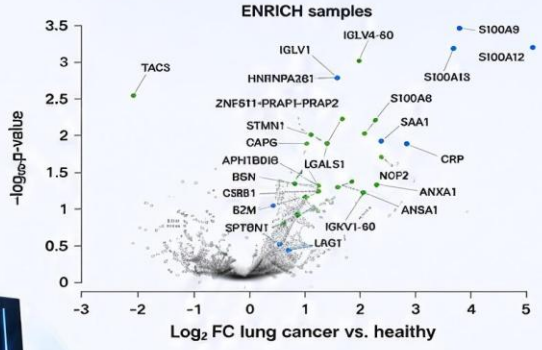
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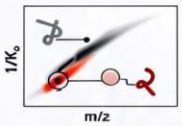


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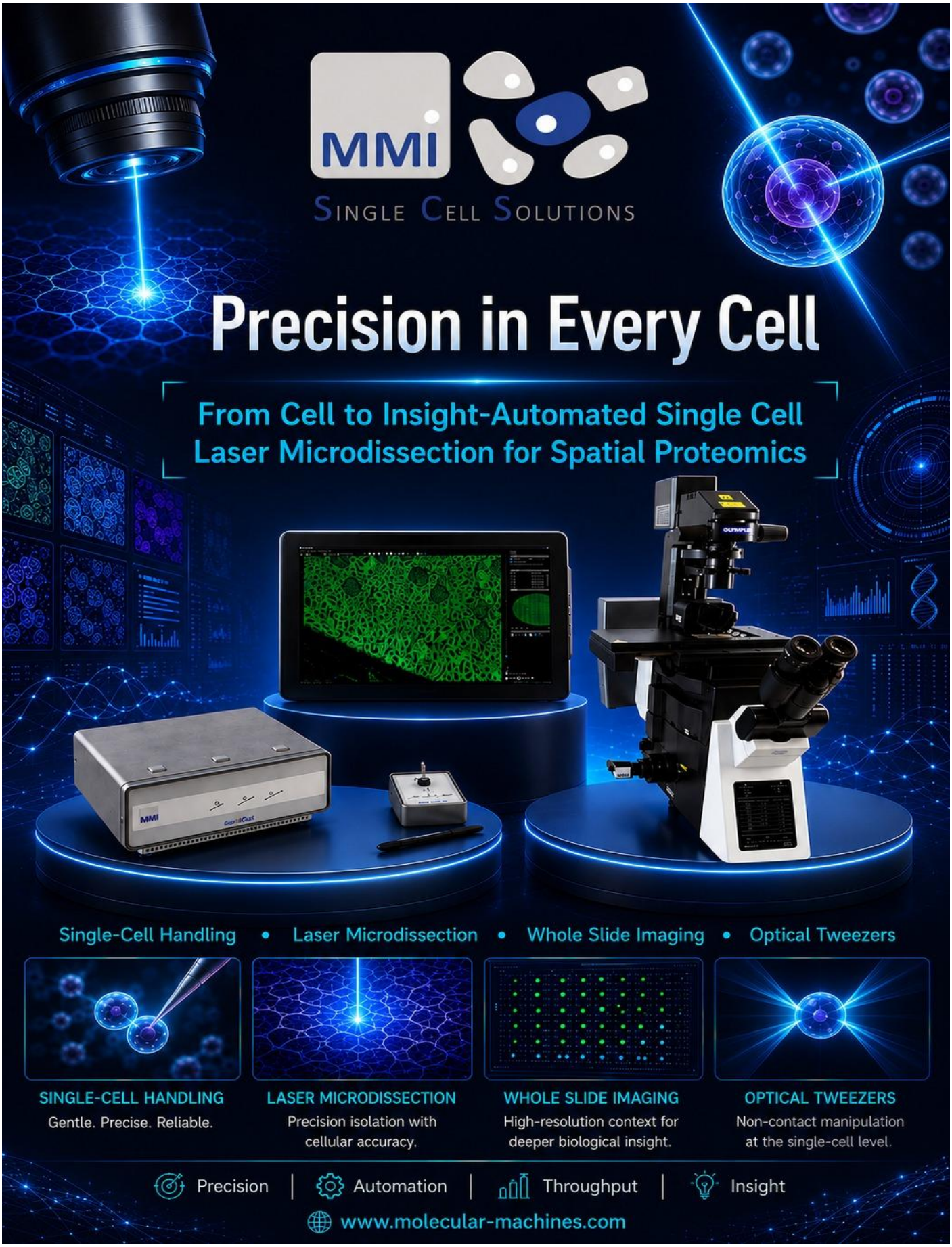
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PRE-CONFERENCE INTERNSHIP PROGRAM SCHEDULE

Day 1: Monday, 22 June

Theme: Fundamentals of Proteomics & Sample Preparation

TIME	SESSION / ACTIVITY
08:30 AM – 09:00 AM	Registration
09:00 AM – 10:00 AM	**Convener's Keynote Address** *Speaker: Dr. Sanjeeva Srivastava (IIT Bombay)*
10:00 AM – 11:00 AM	**Hands-On: Proteomics Sample Preparation** *Syllabus: Brief Overview of Digestion Workflow, Lysate Preparation and Protein Quantification* *Instructors: Avinash Singh, Dr. Shambhu Kumar Prasad, Pratibha Sharma (TAs)*
11:00 AM – 11:30 AM	Tea Break
11:30 AM – 12:00 PM	**Hands-On: Electrophoretic Separations** *Syllabus: Pouring and loading sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) systems.* *Instructors: Avinash Singh, Vaishali Singh (TAs)*
12:00 PM – 01:00 PM	**Hands-On: In-Gel Proteolytic Digestion (Part 1)** *Syllabus: Chemical lysis, disulfide bond reduction, and fast gel staining/destaining techniques.* *Instructors: Dr. Shambhu Kumar Prasad, Vaishali Singh (TAs)*
01:00 PM – 02:15 PM	Lunch Break & Sample Incubation
02:15 PM – 03:00 PM	**Hands-On: In-Gel Proteolytic Digestion (Part 2)** *Syllabus: Free thiol alkylation, trypsin addition, and setting up overnight digestion profiles.* *Instructors: Avinash Singh, Dr. Shambhu Kumar Prasad (TAs)*
03:00 PM – 03:30 PM	**Clinical Sample Types & Digestion Challenges** *Syllabus: Methodological hurdles, recovery issues, and handling strategies for biofluids, biopsies, and challenging sample matrices.* *Instructors: TAs*
03:30 PM – 04:00 PM	**Application Talk / Case Study** *Speaker: Avinash Singh (Research Scholar)*
04:00 PM – 04:30 PM	Tea Break
04:30 PM – 05:00 PM	**Application Talk / Case Study** *Speaker: Dr. Shambhu Kumar Prasad (Postdoc)*
05:00 PM – 05:30 PM	**Discussion** *Moderator: Vaishali Singh (TA)*

Day 2: Tuesday, 23 June

Theme: Sample Processing & Mass Spectrometry Workflows

TIME	SESSION / ACTIVITY
09:00 AM – 09:45 AM	**Hands-On: Peptide Clean-Up Operations** *Syllabus: Proteolysis quenching techniques and sample concentration using centrifugal vacuum concentrators (SpeedVac).* *Instructors: Dr. Vishal Vikram Singh, Vaishali Singh (TAs)*
09:45 AM – 11:00 AM	**Hands-On: Solid-Phase Extraction Desalting** *Syllabus: Reversed-phase stage-tip desalting, column conditioning, sample loading, peptide reconstitution, and micro-volume spectroscopic quantification.* *Instructors: Dr. Vishal Vikram Singh, Vaishali Singh (TAs)*
11:00 AM – 11:30 AM	Tea Break
11:30 AM – 12:00 PM	**Hands-On: High-Performance LC-MS/MS System Setups** *Syllabus: Autosampler alignment, nano-LC fluidics configuration, and parameter assembly for DDA, DIA, and PRM acquisition modes.* *Instructors: Avinash Singh, Vaishali Singh (TAs)*
12:00 PM – 01:00 PM	**Instrument Calibration & Quality Control and Data Acquisition** *Syllabus: Mass spectrometer calibration sequences, multi-system suitability testing (SST), and initiating the automated sample queue run.* *Instructors: TAs*
01:00 PM – 02:15 PM	Lunch Break
02:15 PM – 02:45 PM	**Hands-On: Proteomics Primary Analysis** *Syllabus: High-throughput database searching, spectrum annotation, and spectral library generation using FragPipe and DIA-NN platforms.* *Instructors: Amit Karmakar, Zeenat (TAs)*
02:45 PM – 03:45 PM	**Hands-On: Secondary Analysis** *Syllabus: Data filtering, missing value imputation, normalization, and expression profiling using Perseus and MetaboAnalyst tools.* *Instructors: Amit Karmakar, Zeenat (TAs)*
03:45 PM – 04:15 PM	**Hands-On: Pathway Analysis and Interpretation** *Speaker: Dr. Vishal Vikram Singh (Postdoc)*
04:15 PM – 04:30 PM	Tea Break
04:30 PM – 05:00 PM	Project Allocation & Dataset Briefing
05:00 PM – 05:30 PM	**Discussion** *Moderator: Zeenat (TA)*

Day 3: Wednesday, 24 June

Theme: Data Analysis & Systems Biology Interpretation

TIME	SESSION / ACTIVITY
09:00 AM – 10:00 AM	**Hands-On: Metabolomics Sample Preparation** *Instructors: Vaishali Singh (Research Scholar)*
10:00 AM – 11:00 AM	**Hands-On: Metabolomics Sample Reconstitution, MS Data Acquisition** *Instructors: Amit Karmakar (Research Scholar)*
11:00 AM – 11:30 AM	Tea Break

11:30 AM – 12:00 PM	**Statistical Methods in Omics Data Analysis and Visualization** *Syllabus: Executing principal component analysis (PCA), hierarchical cluster mapping (heatmaps), and differential expression tracking (volcano plots).* *Instructors: TAs*
12:00 PM – 01:00 PM	**Lab Visit: Proteomica** *Instructors: TAs*
01:00 PM – 02:00 PM	Lunch Break
02:15 PM – 03:00 PM	**Hands-On: Targeted Proteomics and Metabolomics** *Syllabus: Skyline Hands-On Demo and Acquisition* *Instructors: TAs*
03:00 PM – 03:30 PM	**Hands-On: Skyline Result Refinement** *Instructors: TAs*
03:30 PM – 04:00 PM	**Application Talk / Case Study** *Speaker: Zeenat (Research Scholar)*
04:00 PM – 04:30 PM	Tea Break
04:30 PM – 05:00 PM	**Application Talk / Case Study** *Speaker: Vaishali Singh (Research Scholar)*
05:00 PM – 05:30 PM	**Discussion** *Moderator: Amit Karmakar (TA)*

Day 4: Thursday, 25 June

Theme: Targeted Assays & Supervised Machine Learning

TIME	SESSION / ACTIVITY
09:00 AM – 10:00 AM	**Hands-On: Metabolomics Data Processing & Annotation, and Analysis** *Syllabus: Feature extraction, deconvolution, compound annotation, and spectral alignment of small molecule datasets.* *Instructors: TAs*
10:00 AM – 11:00 AM	**Hands-On: Skyline-based Targeted Proteomics/Metabolomics** *Instructors: TAs*
11:00 AM – 11:30 AM	Tea Break
11:30 AM – 12:00 PM	**Machine Learning-based Biomarker Identification** *Syllabus: Application of machine learning algorithms (Random Forest, SVM, logistic regression) for clinical marker optimization.* *Instructors: TAs*
12:00 PM – 01:00 PM	**Lab Visit: Proteomics Lab** *Instructors: TAs*
01:00 PM – 02:00 PM	Lunch Break
02:15 PM – 03:00 PM	**Post Translation Modification Session: Basic and Applications** *Instructor: Dr. Rohit Budhraja*
03:00 PM – 03:30 PM	**PTM Hands-On: Sample Preparation for Phospho Enrichment** *Instructor: Dr. Rohit Budhraja*
03:30 PM – 04:00 PM	**PTM Hands-On: MS Analysis and Data Acquisition** *Instructor: Dr. Rohit Budhraja*
04:00 PM – 04:30 PM	Tea Break

04:30 PM – 05:00 PM	**Guided Project Analysis (Mentored Session)** *Instructors: TAs*
05:00 PM – 05:30 PM	**Discussion** *Instructors: Pratibha Sharma, Esha Ghosh (TAs)*

Day 5: Friday, 26 June

Theme: Internship Project Evaluations & Special Topics

TIME	SESSION / ACTIVITY
09:00 AM – 10:00 AM	**Internship Presentation Panel: Session A** *Evaluation of student group project data processing, outcome modeling, and conclusions.* *Reviewers: TAs Panel*
10:00 AM – 11:00 AM	**Internship Presentation Panel: Session B** *Evaluation of student group project data processing, outcome modeling, and conclusions.* *Reviewers: TAs Panel*
11:00 AM – 11:30 AM	Tea Break
11:30 AM – 12:30 PM	**PTM Hands-On Session: PTM Analysis for Phosphorylation and Glycosylation** *Instructor: Dr. Rohit Budhraja*
12:30 PM – 01:00 PM	**Application Talk / Case Study** *Speaker: Dr. Bipin Nair*
01:00 PM – 02:00 PM	Lunch Break
02:15 PM – 03:00 PM	**MMI: Deep Visual Proteomics Workflow** *Syllabus: Demonstration of precision cellular and spatial sample processing layouts using Molecular Machines & Industries (MMI) workflows.* *Instructors: MMI*
03:00 PM – 03:30 PM	**MMI: Deep Visual Proteomics Workflow – Hands-On Demo** *Instructors: MMI*
03:30 PM – 04:00 PM	**Application Talk / Case Study** *Speaker: Dr. Deepa Bisht*
04:00 PM – 04:30 PM	Tea Break
04:30 PM – 05:00 PM	**Application Talk / Case Study** *Speaker: TBA*
05:00 PM – 05:30 PM	**Final Comprehensive Assessment & Program Wrap-Up** *Instructors: Mayank Singh, Kartikey Gaur (TAs)*



CONFERENCE SCHEDULE

Conference Schedule – Day 1

TIME	SESSION / ACTIVITY
08:00 AM – 08:40 AM	Registration
08:40 AM – 09:00 AM	**Invocation & Conference Opening Remarks** *Speaker: Dr. Sanjeeva Srivastava (IIT Bombay)*
Session I: Cancer Proteomics	
	Session Chairs: Dr. Geetanjali Sachdeva (NIRRCH, Mumbai) & Dr. Nattawadee Panyain (Mahidol Univ, Thailand)
09:00 AM – 09:25 AM	**Plenary Talk** *Dr. Joshua LaBaer (ASU, USA)*
09:25 AM – 09:50 AM	**Plenary Talk** *Dr. Arun Wiita (UCSF, USA)*
09:50 AM – 10:20 AM	**Plenary Talk** *Dr. Harish Vasudevan (UCSF, USA)*
Session II: Clinical Proteomics & Multi-omics	
	Session Chairs: Dr. Ashok K Varma (ACTREC, Navi Mumbai) & Dr. Hem Chandra Jha (IIT Indore)
10:20 AM – 10:45 AM	**Plenary Talk** *Dr. Shourjo Ghose (Bruker, USA)*
10:45 AM – 11:10 AM	**Plenary Talk** *Dr. Sanjiv Dhingra (UM, Canada)*
11:10 AM – 11:40 AM	Tea Break
Session III: Proteomics in India	
	Moderators: Dr. Subhra Chakraborty (NIPGR, Delhi) & Dr. Srikanth Rapole (NCCS, Pune)
11:40 AM – 12:25 PM	**Panel Discussion #1: Reflection of Nearly Two Decades of Proteomics – Through the Lens of Proteomics Society of India (PSI)** *Panelists: Dr. Amit Kumar Yadav (THSTI, Faridabad), Dr. Amol Suryawanshi (ILS, Bhubaneswar), Dr. Deepa Bisht (ICMR-NICPR, Noida), Dr. Mahesh Kulkarni (NCL, Pune), Dr. Mukunda Goswami (ICAR-CIFE, Mumbai), Dr. Niranjan Chakraborty (NIPGR, Delhi), Dr. Rashmi Rana (SGRH, Delhi), Dr. Sandipan Ray (IIT Hyderabad) & Dr. Suman Thakur (CCMB, Hyderabad)*
12:25 PM – 01:10 PM	Poster Session
01:10 PM – 02:00 PM	Lunch Break

Session IV: Challenges & Opportunities for Young Investigators	
	Moderators: Dr. Arup Acharjee (AU, Prayagraj) & Dr. Rajeev Kumar (CCHRC, Assam)
02:00 PM – 02:45 PM	**Panel Discussion #2: Navigating Omics Research in India – Opportunities and Challenges for Young Investigators** *Panelists: Dr. Kamal Mandal (GBU, Gujarat), Dr. Kaushik Kumar Dey (ICMR-NIRBI, Kolkata), Dr. Litika Vermani (CCHRC, Assam), Dr. Manisha Choudhary (ARGU, Assam), Dr. Papia Acharjee (BHU, Varanasi), Dr. Pratibha Sharma (IHBAS, Delhi), Dr. Surya Pratap Singh (IIT Dharwad) & Dr. Vineeta Rai (CDRI, Lucknow)*
Session V: Advances in Proteomics Research	
	Chairs: Dr. Purvi Bhatt (NMIMS, Mumbai) & Dr. Siddhartha P Duttagupta (IIT Bombay)
02:45 PM – 03:10 PM	**Plenary Talk** *Dr. Jochen Schwenk (KTH, Sweden)*
03:10 PM – 03:25 PM	**Invited Talk** *Dr. Vel Murugan (ASU, USA)*
03:25 PM – 03:40 PM	**Invited Talk** *Dr. Wen Donq Looi (Bruker, Singapore)*
03:40 PM – 03:55 PM	**Invited Talk** *Dr. Jaswinder Singh Maras (ILBS, New Delhi)*
03:55 PM – 04:10 PM	**Invited Talk** *Dr. Pratik Jagtap (UMN, USA)*
04:10 PM – 04:30 PM	Tea Break
Session VI: Academia Meets Industry – Future of Omics in India	
	Moderators: Dr. Ravi Trivedi (Zydus, Ahmedabad) & Dr. Ritu Kulshrestha (VPCI, Delhi)
04:30 PM – 05:10 PM	**Panel Discussion #3: Where Academia Meets Industry – Shaping the Future of Omics in India** *Panelists: Dr. Ashok Sharma (AIIMS Delhi), Dr. Ashutosh Kumar (IIT Bombay), Dr. Ashutosh Shrivastava (KGMU, Lucknow), Dr. Balaji Sitharaman (Millennial Scientific, India), Dr. Bipin Nair (Amrita Univ. Kerala), Dr. C Murali Krishna (ACTREC, Navi Mumbai), Dr. Chris Swift (Bruker, Germany), Dr. Hem Chandra Jha (IIT Indore), Dr. Kshitij Jadhav (IIT Bombay), Dr. Swapnil Rohidas Shinde (IIT Bombay), Dr. Swati Chitrangi (Thermo Fisher Scientific, India) & Dr. Vadiraja Bhat (Sciex, India)*
05:10 PM onwards	Student Oral Presentation (Selected from Poster Session)



CONFERENCE SCHEDULE

Conference Schedule – Day 2

TIME	SESSION / ACTIVITY
08:45 AM – 09:00 AM	**Convener's Technical Overview** *Dr. Sanjeeva Srivastava (IIT Bombay)*
Session VII: Journey from Genome to Proteome	
	Chairs: Dr. Deepak Agrawal (IIT Bombay) & Dr. Poonam Deshpande (DES Pune Univ., Pune)
09:00 AM – 09:25 AM	**Plenary Talk** *Dr. K Thangaraj (CCMB, Hyderabad)*
09:25 AM – 09:50 AM	**Plenary Talk** *Dr. Peter Nilsson (KTH, Sweden)*
09:50 AM – 10:15 AM	**Plenary Talk** *Dr. Jonathan Blackburn (UCT, South Africa)*
Session VIII: OMICS in Modern Medicine	
	Moderators: Dr. Soumil Vyas (Sir H.N. Reliance Foundation Hospital, Mumbai) & Dr. Jerene Mathews (AIIMS Bhopal)
10:15 AM – 10:55 AM	**Panel Discussion #4: Omics in Healthcare – Opportunities and Challenges** *Panelists: Dr. Abhishek Anand (Paras Health, Patna), Dr. Amarendra Amar (Medanta Hospital, Patna), Dr. Apurva Prasad (KJSMC, Mumbai), Dr. Kunal Goyal (Kokilaben Hospital, Mumbai), Dr. Natasha Lalwani (Shalby Hospital, Ahmedabad), Dr. Prasanna Venkatraman (ACTREC, Navi Mumbai), Dr. Pramod Wangikar (IIT Bombay), Dr. Rajiv Kumar Kaushal (TMH, Mumbai), Dr. Sangeeta Choudhury (SGRH, Delhi), Dr. Satish Sharma (Manipal Hospital, Ranchi) & Dr. Sudhir Nair (ACTREC, Navi Mumbai)*
10:55 AM – 11:15 AM	Tea Break
Session IX: Clinical Multi-omics	
	Chairs: Dr. Syed Hasan (ACTREC, Navi Mumbai) & Dr. Sudhir Nair (ACTREC, Navi Mumbai)
11:15 AM – 11:40 AM	**Plenary Talk** *Dr. Rajiv Sarin (TMC, Mumbai)*
11:40 AM – 12:05 PM	**Plenary Talk** *Dr. Harpreet Singh (ICMR, Delhi)*
12:05 PM – 12:30 PM	**Plenary Talk** *Dr. Sewanti Limaye (Sir H.N. Reliance Foundation Hospital, Mumbai)*
12:30 PM – 01:30 PM	Lunch Break

MOOD-OMICS Special Session	
Session X: Bridging Omics and Clinical Care	
	Moderators: Dr. Sewanti Limaye (Sir H.N. Reliance Foundation Hospital, Mumbai) & Dr. Prashant Kumar (Datar Cancer Genetics, India)
01:30 PM – 02:10 PM	**Panel Discussion #5: Bridging Omics and Clinical Care – Perspectives from Clinicians and Researchers** *Panelists: Dr. Bharat Sinha Bhosale (BB Precision Oncocare Centre, Mumbai), Dr. Harish Vasudevan (UCSF, USA), Dr. Jochen Schwenk (KTH, Sweden), Dr. Jyoti Bajpai (Apollo Hospital, Mumbai), Dr. Peter Nilsson (KTH, Sweden), Dr. Rajiv Sarin (TMC, Mumbai), Dr. Saikat Das (AIIMS Bhopal), Dr. Sanjiv Dhingra (UM, Canada), Mr. Sunil Kumar (ISRO, Bangalore) & Dr. Vijay Mahadik (RDG Medical College, Ujjain)*
Spotlight Talks	
02:10 PM – 02:18 PM	**Talk: OMICS and AI/ML in Precision Healthcare** *Dr. Sanjeeva Srivastava (IIT Bombay)*
02:18 PM – 02:24 PM	**Talk: Cancer Biology and Precision Medicine** *Dr. Joshua LaBaer (ASU, USA)*
02:24 PM – 02:30 PM	**Talk: Advances in Cancer Immunotherapy** *Dr. Arun Wiita (UCSF, USA)*
MOOD-OMICS & Cultural Event	
02:45 PM – 03:00 PM	Melodic Harmonies
03:00 PM – 03:15 PM	Classical Expressions
03:15 PM – 03:30 PM	Rhythmic Fusion
03:30 PM – 04:55 PM	Cultural Heritage
05:00 PM onwards	Felicitation and Award Ceremony



WORKSHOP SCHEDULE

DHR-ICMR Workshop (W1): Clinical Proteomics – Day 1

TIME	SESSION / ACTIVITY
08:00 AM – 08:30 AM	Registration
08:30 AM – 09:00 AM	**Workshop Overview** *Dr. Vishal Vikram Singh (IIT Bombay)*
Session I: Clinical Proteomics	
09:00 AM – 11:10 AM	**Hands-On: Sample Preparation** *Proteomics Sample Preparation: Lysate Preparation and Protein Quantification, SDS-PAGE, Protein Digestion and Desalting.*
11:10 AM – 11:30 AM	Tea Break
Session II: Metabolomics and Lipidomics Sample Preparation	
11:30 AM – 12:45 PM	**Metabolomics and Lipidomics Sample Preparation – Metabolite Extraction**
12:45 PM – 02:00 PM	Lunch Break / Guided Facility Visit: MASFIITB & Proteomica | Poster Session
Session III: Mass Spectrometry Data Acquisition	
02:00 PM – 02:15 PM	**Live Demo of MS Data Acquisition**
Concurrent Clinical Invited Talks	
02:15 PM – 02:30 PM	**Application Talk** *Dr. Deepa Bisht (ICMR-NICPR, Noida)*
02:30 PM – 02:45 PM	**Application Talk** *Dr. Srikanth Rapole (NCCS, Pune)*
02:45 PM – 03:00 PM	**Application Talk** *Dr. Mahesh Kulkarni (NCL, Pune)*
03:00 PM – 03:15 PM	**Application Talk** *Dr. Saikat Das (AIIMS, Bhopal)*
03:15 PM – 03:30 PM	**Application Talk** *Dr. Rashmi Rana (SGRH, Delhi)*
03:30 PM – 03:45 PM	**Application Talk** *Dr. Suman Thakur (CCMB, Hyderabad)*
03:45 PM – 04:00 PM	**Application Talk** *Dr. Amol Suryavanshi (ILS, Bhubaneswar)*

04:00 PM – 04:15 PM	**Application Talk** *Dr. Amit Kumar Yadav (THSTI, Faridabad)*
04:15 PM – 04:30 PM	Tea Break
04:30 PM – 04:45 PM	**Application Talk** *Dr. Wen Donq Looi (Bruker, Singapore)*
04:45 PM – 05:00 PM	**Application Talk** *Dr. Barnali Das (Kokilaben Hospital, Mumbai)*
05:00 PM – 05:15 PM	**Application Talk** *Dr. Deepalakshmi PD (Neuberg Diagnostics, Bangalore)*
05:15 PM – 05:30 PM	**Application Talk** *Dr. Jerene Mathews (AIIMS Bhopal)*
05:30 PM onwards	Evaluation of MS Data (TA) and Discussion

DHR-ICMR Workshop (W1): Clinical Proteomics – Day 2

TIME	SESSION / ACTIVITY
08:45 AM – 09:15 AM	**Opening Remarks** *Speakers: Dr. Santosh Varma (GMC, Ambernath) & Dr. Vijay Mahadik (RGD Medical College, Ujjain)*
Session IV: Multi-Omics Data Analysis Session	
09:15 AM – 10:55 AM	**Multi-Omics Data Analysis: Hands-On**
10:55 AM – 11:15 AM	Tea Break
Session V: Multi-Omics Clinical Application	
	Chairs: Dr. Santosh Varma (GMC, Ambernath) & Dr. Anupama Varma (GMC, Ambernath)
11:15 AM – 11:45 AM	**Plenary Talk** *Dr. Ginu S Khan (ICMR, Delhi)*
11:45 AM – 12:15 PM	**Plenary Talk** *Dr. Prashant Kumar (Datar Cancer Genetics)*
12:15 AM – 12:30 PM	**Invited Talk** *Dr. Venkatesh Sankarasetty (Bruker)*
12:30 PM – 01:30 PM	Lunch Break
Session VI: Bridging Omics and Clinical Care	
	Moderators: Dr. Sewanti Limaye (Sir H.N. Reliance Foundation Hospital, Mumbai) & Dr. Prashant Kumar (Datar Cancer Genetics, India)
01:30 PM – 02:10 PM	**Panel Discussion #5: Bridging Omics and Clinical Care – Perspectives from Clinicians and Researchers** *Panelists: Dr. Bharat Sinha Bhosale (BB Precision Oncocare Centre, Mumbai), Dr. Harish Vasudevan (UCSF, USA), Dr. Jochen Schwenk (KTH, Sweden), Dr. Jyoti Bajpai (Apollo Hospital, Mumbai), Dr. Peter Nilsson (KTH, Sweden), Dr. Rajiv Sarin (TMC, Mumbai), Dr. Saikat Das (AIIMS Bhopal), Dr. Sanjiv Dhingra (UM, Canada), Mr. Sunil Kumar (ISRO, Bangalore) & Dr. Vijay Mahadik (RDG Medical College, Ujjain)*
Spotlight Talks	
02:10 PM – 02:18 PM	**Talk: OMICS and AI/ML in Precision Healthcare** *Dr. Sanjeeva Srivastava (IIT Bombay)*
02:18 PM – 02:24 PM	**Talk: Cancer Biology and Precision Medicine** *Dr. Joshua LaBaer (ASU, USA)*

02:24 PM – 02:45 PM	**Talk: Advances in Cancer Immunotherapy** *Dr. Arun Wiita (UCSF, USA)*
Session VII: Advanced Data Analysis	
02:45 PM – 05:30 PM	**Bioinformatics Practice: Group Project Activity & Assignment** *Instructors: TAs*



WORKSHOP SCHEDULE

Workshop 2: Mass Spectrometry-based Proteomics

TIME	SESSION / ACTIVITY
08:00 AM – 09:00 AM	Registration
09:00 AM – 09:30 AM	**Basics of Proteomics: Introduction to Proteomics** *Dr. Sanjeeva Srivastava (IIT Bombay)*
09:30 AM – 10:30 AM	**Hands-On: Proteomics Sample Preparation** *Instructors: TAs*
10:30 AM – 10:45 AM	**Mass Spectrometry – Parameters and Method Discussion** *Dr. Amrita Mukherjee (Bruker, India)*
10:45 AM – 11:00 AM	**Mass Spec Live Run and Sample Lineup** *Dr. Amrita Mukherjee (Bruker, India)*
11:00 AM – 11:30 AM	Tea Break / MS Data Acquisition
11:30 AM – 11:45 AM	**Discussion on LC-MS/MS and Chromatogram** *Instructors: TAs*
11:45 AM – 12:00 PM	**Primary Analysis – Hands-On FragPipe/DIANN** *Instructors: TAs*
Keynote Talks	
12:00 PM – 12:25 PM	**Application Talk** *Dr. Niranjan Chakraborty (NIPGR, Delhi)*
12:25 PM – 12:50 PM	**Application Talk** *Dr. Subhra Chakraborty (NIPGR, Delhi)*
12:50 PM – 01:00 PM	**Discussion on FragPipe/DIA-NN Outcomes** *Instructors: TAs*
01:00 PM – 02:00 PM	Lunch Break / MS Facility Visit: MASFIITB & Proteomica
02:00 PM – 02:10 PM	**Mass Spectrometry Data Acquisition – Sample Lineup** *Instructors: TAs*
02:10 PM – 03:10 PM	Mass Spectrometry Data Acquisition – Live Run (In Progress)
Invited Talks	
02:10 PM-02:30 PM	**Application Talk** *Dr. Ravi Sirdeshmukh (Mazumdar Shaw Medical Centre & IOB, Bangalore)*
02:30 PM – 02:50 PM	**Application Talk**

	Dr. Hem Chandra Jha (IIT, Indore)
02:50 PM – 03:10 PM	**Application Talk** *Dr. Rajeev Kumar (CCHRC, Assam)*
03:10 PM – 03:30 PM	**Mass Spec Data Analysis – Hands-On** *Instructors: TAs*
03:30 PM – 04:00 PM	Tea Break
04:00 PM – 04:20 PM	**Application Talk** *Dr. Rohit Budhraja (Zydus, Ahmedabad)*
04:20 PM – 04:40 PM	**Hands-On: Pathway Analysis** *Instructors: TAs*
04:40 PM – 05:00 PM	**Hands-On: Targeted Proteomics (Skyline-based Peak Refinement and Analysis)** *Instructors: TAs*
05:00 PM – 05:20 PM	**Hands-On Demo: Machine Learning-based Feature Identification** *Instructors: TAs*
05:20 PM – 05:30 PM	**Discussion** *Instructors: TAs*
05:30 PM onwards	Q/A and Closing Remarks / Lab Visit – BSBE & Proteomica



WORKSHOP SCHEDULE

Workshop 3: Cell Surface Proteomics

TIME	SESSION / ACTIVITY
08:00 AM – 09:00 AM	Registration
09:00 AM – 09:30 AM	**Basics of Proteomics: Introduction to Proteomics** *Dr. Sanjeeva Srivastava (IIT Bombay)*
09:30 AM – 10:30 AM	**Hands-On: Proteomics Sample Preparation** *Instructors: TAs*
10:30 AM – 10:45 AM	**Mass Spectrometry – Parameters and Method Discussion** *Dr. Amrita Mukherjee (Bruker, India)*
10:45 AM – 11:00 AM	**Mass Spec Live Run and Sample Lineup** *Dr. Amrita Mukherjee (Bruker, India)*
11:00 AM – 11:30 AM	Tea Break / MS Data Acquisition
11:30 AM – 11:55 AM	**Application Talk: Advances in Cancer Immunotherapy** *Dr. Arun Wiita (UCSF, USA)*
11:55 AM – 12:20 PM	**Application Talk: Proteomics for Diagnostic and Therapeutic Discovery** *Dr. Harish Vasudevan (UCSF, USA)*
12:20 PM – 12:50 PM	**Cell Surface Capture: Hands-On** *Dr. Kamal Mandal (GBU, Gujarat) and TAs*
12:50 PM – 01:00 PM	**Sample QC Check** *TAs and Merck Team*
01:00 PM – 02:00 PM	Lunch Break
02:00 PM – 02:30 PM	**Hands-On: Sample Preparation** *Instructors: TAs*
02:30 PM – 03:00 PM	**Application Talk** *Dr. Kamal Mandal (GBU, Gujarat)*
03:00 PM – 03:30 PM	**Data Analysis** *Instructors: TAs*
03:30 PM – 04:00 PM	Tea Break
04:00 PM – 04:20 PM	**Application Talk** *Dr. Amrita Mukherjee (Bruker, India)*
04:20 PM – 05:00 PM	**Data Interpretation and Discussion** *Instructors: TAs*
05:00 PM onwards	Quiz & Q&A Session / Lab Visit – BSBE & Proteomica

WORKSHOP SCHEDULE

Workshop 4: Metabolomics & Lipidomics

TIME	SESSION / ACTIVITY
08:30 AM – 09:00 AM	Registration
09:00 AM – 09:30 AM	**Introduction to Metabolomics** *Proteomics Lab IITB (TAs)*
09:30 AM – 10:30 AM	**Metabolomics & Lipidomics Sample Preparation** *Instructors: TAs*
10:30 AM – 11:00 AM	**Mass Spectrometry – Parameters and Live Demonstration of Data Acquisition** *Instructors: TAs*
11:00 AM – 11:30 AM	Tea Break / MS Data Acquisition
11:30 AM – 12:00 PM	**Application Talk** *Dr. Saravanan Kumar (Thermo Fisher, India)*
12:00 PM – 12:45 PM	**Primary Analysis for Metabolomics – Hands-On Demo Compound Discoverer** *Instructors: TAs*
12:45 PM – 01:00 PM	**Introduction to Lipidomics** *Instructors: TAs*
01:00 PM – 02:00 PM	Lunch Break
02:00 PM – 02:30 PM	**Application Talk** *Dr. Ratnasekhar CH (CSIR-CIMAP, Lucknow)*
02:30 PM – 03:10 PM	**MS Data Analysis – Hands-On** *Instructors: TAs*
03:10 PM – 03:30 PM	**Primary Analysis for Lipidomics – Hands-On LipidSearch** *Instructors: TAs*
03:30 PM – 04:00 PM	Tea Break
04:00 PM – 04:15 PM	**Secondary Analysis using LipidSig** *Instructors: TAs*
04:15 PM – 04:45 PM	**Application Talk** *Dr. Ravi Trivedi (Zydus, Ahmedabad)*
04:45 PM – 05:30 PM	**Multi-Omics: Pathway Analysis and Interpretation** *Instructors: TAs*
05:30 PM onwards	Discussion & Closing Remarks (TAs)



WORKSHOP SCHEDULE

Workshop 5: 4D-Omics

TIME	SESSION / ACTIVITY
08:00 AM – 09:00 AM	Registration
09:00 AM – 09:30 AM	**Basics of Proteomics: Introduction to Proteomics** *Dr. Sanjeeva Srivastava (IIT Bombay)*
09:30 AM – 10:30 AM	**Hands-On: Proteomics Sample Preparation** *Instructors: TAs*
10:30 AM – 10:45 AM	**Mass Spectrometry – Parameters and Method Discussion** *Dr. Amrita Mukherjee (Bruker, India)*
10:45 AM – 11:00 AM	**Mass Spec Live Run and Sample Lineup** *Dr. Amrita Mukherjee (Bruker, India)*
11:00 AM – 11:30 AM	Tea Break / MS Data Acquisition
11:30 AM – 12:00 PM	**Application Talk** *Dr. Shourjo Ghose (Bruker, USA)*
12:00 PM – 12:30 PM	**Application Talk** *Dr. Arghya Banerjee (Proteomica, Mumbai)*
12:30 PM – 01:00 PM	**Primary Analysis – Hands-On FragPipe/DIANN** *Instructors: TAs*
01:00 PM – 02:00 PM	Lunch Break
02:00 PM – 02:30 PM	**Application Talk** *Dr. Peter Nilsson (KTH, Sweden)*
02:30 PM – 03:00 PM	**Application Talk** *Dr. Sandipan Ray (IIT Hyderabad)*
03:00 PM – 03:30 PM	**Secondary Analysis – Hands-On MetaboAnalyst** *Instructors: TAs*
03:30 PM – 04:00 PM	Tea Break
04:00 PM – 04:30 PM	**Hands-On: Pathway Analysis** *Instructors: TAs*
04:30 PM – 05:00 PM	**Application Talk** *Dr. Vineeta Rai (CDRI, Lucknow)*
05:00 PM – 05:25 PM	**Application Talk** *Dr. Harsh Pawar (IOB, Bangalore)*
05:25 PM – 05:35 PM	**Discussion**

	Instructors: TAs
05:35 PM onwards	Q/A and Closing Remarks / Lab Visit – BSBE & Proteomica



WORKSHOP SCHEDULE

Workshop 6: Single Cell & Deep Visual Proteomics

TIME	SESSION / ACTIVITY
08:00 AM – 09:00 AM	Registration
09:00 AM – 09:30 AM	**Basics of Proteomics: Introduction to Proteomics** *Dr. Sanjeeva Srivastava (IIT Bombay)*
09:30 AM – 10:30 AM	**Hands-On: Proteomics Sample Preparation** *Instructors: TAs*
10:30 AM – 10:45 AM	**Mass Spectrometry – Parameters and Method Discussion** *Dr. Amrita Mukherjee (Bruker, India)*
10:45 AM – 11:00 AM	**Mass Spec Live Run and Sample Lineup** *Dr. Amrita Mukherjee (Bruker, India)*
11:00 AM – 11:30 AM	Tea Break / MS Data Acquisition
11:30 AM – 12:00 PM	**Application Talk** *Dr. Jochen Schwenk (KTH, Sweden)*
12:00 PM – 01:00 PM	**Sample Prep: SCP – Single Cell Proteomics** *Instructors: TAs*
01:00 PM – 02:00 PM	Lunch Break
02:00 PM – 03:00 PM	**Deep Visual Proteomics Workflow – Demonstration** *Dr. Martin Breitkreuz (MMI, Germany)*
03:00 PM – 03:30 PM	**Deep Visual Proteomics Workflow – Demonstration** *Dr. Asif Khan (MMI, Germany)*
03:30 PM – 04:00 PM	Tea Break
04:00 PM – 04:30 PM	**Data Analysis: SCP** *Instructors: TAs*
04:30 PM – 05:00 PM	**Application Talk** *Dr. Deeptarup Viswas (Online)*
05:00 PM – 05:30 PM	**Data Interpretation and Discussion** *Instructors: TAs*
05:30 PM onwards	Quiz & Discussion



WORKSHOP SCHEDULE

Workshop 8: Metaproteomics Workshop

TIME	SESSION / ACTIVITY
08:00 AM – 09:00 AM	Registration
09:00 AM – 09:30 AM	**Introduction to Metaproteomics** *Dr. Pratik Jagtap (UMN, USA)*
09:30 AM – 10:30 AM	**Sample Preparation and Study Design in Metaproteomics** *Dr. Leyuan Li (BPRC, China)*
10:30 AM – 11:00 AM	Tea Break
11:00 AM – 11:30 AM	**Mass Spectrometry & Metaproteomics** *Dr. Pratik Jagtap (UMN, USA)*
11:30 AM – 01:00 PM	**Bioinformatics: Hands-On Metaproteomics Session using Galaxy Platform** *Dr. Pratik Jagtap (UMN, USA)*
01:00 PM – 02:15 PM	Lunch Break
02:15 PM – 02:45 PM	**Bioinformatics: Metapilot Introduction** *Dr. Kai Cheng (Quadram Institute, UK)*
02:45 PM – 03:30 PM	**Power Analysis and Data Interpretation** *Dr. Luman Wang (Peking University, China)*
03:30 PM – 04:00 PM	Tea Break
04:00 PM – 04:30 PM	**Clinical Metaproteomics** *Dr. Daniel Figeys (Quadram Institute, UK)*
04:30 PM – 05:00 PM	**Wrap-Up and Questions & Answers** *Dr. Pratik Jagtap (UMN, USA)*
05:00 PM onwards	Lab Visit – BSBE & Proteomica



SCHOOL OUTREACH PROGRAM SCHEDULE

MOOD-OMICS: School Outreach Program Schedule

Room 1

TIME	SESSION / ACTIVITY
Session I: Career Development	
08:30 AM	Mr. Girish Dalvi
08:40 AM	Mrs. Sandhya Srivastava
08:50 AM	Dr. Bipin Nair
09:00 AM	Discussion & Q&A
09:10 AM – 09:40 AM	**Session II: AI/ML in Healthcare** *Dr. Ganesh Ramakrishnan*
09:50 AM – 10:00 AM	Transition Break
Session III: Application of Multi-Omics, Big Data, and AI in Healthcare	
10:00 AM	Dr. Harpreet Singh
10:10 AM	Dr. Arun Wiita
10:20 AM	Dr. Sanjiv Dhingra
10:30 AM	Dr. Joshua LaBaer
10:40 AM	Group Photograph & Photo Session
10:50 AM	Dr. Prashant Kumar
11:00 AM – 11:20 AM	Tea Break
11:20 AM – 11:30 AM	Seating & Transition
Session IV: School Presentations	
11:30 AM	Dr. Jochen Schwenk
11:45 AM	School 1 Presentation
12:00 PM	Prof. Sanjeeva Srivastava
12:10 PM	Transition
12:15 PM	School 2 Presentation
12:30 PM	School 3 Presentation

12:45 PM	School 4 Presentation
01:00 PM	Cultural Performance

Room 2

TIME	SESSION / ACTIVITY
Session I: Career Development	
08:30 AM	Mr. Rajiva Srivastava
08:40 AM	Mrs. Vasanti Anand
08:50 AM	Dr. Nirupama Srivastava
09:00 AM	Discussion & Q&A
Session II: Application of Multi-Omics, Big Data, and AI in Healthcare	
09:10 AM	Dr. Vijay Mahadik
09:20 AM	Dr. Harish Vasudevan
09:30 AM	Dr. Sewanti Limaye
09:40 AM	Dr. Ginu S Khan
09:50 AM	Transition Break
10:00 AM – 10:40 AM	**Session III: AI/ML in Healthcare** *Dr. Ganesh Ramakrishnan*
10:40 AM – 11:00 AM	Group Photograph & Photo Session
11:00 AM – 11:20 AM	Tea Break
11:20 AM – 11:30 AM	Seating & Transition
Session IV: School Presentations	
11:30 AM	Dr. Peter Nilsson
11:45 AM	School 5 Presentation
12:00 PM	School 6 Presentation
12:15 PM	School 7 Presentation
12:30 PM	Prof. Sanjeeva Srivastava
12:40 PM	Transition
12:45 PM	School 8 Presentation
01:00 PM	Cultural Performance

SECTION I

APT-2026

Distinguished Plenary Speakers Biography



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Distinguished Plenary Speakers Biography

Dr. Vijay Mahadik, RDG Medical College, Ujjain



Dr. Vijay K. Mahadik is a renowned physician, pediatrician, healthcare visionary, and social reformer who has dedicated more than five decades to advancing healthcare, medical education, and public health in India. He currently serves as the Medical Director of Ruxmaniben Deepchand Gardi Medical College (RDGMC) and Ujjain Charitable Trust Hospital & Research Centre, Ujjain, Madhya Pradesh.

A graduate in Medicine with a Diploma in Child Health (DCH), Dr. Mahadik began his medical practice in 1974 and has since provided compassionate and affordable healthcare to millions of patients. Recognizing the burden of tuberculosis among underserved communities, he pioneered free tuberculosis treatment programs and has contributed significantly to improving public health outcomes in the region.

Dr. Mahadik played a pivotal role in shaping private medical education in Madhya Pradesh and was instrumental in the establishment of R.D. Gardi Medical College in 2001, the first private medical college in the state. Under his leadership, the institution has evolved into a major center for medical education, clinical care, research, and community outreach, serving patients from across Central India.

A strong advocate of charitable healthcare, Dr. Mahadik has led numerous initiatives aimed at expanding access to quality medical services, strengthening rural healthcare systems, promoting medical research, and supporting healthcare innovation. His vision has helped establish advanced specialty services, cancer care facilities, public health programs, and collaborative research initiatives that continue to benefit underserved populations.

Widely respected for his commitment to patient care, medical education, and social service, Dr. Mahadik's contributions have had a lasting impact on healthcare delivery and medical training in Madhya Pradesh and beyond. Through his leadership and humanitarian efforts, he continues to inspire generations of healthcare professionals dedicated to serving society.

Dr. Suresh Advani, Sir H.N. Reliance Foundation Hospital, Mumbai



Dr. Suresh Advani is one of India’s most distinguished medical oncologists and hematologists, with over five decades of experience in cancer care, research, and medical education. He currently serves as Mentor, Department of Medical Oncology, at Sir H. N. Reliance Foundation Hospital and is widely recognized as a pioneer of bone marrow transplantation in India.

He completed his MBBS from Bombay University and earned his M.D. in General Medicine in 1973. Dr. Advani received specialized training in Bone Marrow Transplantation and Medical Oncology at the Fred Hutchinson Cancer Research Center, Seattle, USA, under the International Cancer Research Technology Transfer (ICRETT) program in 1981, followed by a fellowship under the International Union Against Cancer (UICC) in 1986.

A visionary clinician-scientist, Dr. Advani played a seminal role in establishing Bone Marrow Transplantation (BMT) programs in India and has made significant contributions to the advancement of medical, pediatric, and hematological oncology. His research interests include biological therapeutics, targeted cancer therapies, clinical oncology, and

translational cancer research. He has authored more than 600 scientific publications and has served on the editorial boards of several leading medical journals.

Mr. Rajan Datar, Datar Cancer Genetics, India



Mr. Rajan Datar is the Founder of Datar Cancer Genetics, a pioneering molecular oncology company dedicated to advancing precision cancer diagnostics and personalised healthcare. With a strong multidisciplinary background in engineering, science, and business, he has led the development of innovative technologies that enable early cancer detection, treatment monitoring, and precision oncology solutions.

Under his leadership, Datar Cancer Genetics has emerged as a global leader in liquid biopsy and molecular diagnostics, offering cutting-edge tests for cancer screening, prognostication, and therapy guidance. A significant recent milestone has been the **US FDA clearance of CellDx-Tissue**, a comprehensive genomic profiling (CGP) assay for solid tumors that integrates both DNA and RNA analysis, enabling enhanced molecular characterization and supporting precision treatment decisions for cancer patients. This landmark achievement highlights the company's commitment to developing globally recognized, clinically validated diagnostic solutions.

Through his visionary leadership, Mr. Datar has championed the translation of advanced genomic research into clinically actionable technologies. His efforts have contributed significantly to expanding the role of precision oncology in routine clinical practice, enabling more informed treatment decisions and improving patient outcomes across diverse cancer types. His work continues to drive innovation in molecular diagnostics and shape the future of personalized cancer care on a global scale.

APT-2026

Plenary Speakers
Biography and Abstract

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Plenary Speakers Biography and Abstracts

Dr. Arun Wiita, University of California, San Francisco, USA



Dr. Arun Wiita is a physician-scientist and Professor in the Dept of Laboratory Medicine and Dept of Bioengineering & Therapeutic Sciences at the University of California, San Francisco. He is also currently serving as Interim Chair of the Dept. of Laboratory Medicine. Dr. Wiita's research laboratory focuses on mass spectrometry-based proteomics, target discovery, protein engineering, and cellular engineering toward the development of novel immunotherapies for hematologic malignancies, while his clinical duties center on molecular genomic pathology. Dr. Wiita also directs the UCSF Stephen and Nancy Grand Multiple Myeloma Translational Initiative (MMTI) Laboratory. Dr. Wiita is a prior recipient of the NIH Director's New Innovator Award, a Clinical Scientist Development Award from the Doris Duke Charitable Foundation, and a Chan Zuckerberg Biohub Investigator Award, among others. He is also an elected member of the American Society for Clinical Investigation. He completed his residency in Clinical Pathology at UCSF, his MD and PhD at Columbia, with graduate training in single molecule biophysics, and undergraduate studies in Chemistry at Princeton.

Abstract: Advances in Cancer Immunotherapy

Despite advancements, 5-year survival for AML remains ~30%. Unlike other hematologic cancers, surface protein-targeting immunotherapies have shown limited efficacy in AML, largely due to the lack of surface antigens that clearly distinguish malignant cells from normal hematopoietic counterparts. Conventional transcriptomics and proteomics have only found targets lacking clear distinction between AML, myeloid cells, and stem cells. Here, we employed high-resolution surface proteomics to identify both tumor-enriched annotated plasma membrane proteins as well as a new class of "non-canonical" surface proteins, i.e. typically intracellular proteins aberrantly presented on the AML cell surface, as potential immunotherapy candidates.

Methods: We used periodate-based CSC and NHS-sulfo labeling, with both DDA and DIA proteomic methods, to profile surface proteins in newly diagnosed (n=35), relapsed (n=25), and remission (n=16) primary AML samples. Potential AML-specific targets were identified in comparison to multiple gene expression databases. An independent cohort (n=38) was used for target validation, with assessment in PBMCs and HSPCs for off-tumor expression.

Results: Among "canonical" targets, CD209 was validated as a uniquely expressed AML surface protein. An antibody-drug conjugate developed against CD209 demonstrated strong preclinical efficacy. Several non-canonical proteins were validated to be aberrantly presented on the AML cell surface through both flow cytometry and microscopy. Bioinformatic analysis confirmed a preponderance of RNA-binding proteins in the primary AML non-canonical surfacome, consistent with our recent findings in other cell lines (Perr et al, Cell (2025)), but also several other classes of typically intracellular proteins.

Conclusion: Our study provides a comprehensive surfaceome map of AML, identifying both canonical and non-canonical proteins as promising immunotherapy targets. The successful validation and preclinical efficacy of CD209-targeting ADC, along with surface localization of several previously-unrecognized proteins, underscore the potential for developing novel AML-selective therapies. This work will also drive investigation into new areas of tumor biology and surface protein trafficking.

Dr. Ganesh Ramakrishnan, IIT Bombay



Dr. Ganesh Ramakrishnan is a Professor at the Indian Institute of Technology (IIT) Bombay and a leading expert in artificial intelligence, machine learning, natural language processing, and data science. His research focuses on developing advanced computational methods for extracting knowledge from large and complex datasets, with applications spanning healthcare, biomedical informatics, education, and intelligent systems. He has led several innovative research projects in AI-driven analytics and decision-support systems, contributing significantly to both academic research and real-world applications. An accomplished educator and researcher, Dr. Ramakrishnan has published extensively, mentored numerous students, and played a key role in advancing AI and data-driven technologies in India and globally.

Dr. Ginu S Khan, DHR-ICMR, Delhi



Dr. Ginu S. Khan is a Scientist-D in the Division of Human Resource Development (HRD) at the **Indian Council of Medical Research (ICMR),** Department of Health Research, Government of India, New Delhi. She is actively involved in the formulation, coordination, and implementation of national programs to strengthen biomedical and health research capacity across the country. In her current role, Dr. Khan contributes significantly to the development of research manpower through various ICMR-supported fellowship schemes, training initiatives, career development programs, and capacity-building activities.

With extensive experience in research administration and scientific program management, Dr. Khan has played an important role in fostering a vibrant research ecosystem by supporting young investigators, early-career scientists, and healthcare professionals. Her work focuses on promoting excellence in medical research, facilitating interdisciplinary collaborations, and enhancing opportunities for scientific training and mentorship.

Dr. Khan is committed to advancing translational and public health research by encouraging innovation, skill development, and evidence-based scientific inquiry. Through her leadership and contributions at ICMR, she continues to support initiatives that strengthen India's biomedical research landscape and nurture the next generation of researchers dedicated to addressing national and global health challenges. Her efforts have contributed to the growth of a skilled and dynamic scientific workforce that supports the country's evolving healthcare and research priorities.

Abstract Title: Strengthening Research Capacity and Its Dissemination - Awareness Among Medical and Non-Medical Researchers

Dr. Harish Vasudevan, University of California, San Francisco, USA



Dr. Harish Vasudevan is a physician scientist in the Departments of Radiation Oncology, Neurological Surgery, and Cell and Tissue Biology at the University of California San Francisco. His laboratory studies growth factor signaling and tumor suppressor biology in development and cancer using neurofibromatosis and nervous system tumors as a model system to understand how tumor suppressor loss produces dramatically different outcomes across tissues, developmental contexts, and cancers. As a radiation oncologist, Dr. Vasudevan maintains an active clinical practice specialized in providing radiotherapy for pediatric and adult nervous system tumors. His work has directly informed the development of multiple clinical trials and led to multiple patents and the licensing of technologies to academic and commercial entities. Dr. Vasudevan obtained his undergraduate degree at the California Institute of Technology, his MD and PhD degrees from the Mount Sinai School of Medicine and completed his residency and postdoctoral fellowship at the University of California, San Francisco. He is a past recipient of the Francis Collins Scholar Award and the Department of Defense New Investigator Award, and his work is funded by the National Institutes of Health, Department of Defense, multiple foundations, and industry collaborators.

Abstract: Imaging-defined spatial niches reveal proteomic intratumor heterogeneity in nerve sheath tumors

Purpose/Objectives: Nerve sheath tumors (NSTs) span a spectrum from benign schwannomas and neurofibromas to malignant peripheral nerve sheath tumors (MPNSTs), yet the extent of intratumor heterogeneity and biological variation across spatial compartments remain unclear. We hypothesized that radiographically distinct tumor regions harbor distinct proteomic profiles associated with tumor biology and malignant progression.

Methods: We performed LC-MS/MS proteomics on 72 spatially mapped intratumor samples from 12 human NSTs comprising histopathologic neurofibromas (n=1), atypical neurofibromatous neoplasms of uncertain biologic potential (ANNUBPs) (n=2), MPNST (n=1), and schwannomas (n=8) with patient-matched targeted DNA sequencing data. For patients with preoperative MR neurograms (n=48 sites from 9 tumors), apparent diffusion coefficients (ADCs) were used to define high-ADC versus low-ADC spatial niches.

Results: Recurrent variants included *NF2* (n=7), chr22q loss (n=7), *NF1* (n=4), *SMARCB1* (n=3), and *CDKN2A/B* deletion (n=2) while germline variants included *NF1* (n=4), *ABCB11* (n=1) or *WRN* (n=1). Principal component analysis (PCA) revealed that while proteomic profiles predominantly grouped samples by patient, spatial sites within a single tumor also showed separation in PCA space. Differential protein analysis identified distinct proteomic signatures between high versus low ADC compartments in neurofibromas/ANNUBPs/MPNSTs (n=12 enriched proteins in low-ADC regions, n=23 proteins in high-ADC regions; p-value<0.05, $|\log_2 FC| > 1.2$). Gene set enrichment analysis revealed high-ADC proteins were enriched for oxidative phosphorylation while low-ADC proteins were enriched for glycolysis, which reflects spatial metabolic divergence across imaging-defined niches. Five low-ADC proteins were enriched in MPNSTs compared to benign NSTs in independent transcriptomic datasets, suggesting that ADC-defined NST compartments are associated with focal malignant progression.

Conclusions: Proteomics across radiographically defined sites within NSTs reveals intratumor heterogeneity that corresponds to divergent metabolic states and markers of malignant transformation. Future work will integrate genomic, transcriptomic, and epigenetic signatures across imaging-defined niches to build a multi-modal atlas of NST heterogeneity.

Dr. Harpreet Singh, ICMR, Delhi



Dr. Harpreet Singh is a distinguished scientist and research leader associated with the Indian Council of Medical Research (ICMR), New Delhi, India. With extensive experience in biomedical research, public health, and translational medicine, he has made significant contributions to advancing healthcare research and innovation in India. His work focuses on strengthening research ecosystems, promoting interdisciplinary collaborations, and translating scientific discoveries into improved healthcare outcomes.

Dr. Singh has been actively involved in the development and implementation of national research programs addressing critical health challenges, including infectious diseases, non-communicable diseases, precision medicine, and emerging healthcare technologies. He has played a key role in fostering collaborations among academic institutions, healthcare organizations, government agencies, and industry partners to accelerate biomedical research and innovation.

Throughout his career, Dr. Singh has contributed to policy development, research capacity building, and the promotion of evidence-based healthcare practices. He has supported numerous initiatives aimed at advancing clinical research, genomics, diagnostics, and translational science to address public health priorities. As a respected scientific leader, he continues to guide and mentor researchers while contributing to the growth of India's biomedical research landscape. His dedication to scientific excellence and healthcare innovation has earned him recognition as an influential figure in advancing medical research and public health in India.

Abstract: From Protein Design to Self-Evolving AI: Rethinking Trust in Biomedical Science

Artificial intelligence is now deeply embedded in modern proteomics, supporting protein-structure prediction, de novo peptide sequencing, generative protein design, and clinical biomarker discovery. As these systems move from assistive tools to increasingly autonomous scientific agents, the meaning of "trust" must extend beyond accuracy, reproducibility, bias, and privacy. This keynote examines a narrower, but increasingly urgent, question: can biomedical science trust frontier AI systems when their behavior begins to suggest self-reference, limited introspection, long-horizon agency, strategic deception, and evolution-like adaptation?

Dr. Jochen Schwenk, KTH Royal Institute of Technology, Sweden



Jochen M. Schwenk is Professor of Translational Proteomics at the KTH Royal Institute of Technology in Stockholm. He holds a Ph.D. in Biochemistry from the University of Tübingen, Germany. Since 2010, he has led a research group at SciLifeLab, focusing on the development and application of proteomics technologies to study circulating proteins in human blood. His research aims to elucidate how the molecular composition and dynamics of the plasma proteome relate to human health and disease. In addition to his academic work, he contributes to the Human Protein Atlas (HPA), serves as Scientific Director of the Proteomics Platform at SciLifeLab, is an elected council member of the Human Proteome Organization (HUPO), and chaired HUPO's Plasma Proteome Project during the last decade.

Abstract: Microsampling Blood Proteomes for Molecular Health Monitoring

Recent advances in omics technologies now enable the measurement of thousands of molecules across large populations, fueling expectations for transformative progress in precision medicine. However, translating these data into actionable health insights requires moving beyond testing observational associations and addressing the biological, technical, and analytical complexities that shape molecular measurements.

Advancing precision medicine through blood-based proteomics will require integrated strategies that consciously address pre-analytical variability, embrace biological heterogeneity, critically evaluate technology-dependent findings, and account for donor-specific conditions at the time of sampling.

In this presentation, I will highlight our experience and efforts to characterize the dynamics of circulating blood proteins and elucidate their relationships with health and disease states. I will also present self-sampling approaches for blood collection that enable frequent, person-centric measurements and population-scale studies beyond traditional clinical settings. Together, these microsampling strategies offer new opportunities to transform molecular snapshots into longitudinal molecular movies, providing a more granular understanding of human health trajectories and supporting the development of proactive precision medicine.

Dr. Jonathan Blackburn, University of Cape Town, South Africa



Dr Blackburn holds the Chair of Proteomics at the University of Cape Town, where he directs infectious disease, autoimmune and cancer research using combinations of mass spectrometry-based proteomics, phosphoproteomics, metaproteomics, affinity proteomics, and antibody profiling, together with advanced imaging, to unravel disease mechanisms & disease heterogeneity, to define immune landscapes at the site of disease, and to identify novel biomarkers of disease and treatment response. Jonathan in also a Principal Scientist (Proteomics) at Illumina. He was previously the academic founder and Chief Scientific Officer of Sengenics, which commercialized the KREX protein array technology spun-out from his academic lab at the University of Cambridge, UK, and which was recently acquired by Illumina. He holds undergraduate and doctoral degrees in Chemistry from the University of Oxford. Jonathan has published ~150 articles, 10 book chapters, and is lead inventor on 35 granted patent families. His contributions span bioorganic chemistry, enzymology, protein engineering, in vitro evolution of new protein activities, development of protein- and glycan- arrays, surface chemistry, proteomics, computational biology, and biophysical characterization of protein-ligand interactions.

Abstract: Discovery and validation of early diagnostic markers of pancreatic cancer through autoantibody- & proteome profiling

Introduction: Pancreatic ductal adenocarcinoma (PDAC) is a lethal malignancy, ranked the 2nd leading cancer with the lowest 5-year survival rate. This is in part, due to late diagnosis, as 80% of PDAC cases are diagnosed at stage 4, and only 20% of patients are suitable for surgical resection - the only treatment considered potentially curative. Furthermore, there is an absence of sensitive, specific biomarkers for early detection. To address this gap, we profiled serum autoantibody responses in PDAC patients using a protein microarray platform to identify an autoantibody-based signature against cancer antigens, and to evaluate their diagnostic potential in PDAC.

Methods: We used DIA-based mass spectrometry to analyse tumour and adjacent normal samples obtained from PDAC patients undergoing resection surgery. We also analysed serum samples from PDAC patients comprising a discovery cohort (n=30), an independent validation cohort (n=180), and a non-cancer chronic pancreatitis (n=16) cohort. In the discovery phase, a protein microarray platform consisting of 262 tumour-associated, and cancer testis antigens was used to quantify antigen-specific IgA and IgG autoantibody responses in PDAC compared to chronic pancreatitis. A panel of candidate markers was selected based on differential signal intensity, statistical significance, and receiver operating characteristics (ROC) analysis. In the validation phase, we developed a

custom array comprising of the select antibody markers and evaluated their diagnostic performance. FFPE sections from the PDAC cohort were analysed by multiplexed immunohistochemistry and imaging mass cytometry.
Results: DIA proteomic data distinguished PDAC from adjacent normal samples and revealed enriched pathways associated amongst others with humoral immune responses in the tumour. The proteomic data also identified multiple PDAC subtypes that have different progression and survival characteristics. In the discovery cohort, we identified 5-marker IgG and IgA autoantibody panels able to distinguish PDAC from controls with ROC AUC of 0.91 and 0.95, respectively. The optimal 10 autoantibody panel was reproducibly detected in the independent validation cohort and the target autoantigens were further localised in the tumour tissue by imaging methods.
Conclusions: Our study revealed the presence of autoantibodies against specific cancer antigens in peripheral blood from PDAC patients, which are distinguishable by antibody isotype. Collectively, our integrated proteomic, serological profiling and imaging strategy reveals novel antibody signatures that improve diagnostic performance in PDAC and offer promise of pre-symptomatic detection of PDAC.

Dr. Joshua LaBaer, Arizona State University, USA



Dr. LaBaer is one of the nation's foremost investigators in the rapidly expanding field of personalized diagnostics. His efforts focus on the discovery and validation of biomarkers — unique molecular fingerprints of disease that provide early warning for those at risk or with occult major illnesses, including cancer and diabetes. Formerly founder and director of the Harvard Institute of Proteomics, LaBaer was recruited to ASU's Biodesign Institute as the first Piper Chair in Personalized Medicine in 2009. The Virginia G. Piper Center for Personalized Diagnostics has a highly multidisciplinary staff of molecular biologists, cell biologists, biochemists, software engineers, database specialists, bioinformaticists, biostatisticians, and automation engineers. This team has prepared copies of nearly all human genes, which it employs to produce and study the function of all human proteins. They invented a novel protein microarray technology, Nucleic Acid Programmable Protein Array, which has been used widely for biomedical research, including the recent discovery of biomarkers that aid the early diagnosis of breast cancer. To accomplish this, LaBaer and his colleagues exploited the body's own molecular sentinel, called the immune system, which constantly monitors the body for evidence of foreign invasion. When the immune system encounters something that does not belong there, it will produce antibodies against it, which then flag the foreigner for elimination or isolation. Most often, this is used to find bacteria, viruses and other pathogens. But it can also be used to find abnormal proteins produced by chronic diseases such as autoimmune diseases (like diabetes) or chronic diseases (like cancer). By studying several groups of women, including healthy women, women with breast cancer and women with benign breast diseases, LaBaer's team discovered of a panel of 28 autoantibody biomarkers that led to Videssa™, the first CLIA-certified diagnostic test for the detection of breast cancer.

Abstract 1: The Mug Shot of Cancer: Finding Cancer Before It Finds Us

Despite major advances in medicine, cancer still takes too many lives because it is often detected after it has already spread. Early diagnosis improves survival, but current screening methods are not always accurate and can lead to unnecessary procedures. This presentation describes a new way to find cancer that uses the body's own surveillance system, the natural immune response to abnormal proteins produced by cancer cells. We developed a protein microarray technology capable of testing thousands of human proteins simultaneously. Using this platform, blood samples from healthy individuals and cancer patients were compared to identify antibody responses linked to cancer. We identified antibody signatures that distinguished cancer patients from healthy controls. In clinical trials, these signatures detected cancers while reducing unnecessary biopsies. Because the approach relies on the body's natural immune surveillance system, it can be used for multiple cancer types. These findings demonstrate the promise of protein-based blood tests for earlier and more accurate cancer detection. Continued advances in proteomics and immune profiling may lead to new screening tools that improve outcomes by identifying cancer before symptoms develop.

Abstract 2: Advances in Proteomic Technologies

The immune response to vaccination varies widely in populations, affected by general health, underlying medical conditions including immunosuppressive illnesses as well as medication and diet. The ability to predict who will have blunted vaccine responses will improve clinical management. The COVID-19 pandemic created a unique opportunity to assess naïve vaccine responses to a novel microbe. We developed a new proteomics tool that quantifies immune responses to hundreds of antigens in population-sized studies. We conducted a national study assessing humoral immune responses to 185 antigens including SARS-CoV-2 (n=3), common pathogens and microbes (n=157), and autoantigens (n=25), in immunosuppressed patients (n=1,644) and healthy controls (n=2,445), before and

after COVID-19 vaccination. In longitudinal samples, we quantified immune response to 185 common infection related antigens, including SARS- CoV-2 antigens, seasonal coronavirus antigens, other pathogens or microbes (n=148), autoantigens (n=25), resulting in over 2 million serological data points. Although blunted COVID-19 vaccine responses were observed in groups with solid organ transplants, multiple myeloma, autoimmune diseases, inflammatory bowel disease, and human immunodeficiency virus, responses were highly heterogeneous in all groups. About 5- 6% of healthy individuals had weak vaccine responses. We are applying this tool to study pre-existing antibodies to determine if they can predict individuals with blunted immune responses to vaccination. This would enable clinicians to monitor their patients and determine who may need more attentive boosting and who may be prone to infection.

Dr. K Thangaraj, CCMB, Hyderabad



K. Thangaraj is a CSIR Bhatnagar Fellow at the CSIR-Centre for Cellular and Molecular Biology, Hyderabad. He was the Director of Centre for DNA Fingerprinting and Diagnostics, Hyderabad during 2020 - 2023. He was also holding Director-Additional Charge of the Institute for Stem Cell Science and Regenerative Medicine (inStem), Bengaluru during February 2022 - August 2022. His main research interest for the last three decades has been in the field of population and medical genomics. He has published more than 300 research articles. He is an elected Fellow of - Indian National Science Academy, Indian Academy of Sciences, and National Academy of Sciences. He is a recipient of several awards, including Padma Shri, Rashtriya Vigyan Puraskar - Vigyan Shri, J C Bose Fellowship, Sun Pharma Research Award in Medical Sciences, Legend of Hyderabad, Raman Research Fellowship, Life-time achievement Award, Excellence in Science Award, Distinguished Scientist Award, Sir CV Raman Memorial Lecture Award, Sir Dr. UN Brahmachari Award, etc. He had also delivered several Orations. He is a Board Editor of Mitochondrion; Associate Editor of BMC Medical Genomics, Tropical Medicine and International Health, and Editorial Board member of Human Genetics and Clinical Genetics. He was the President of the “Indian Society of Human Genetics” (2011 - 2015), and the founder & President of “Society for Mitochondrial Research and Medicine”.

Abstract: Population genomics for public health

Indian subcontinent is a region of remarkable cultural, linguistic, and genetic diversity with over 4,500 anthropologically well-defined groups. We have been studying various South Asian populations to understand their origin, affinities, and impact of endogamy. Our genetic study revealed that the enigmatic tribal populations of Andaman Islands are the first modern humans, who migrated out of Africa (Science, 2005). Subsequently, we demonstrated that the contemporary Indian populations have descend from two divergent groups (Nature, 2009), and these two groups have admixed during the past 2000 – 4000 years (Am. J. Hum. Genet., 2013). Since then, almost all the populations in Indian subcontinent have been practicing endogamy. To assess the impact of endogamy, we have analysed 275 distinct South Asian groups and found 81 groups with strong founder event (Nat. Genet., 2017). Further, we revisited the populations that have strong founder event, and found that they have high prevalence of recessive and pathogenic mutation (J. Genet. Genomics, 2025), leading to population-specific diseases (unpublished). Our strategy is to provide prenatal and premarital counseling to such populations and reduce disease burden.

Dr. Peter Nilsson, KTH Royal Institute of Technology, Sweden



Peter Nilsson is Professor in Proteomics since 2011 at the Department of Protein Science at SciLifeLab and KTH Royal Institute of Technology in Stockholm. He is head of Protein Array Technologies within Human Protein Atlas since 2003, Deputy head of Division of Biomedical Proteomics, Platform Scientific Director in the Proteomics platform at SciLifeLab and KTH Scientific Director for SciLifeLab. The research is devoted to highly multiplex and high-throughput protein and antibody profiling in body fluids based on various aspects of affinity proteomics. This is enabled through the development and utilization of bead-based and planar protein array formats using proteins and antibodies from the Human Protein Atlas. The protein, autoantibody and serology profiling has mainly been applied within autoimmune, neurodegenerative, psychiatric and infectious diseases, which has generated more than 260 co-authored publications. To enable broad and large-scale seroprevalence studies, a current emphasis is on the development of an extensive resource for multi-disease serology. This is including a wide range of antigens representing various respiratory and infectious diseases, such as coronas, influenza, RSV, EBV, CMV, Mpox, Zika, Dengue, West Nile, Yellow fever, Chikungunya, Oropouche, Mayaro etc.

Abstract: Multiplex protein and antibody profiling in infectious diseases

The successful development of affinity proteomics for the analysis of the circulating proteome has been based on the combination of the access to affinity reagents and technologies enabling high sample throughput as well as a high degree of multiplexing. Within the Human Protein Atlas, (www.proteinatlas.org), we have explored this for many years in large scale, with in-house generated antigens and antibodies for bead-based assays, but also recently with very extensive pan-disease protein profiling in blood utilizing Olink Explore HT and Somascan assays (1,2).

The focus has mainly been devoted to protein and antibody profiling within neurodegenerative and autoimmune diseases but during the first phase of the pandemic, we converted the autoantibody profiling setup to a high-throughput multiplex SARS-CoV-2 serology assay (3) and followed up with analysis of autoantibodies associated to post-COVID (4). We have extended the serology assay to provide a platform for multi-disease serological studies including a wide range of antigens representing various respiratory and infectious diseases. This includes antigens representing influenza virus, respiratory syncytial virus, Mpox, Epstein–Barr virus, cytomegalovirus. We are now expanding into the area of arboviruses, targeting infections such as Dengue, Zika, West Nile, Yellow fever, Japanese encephalitis, Chikungunya, Oropouche, Mayaro etc.

The aim is to enable broad and large-scale seroprevalence studies with high specificity and sensitivity and with thousands of samples analysed on hundreds of antigens. Enabled through international collaborations, eg with Brazil, Singapore, Rwanda and Uganda, we are exploring the potential of the combination of high-throughput and highly multiplex profiling of circulating proteins, autoantibodies and arbovirus targeting antibodies with the aim to develop signatures of diagnostic and prognostic values.

Dr. Prashant Kumar, Datar Cancer Genetics, Nashik



Dr. Prashant Kumar is a leading expert in cancer genomics and precision oncology, associated with DATAR Cancer Genetics, India. His work focuses on molecular diagnostics, liquid biopsy technologies, translational cancer research, and personalized medicine. He has contributed significantly to the development and implementation of advanced genomic platforms for early cancer detection, disease monitoring, and individualized treatment strategies.

Dr. Kumar has played a key role in integrating next-generation sequencing (NGS) and liquid biopsy approaches into clinical oncology, enabling non-invasive and highly sensitive methods for cancer diagnosis and therapeutic decision-making. His research emphasizes the identification of clinically relevant biomarkers that support precision medicine and improve patient outcomes.

Through collaborations with clinicians, researchers, and industry partners, Dr. Kumar has advanced the translation of genomic discoveries into practical healthcare solutions. His contributions have helped expand access to innovative cancer diagnostics and personalized treatment approaches. Recognized for his scientific leadership and commitment to innovation, Dr. Kumar continues to drive advancements in genomics-based cancer care and precision oncology.

Abstract: Advances in Cellular Therapy: Shaping the Future of Cancer Management

Cellular therapies have emerged as a transformative pillar of cancer treatment, offering novel strategies to harness the immune system for the targeted elimination of malignant cells. The remarkable success of adoptive cell therapies, particularly chimeric antigen receptor (CAR)-T cells, has demonstrated the potential of engineered immune cells to achieve durable clinical responses in patients with otherwise refractory cancers. These achievements have catalyzed the development of a diverse range of cellular platforms, including tumor-infiltrating lymphocyte (TIL) therapy, T-cell receptor (TCR)-engineered therapies, natural killer (NK) cell therapies, and gene-edited immune cell products. Advances in cell engineering, genome editing, manufacturing technologies, and multi-omics profiling are driving the next generation of cellular therapeutics with improved efficacy, safety, and scalability. The integration of precision medicine approaches, including biomarker-guided patient selection and treatment monitoring, is further enhancing the clinical impact of these therapies. At the same time, significant challenges remain, including treatment-associated toxicities, tumor heterogeneity, antigen escape, and the immunosuppressive tumor microenvironment, particularly in solid tumors. Ongoing innovations such as allogeneic 'off-the-shelf' cellular products, combination immunotherapies, and synthetic biology-driven cell engineering are expanding therapeutic possibilities and improving accessibility. Collectively, these developments are redefining the landscape of cancer management and advancing the vision of personalized, durable, and potentially curative therapies for a wide range of malignancies.

Dr. Rajiv Sarin, Tata Memorial Centre, Mumbai



Dr. Founding Director of fully commissioned ACTREC, Tata Memorial Centre, Mumbai from 2005–2013. Clinician Scientist working at TMC since 1996. Has extensive experience in the management of Breast Cancer, Brain tumours & Cancer Genetics. Trained in oncology at TMH and Royal Marsden Hospital, London. Established India's first Comprehensive Cancer Genetics Unit. Established TMH multidisciplinary Neuro-oncology unit, the Joint Neuro-Oncology Meeting and the Brain Tumour Foundation in 1999. Provide national leadership and chaired the ICMR committee for National Guidelines in Breast Cancer Management. Through the ICMR Centre for Advanced Research in Cancer Genetics and Genomics, established a comprehensive clinical & Lab cancer genetics programme, 1st in any LMIC that has 24000 cancer prone families and identified germline mutation in over 6000 individuals. It is now the national referral lab serving other hospitals across the country for their difficult cases or solving their ambiguous NGS reports. Started 1st Indian PG Diploma in Cancer Genetics & Counselling.

Abstract: TBA

Dr. Sanjeeva Srivastava, IIT Bombay



Dr. Dr. Sanjeeva Srivastava is a Professor of Biosciences and Bioengineering at IIT Bombay and a Visiting Professor at the University of California, San Francisco (UCSF). A Fellow of the Royal Society of Biology (FRSB), the Royal Society of Chemistry (FRSC), and the Royal Society of Medicine (FRSM), he has over 17 years of academic leadership at IIT Bombay. He currently serves as the Convener of the MASSFIITB National Proteomics Facility and is an associate faculty member at the Koita Centre for Digital Health.

Dr. Srivastava's research focuses on multi-omics biomarker discovery for cancer and infectious diseases. A key contributor to global initiatives like the Human Proteome Project (HPP) and the π-HuB Project Council, he has published over 200 papers, holds 15 granted patents (with 60 filed), with an h-index of 49 and an i10-index of 143.

Recognized with IIT Bombay's highest teaching honors, Dr. Srivastava has mentored 33 Ph.D. graduates and educated more than 50,000 students globally via NPTEL-MOOCs. He is also an active entrepreneur, founding the SINE-incubated startup Proteomica International Pvt. Ltd. to bring affordable, multi-omics-driven diagnostics to healthcare.

Abstract: Translational Proteomics and Multi-Omics Frameworks: Accelerating Biomarker Discovery and Target Identification in Oncology

While genomic sequencing has fundamentally reshaped our understanding of oncogenesis, genomic alterations often fail to capture the dynamic, functional protein networks and structural phenotypes that drive tumor progression and therapeutic resistance. Bridging this gap requires a transition toward high-throughput clinical proteomics and integrated multi-omics pipelines that translate complex biological datasets into actionable clinical insights. This talk highlights recent advancements in leveraging mass spectrometry, structural interactomics, and advanced computational frameworks to decode complex tumor microenvironments and accelerate target discovery. Demonstrating this translational pipeline, we present India's first high-grade glioma proteogenomics map, a landmark cohort study that unravels distinct molecular subtypes, targetable signaling hubs, and novel biomarker signatures unique to the Indian population to deliver affordable precision oncology solutions at the bedside. Crucially, the scalability of this ecosystem is driven by advanced computational tools and AI integration developed in our laboratory. We introduce a suite of newly engineered platforms: BrainProt, a specialized multi-omics data portal for deep proteomic phenotyping; AlphaCross-XL, an advanced platform integrating chemical cross-linking mass spectrometry (XL-MS) with structural modeling to map intact protein-protein

interactions; and DrugProt AI, a computational engine that simulates drug-protein networks to predict therapeutic efficacy and accelerate precision candidate selection.

Dr. Sanjiv Dhingra, University of Manitoba, Canada



Dr. Sanjiv Dhingra is a Professor and Associate Head Research of the Department of Physiology and Pathophysiology, University of Manitoba. He is also the Director of the Canada Italy Tissue Engineering Program at the St. Boniface Hospital Research Centre, Winnipeg, Canada. His research interests are focused on the post- myocardial infarction cardiac regeneration and tissue engineering using stem cells and biomaterials. The current research in Dhingra lab focuses on understanding the host immune response against transplanted stem cells. Another major area of interest in Dhingra lab is to develop MXene based immunomodulatory materials to prevent rejection of transplanted stem cells and solid organs. Dr. Dhingra has published several papers in this area in prominent journals. Dr. Dhingra has been actively involved in promoting the field of cardiac stem cell therapy and tissue engineering. He has organized several national and international conferences and symposia. He was the Chair of International Conferences on Future of Regenerative Medicine, which were held in different parts of Europe, in Tuscania (2017), Ostuni (2018), Rome (2023) and Bratislava (2025). Dr. Dhingra has been recognized nationally and internationally for his accomplishments in research. He received Outstanding Leadership Award in Cardiovascular Research from the Life Science Association of Manitoba. Previously he has been recognized by the American Heart Association (AHA) in 2012 and Canadian Cardiovascular Society in 2017 for his efforts in the field of cardiac regenerative medicine. Recently Dr. Dhingra received Dennis McNmara Oration (2025) and J. Mehta Oration Awards (2024) at the Annual Meeting of the International Academy of Cardiovascular Sciences (North and South American Sections), and Dr. Guido Tarone Lecture Award (2023) at the Annual Congress of the Italian Society of Cardiovascular Sciences. Dr. Dhingra's laboratory is currently funded by multiple agencies including CIHR, NSERC and European Union. He continues to serve as committee member on several granting agency review panels such as CIHR, Heart and Stroke Foundation of Canada, NSERC, NFRF, European Science Foundation, Italian Ministry of Health and Medical Research Council of England.

Abstract: Multi-omics in cardiac regenerative medicine

Institute of Cardiovascular Sciences, St. Boniface Hospital Albrechtsen Research Centre, Department of Physiology and Pathophysiology, Rady Faculty of Health Sciences, Biomedical Engineering Program, University of Manitoba, Winnipeg, Canada

Allogeneic stem cells including bone marrow derived mesenchymal stem cells (MSC) and induced pluripotent stem cells (iPSC) have shown potential for cardiac regenerative medicine. However, poor survival of transplanted allogeneic stem cells in the ischemic heart and immature nature of iPSC derived cardiomyocytes has impaired the clinical translation of stem cells-based therapies. We reported that allogeneic stem cells after transplantation in the ischemic heart turned immunogenic and were rejected by host immune system. In our ongoing studies we use multi-omics-based approaches to understand the mechanisms of transplanted allogeneic stem cells rejection in the heart. My research program also focuses on developing strategies to generate mature iPSC derived cardiomyocytes (iPSC-CM). We hypothesized that mimicking electroconductive environment of the heart in iPSC-CM culture conditions using electrically conductive nanomaterials will provide essential stimulation to promote maturation of iPSC-CM. One of the nanomaterials my lab has been interested in is tantalum carbide MXene quantum dots. We synthesized highly biocompatible Ta4C3Tx MXene quantum dots (MQD) using a facile hydrofluoric acid-free protocol and tested the efficacy of MQD for maturation of iPSC-CM. Our data demonstrate that MQD treated iPSC-CM exhibit a mature phenotype with significantly improved beat rates and calcium handling, enhanced electrophysiological and metabolic activity. Furthermore, the integrative analysis of our transcriptomic, proteomic and metabolomic data using OmicsNET suggest that MQD driven maturation of iPSC-CM is mediated through the focal adhesion kinase (FAK) pathways such as organelle & cytoskeletal organization and cell development.

Dr. Sewanti Limaye, Sir H.N. Reliance Foundation Hospital, Mumbai



Dr. Sewanti Limaye is a distinguished medical oncologist and a pioneer in precision oncology in India. She serves as the Director of Medical & Precision Oncology and Director of Clinical and Translational Oncology Research at Sir H. N. Reliance Foundation Hospital and Research Centre, Mumbai. With over two decades of experience in oncology, she specializes in treating solid tumors, including breast, lung, head and neck, gastrointestinal, genitourinary, and gynecological cancers.

Dr. Limaye completed her MBBS from Jawaharlal Nehru Medical College, India, followed by an MD in Internal Medicine from New York University and a Master's degree in Patient-Oriented Research from Columbia University, USA. She subsequently pursued advanced training and fellowship in Hematology and Medical Oncology in the United States and has held academic and research positions at prestigious institutions including Harvard Medical School, Columbia University Medical Center, Dana-Farber Cancer Institute, and Memorial Sloan Kettering Cancer Center.

A recognized leader in precision medicine and translational cancer research, Dr. Limaye has led numerous national and international clinical trials and has been instrumental in establishing one of India's leading precision oncology programs. Her contributions to cancer genomics, biomarker-driven therapies, immunotherapy, and personalized cancer care have significantly advanced oncology practice and research in India and globally.

Abstract: TBA

Dr. Shourjo Ghose, Bruker Daltonics, USA



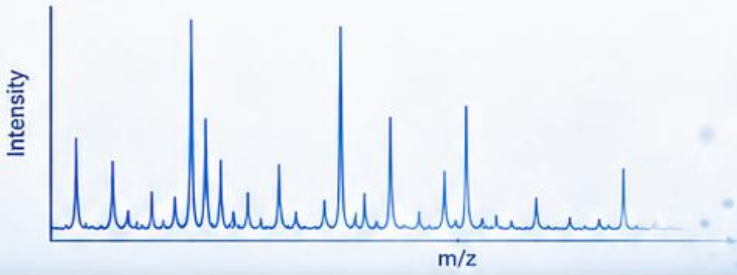
Dr. Shourjo Ghose is a Proteomics Business Development Manager— North America at Bruker Daltonics, where he plays a key role in advancing proteomics applications and business strategies. Dr. Ghose earned his Ph.D. in Biochemistry from Montana State University, where he developed a strong foundation in molecular and structural biology. He then pursued postdoctoral research at the Scripps Research Institute, further expanding his expertise in advanced biochemical and analytical techniques. To complement his scientific background with business acumen, he completed a business certification at Harvard Business School, equipping him with the strategic and leadership skills needed to drive innovation in the industry. In 2017, he joined Bruker as an Application Scientist, focusing on proteomics workflows for the timsTOF line of mass spectrometry systems. His expertise in proteomics and mass spectrometry, combined with his ability to bridge the gap between research and commercialization, led him to his current leadership role. As the North America Proteomics Business Manager, Dr. Ghose is responsible for overseeing business growth, strategic partnerships, and the development of cutting-edge proteomics solutions. His extensive scientific and business experience makes him a key figure in the advancement of proteomics technologies and applications in the life sciences industry.

Abstract: Single-cell to chemoproteomics, scale deep bioinsights with Trapped Ion Mobility

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Keynote Speakers

Biography and Abstract



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Keynote Speakers and Abstracts

Dr. Bipin Nair, Amrita University, Kerala



Bipin Nair received his Ph.D. in Microbiology in 1986 from the Department of Microbiology, M.S. University of Baroda, India and received post-doctoral training at the University of Tennessee, Memphis, USA, in the Dept. of Pharmacology from 1987-1992. His major contributions during that phase were in the areas of growth factor receptor signaling, GTP binding proteins and second messenger pathways. Dr. Nair then moved to the Biotechnology industry in 1993 as Senior Scientist- Lead Discovery at MDS Pharma Services in Seattle, Washington, USA. His experience with High Throughput Screening and application of novel technologies to a wide range of target areas, resulted in many significant achievements for MDS, during his tenure as Research Manager--Lead Discovery, at MDS Pharma Services.

In Dec. 2004, Dr. Nair took over as Professor and Chairman of the School of Biotechnology, Amrita University, India. Under his leadership, the School of Biotechnology has been a trail- blazer in the Biotechnology arena for both undergraduate and postgraduate academic programs as well as an active PhD program at the school. With active national and international collaborations, Dr. Nair's laboratory also has well-funded (DST, DBT, CSIR, MHRD, Bill and Melinda Gates Foundation) and SDG centric research initiatives, in Natural Products Lead Discovery, Multidrug Resistance and Sanitation. Dr. Nair also leads the group at Amrita University that was funded by the Tata Trust as part of the Tata Institute for Genetics and Society, to address the critical global problem of Antimicrobial Resistance [AMR], in collaboration with the University of California, San Diego, USA. More recently (2024), the Amrita School of Biotechnology has also been recognized by the Dept. Of Science and Technology (DST), Govt. of India, as a Centre of Excellence for AMR research in collaboration with Indian Institute of Technology, Kanpur and Central Drug Research Institute, Lucknow. He has numerous publications in national and international scientific journals [Total 275, Citations 4313, h-index 34, i10 index 89, Research Gate score 2577], He is an Editor for Journal of Medical Microbiology (Microbiology Society, London) and an Associate Editor for the International Journal 'Current Pharmacogenomics and Personalized Medicine'. Dr. Nair has also served on several national and international advisory committees. Some other notable achievements include: Recipient of Bill and Melinda GATES Foundation–Department of Biotechnology, GOI/BIRAC Grand Challenge Award, March 2014. Recipient of the Aegis International Graham Bell Award for 'Innovation in Mobile Health, Sept 2016. Nominated as Vice-Chair for Special Interest Group on Antimicrobial Resistance in the Environment as part of India AMR Innovation Hub (IAIH), under the Principal Scientific Advisor to the PM Office, Govt. of India, November 2022 Recipient of Careers 360 National Outstanding Faculty Award – Biotechnology, September 2023.

Abstract- Beyond Venomics: Translating Proteomic Insights into Next-Generation Diagnostics and Therapeutics for Snakebite Envenomation

Snakebite envenoming is a neglected tropical disease that continues to impose a significant burden on public health, particularly in tropical and subtropical regions. Despite advances in antivenom therapy, challenges related to species identification, timely diagnosis, treatment efficacy, and accessibility remain major obstacles to effective clinical management. Over the past two decades, proteomics-driven venomics has transformed our understanding of snake venom composition, revealing remarkable complexity and variability in toxin repertoires and their contributions to envenomation pathology. Recent developments in quantitative venomics, proteotranscriptomics, antivenomics, and functional toxin characterization have enabled the identification of clinically relevant toxins, species-specific biomarkers, and novel therapeutic targets. These advances are facilitating the development of rapid diagnostic platforms capable of accurately identifying the offending snake species and guiding evidence-based treatment decisions. At the same time, proteomic insights are driving the discovery of next-generation therapeutics, including toxin-targeted inhibitors, recombinant

biologics, and adjunct therapies designed to complement conventional antivenoms. The integration of multi-omics technologies with artificial intelligence and machine learning is further accelerating biomarker discovery, epitope prediction, venom classification, and therapeutic target identification. Collectively, these advances are moving the field beyond descriptive venomics toward precision diagnostics and targeted interventions, establishing a translational framework for improving snakebite management and reducing the global burden of envenomation.

Dr. Niranjan Chakraborty, NIPGER, Delhi



Dr. Niranjan Chakraborty earned his master's degree from the University of Dhaka, Bangladesh and PhD from the Jawaharlal Nehru University, New Delhi, India. He did post-doctoral research at the University of California, Riverside, USA. He then joined the Centre for Plant Molecular Biology (CPMB) at the Jawaharlal Nehru University, New Delhi, and later moved to the National Institute of Plant Genome Research (NIPGR), New Delhi, India. His research interest has been exploring the stress-responsive organelle proteomes of economically important crop species, and the molecular mechanisms of stress resilience. He is an elected fellow of National Academy of Sciences, India (NASI); Indian National Science Academy (INSA); and National Academy of Agricultural Sciences (NAAS), India and a member of International Plant Proteomics Organization (INPPO).

Abstract: Mitochondria function as the cellular motherboard empowering stress adaptation and resilience

Mitochondria perceive inputs from the environment, send signals, and communicate constantly with the nucleus and other cell organelles to initiate adaptive responses. When exposed to environmental stresses, mitochondrial redox potential is greatly influenced by stress-induced reactive oxygen species (ROS). Therefore, we investigated the stress-induced alterations in the mitochondrial proteome of a resilient rice cultivar, Rasi, generating a proteome map representing the largest inventory of stress-responsive mitochondrial proteins from any plant species. iTRAQ-based quantitative proteomic analysis led to the identification of an array of stress-responsive proteins (SRPs), associated with various cellular functions, conceivably impinging on the molecular mechanism of stress resilience. A critical screening of the SRPs revealed an uncharacterized DUF (domain of unknown function) protein, henceforth designated OsDUF2488. We demonstrated that OsDUF2488 localizes to the mitochondria and preferentially interacts with peroxiredoxin, OsPrx1.1. The overexpression of OsDUF2488 in rice caused enhanced tolerance to dehydration and oxidative stress, while CRISPR/Cas9 knockout mutants of OsDUF2488 showed hypersensitivity to dehydration. Interestingly, upon exposure to dehydration, OsDUF2488 could rescue mitochondrial dysfunction, contributing to increased ATP production and oxygen concentration in OsDUF2488-overexpressing rice plants. Most significantly, coexpression of OsDUF2488 and OsPrx1.1 in yeast demonstrated a mutual effect on enhanced ROS catabolism, suggesting a cross-kingdom adaptive response of OsDUF2488. Together, the results suggest that OsDUF2488 acts synergistically with OsPrx1.1 to regulate redox homeostasis and promote stress tolerance.

Dr. Ravi Sirdeshmukh, Institute of Bioinformatics & MSCTR, Bangalore



Dr Ravi Sirdeshmukh is presently the incumbent Associate Director in the Institute of Bioinformatics, Principal Advisor at Mazumdar Shaw Center for Translational Research, Bangalore, India and an Adjunct Faculty at MAHE, Manipal. He is also the Founder President of Proteomics Society, India (PSI). Dr Ravi Sirdeshmukh received his Ph. D in Biochemistry from the Centre for Cellular and Molecular Biology (CCMB), Hyderabad and later served on the staff of the CCMB, for over 25 yrs. While at the CCMB, he was responsible for starting and promoting proteomics research in India. His research interest has been in on brain tumors and Head and Neck cancer and he is using integrated multi omics approaches to understand expression of novel protein variants as well as novel ORFs. He served as a council member of Human Proteome Organization (HUPO) and Asia Oceania HUPO for many years and as the designated PI for Chromosome 12 under Chromosome centric - Human Proteome Project (C- HPP) of HUPO.

Abstract: **Exploring alternatively spliced and other non-canonical protein expressions with biological and tumorigenic implications**

Molecular alterations in cancer revealed by multi omics and spatial omics approaches have undoubtedly improved our understanding of the pathogenesis of cancer including tumor heterogeneity and microenvironment. However, most studies remained limited to known pathways and processes. In recent years, protein variants due to alternative splicing or other non-canonical expressions involved in growth and differentiation are increasingly being implicated in the molecular repertoire underlying cancer pathogenesis. These events may be more specific to a given cancer offering

important molecular and mechanistic insights. Our studies on Glioblastoma, a very aggressive primary brain tumor, offer some examples of known and novel protein forms that may contribute to further disease insights and biomarker pursuits.

G protein-coupled receptor 56 (GPR56/ADGRG1) is an adhesion GPCR with a key role in brain development and cancer including Glioblastoma. Using multiomics approaches, we reported that the dynamic interaction between the receptor and its ligand Transglutaminase 2 (TG2) contributes to epithelial (pro neural) to mesenchymal transition involved in Glioblatoma progression and recurrence. For deeper understanding of the mechanics of this interaction, we further explored the role of alternatively spliced forms of GPR 56 and found that the differential expression of two isoforms of the receptor with or without the extracellular, ligand biding domain that may determine the dynamics of this interaction and downstream molecular and cellular events. This has motivated us to explore, at a broader scale, novel non-canonical molecular events and expressions, that may expand our understanding of isoform biology in the context of Glioblastoma and cancer in general.

Proteogenomic approaches integrating RNA Seq and mass spectrometry (MS) data allow identification of such novel translated sequences, many of them may be relevant and specific to tumor pathology. In the background of deep transcriptomic and proteomic data encompassing thousands of canonical genes and protein expressions in Glioblastoma, we have carried out integrated proteogenomic analysis that consisted of *de novo* transcript assembly, in silico translation in six frames to build a custom database of tryptic peptides followed by querying with residual mass spectrometry data unassigned to canonical sequences. We have thus identified, novel peptide sequences which could be assigned to hitherto unreviewed or unreported expression of protein variants using bioinformatic approaches. A snap shot of the kind of variants observed will be presented that may potentially contribute to the pathobiology of Glioblastoma that is still evading effective clinical management.

Dr. Subhra Chakraborty, NIPGER, Delhi



Prof. Subhra Chakraborty, Distinguished Scientist & Former Director at BRIC-NIPGR, India. She obtained her Ph D from JNU, India and worked as Visiting Scientist at Yale University, USA. The central aim of her research is to elucidate the molecular mechanism, translational remodeling, protein-proteoform networks & proteomic pathways, and metabolic fingerprints involved in nutrient-response and multi-host resistance using proteome scale analyses of organeller, quantitative and PTM proteomics and system biology. Her targeted research has direct implications in plant and human health and vital to food and nutritional security. She has authored more than 100 publications, hold 28 international and national patents, mentored a large number of doctoral, post-doctoral students. She is actively associated with national and international proteomics societies as Former President, PSI; Council Member, HUPO and AOAPO; Former Co-chair of Food & Nutrition Initiative and HPP-SAB. She is an elected Fellow of all four National Academies of Sciences, India. Her achievements have been attested by several Awards and Honours, namely, JC Bose National Fellowship, TATA Innovation Award, NASI-Reliance Industries Platinum Jubilee Award, Technology Development Award, Vivek Jyoti Samman Life time achievement award, Platinum Jubilee Lecture Award, National Young Women Bioscientist Award, Young Scientist Award, IUBMB, Professor Hiralal Chakraborty Award.

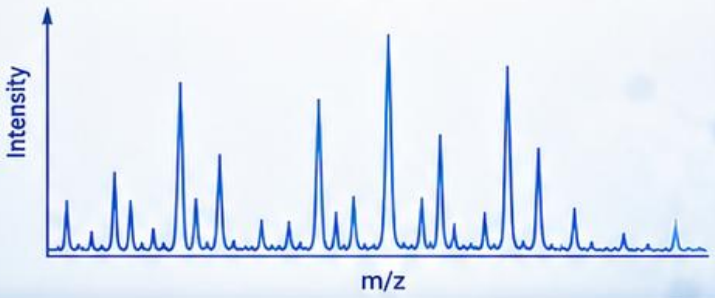
Abstract: Beyond a bird's eye view towards One Health: Demystifying proteogenomic landscape and cellular control of health to disease linking multi-host response

Complex nature of the interactions between plant, animal, human and ecosystem renders multisectoral transdisciplinary approaches critical to address future food and health risks and challenges. Proteo-genomics and spatial proteomics uncover new strategies for one health problems by facilitating discovery of molecular signature of disease and protein biomarkers to multi-host resistance. *Fusarium* sp., an ascomycetes fungus and multi-host pathogen is a causal agent of vascular wilt in plants, neuronal stress in worm and fusariosis in humans. Although precisely controlled innate immune response is governed by conserved cellular events in phylogenetically diverse hosts, underlying molecular mechanisms by which this process is regulated against multi-host pathogen remain unknown. We have established the proteo-genomics landscape of a food legume, chickpea and reanalysed the data for worm in healthy and disease state based on DDA library and SWATH-MS with a high-quality spectral library for rapid and deep profiling. Further, with the label-free based proteomics workflow combining integrated transcriptomics and metabolomics, we also demonstrated multilayered analyses at the resolution of spatial proteomics and their application to reveal new insight on the immune signature and pathogenesis during fusariosis. Most excitingly, network analysis identified significant functional modules pointing toward fusarium responsive common mechanism of remodelling, homeostasis and cell death response through divergent regulatory pathways across kingdom.

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Invited Speakers

Biography and Abstract



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Invited Speakers Biography and Abstracts

Dr. Abhishek Anand, Paras Health, Patna



Dr. Abhishek Anand is a renowned Medical Oncologist and currently serves as the **Director and Head of the Department of Medical Oncology at Paras HMRI Hospital, Patna**. He is recognized for his expertise in the diagnosis and treatment of a wide spectrum of solid tumors and hematological malignancies, including leukemia, lymphoma, and multiple myeloma. His clinical practice integrates precision medicine, targeted therapies, immunotherapy, and stem cell transplantation to provide personalized cancer care.

Dr. Anand completed his MBBS and MD in Medicine before pursuing a **DM in Medical Oncology**, receiving advanced oncology training at the prestigious **Kidwai Memorial Institute of Oncology, Bengaluru**. Over the years, he has gained extensive experience in managing complex cancer cases and implementing evidence-based treatment strategies tailored to individual patient needs.

His areas of interest include breast cancer, lung cancer, gastrointestinal malignancies, genitourinary cancers, hematological cancers, targeted therapies, precision oncology, and stem cell transplantation. Dr. Anand is actively involved in clinical research, academic activities, and cancer awareness initiatives aimed at improving access to advanced oncology care.

Through his leadership at Paras Health, Patna, Dr. Anand continues to advance comprehensive cancer care by combining cutting-edge therapies with compassionate, patient-centered treatment. His contributions have helped strengthen oncology services and improve outcomes for cancer patients across eastern India.

Dr. Amarendra Amar, Medanta Hospital, Patna



Dr. Amarendra Amar is an accomplished Medical Oncologist and currently serves as **Associate Director, Medical Oncology** at **Jay Prabha Medanta Super Speciality Hospital, Patna.** With extensive experience in cancer diagnosis, treatment, and clinical research, he is recognized for his expertise in precision oncology, immunotherapy, targeted therapies, and comprehensive cancer care. cancer treatment. the **American Society of Clinical Oncology (ASCO)** and the **European Society for Medical Oncology (ESMO).** a vital role in advancing cancer care and improving outcomes for patients across eastern India.

Dr. Amit Kumar Yadav, THSTI, Faridabad



Dr. Amit Kumar Yadav is Principal Scientist-II at the Translational Health Science and Technology Institute (THSTI), Faridabad. He obtained his Ph.D. in Computational Biology from CSIR-IGIB, where he developed MassWiz, one of India's first proteomics database search algorithms for peptide identification from mass spectrometry data. This work earned him recognition as an MIT Technology Review Innovator Under 35 (TR35). Later, he joined THSTI and received the Innovative Young Biotechnologist Award (IYBA) from the Department of Biotechnology, Government of India. His research has led to the development of several computational and experimental innovations in proteomics, including BONplex, a multiplexed quantitative proteomics platform enabling simultaneous analysis of 18 biological conditions in a single mass spectrometry experiment. Dr. Yadav leads research at the intersection of proteomics, proteogenomics, post-translational modifications (PTMs), artificial intelligence, and translational bioinformatics. His group develops computational tools and multi-omics frameworks for biomarker discovery and disease biology, with current applications in metabolic dysfunction-associated steatotic liver disease (MASLD), chronic pancreatitis, and cardiovascular and infectious diseases. His current interests include proteoform mapping, AI-driven biomarker discovery, knowledge graphs, and digital twin frameworks for predictive and precision medicine.

Abstract: From PTM Knowledge Bases to AI-Driven Disease Knowledge Graphs: Advancing PTM Informatics for MASLD Research

Post-translational modifications (PTMs) constitute a critical layer of biological regulation that regulates protein activity, signaling, interactions and subcellular localization. Despite their importance in disease progression and regulation, PTM knowledge remains fragmented across databases and the biomedical literature, limiting its systematic exploration and application. To address this, we have developed complementary PTM informatics resources. First, we created PTM-WEB, a curated knowledge base of PTM writer and eraser enzymes spanning both well-characterized and emerging PTMs. PTM-WEB enables exploration of PTM regulatory networks, enzyme relationships, and pathway-level interactions. Second, we developed a PTM-specific named entity recognition (NER) framework based on fine-tuning a large language model (LLM) for automated extraction of PTM knowledge from biomedical literature. Integrating PTM NER with PubTator-derived annotations for genes, diseases, chemicals, and other biomedical entities, we further performed relation extraction (RE) to identify biologically meaningful associations from PubMed literature. We applied this framework to Metabolic Dysfunction-Associated Steatotic Liver Disease (MASLD), a disease in which PTM dysregulation contributes to metabolic dysfunction, inflammation, and fibrosis. The extracted entities and relationships were assembled into a MASLD-specific knowledge graph (MASLD-KG), enabling exploration of connections among PTMs, regulatory enzymes, pathways, and disease phenotypes. Together, PTM-WEB and MASLD-KG demonstrate how curated knowledge resources, AI-driven entity recognition, and relation extraction can transform dispersed PTM information into actionable biological knowledge, providing a foundation for hypothesis generation, biomarker discovery, and mechanistic studies in MASLD and beyond.

Dr. Amol Suryavanshi, ILS, Bhubaneswar



Dr. Amol Suryawanshi is an eminent senior scientist working in the field of Clinical Proteomics at the BRIC-Institute of Life Sciences (ILS), Bhubaneswar. He is a Veterinary clinician transformed into a research scientist. His research focus is clinical proteomics for understanding disease biology through Disease Proteome Mapping, Bio-marker discovery in various diseases, decipher the role of important protein/s in disease pathogenesis and identification of post-translational modifications (PTMs) with respect to their role in disease pathogenesis. Currently his group works on understanding Cancer and viral diseases particularly Rabies, SARS-CoV-2, Chikungunya, Dengue, etc. He has many extramural project grants. His research findings have been published in various reputed peer-reviewed journals. He is a peer-reviewer for many national and international scientific journals. He is an

Executive council member of the Proteomics Society of India (PSI) where his main interest is to carry educational activities towards the popularization of proteomics.

Abstract: Deciphering Pathogenesis and Biomarker Landscapes via Mass Spectrometry-Based Clinical Proteomics

High-throughput clinical proteomics offers unprecedented capabilities to elucidate cellular phenotypes through comprehensive protein identification, deep quantification, and the characterization of post-translational modifications. Delineating how these qualitative and quantitative proteomic alterations drive cellular behavior across diverse physiological and pathological states is essential for modern translational medicine. To this end, mass spectrometry (MS)-based methodologies have emerged as indispensable platforms, enabling highly sensitive, accurate quantification and robust multiplexing of complex clinical biospecimens, thereby serving as a cornerstone for biomarker discovery.

Depending on the target clinical context of use (COU), tailored proteomic workflows can be strategically deployed to map differentially expressed proteins and specific proteoforms. These candidate biomarkers hold significant utility for deconstructing disease biology, optimising diagnostic and prognostic stratification, and guiding targeted therapeutic development. The overarching objective of our laboratory is to implement advanced MS-based proteomic architectures to discover robust protein signatures that drive disease pathogenesis and to decipher their mechanistic roles. Currently, we are profiling the proteomic landscapes of distinct oncology cohorts (including nasopharyngeal, cervical, and ovarian malignancies) as well as critical viral pathologies (e.g., Rabies, SARS-CoV-2, Chikungunya, and Dengue). This presentation will outline the current state of MS-based clinical proteomics and detail our laboratory's recent initiatives to map disease-specific protein signatures, evaluating their translational viability as clinical biomarkers.

Dr. Amrita Mukherjee, Bruker, India



Dr. Amrita Mukherjee is an Application Specialist at Bruker, India, with expertise in proteomics, mass spectrometry, biomarker discovery, and multi-omics data analysis. She earned her Ph.D. from the Department of Biosciences and Bioengineering, IIT Bombay, where her research focused on understanding the molecular mechanisms and identification of biomarkers of cervical cancer using advanced proteomics and systems biology approaches.

Through her current role, Dr. Mukherjee works closely with academic, clinical, and industrial researchers, supporting the application of cutting-edge mass spectrometry technologies to advance biomedical research and healthcare innovation.

Dr. Anupama Varma, GMC, Ambernath



Dr. Anupama Varma is a clinician-scientist and academic leader at Government Medical College (GMC), Ambernath. Her professional interests include clinical research, medical education, public health, and translational medicine. She has actively participated in multidisciplinary research initiatives focused on improving healthcare outcomes and advancing evidence-based clinical practices. Dr. Varma is committed to mentoring future healthcare professionals and promoting research-driven medical education. Her contributions to patient care, academic development, and collaborative research have strengthened healthcare and biomedical research initiatives within the region.

Dr. Apurva Prasad, KJSMC, Mumbai



Dr. Apurva Prasad is a distinguished Neurologist and academician associated with **K. J. Somaiya Medical College and Research Centre (KJSMC), Mumbai**. With extensive experience in clinical neurology, neuroscience research, and medical education, he is recognized for his contributions to the diagnosis and management of complex neurological disorders. His clinical practice integrates evidence-based medicine with advanced diagnostic approaches to deliver comprehensive patient care.

Dr. Prasad completed his medical training and specialized education in Neurology at leading institutions in India. Over the years, he has developed expertise in the management of stroke, epilepsy, movement disorders, headache disorders, neuromuscular diseases, neuroimmunological conditions, and neurodegenerative disorders. His research interests include clinical neuroscience, neurophysiology, neuroimaging, and the application of emerging technologies in neurological diagnosis and treatment.

In addition to his clinical responsibilities, Dr. Prasad is actively involved in teaching undergraduate and postgraduate medical students, mentoring young clinicians, and promoting neurological awareness through academic and public engagement initiatives. He has contributed to scientific publications, national conferences, and professional training programs aimed at advancing neurological care and research.

Through his dedication to patient care, research, and education, Dr. Prasad continues to contribute significantly to the field of neurology. His work focuses on improving neurological health outcomes through innovation, interdisciplinary collaboration, and the translation of scientific advances into clinical practice.

Dr. Arghya Banerjee, Proteomica, Mumbai



Dr. Arghya Banerjee is a cancer biologist and proteomics researcher with expertise in mass spectrometry-based approaches for studying brain tumors and advancing biomarker discovery. He earned his Ph.D. in Cancer Biology from the Indian Institute of Technology Bombay (IIT Bombay), where his research focused on the molecular characterization of pituitary adenomas and other brain tumors using advanced analytical technologies. His scientific interests encompass proteomics, mass spectrometry, ATR-FTIR spectroscopy, Raman spectroscopy, and translational cancer research to identify clinically relevant biomarkers. Dr. Banerjee has made significant contributions to understanding the molecular mechanisms underlying brain tumors by applying cutting-edge proteomic and vibrational spectroscopy techniques. His work has helped advance the use of mass spectrometry in both research and clinical settings, contributing to improved disease characterization and biomarker identification. In addition to his academic achievements, Dr. Banerjee founded Proteomica International Private Limited, a company dedicated to providing high-quality proteomics and mass spectrometry services. Through this initiative, he has supported researchers worldwide with customized solutions for protein profiling, biomarker discovery, quantitative proteomics, and advanced data analysis, further promoting the adoption of modern proteomics technologies across diverse biomedical research fields.

Dr. Arup Acharjee, Allahabad University, Prayagraj



Dr. Arup Acharjee is an Assistant Professor in the Department of Zoology, University of Allahabad, India, specializing in proteomics and molecular neuroscience. His research focuses on proteomics-based biomarker discovery, multi-omics integration, and AI-driven approaches to disease modelling. Dr. Acharjee earned his Ph.D. in Zoology from Banaras Hindu University (BHU). His postdoctoral work at BHU and IIT Bombay expanded into mass spectrometry-based proteomics, neuroproteomics, and biomarker discovery, particularly in hepatic encephalopathy and neurodegenerative disorders. As a Research Scientist at IIT Bombay's Proteomics Lab, he contributed to large-scale COVID-19 proteomics studies, identifying novel diagnostic markers and variant-specific immune responses. His expertise in quantitative proteomics, high-resolution mass spectrometry (HRMS), and protein microarrays has led to impactful research in neuroproteomics, host-pathogen interactions, and metabolic disorders. Dr. Acharjee has co-authored multiple high-impact publications and book chapters, contributing significantly to the application of proteomics in biomedical research. His work integrates big data analytics, machine learning, and computational proteomics for better understanding disease mechanisms.

Beyond research, he is actively involved in mentoring students and organizing training program such as GIAN on advanced proteomics technologies and data analysis. His leadership in proteomics education in India extends as a mentor at various faculty training programs and interdisciplinary collaborations aimed at bridging basic science with translational applications.

Currently, Dr. Acharjee's work is focused on unraveling proteomic alterations in neurological disorders such a hepatic encepatholpathy developing next-generation proteomics workflows, and applying AI in proteome data interpretation. Through his research and teaching, he continues to advance the role of proteomics in personalized medicine and clinical diagnostics.

Dr. Ashok K Varma, ACTREC, Navi Mumbai



Dr. Ashok K Varma is a Professor of Translational Research and scientific officer 'H' in ACTREC where he maintains an active & result oriented research laboratory. Dr. Varma obtained his Ph D degree on the topic "X-ray crystallographic studies of biomolecules", from Jiwaji University, Gwalior. Soon after PhD, he joined world renowned scientists like Prof. G R Desiraju (Central University Hyderabad) and Prof. T. P. Singh in AIIMS. He has received very good postdoctoral research experiences at Harvard Medical School, Boston Biomedical Research Institute (BBRI), Boston, USA. Dr Varma has excellent research experiences in molecular biology, protein biochemistry, structural biology and Bioinformatics. He has supervised Twelve – PhDs students and eight are registered under him working on structural and functional basis of cancer- associated proteins. He also supervised > fiftly, M.Phil / M.Sc. /M.Tech /B.Tech students for their degree dissertation. He has more than 50 international publications to his credit. He is very good team-leader and received grants from DBT, DST, ICMR.

Dr. Ashok Sharma, AIIMS Delhi



Dr. Ashok Sharma is a Professor in the Department of Biochemistry and head of Neurobiochemistry Division & Molecular Diagnostic Lab at Neuroscience Center & National Cancer Institute, AIIMS, New Delhi. He is the president of the DNA Society of India. He is the recipient of multiple awards, including the prestigious "DBT-Ramalingaswami" and "DST-Ramanujan fellowship" from the Government of India, and the Outstanding Immunologist Award from Immunocon, the Indian Immunologist Society, and BHU.

He received a Ph.D. in Cancer Biology at the Department of Biochemistry at All India Institute of Medical Sciences (AIIMS), New Delhi, in 2009. In 2009, he joined the Vanderbilt Medical Center, Vanderbilt University, Nashville, TN, USA as a postdoctoral fellow. In 2012, he joined the group of Adam R. Karpf at the Eppley Institute at UNMC as a senior postdoctoral researcher. He is working on the epigenetics and regulation of the Cancer-Testis/germline antigen and its biomarkers/therapeutic potential.

At present, his team is exploring the potential of Artificial Intelligence to unveil indigenously developed technology iOncology.ai for early detection and personalized treatment for Indian cancer patients in a joint venture with Center for Development of Advanced Computing, Pune, India. He has published multiple research articles, abstracts, and book chapters in national and international journals. He is actively involved in ePG-Pathshala, an MHRD National Mission on Education through ICT (NME-ICT) venture to develop e-content at the postgraduate level to help improve the education system in India. Dr. Sharma has served as the principal investigator and co-investigator on multiple projects focused on gynecological cancer. He is the coordinator for the Indian Cancer Research Consortium and a member of the National Consultation on strengthening cancer screening interventions. Dr. Sharma has been actively involved in establishing the National Cancer Institute (NCI)-AIIMS, Jhajjar Campus.

Dr. Ashutosh Kumar, IIT Bombay



Dr. Ashutosh Kumar is a Professor in the Department of Biosciences and Bioengineering at the Indian Institute of Technology (IIT) Bombay and a leading expert in structural biology and biomolecular NMR spectroscopy. He heads the NMR-Based Structural Biology Laboratory and is recognized internationally for his research on the structure, dynamics, and mechanisms of biomolecular assemblies using advanced solution-state and solid-state Nuclear Magnetic Resonance (NMR) spectroscopy. His research focuses on protein–protein, protein–lipid, and protein–drug interactions, as well as the structural characterization of complex biological systems, including nucleosomes, amyloid fibrils, and multiprotein regulatory complexes.

Dr. Kumar's work has significantly advanced the understanding of chromosome organization, centromere assembly, ubiquitin-mediated protein degradation, and protein aggregation associated with human diseases. By integrating NMR spectroscopy with complementary biophysical and structural biology techniques, his laboratory investigates fundamental molecular mechanisms underlying cellular regulation and disease pathogenesis.

An accomplished researcher, educator, and mentor, Dr. Kumar has authored numerous high-impact publications and has played a key role in developing advanced NMR infrastructure and training programs in India. His contributions to structural biology, biophysics, and biomolecular spectroscopy continue to influence both fundamental biological research and translational biomedical science.

Dr. Ashutosh Shrivastava, KGMU, Lucknow



Dr. Ashutosh Shrivastava is an Additional Professor at the Centre for Advanced Research, King George's Medical University, Lucknow, India. Dr Shrivastava completed his Ph.D. from the Sanjay Gandhi Postgraduate Institute of Medical Sciences, Lucknow. He pursued postdoctoral fellowships at Harvard Medical School, Boston, USA, where he worked in the area of experimental medicine. His research focuses on cancer biology, metabolomics and biomarker discoveries. He has extensive experience in investigating the molecular mechanisms of cancer progression, drug resistance, and metabolic reprogramming, particularly in glioblastoma and breast cancer.

Dr Shrivastava has authored numerous peer-reviewed publications and has contributed significantly to the fields of translational research and multi-omics integration. His work focuses on using advanced analysis methods, like GC-MS-based metabolomics, to find important biomarkers and targets in various diseases. In this

regard, he has filed two patent applications. He has established interdisciplinary collaborations with clinicians and researchers to conduct research of translational value. His current research interests include circulating tumour cells, liquid biopsy, organoid models, AI-assisted biomarker discovery, and personalised medicine.

Dr. Asif Khan, MMI, Germany



Dr. Asif Khan is a life science technology specialist and international business leader currently serving as Head and Director of Sales for Europe, India, and Asia-Pacific at MMI – Molecular Machines & Industries, Germany. He has extensive experience in advanced bioinstrumentation, single-cell technologies, laser microdissection, optical tweezers, micromanipulation, and high-resolution imaging solutions that support cutting-edge biomedical research.

Dr. Khan earned his Ph.D. from Ben-Gurion University of the Negev, Israel, where his research focused on molecular genetics and plant biology. Following his academic training, he built a successful international career spanning scientific research, technical applications, sales leadership, and business development across Europe, the Middle East, Africa, India, and the Asia-Pacific region.

Prior to joining MMI, Dr. Khan held key roles at Bruker, Curiox Biosystems, and Dispendix, where he supported innovative technologies in microbial diagnostics, flow cytometry, laboratory automation, and life science instrumentation. At MMI, he leads global market development and commercial strategy for advanced single-cell isolation and laser microdissection platforms, helping researchers accelerate discoveries in spatial biology, genomics, transcriptomics, and proteomics.

Combining scientific expertise with strong commercial leadership, Dr. Khan is passionate about enabling researchers with innovative technologies that advance precision medicine and next-generation life science research.

Dr. Balaji Sitharaman, Millennial Scientific, India



Dr. Balaji Sitharaman is a scientist-entrepreneur at Millennial Scientific, a deep-tech life science tools company developing custom chromatography media and bioprocess materials for next-generation biologics manufacturing, including peptides, large proteins, nucleic acids, and cells.
He received his B.Sc. from the Indian Institute of Technology at Kharagpur, M.A., and Ph.D. from Rice University in Houston, Texas, where he also completed his postdoctoral research at the Richard E. Smalley Institute for Nanoscale Science and Technology. He was a tenured faculty member in the Department of Biomedical Engineering at the State University of New York at Stony Brook, USA. To date, he has published over 100 peer-reviewed scientific articles. Together, these articles have received over 10,000 citations. In addition, he has received awards and funding for innovative basic and translational research from U.S. federal agencies and private foundations, including the prestigious NIH Director's New Innovator Award and the Wallace H. Coulter Translational Research Award. He is an inducted member of the National Academy of Inventors, USA.

Dr. Barnali Das, Kokilaben Hospital, Mumbai



Dr. Barnali Das is the Lead Consultant in Biochemistry, Immunology, and Toxicology at Kokilaben Dhirubhai Ambani Hospital, Mumbai, India. She holds an MBBS, MD, DNB in Biochemistry, a Postgraduate Diploma in Hospital and Healthcare Management (PGDHHM), and is a Fellow of the American Association of Clinical Chemistry (FAACC). A highly respected expert in laboratory medicine, her research focuses on clinical chemistry, immunology, and biomarker discovery, with particular emphasis on autoimmune markers, high-sensitivity cardiac troponins, neuroimmune biomarkers, and biomarkers for traumatic brain injury (TBI) and intracerebral hemorrhage (ICH). Her work is dedicated to enhancing diagnostic precision, disease monitoring, and patient outcomes through the standardization and harmonization of advanced immunoassays. In addition to leading the Biochemistry, Immunology, and Toxicology divisions at Kokilaben Dhirubhai Ambani Hospital, Dr. Das has served as the institution's Quality Improvement Champion since 2021 and has been a member of the Institutional Ethics Committee (Academics) since 2018. Recognized internationally for her contributions to laboratory medicine, she was featured in *The Pathologist Power List 2023* and has received the prestigious Seth G. S. Medical College & KEM Hospital Oration Award for her outstanding achievements in clinical diagnostics and healthcare excellence.

Abstract: Enhancing Clinical Services with Proteomics

Clinical proteomics is increasingly enabling the translation of molecular discoveries into clinically actionable diagnostic tests. Among its most impactful applications is the development of targeted mass spectrometry assays capable of delivering highly specific and multiplexed protein measurements for disease diagnosis and patient stratification. I will showcase few examples of standardizing LC-MS/MS assays for hormone analysis, proteomic analysis in NMDA receptor Autoimmune Encephalitis, Hemoglobinopathies and Acute Kidney Injury etc.

As an example, one of our collaborative works with Prof. Akhilesh Pandey from Mayo Clinic and Dr. Anikha Bellad from Institute of Bioinformatics, we describe a multiplexed targeted mass spectrometry assay for the diagnosis of hemoglobinopathies and thalassemias from dried blood spots using a triple quadrupole platform.

The assay simultaneously quantifies globin chain peptides and detects mutation-specific peptides, enabling direct identification of common and rare hemoglobin variants while also assessing globin chain imbalances associated with thalassemia. Evaluated in more than 700 individuals, the assay accurately identified heterozygous, homozygous, and compound heterozygous states.

A unique advantage of this approach is its ability to identify the mutant amino acid at the protein level, effectively providing sequence-level confirmation of hemoglobin variants. This enables the assay to serve not only as a screening test but also as a confirmatory test, reducing the need for multiple sequential investigations. The assay resolves ambiguities encountered with conventional methods, provides clinically relevant globin-chain ratios for thalassemia assessment, and offers a scalable solution for newborn screening, carrier detection, and precision diagnosis of hemoglobin disorders.

As another example, one of our collaborative works with Ms. Zeenat Parween, Prof. Sanjeeva Srivastava from IIT Bombay, We found six fibro-inflammatory proteins — BMP1, COL1A, MMP14, SPP1, IL1RL1, and SULF2 — that went up steadily as AKI got worse across the KDIGO stages (ANOVA $p \leq 1\times10^{-12}$).

This talk will explore the journey from guideline-based AKI detection and electronic alert implementation to artificial intelligence-driven prediction models and multi-omics-enabled precision medicine, highlighting opportunities and challenges in transforming AKI care in India.

Therefore, Clinical Proteomics is revolutionizing healthcare by translating complex protein signatures into actionable insights, enabling earlier diagnosis, precise risk stratification, and truly personalized patient care.

Dr. Bharat Sinha Bhosale, BB Precision Oncocare Centre, Mumbai



Dr. Bharat Bhosale, MD, DM (Medical Oncology), is a distinguished medical oncologist with extensive experience in the diagnosis and treatment of cancer. He previously served as a Consultant Medical Oncologist at Tata Memorial Hospital, Mumbai, one of India's premier cancer care and research institutions.

Dr. Bhosale is the Founder and Director of BB Precision Oncocare Centre, Mumbai, where he focuses on delivering personalized and precision oncology care by integrating advanced diagnostics, targeted therapies, and evidence-based treatment approaches.

In addition to his leadership role, he serves as a Visiting Consultant at several leading healthcare institutions, including Bombay Hospital, Jaslok Hospital, Sir H. N. Reliance Foundation Hospital, S. L. Raheja Hospital, and Holy Spirit Hospital.

His clinical interests encompass precision oncology, targeted therapies, immunotherapy, and the translation of emerging cancer research into improved patient care. Through his commitment to clinical excellence and innovation, Dr. Bhosale continues to contribute significantly to advancing cancer treatment and personalized medicine in India.

Dr. C Murali Krishna, ACTREC, Navi Mumbai



Dr. C. Murali Krishna is a distinguished scientist and Head of the **Chilakapati Laboratory at the Advanced Centre for Treatment, Research and Education in Cancer (ACTREC), Tata Memorial Centre, Mumbai**. He is internationally recognized for his pioneering contributions to **biomedical optics, Raman spectroscopy, and translational cancer diagnostics**. With more than three decades of research experience, Dr. Krishna has been at the forefront of developing innovative optical technologies for the early detection and characterization of cancer and other diseases.

His research focuses on the application of **in vivo and ex vivo Raman spectroscopy, optical imaging, vibrational spectroscopy, and biophotonics** for disease diagnosis and therapeutic monitoring. Through interdisciplinary collaborations involving physicists, biologists, clinicians, and engineers, his laboratory has developed novel spectroscopic approaches that enable non-invasive, rapid, and accurate detection of cancer-associated molecular changes.

Dr. Krishna has authored over 200 peer-reviewed publications in leading international journals and has mentored numerous students, postdoctoral fellows, and young investigators. His work has significantly advanced the translation of laboratory-based optical technologies into clinically relevant diagnostic tools. He is a Fellow of several prestigious scientific societies and has received widespread recognition for his contributions to biomedical spectroscopy and cancer research.

Through his scientific leadership at ACTREC, Dr. Krishna continues to drive innovation in precision diagnostics and translational oncology, thereby improving cancer detection, patient management, and healthcare outcomes.

Dr. Chris Swift, Bruker, Germany



Dr. Chris Swift is a distinguished scientist and technology leader at **Bruker, Germany**, where he plays a key role in advancing next-generation mass spectrometry and proteomics technologies. With extensive expertise in analytical chemistry, proteomics, and life science instrumentation, Dr. Swift has contributed significantly to the development and application of high-performance mass spectrometry platforms for biomedical, pharmaceutical, and translational research.

Throughout his career, Dr. Swift has worked closely with academic institutions, clinical researchers, and industry partners to accelerate the adoption of innovative omics technologies. His scientific

interests encompass mass spectrometry-based proteomics, biomarker discovery, systems biology, clinical research applications, and emerging technologies that support precision medicine. He has been actively involved in translating advanced analytical tools into practical solutions to understand complex biological systems and improve healthcare outcomes.

At Bruker, a global leader in scientific instrumentation, Dr. Swift supports the development of cutting-edge technologies that enable researchers to explore proteins, metabolites, and other biomolecules with unprecedented sensitivity and accuracy. His work has contributed to strengthening collaborations between technology developers and the scientific community, fostering innovation across life sciences research.

A frequent speaker at international conferences and scientific forums, Dr. Swift is recognized for his ability to bridge technological innovation with biological and clinical applications. Through his leadership and scientific contributions, he continues to advance the fields of proteomics, translational research, and precision healthcare.

Dr. Daniel Figeys, Quadram Institute, UK



Dr. Daniel Figeys is an internationally renowned scientist, entrepreneur, and leader in the fields of **proteomics, systems biology, microbiome research, and precision health**. He currently serves as the **Director and Chief Executive Officer of the Quadram Institute, United Kingdom**, one of the world's leading centers dedicated to food, microbiome, and health research. Prior to joining the Quadram Institute, he was a Professor at the University of Ottawa and a Senior Scientist at the Ottawa Hospital Research Institute, where he established globally recognized research programs in proteomics and systems medicine.

Dr. Figeys earned his Ph.D. in Chemistry and has pioneered numerous technological advances in mass spectrometry-based proteomics, contributing significantly to the development of high-throughput analytical platforms for studying complex biological systems. His research focuses on understanding host–microbiome interactions, systems biology, biomarker discovery, personalized medicine, and the molecular mechanisms underlying human health and disease.

Over the course of his distinguished career, Dr. Figeys has authored more than 400 peer-reviewed publications, holds numerous patents, and has co-founded several biotechnology companies translating scientific discoveries into healthcare innovations. His contributions have been recognized through prestigious international awards, fellowships, and leadership positions within the global scientific community.

At the Quadram Institute, Dr. Figeys leads multidisciplinary programs that integrate microbiology, nutrition, genomics, metabolomics, proteomics, and clinical research to advance precision health and improve human well-being. Through his scientific leadership and innovation, he continues to shape the future of systems medicine, microbiome science, and translational biomedical research globally.

Dr. Deepa Bisht, ICMR-NIPCR, Noida



Dr. Deepa Bisht is a distinguished scientist at the ICMR–National JALMA Institute for Leprosy and Other Mycobacterial Diseases, Agra, India, and is widely recognized for her pioneering contributions to infectious disease research, proteomics, microbiology, and translational medicine. Her research focuses on understanding the molecular basis of mycobacterial diseases, particularly tuberculosis and leprosy, through the application of advanced proteomic, genomic, and immunological approaches. She has made significant contributions to deciphering host–pathogen interactions, identifying disease-associated biomarkers, and uncovering molecular mechanisms involved in pathogenesis, immune responses, and drug resistance.

Over the years, Dr. Bisht has led several nationally and internationally funded research projects aimed at improving the diagnosis, prognosis, and treatment of mycobacterial diseases. Her work has advanced the application of proteomics and systems biology in infectious disease research, resulting in the identification of novel therapeutic targets and biomarkers with potential clinical utility. She has published extensively in high-impact international journals and has established numerous scientific collaborations across India and abroad.

An accomplished researcher, mentor, and scientific leader, Dr. Bisht has played a pivotal role in strengthening translational research and capacity building in infectious disease sciences. Through her innovative research and commitment to public health, she continues to contribute significantly to the global fight against tuberculosis, leprosy, and other mycobacterial diseases.

Dr. Deepak Agrawal, IIT Bombay



Dr. Deepak K. Agrawal is an Assistant Professor in the Department of Biosciences and Bioengineering at the Indian Institute of Technology (IIT) Bombay, where he leads the Computational Medicine and Technology (CMT) Laboratory. His research lies at the interface of biomedical engineering, computational medicine, data science, physiological modeling, artificial intelligence, and medical device development. Dr. Agrawal is dedicated to advancing translational healthcare technologies by integrating computational tools, machine learning, and quantitative modeling with clinical and biological sciences.

Prior to joining IIT Bombay in 2024, he served as an Assistant Professor at the Centre for Biomedical Engineering, IIT Delhi. He earned his Ph.D. in Engineering from the University of Cambridge, UK, and subsequently held research positions at leading institutions in the United States, including Johns Hopkins University, Boston University, Northeastern University, and the University of Colorado. His research has contributed to the development of synthetic biological systems, DNA nanotechnology platforms, computational diagnostics, and biomolecular feedback control systems.

Dr. Agrawal's current work focuses on developing innovative computational and engineering solutions for disease prediction, critical care, personalized medicine, healthcare analytics, and next-generation medical technologies. Through interdisciplinary collaborations spanning engineering, biology, and medicine, he continues to advance the application of artificial intelligence and biomedical informatics in healthcare. He has authored numerous scientific publications and actively mentor students and researchers in the fields of computational medicine and biomedical innovation.

Dr. Deepalakshmi PD, Neuberg Diagnostics, Bangalore



Dr. Deepalakshmi P.D. is a Clinical Scientist at Neuberg Diagnostics, Bengaluru, with extensive experience in clinical and translational mass spectrometry. Her work focuses on developing and implementing advanced diagnostic applications in multiple myeloma, hemoglobinopathies, therapeutic drug monitoring, and microbial identification using LC–Tandem Quad MS and MALDI-MS. She has contributed to the translation of mass spectrometry technologies into routine clinical practice, supporting precision diagnostics and evidence-based patient care. Her expertise spans proteomics, metabolomics, top-down and bottom-up protein analysis, native mass spectrometry, hydrogen–deuterium exchange mass spectrometry (HX-MS), ion mobility, biopharmaceutical characterization of monoclonal antibodies, and emerging targeted omics applications in healthcare. Dr. Deepalakshmi played a key role in establishing Proteomics and LC/GC-MS laboratories at the Indian Institute of Science (IISc), Bengaluru. She has actively promoted scientific education and technology adoption through training programs and workshops across India, particularly in the field of high-resolution mass spectrometry. She has authored over 35 peer-reviewed publications, contributed a book chapter on proteomics, and published two Indian patents on novel LC-MS-based diagnostic methods. Her professional interests include diagnostic innovation, laboratory quality, and the clinical translation of advanced analytical technologies at affordable cost.

Abstract: Proteins in Clinical Mass Spectrometry: Translating Targeted Proteomics into Routine Diagnostics

Introduction: Proteins are clinically actionable biomarkers that directly reflect disease biology and therapeutic response. Recent advances in mass spectrometry have enabled highly selective, sensitive, and multiplexed protein analysis, creating opportunities for clinical proteomics beyond research laboratories. This talk highlights two translational applications of protein mass spectrometry implemented in routine diagnostics: monoclonal protein characterization in multiple myeloma and globin chain analysis for hemoglobinopathies. Methods Project 1: Monoclonal Proteins in Multiple Myeloma Immunoglobulins were enriched from patient serum using isotype-specific affinity capture. Following elution and reduction, heavy and light chains were separated on LC and mass measured using low-resolution tandem quadrupole mass spectrometry (LC-TQMS). Detection of monoclonal proteins was based on identification of unique light-chain masses and comparison with conventional immunofixation electrophoresis (IFE).

Project 2: Hemoglobinopathies Hemoglobin was extracted from whole blood or dried blood spot specimens and analyzed using Flow Injection analysis (FIA) TQMS) with or without tryptic digestion. Globin chains were measured using a dual mass spectrometry approach to detect both β-thalassemia and rare hemoglobin variants. Clinically significant variants were confirmed by tryptic digestion of globin chains followed by targeted MS/MS analysis of diagnostic peptides.

Results: For monoclonal proteins, LC-TQMS demonstrated high concordance with IFE, achieving 89.7% agreement in IFE-positive samples and 90.9% agreement in IFE-negative samples. Isotype-specific agreement ranged from 75–88%, supporting the utility of LC-TQMS for M-protein detection and monitoring. For hemoglobinopathies, the combined assessment of globin chain ratios demonstrated robust diagnostic performance. The approach facilitated identification of β-thalassemia carriers during family cascade screening, sub-classification of sickle cell disorders, and confirmation of rare structural hemoglobin variants. In newborn screening, clinically significant hemoglobin variants were detected from dried blood spots by FIA-MS with 100% sensitivity and specificity.

Conclusion: LC-TQMS can be translated into routine diagnostic laboratories, enabling precision diagnostics for protein-based diseases while supporting future applications such as targeted proteomics, therapeutic drug monitoring, and biomarker quantification.

Dr. Deeptarup Biswas, HMS, USA



Dr. Deeptarup Biswas is a Postdoctoral Researcher in the Department of Neurology at Boston Children's Hospital, Harvard Medical School, specializing in Single-Cell Omics, Artificial Intelligence and Machine Learning, Neuroscience, and Biomarker Discovery. His research focuses on developing high-throughput quantitative workflows and computational pipelines for single-cell proteomics, aiming to unravel molecular mechanisms and disease-associated proteomic profiles in neurodegenerative disorders. Dr. Biswas earned his Ph.D. in Biosciences and Bioengineering from the Indian Institute of Technology Bombay (IIT Bombay), where he developed robust big data analysis pipelines to investigate the pathophysiology and therapeutic mechanisms of high-grade meningioma tumors. His doctoral research was recognized with the Dr. Gargi Vishnoi Memorial Prize for the Best Ph.D. Thesis. He holds a Master's degree in Biotechnology from Pondicherry University, where he graduated with First Class with Distinction.

Throughout his career, Dr. Biswas has worked in the intersection of healthcare, technology and data analytics to tackle complex clinical questions. He has developed several databases, automated tools, and computational platforms, including BrainProt (India's first brain disease omics database), CoVProt, IBPM, PhosphoMap, Brain Disease Marker Curator (BDMC), and Clustome. His work has resulted in multiple peer-reviewed publications, book chapters, copyrights, and patents, including a biomarker panel for grade-specific diagnosis of meningioma brain tumors.

During the COVID-19 pandemic, Dr. Biswas contributed to government-funded research projects, earning an Institutional Appreciation Certificate for his efforts. His commitment to education is reflected in his extensive teaching and mentorship experience, including as 5 years of mentorship and teaching instructor on NPTEL MOOC (funded by MHRD), Koita Centre for Digital Health (KCDH) - IIT Bombay. He has also served as an expert in Big Data Analysis, AI applications in clinical research and Omics across several national and international workshops. Dr. Biswas represented IIT Bombay at the Inter-IIT Scientific Conclave (2023), where he won a gold medal, competing against over 15 IITs across India.

Abstract: Single-Cell Proteomics Unlocking Cellular Heterogeneity for Precision Medicine

Single-cell proteomics (SCP) is transforming our ability to investigate cellular heterogeneity and unravel the molecular complexity of disease. Traditional bulk tissue proteomics averages signals across diverse cell populations, masking cell-specific biological processes and limiting our understanding of disease mechanisms. Although recent advances in mass spectrometry have significantly improved proteome coverage, sensitivity, and throughput, challenges remain in achieving robust quantification, reproducibility, and post-translational modification (PTM) analysis at the single-cell level. Recent innovations in SCP technologies are enabling increasingly sensitive and comprehensive characterization of proteins and PTMs from individual cells and low-input samples. Emerging approaches such as TimePlex time-encoded sample multiplexing are enhancing analytical depth, throughput, and scalability, while advances in sample preparation, instrumentation, and computational analysis continue to push the boundaries of single-cell measurements. In parallel, the rapid expansion of single-cell proteomics software platforms, databases, and bioinformatics tools is accelerating biological discovery and improving data interpretation. Together, these developments are opening new opportunities to understand cellular heterogeneity, molecular signaling, and disease biology with unprecedented resolution, ultimately contributing to more precise diagnostic, prognostic, and therapeutic strategies in the era of precision medicine.

Dr. Geetanjali Sachdeva, NIRRCH, Mumbai



Dr. Geetanjali Sachdeva is a distinguished reproductive biologist and senior scientist at the ICMR–National Institute for Research in Reproductive and Child Health (NIRRCH), Mumbai, India. She is widely recognized for her pioneering contributions to reproductive biology, developmental biology, stem cell research, and women's health. Over the course of her career, Dr. Sachdeva has led several innovative research programs aimed at understanding the molecular and cellular mechanisms underlying embryo implantation, placental development, pregnancy-related disorders, and reproductive health.

Her research integrates advanced molecular biology, genomics, proteomics, and cell biology approaches to investigate critical processes involved in fertility, maternal health, and fetal development. She has made significant contributions to understanding the role of signaling pathways, stem cells, and molecular biomarkers in reproductive disorders and pregnancy outcomes. Her work has provided valuable insights into reproductive diseases and has supported the development of novel diagnostic and therapeutic strategies.

An accomplished researcher, mentor, and scientific leader, Dr. Sachdeva has authored numerous high-impact publications in leading international journals and has guided many students and young investigators. She has also played an important role in national and international collaborative research initiatives focused on reproductive and child health. Through her scientific excellence and leadership, Dr. Geetanjali Sachdeva continues to advance reproductive health research and contribute to improving maternal and child healthcare in India and globally.

Dr. Harsh Pawar, IOB Bangalore



Dr. Harsh Pawar is a Faculty Scientist at the Institute of Bioinformatics (IOB), Bengaluru, with expertise in proteomics, proteogenomics, parasitology, infectious diseases, and systems biology. He earned his Ph.D. in Pathology from Rajiv Gandhi University of Health Sciences, Bengaluru, where his research focused on biomarker discovery in cancer and the application of multi-omics approaches to disease biology.

Following his doctoral training, Dr. Pawar was awarded the prestigious Dr. D. S. Kothari Postdoctoral Fellowship and conducted pioneering research on the biology of *Leishmania donovani* and its insect vectors using proteomic and proteogenomic approaches. He subsequently held postdoctoral positions at Technion – Israel Institute of Technology and Lancaster University, United Kingdom, where he investigated nutrient sensing, cellular signaling, and host–pathogen interactions in kinetoplastid parasites.

Dr. Pawar has extensive experience in next-generation sequencing, quantitative proteomics, phosphoproteomics, genome annotation, and parasite biology. His research integrates genomics and proteomics to understand infectious diseases, vector biology, and molecular mechanisms underlying pathogen adaptation and survival. He has authored numerous peer-reviewed publications and has contributed significantly to advancing multi-omics research in parasitology and infectious disease biology.

At the Institute of Bioinformatics, Bengaluru, Dr. Pawar leads research efforts focused on applying advanced omics technologies to study parasites and insect vectors of medical importance, with the goal of identifying novel biomarkers, therapeutic targets, and mechanisms of disease transmission relevant to the Indian subcontinent.

Abstract: Proteogenomic Analysis of *Angomonas deanei* to improve its genome annotations

Introduction: *Angomonas deanei* is a monoxenous trypanosomatid parasite of insects belonging to the subfamily *Strigomonadinae*, notable for harbouring an obligate endosymbiotic bacterium of the *Candidatus Kinetoplastibacterium* genus. This endosymbiotic relationship confers unique metabolic capabilities to the host parasite, making *A. deanei* an

important model organism for studying co-evolutionary dynamics. Despite the availability of a sequenced genome, the proteome of *A. deanei* remains poorly characterised, with a substantial proportion of predicted protein-coding genes lacking experimental validation. Proteogenomics is a powerful strategy to extend proteome coverage, validate gene models, and discover novel coding regions beyond the reach of computational annotation alone.

Methods: Publicly available mass spectrometry proteomics datasets for *A. deanei* were retrieved from repositories including PRIDE and MassIVE. Raw spectral data were processed and searched against a six-frame translated genome database of *A. deanei*. Unique peptides identified post database dependent searches were mapped to the annotated *A. deanei* protein database. Those that mapped were discarded but peptides that didn't match to the annotated protein database but mapped to six-frame translated genome database of *A. deanei* were referred to as Genome Search Specific Peptides (GSSPs). These GSSPs resulted in identification of novel protein coding genes and corrections to existing gene models in *A. deanei.*

Results: Proteogenomic database searching substantially expanded the experimentally supported proteome of *A. deanei* beyond canonical annotation-based searches. We identified 950 novel protein-coding genes were identified with reproducible peptide evidence, including unannotated intergenic regions. Additionally, we corrected annotation of >2000 annotated genes which included N- and C-terminal extensions.

Conclusions: This study demonstrates that publicly available proteomics data constitute a valuable and underutilised resource for proteogenomic discovery in *Angomonas deanei*, enabling genome annotation refinement and expanding knowledge of both the parasite. These findings provide a foundation for future functional studies exploring the metabolic and co-evolutionary relationship in *A. deanei*.

Dr. Hem Chandra Jha, IIT Indore



Dr. Hem Chandra Jha, an Associate Professor at Mehta Family School of Biosciences and Biomedical Engineering, IIT Indore, earned his Ph.D. in 2010 from the Institute of Pathology, Delhi, focusing on Chlamydia pneumoniae in coronary artery disease, and completed his degree at BITS Pilani. He conducted postdoctoral research at the University of Pennsylvania on tumour viruses, including Epstein-Barr Virus (EBV) and Kaposi's Sarcoma-associated Herpesvirus. He joined IIT Indore as a Ramanujan Fellow in 2016, became Assistant Professor in 2017, and is currently serving as an Associate Professor in the same department. He currently leads Infection Bioengineering Group, which integrates molecular biology, and multi-omics to investigate host-pathogen interaction and disease pathogenesis. Dr. Jha's research focuses on deciphering molecular mechanisms underlying pathogen-associated cancers, neurodegenerative disorders, antimicrobial resistance (AMR), and emerging infectious diseases. His laboratory made significant contributions towards understanding of EBV, Helicobacter pylori, SARS-CoV-2, and associated coinfections drive gastric carcinogenesis and neurodegenerative disorders through multi-organ axes including gut-brain axis, lung-colon axis, etc. Recent studies from his group have employed lipidomic, metabolomics, proteomics, Raman spectroscopy, and machine-learning frameworks to identify biomarkers and therapeutic targets in gut-brain axis-mediated neurodegeneration and oral cancer progression. A major focus of his current research is the development of omics-driven diagnostic and prognostic platforms for infectious and neurological diseases. His group has utilized multi-omics and artificial intelligence approaches to characterize molecular signatures associated with Long COVID, and infection-induced neurological complications. These studies have identified critical metabolic, hormonal, and inflammatory pathways disrupted during disease progression and have provided novel opportunities for precision diagnostics and therapeutic interventions.

Dr. Jha's interdisciplinary research program also investigates antimicrobial resistance, microbiome-host interactions, environmental toxicants, and phytochemical therapeutics. His laboratory is actively involved in biomarker discovery for antibiotic-resistant infections, neurodegenerative disorders, and oral cancer progression, supported by multiple national and international research grants. His translational research has resulted in several patents related to EBV-mediated

neurological disorders and peptide-based therapeutic interventions. Till now his lab contributed more than 150 research articles, reviews, 16 book chapters, six extramural grants completed and five research grants are on-going along with one patent approved and 14 patents filed. Research work appeared in reputed journals such as Apoptosis, IEEE-JBHI, mSphere, J of Proteome Research, etc. Dr. Jha is also a part of theme lead of Hub-Spoke model in Health Medical Technology in which 29 projects are running in six University/Institute related to AMR and a co-project director in Technology Translational Research Park at Drishti-CPS, IIT Indore.

Abstract: Infection-Induced Host Responses Revealed by Multi-Omics: Implications for Neurodegeneration, Cancer, and Precision Medicine

Microbial infections drive complex host responses that influence neurological disorders, cancer progression, and systemic diseases through interconnected immune, metabolic, and signalling networks. Our research employs integrated multi-omics approaches, including proteomics, lipidomics, metabolomics, to decipher host-pathogen interactions and identify clinically relevant biomarkers and therapeutic targets. A major focus of our work is the gut-brain axis, where antimicrobial-resistant (AMR) *Helicobacter pylori* and its coinfection with Epstein-Barr virus (EBV) disrupt gut and blood–brain barrier integrity, induce neuroinflammation, and promote synaptic dysfunction. Multi-omic analyses revealed STAT3-dependent signalling, metabolic reprogramming, alterations in Alzheimer's disease-associated markers such as APP and APOE4. Proteomic characterization of coinfection-derived secretome further identified mechanistic targets associated with GRM1-mediated signalling in brain organoids.

Beyond neuroinfectious disorders, the laboratory has applied multi-omics approaches to oral carcinogenesis and COVID-19 pathogenesis. Studies in oral submucous fibrosis (OSMF) and oral squamous cell carcinoma (OSCC) identified disease-associated molecular signatures with diagnostic and prognostic potential. In parallel, COVID-19 investigations revealed variant-specific metabolic, lipidomic, proteomic, and hormonal perturbations linked to disease severity, long-COVID manifestations, thyroid dysfunction, and silent heart failure. Collectively, these studies provide a systems-level framework for biomarker discovery, precision medicine, and therapeutic intervention in infection-associated diseases.

Keywords: Multi-omics, host-pathogen interactions, gut-brain axis, oral cancer, COVID-19.

Dr. Jaran Jainhuknan, Bruker Daltonics, Thailand



Dr. Jaran Jainhuknan earned his Ph.D. in Analytical Chemistry, focusing on peptide structures in the gas phase and peptide fragmentation under MALDI-PSD conditions. In 1998, he joined Bruker as an application scientist, where he has spent over two decades advancing mass spectrometry techniques and supporting researchers in method development. Dr. Jainhuknan specializes in LC-MS applications across a broad spectrum of scientific areas, including proteomics, protein characterization, metabolite profiling, biomarker discovery, and small-molecule analysis. His expertise spans biological and polymer applications of MALDI-TOF, small-molecule X-ray crystallography, and metabolite quantification and screening. Over the past decade, he has collaborated with scientists worldwide, helping them design and optimize LC-MS workflows for diverse applications, from protein identification to drug metabolism studies. He finds great satisfaction in witnessing well-planned experiments produce meaningful results. With a deep passion for analytical chemistry and mass spectrometry, Dr. Jainhuknan continues to drive innovation in the field, providing valuable insights into complex biological systems. His contributions have played a crucial role in advancing mass spectrometry as a powerful tool for scientific discovery and application.

Dr. Jaswinder Singh Maras, ILBS, New Delhi



Dr. Jaswinder Singh Maras is a translational scientist whose research focuses on hepatology, systems biology, immunometabolism, multi-omics, and host–microbial interactions. His work integrates metabolomics, proteomics, lipidomics, metaproteomics, transcriptomics, and functional experimental models to uncover molecular mechanisms and clinically relevant biomarkers in liver diseases. His research has significantly advanced understanding of alcohol-related liver disease (ALD), acute liver failure (ALF), acute-on-chronic liver failure (ACLF), gallbladder carcinoma, and cirrhosis-associated immune dysfunction.

A major contribution of Dr. Maras's work has been the identification of hyperoxidized albumin as an active mediator of inflammation, oxidative stress, neutrophil dysfunction, and platelet activation in severe alcoholic hepatitis. His studies have also uncovered novel microbial, fungal, metabolic, and lipid signatures associated with disease progression, mortality, and corticosteroid non-response. Using integrated multi-omics approaches, he has developed biomarker panels with potential applications in precision diagnostics and patient stratification.

Dr. Maras has pioneered bile-based multi-omics profiling for gallbladder carcinoma and identified fungal–lipid interactions that influence outcomes in liver failure. His research has further led to the discovery of therapeutic targets, including kinase- and platelet-mediated pathways, with translational potential for treating inflammatory and fibrotic liver diseases. He has published extensively in leading journals including Journal of Hepatology, Hepatology, Molecular Therapy, Redox Biology, Clinical and Molecular Hepatology, and Liver International. His work bridges fundamental biology and clinical medicine, contributing to the development of precision medicine approaches in hepatology and translational healthcare.

Abstract

Severe alcohol-associated hepatitis (SAH) is a life-threatening condition with high mortality rates and poor response to prednisolone therapy. Identifying reliable early predictors of therapy response and survival is critical. Plasma metabolomics was conducted on 70 SAH patients (50 responders and 20 non-responders) to identify biomarkers for non-response and early mortality. These findings were validated in a cohort of 153 patients and an independent cohort of 245 patients using high-resolution mass spectrometry, machine learning, and severity indices. Temporal metabolic changes indicated interactions between the host and microbiome, with a focus on inflammation and intestinal permeability. Plasma metabolomics revealed that non-responders had significantly higher urobilinogen levels (3.6-fold change). Additionally, a decrease in alpha/beta diversity and temporal metabolic inactivity characterized non-responders. Plasma urobilinogen levels predicted non-response (area under the curve [AUC] > 0.97) and identified non-survivors (AUC = 0.94) with a threshold of >0.07 mg/mL. Urobilinogen levels correlated with bacterial peptides belonging to Firmicutes and Proteobacteria, neutrophil activation, oxidative stress, and pro-inflammatory cytokine production. These changes contributed to non-response by increasing glucocorticoid receptor β expression and compromising intestinal permeability. Fecal microbiota transplantation decreased urobilinogen levels by reducing bilirubin reductase gene-containing microbiota. Plasma urobilinogen >0.07 mg/mL could predict early mortality, and modulation of the gut microbiome may improve outcomes in SAH patients.

Dr. Jerene Mathews, AIIMS Bhopal



Dr. Jerene Mathews is Assistant Professor of Dermatology at AIIMS Bhopal, India. Her clinical and research interests include paediatric dermatology, rare genetic skin diseases, and inflammatory dermatoses, with a particular focus on psoriasis. Her work includes severe and genetically defined phenotypes such as pustular and monogenic psoriasis. She aims to better define the burden and spectrum of rare skin diseases in India and to develop context-appropriate screening, diagnostic, referral, and care pathways for patients.

Abstract: Endotyping in Psoriasis: Toward Practical Precision Care in India

Psoriasis is a chronic inflammatory disease marked by substantial clinical and biological heterogeneity. Uniform approaches to treatment, prognostication, and surveillance for complications are therefore of limited value. Advances in clinical phenotyping and omics now offer an opportunity to move beyond descriptive labels toward biologically informed endotypes that more faithfully reflect underlying disease mechanisms and individual patient trajectories.

In settings such as India, the value of endotyping lies not only in molecular refinement but in its translational practicality. A central question is how endotypes defined through cost-intensive omics can be justified in a low-resource context. The proposed answer is that omics-derived endotypes need not be deployed directly at the point of care; rather, they can be used to identify robust phenotypic markers and affordable biomarker panels that serve as practical surrogates. Such low-cost proxies may support risk stratification, strengthen referral pathways, and help flag patients who require closer monitoring for complications such as psoriatic arthritis and metabolic comorbidity. This approach is especially relevant in low-resource settings, where prioritising high-risk patients at peripheral centres could prevent delayed referral, prolonged uncontrolled disease, permanent disability, and high burden on tertiary care centres.

Translation into routine practice in India will depend on rigorous validation, demonstration of feasibility and affordability, and successful integration in existing patient-care pathways.

Dr. Jyoti Bajpai, Apollo Hospital, Mumbai



Dr. (Prof.) Jyoti Bajpai is a Medical and Precision Oncologist with over 20 years of experience, including 15 years at the Tata Memorial Centre, and currently serves as Lead-Medical and Precision Oncologist at Apollo Hospitals, Mumbai. Trained at the All India Institute of Medical Sciences, Memorial Sloan Kettering Cancer Center, and Johns Hopkins Cancer Center, and a graduate of the European Society for Medical Oncology Leaders Generation Program, she is internationally recognized for advancing precision medicine and immunotherapy across common and rare cancers. She has contributed to global clinical practice guidelines with the European Society for Medical Oncology, the Society for Immunotherapy of Cancer, ABC, EURACAN, and ARIA, and has authored more than 200 peer-reviewed publications. Founder of the Indian Immuno-Oncology Society and a leader within Indian Society of Medical and Pediatric Oncology and Women in Oncology initiatives, she integrates research, education, and policy to strengthen equitable cancer care. Her pioneering work in young and pregnancy-associated breast cancer, national registries, AYA oncology, and cost-effective protocols for low–middle income countries reflect a singular commitment to scientific excellence, survivorship, and global impact.

Dr. Kai Cheng, Quadram Institute, UK



Dr Kai Cheng is a Career Track Group Leader at the Quadram Institute Bioscience. His research focuses on computational metaproteomics, microbiome bioinformatics and AI-enabled analysis of mass spectrometry data. He developed MetaLab, a widely used metaproteomics analysis platform, and is now leading the development of MetaPilot: an integrated research programme designed to make human gut metaproteomics easier to analyse, interpret and reuse. His work aims to connect microbial genetic potential with realised protein-level function and to establish metaproteomics as a routine functional read-out in microbiome research.

Abstract - Bioinformatics: Metapilot Introduction

Metaproteomics directly measures microbial protein expression in complex communities, but analysis is constrained by large, poorly structured search spaces. Microbial gene catalogues provide broad coverage, but their pooled organisation hinders genome-level evidence accumulation, limiting sample-specific refinement and consistent DDA and DIA analysis. Here, we present MetaPilot, a genome-aware workflow using conserved marker-protein evidence to guide adaptive genome-resolved search-space refinement. MetaPilot maps identifications to candidate genomes, ranks them by marginal

peptide contribution, and constructs refined sample-specific search spaces for final identification, quantification and multi-layer reporting.

We evaluated MetaPilot across DDA and DIA datasets from defined mixtures and fecal microbiomes. MetaPilot adapted genome selection to sample complexity while preserving substantial overlap with published peptide identifications and expanding the detectable peptide space. For DIA analysis, iterative refinement increased peptide identification while controlling search-space expansion. In DDA-independent reanalysis of Orbitrap human gut metaproteomes, MetaPilot identified 24.4% more peptides than the published DDA-derived library and more than twice the number identified by the matched DDA-assisted workflow. In the timsTOF DIA-PASEF mouse intestinal dataset, MetaPilot outperformed uMetaP in identification depth and enabled genome-resolved functional interpretation. Together, these results establish that DDA-independent DIA metaproteomics, guided by genome-resolved marker evidence, can exceed DDA-assisted workflows in identification depth.

Dr. Kamal Mandal, GBU, Gujarat



Dr. Kamal Mandal is an Assistant Professor in the Department of Animal Biotechnology, at Gujarat Biotechnology University. Dr. Mandal did his PhD from National Institute of Immunology (NII), New Delhi where he worked on integrative multi-omics strategies to understand cellular differentiation using Sertoli cells as a model system. He then moved to University of California San Francisco (UCSF), for his postdoctoral training and started working synthetic immunology to address novel immunotherapeutics development. Leveraging his extensive proteomics expertise, he developed a new technology platform called “structural surfaceomics” to enable identification of protein conformation-based cancer antigens for CAR-T therapy development. Using this technology, he successfully developed a novel CAR-T therapy against Acute Myeloid Leukemia. Dr. Mandal was recognized with the prestigious “Michelson Prize-2019” for his contribution to the field of synthetic immunology. He also received “Abstract Achievement Award-2022” from American Society of Hematology. Currently, Dr. Mandal works on cross-linking mass spectrometry method developments and its applications in developing antibody/nanobody based therapeutics against infectious diseases.

Abstract

Immunotherapy has emerged as a promising modality of modern medicine. Successful immunotherapeutics development involves identification of a specific cell surface marker against the target cell such tumor cell or pathogen. Cell surface proteins are the portal for the cell to the outside world, making them particularly attractive for therapeutic targeting. More than 70% of the pharmaceutical drugs are targeted to cell surface proteins emphasizing their importance in medicine. However, cell surface proteins are in extremely low abundance (<2%) resulting in their poor representation in typical whole cell proteomics experiments. This necessitates chemical enrichment of cell surface proteins for their reproducible and high confidence identification in mass spectrometers. The cell surface proteins are heavily N-glycosylated, unlike the intracellular proteins. This molecular feature has been successfully exploited to install an enrichment handle exclusively on the cell surface. Such chemical labelling of the cell surface proteins involves glycol-oxidation of the N-glycosylated sugar residues using sodium metaperiodate, followed by installation of biotin using biocytin hydradize. Alternatively, the cells may also be treated with cell impermeable Sulfo-NHS ester chemical biotin probe, to install biotin on the cell surface proteins. In either case, once biotin is installed, the cells may be lysed and the surface proteins may be enriched using streptavidin beads, followed by mass spectrometry and data analysis for protein identification. The identified cell surface proteins may be targeted for immunotherapy with therapeutic antibodies or nanobodies. This strategy may be used for therapeutic targeting of cancer cells as well as pathogen.

Dr. Kaushik Kumar Dey, ICMR-NIRBI, Kolkata



Dr. Kaushik Kumar Dey is a Scientist (Proteomics) at the ICMR–National Institute for Research in Bacterial Infections (ICMR–NIRBI), Kolkata, where he leads proteomics and multi-omics research focused on host–pathogen interactions, antimicrobial resistance, infectious diseases, and translational biomarker discovery. He is establishing advanced mass spectrometry-based proteomics and systems biology platforms to address critical challenges in infectious disease research and precision medicine.

Previously, he served as a Postdoctoral Associate at St. Jude Children's Research Hospital, Memphis, USA (2016–2025), where he applied quantitative and integrative multi-omics approaches to investigate neurodegenerative diseases, particularly Alzheimer's disease. He earned his Ph.D. from IIT Kharagpur in 2016, focusing on proteomics-based biomarker discovery and molecular mechanisms of oral cancer.

With over 15 years of academic and industrial research experience, Dr. Dey has authored more than 25 peer-reviewed publications in leading international journals and is a co-inventor on a U.S. patent application related to Alzheimer's disease biomarkers. He is a recipient of the ICMR Senior Research Fellowship, the Ramalingaswami Re-entry Fellowship, and numerous national and international travel awards. His research integrates proteomics, metabolomics, and systems biology to advance biomarker discovery and precision medicine.

Dr. Kshitij Jadhav, IIT Bombay



Dr. Kshitij Jadhav is an Assistant Professor and Core Faculty member at the **Koita Centre for Digital Health (KCDH), Indian Institute of Technology Bombay (IIT Bombay)**. A clinician-scientist and neuroscientist by training, he works at the intersection of medicine, artificial intelligence, machine learning, and digital health, with a mission to develop innovative data-driven solutions for healthcare challenges.

Dr. Jadhav completed his **MBBS** and **MD (Pharmacology)** from premier medical institutions in Mumbai before pursuing a **Ph.D. in Neuroscience** at the **University of Lausanne, Switzerland**. He further enhanced his research expertise through postdoctoral training in neuroscience at the **University of Cambridge, United Kingdom**.

His current research focuses on **Healthcare Analytics, Artificial Intelligence/Machine Learning, Federated Learning, Medical Data-Efficient AI, and Large Language Models (LLMs) for healthcare applications**. At KCDH, he leads interdisciplinary initiatives that bring together clinicians, engineers, and data scientists to develop scalable and impactful digital health technologies.

Dr. Jadhav is also actively involved in translational AI research for medical imaging and cancer diagnostics. His startup, **Rad AI Pvt. Ltd.**, has gained national recognition for developing AI-powered solutions for breast cancer screening and reporting.

Through his research, teaching, and innovation activities, Dr. Jadhav continues to advance the integration of artificial intelligence into healthcare, contributing to more accessible, efficient, and precision-driven medical care.

Dr. Kunal Goyal, Kokilaben Hospital, Mumbai



Dr. Kunal Goyal is a Consultant Haemato-Oncologist, Bone Marrow Transplant (BMT), and Cellular Therapies specialist at **Kokilaben Dhirubhai Ambani Hospital, Navi Mumbai**. He is a highly accomplished clinician with expertise in the diagnosis and management of hematological malignancies, bone marrow transplantation, and advanced cellular therapies, including CAR-T cell therapy.

Dr. Goyal completed his **MBBS (Gold Medalist)**, **MD (Silver Medalist)**, and **DM in Clinical Hematology**, followed by advanced fellowship training in Bone Marrow Transplantation and Cellular Therapies at **Tata Memorial Centre–ACTREC, Mumbai**. Throughout his career, he has remained actively engaged in cutting-edge hematology research and clinical innovation.

His areas of expertise include autologous and allogeneic bone marrow transplantation, CAR-T cell therapy, leukemia, lymphoma, myelodysplastic syndromes, coagulation disorders, hemoglobinopathies, immunodeficiency disorders, and complex hematological conditions. Dr. Goyal has been involved in more than 200 bone marrow transplants and was part of the pioneering team that contributed to the development and clinical implementation of indigenous CAR-T therapy in India through collaborations involving Tata ACTREC and IIT Bombay.

An active member of professional organizations including ISHBT, ISBMT, ASH, and ASCO, Dr. Goyal has presented research at national and international conferences and continues to contribute to advancing the fields of hematology, stem cell transplantation, and cellular immunotherapy. Guided by his personal philosophy, *"There is always hope beyond what you see,"* he remains committed to delivering innovative, compassionate, and patient-centered care.

Dr. Leyuan Li, Beijing Proteome Research Center, China



Dr. Leyuan Li is a Junior Principal Investigator at the National Center for Protein Sciences (Beijing), also known as the Phoenix Center. She is one of three finalists in the HUPO2024 manuscript competition, where she will present her research, "Revealing Proteome-Level Functional Redundancy in the Human Gut Microbiome Using Ultra-Deep Metaproteomics." Her work is being evaluated for the prestigious "Proteomics Highlight of the Year" award. Dr. Li's expertise lies in metaproteomics and microbial systems ecology. From 2016 to 2022, she was a postdoctoral fellow and research associate in Dr. Daniel Figeys's lab at the University of Ottawa, where she developed in vitro culturing techniques and automated metaproteomics workflows for personalized microbiome drug response assessments. In 2022, she established the Proteome-level Microbial Systems Ecology (ProMiSE) Lab at the Phoenix Center, focusing on metaproteomics and advanced analytical techniques to study the complexities of microbial ecosystems within the human body. Her research aims to deepen our understanding of microbial community dynamics, functional redundancy, and their impact on human health, with a vision to enable future personalized therapeutic interventions through microbiome-based strategies.

Dr. Litika Vermani, CCHRC, Assam



Dr. Litika Vermani is a Senior Scientist at Cachar Cancer Hospital and Research Centre, Assam, India, specializing in cancer genetics, hereditary cancer predisposition, multi-omics research, and molecular diagnostics. She established the hospital's Cancer Genetics Clinic and contributes to molecular diagnostic services that support precision cancer care.

She is a Co-Investigator in a multicentre colorectal cancer multi-omics project and a Co-Principal Investigator in the ICMR-funded Pre-Cancer Genome/Transcriptome Atlas project of the oral cavity. She has received the Lady Tata Memorial Trust Research Grant for a collaborative multi-omics study on esophageal cancer in collaboration with Tata Memorial Hospital, Mumbai, and a Department of Health Research Start-Up Grant for research on founder mutations and germline cancer genetics.

Dr. Vermani earned her PhD in colorectal cancer genetics from Mizoram University and a Master's degree in Human Genetics from the University of Jammu, where she graduated as a gold medalist. Her research over the past nine years has focused on the genetic basis of cancer susceptibility.

Previously, she worked at Karolinska University Hospital and Karolinska Institute in Stockholm, Sweden, investigating familial cancers and low-penetrance genetic variants associated with colorectal, gastric, breast, and endometrial cancers. Her work has been presented internationally, and she was selected as the only scientist from India for an advanced data curation course organized by LOVD and UNESCO. She continues to advance cancer genetics through research, diagnostics, and personalized cancer prevention.

Dr. Luman Wang, Peking University, China



Dr. Luman Wang is an Associate Professor at the Department of Health Informatics and Management, School of Health Humanities, Peking University.

Luman Wang's research focuses on intelligent medical data analysis and the development of functional beta diversity for metaproteomics data analysis. She and her colleagues developed a functional beta-diversity method PhyloFunc, that integrates phylogenetic, taxonomic, and functional information to better capture microbial diversity in gut metaproteomes, offering sensitive insights into microbial ecology responses in health and disease applications. They also developed an open-source Python package PhyloFunc. Her research has been published in related journals such as *Microbiome*, *Nature Communications*, and *Proteomics*. Luman Wang has also developed and taught several courses in medical informatics for undergraduate and graduate students and has authored nationally planned textbooks in the field.

Abstract: **Power Analysis and Functional Beta-diversity**

Metaproteomics is a powerful tool for characterizing the functional profiles of microbial communities by directly measuring protein expression. As the application of metaproteomics continues to expand, researchers face two important challenges: designing studies with sufficient statistical power and extracting meaningful biological insights from increasingly complex datasets. This session begins with an introduction to statistical power analysis in metaproteomics. It explains the role of sample size, effect size, and statistical power in study design, and demonstrates how power analysis can help researchers make informed decisions before data collection. Through practical examples, power analysis can improve experimental efficiency, increase the likelihood of detecting biologically relevant signals, and support more reliable conclusions.

The second part focuses on functional beta-diversity, a key concept for understanding differences in microbial community functions across samples. Traditional diversity metrics often emphasize taxonomic composition and may overlook

functionally relevant changes. To address this challenge, this session introduces PhyloFunc, a functional beta-diversity framework that integrates phylogenetic, taxonomic, and functional information to provide a more comprehensive view of metaproteomic variation. Furthermore, this session presents the Python package PhyloFunc to illustrate how this approach can reveal biologically meaningful patterns and environmental responses in real-world cases.

Dr. Mahesh Kulkarni, NCL, Pune



Dr. Mahesh J Kulkarni is a Chief Scientist and Chair, Biochemical Sciences Division at CSIR National Chemical Laboratory, Pune. He is instrumental in setting up a mass spectrometry and proteomics facility at NCL. He has guided more than 20 Ph.D. students and published 118 articles in peer-reviewed journals to date. Dr. Kulkarni has led several important projects as a Principal Investigator and a key team member of the Phenome India Project. Dr. Kulkarni has made significant contributions to understanding protein glycation in diabetes using mass spectrometric and proteomics approaches. He is an editorial member of reputable journals, including Clinical Proteomics and the Journal of Proteins and Proteomics. He was elected Fellow of the Maharashtra Academy of Sciences in 2016. He was awarded the Raman Research Fellowship to visit the University of Turku, Finland, in 2016.

Dr. Manisha Choudhary, ARGU, Guwahati



Dr. Manisha Choudhury currently serves as an Assistant Professor in the Department of Biotechnology at The Assam Royal Global University, Guwahati, Assam. She has extensive experience in proteomics, genomics, Next-Generation sequencing, and computer-aided drug design. Her expertise spans across designing of novel peptide markers using computational approaches and their pre-clinical trials. She works at the intersection of venom proteomics, and identification of novel peptides with therapeutic potential. Her expertise also includes systems biology and big data analysis. Her numerous accolades include the ANRF-National Postdoctoral fellowship (2025-2027), the DBT-RA Postdoctoral fellowship (2023-2025), and the CSIR-Senior Research Fellowship (2016-2018). She also received the Indian Research Initiative (IRI) Fellowship from the National University of Singapore (2013-2014).

Dr. Martin Breitkreuz, MMI, Germany



Dr Martin Breitkreuz is an accomplished bioscientist and industry expert who serves as the Marketing, Product, and Application Manager at Molecular Machines & Industries (MMI), a position he has held since 2022.

Martin completed his academic studies in Biochemistry in Germany and earned his PhD in Cardiovascular Physiology, blending a rigorous research foundation with deep technical expertise.

At MMI, Martin leverages his scientific background to bridge the gap between cutting-edge technology and real-world laboratory applications. Utilizing MMI's state-of-the-art instruments for single-cell isolation, he is dedicated to supporting researchers in establishing highly optimised, custom workflows. Whether the goal is isolating single cells or selecting larger regions of interest (ROI), Martin provides precise guidance on utilising advanced Laser Microdissection or high-precision Cell Picking technologies.

Abstract: Finding "The One": How Microdissection and Cell Picking Uncovers the Hidden World of Single Cells

Understanding single cells is fundamental to unlocking their biological secrets. To this end, Spatial Biology currently leads the forefront in revealing the precise cellular architecture of tissues in situ. For example, by concurrently maximising

multiplexing and resolution, Spatial Omics derive a cell's biomarker co-expression profile and how cells organise and interact to influence the tissue microenvironment.
A deciding factor for such a Spatial Biology study is the need for coherence between spatial and molecular information.
High Resolution Imaging combined with Laser Capture Microdissection (LCM) can convey this coherence, employing microscopy to identify and select cells of interest.
In this presentation, we showcase how MMI's CellCut Laser Microdissection platform provides a fully auditable workflow for single cell biology. We show how our patented CapLift and Predefined Target Positioning (PTP) feature allows high sample integrity and controlled collection of single cells to maximise the number of samples collected for downstream applications.
Finally, we show our systems' versatility and how MMI's High-throughput CellCut HT System enables fast processing of multiple samples in a single run or multiple regions within a single sample, allowing comprehensive analysis of tissue for cellular heterogeneity.

Dr. Natasha Lalwani, Shalby Hospital, Ahmedabad



Dr. Natasha Lalwani is a Consultant Surgical Oncologist at **Shalby Hospital, Ahmedabad**, with specialized expertise in **Head & Neck Oncology, Oral Oncology, and Microvascular Reconstructive Surgery**. She holds a **Bachelor of Dental Surgery (BDS)**, a **Master of Dental Surgery (MDS) in Oral and Maxillofacial Surgery**, and advanced **Fellowship training in Head & Neck Oncology**.

With over nine years of dedicated surgical experience and more than 1,000 successful surgeries to her credit, Dr. Lalwani has established herself as a highly skilled and compassionate cancer surgeon. Her clinical practice focuses on the comprehensive management of head and neck cancers, including complex oral malignancies and advanced oncological procedures requiring intricate reconstruction.

A key area of her expertise is **microvascular reconstructive surgery**, where she employs state-of-the-art techniques to restore form, function, and aesthetics following cancer resection. Her approach combines surgical precision with personalized patient care, ensuring optimal clinical outcomes and enhanced quality of life for cancer survivors.

Beyond the operating room, Dr. Lalwani is deeply committed to raising awareness about cancer prevention, promoting early diagnosis, and supporting rehabilitation initiatives for patients and caregivers. She strongly advocates a holistic approach to cancer care that addresses not only disease treatment but also long-term functional and emotional well-being.

Through her dedication to excellence, innovation, and compassionate care, Dr. Lalwani continues to make significant contributions to the field of surgical oncology and head & neck cancer management.

Dr. Nattawadee Panyain, Mahidol University, Thailand



Dr. Nattawadee Panyain is a Lecturer in the Department of Biochemistry, Faculty of Science, Mahidol University, Thailand. She earned her Ph.D. in Chemical Biology from Imperial College London, followed by a postdoctoral fellowship at EPFL, Switzerland, specialising in mass spectrometry-based proteomics and protein lipidation. Her research bridges chemistry and biology, focusing on mass spectrometry-based proteomic profiling, chemical proteomics, and activity-based protein profiling (ABPP). During her postdoctoral training, she explored the molecular mechanisms of infectious diseases and analysed whole proteomes, interactomes, and palmitomes.

As a Principal Investigator at Mahidol University, Dr. Panyain leads an independent research group applying chemical proteomics and ABPP to investigate disease mechanisms and identify novel drug targets. Her team employs competitive ABPP to profile bioactive natural compounds in disease-relevant cell models and utilises quantitative mass spectrometry to characterise proteome changes in patient-derived samples. A further focus is serine hydrolase profiling using activity-based probes across physiological and pathological contexts. Her research is supported by the National Research Council of Thailand, the UK Biochemical Society, and the Thailand Science Research and Innovation Fundamental Fund. Dr. Panyain is committed to advancing the global proteomics landscape through innovative methodologies and international collaboration.

Dr. Papia Acharjee, BHU, Varanasi



Dr. Papia Acharjee, Assistant Professor, Department of Zoology at Banaras Hindu University, is a domain expert in neuroproteomics and translational neurobiology expert with over a decade of experience in proteomic sample preparation and biological variation interpretation using network analysis. Her work has consistently integrated high-resolution LC-MS/MS with systems-level data interpretation to uncover molecular mechanisms in liver dysfunction led hepatic encephalopathy and related neuroinflammatory states. As PI on multiple funded projects, she has led proteomic investigations from bench to bioinformatics, with recent first/corresponding author publications. Her proven expertise ensures high-quality sample processing and robust biological insights from proteomic datasets.

Dr. Poonam Deshpande, DES Pune Univ. Pune



Dr. Poonam Deshpande is a distinguished academician and researcher at DES Pune University, Pune, with expertise in life sciences, biotechnology, and translational biomedical research. Her research interests include molecular biology, genomics, biomarker discovery, and disease biology, with a focus on translating laboratory findings into meaningful healthcare applications. She has contributed to several research and educational initiatives aimed at strengthening interdisciplinary scientific training and innovation. An accomplished educator and mentor, Dr. Deshpande has guided numerous students and researchers while actively contributing to scientific publications and collaborative research programs.

Dr. Pramod P. Wangikar, IIT Bombay



Prof. Pramod P. Wangikar is a Professor in the Department of Chemical Engineering at Indian Institute of Technology Bombay and a leading researcher in biotechnology, metabolic engineering, and bioprocess development. He earned his Bachelor's degree in Chemical Engineering from Institute of Chemical Technology and completed his Ph.D. at the University of Iowa.

His research focuses on cyanobacterial metabolism, metabolic engineering for the production of biofuels and high-value chemicals, biocatalysis, and industrial bioprocess development. Combining experimental and computational approaches, his work aims to develop sustainable and commercially viable biotechnological solutions. He has published more than 80 research papers, mentored over 18 Ph.D. scholars, and secured numerous grants from government agencies, industry partners, and international funding programs.

Prof. Wangikar currently serves as Professor-in-Charge of the Wadhwani Research Centre for Bioengineering and Coordinator of the DBT-Pan IIT Centre for Bioenergy, where he leads interdisciplinary research and innovation initiatives. He has established extensive collaborations with academic institutions and industries worldwide and actively promotes translational research, entrepreneurship, and industry-academia partnerships. His contributions have significantly advanced biotechnology, bioenergy, and bioprocess engineering in India and beyond.

Dr. Prasanna Venkatraman, ACTREC, Navi Mumbai



Dr. Prasanna Venkatraman is a distinguished scientist at the Advanced Centre for Treatment, Research and Education in Cancer (ACTREC), Tata Memorial Centre, Mumbai, India. She is widely recognized for her contributions to cancer biology, molecular oncology, and translational cancer research. Her research focuses on understanding the molecular mechanisms that drive cancer initiation, progression, and therapeutic resistance, with particular emphasis on signaling pathways, tumor biology, and the identification of novel biomarkers and therapeutic targets.

Dr. Venkatraman has led several innovative research programs integrating molecular biology, genomics, proteomics, and functional studies to investigate cancer pathogenesis and improve precision oncology strategies. Her work has provided valuable insights into the complex interactions between tumor cells and their microenvironment, contributing to the development of more effective diagnostic and therapeutic approaches. She has published extensively in leading international journals and has been actively involved in collaborative research initiatives with national and international institutions.

In addition to her research accomplishments, Dr. Venkatraman is a dedicated mentor and educator who has trained numerous students and young scientists in the fields of cancer biology and biomedical research. Through her scientific leadership and commitment to translational research, she continues to contribute significantly to advancing cancer science and improving patient care through innovative, research-driven solutions.

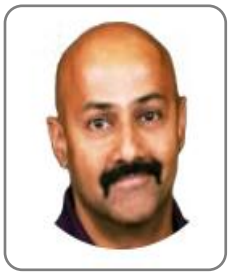
Dr. Pratibha Sharma, IHBAS, Delhi



Dr. Pratibha Sharma is a trained neuroscientist and translational researcher with over 1.5 decades of experience in clinical biomarkers research, including 7+ years as a Principal Investigator. She earned her Ph.D. in Neurosciences from All India Institute of Medical Sciences (AIIMS), New Delhi, specializing in proteomics-driven insights into Alzheimer's and Parkinson's disease. Currently a Senior Scientist and PI at IHBAS, Delhi, she leads multidisciplinary research on Neurodegenerative disorders. Dr. Sharma's expertise lies in bridging traditional proteomics with contemporary molecular omics, including aggregation assay mechanisms and exosome profiling. She has secured several government research grants from ICMR, DHR, DST & CSIR and authored over 25 PubMed-indexed publications. Throughout her career, she has developed innovative methods for isolating neurons and exosomes

and established non-invasive biomarkers for cardiovascular disorders, such as Uromodulin (UMOD) for coronary artery disease. Beyond her research, she is an active mentor and an experienced reviewer for 18+ PubMed-indexed journals, while also serving on the Editorial Boards of the Journal of CNS Diseases and Frontiers in Genetics. She has established an independent lab dedicated to translating clinical biomarkers into "living diagnostics" to deliver bench-to-bedside utility.

Dr. Pratik Jagtap, University of Minnesota, USA



Dr. Pratik Jagtap is a Research Assistant Professor in the Department of Biochemistry, Molecular Biology and Biophysics at the University of Minnesota, USA, and a globally recognized expert in computational proteomics, metaproteomics, proteogenomics, and multi-omics data analysis. Hsutee is a key leader of the Galaxy-P project, an internationally acclaimed open-source platform that develops accessible and reproducible bioinformatics workflows for mass spectrometry-based proteomics and multi-omics research. His research focuses on developing advanced analytical and computational workflows for the analysis of complex biological datasets, with particular emphasis on metaproteomics, proteogenomics, and data-independent acquisition (DIA) proteomics.

Dr. Jagtap has played a pivotal role in advancing bioinformatics tools and community resources that enable researchers worldwide to perform large-scale proteomics and microbiome studies. His work has significantly contributed to understanding the functional dynamics of microbial communities through mass spectrometry-based metaproteomics and integrative multi-omics approaches. He has also been actively involved in international initiatives aimed at standardizing and improving metaproteomics methodologies and data analysis workflows.

With a career spanning academia, industry, and international research institutions, Dr. Jagtap has held research positions at the University of Michigan, the Max Planck Institute for Developmental Biology, and the University of Minnesota. He has authored numerous influential publications and is widely recognized for his contributions to proteomics informatics, open science, and computational biology. Through his research, leadership, and training efforts, he continues to advance the fields of proteomics, metaproteomics, and systems biology globally.

Dr. Purvi Bhatt, NMIMS, Mumbai



Dr. Purvi Bhatt is Associate Professor and Head, Department of Biological Sciences, at SVKM's NMIMS Sunandan Divatia School of Science, Mumbai. She holds a Ph.D. in Biochemistry from the National Institute for Research in Reproductive Health (ICMR), Mumbai, and UG and PG degree in Microbiology from Mithibai College. With over 22 years of academic and research experience, including a postdoctoral fellowship at New York University (NYU) Medical Center (2003-2006), her work primarily focuses on cancer biology with a particular emphasis on breast cancer therapeutics and therapy-induced senescence. Her current work explores therapy-induced senescence in cancer, identification of senescence-associated biomarkers using multi-omics approach, and development of novel therapeutic strategies targeting cancer progression and relapse.

She has guided seven Ph.D. scholars (with two ongoing) and has several publications to her credit in peer-reviewed journals. Her recent publications include work on therapy-induced senescence in breast cancer via cGAS–STING pathway inhibition, and nanoparticle-based methotrexate delivery in breast cancer etc.

Dr. Bhatt is actively engaged in academic leadership, having served as I/C Dean at NMIMS between Nov 2022 to Dec 2023. She is also VC-nominated RRC member for Biotechnology at University of Mumbai, is also on Boards of Studies for several leading colleges in Mumbai and is actively involved in various academic and professional bodies.

Dr. Rajeev Kumar, CCHRC, Assam



Dr. Rajeev Kumar is a distinguished clinician-scientist and healthcare leader associated with the **Cachar Cancer Hospital and Research Centre (CCHRC), Silchar, Assam**, one of the leading cancer care institutions serving northeastern India. With extensive experience in oncology, cancer diagnostics, and patient-centered healthcare, he has played a significant role in advancing cancer treatment and research in the region.

Dr. Kumar has been actively involved in the development and delivery of comprehensive cancer care services, focusing on improving access to quality oncology treatment for patients from underserved and geographically remote communities. His professional interests encompass cancer diagnosis, multidisciplinary oncology care, clinical research, cancer prevention, and community outreach initiatives aimed at promoting early detection and awareness.

At CCHRC, Dr. Kumar collaborates closely with clinicians, researchers, and healthcare professionals to strengthen evidence-based cancer management and improve treatment outcomes. His work emphasizes the integration of modern diagnostic technologies, personalized treatment approaches, and compassionate patient care. In addition to his clinical responsibilities, he actively contributes to academic and research activities that support innovation and capacity building in oncology.

Dr. Kumar is deeply committed to enhancing cancer care infrastructure and expanding research opportunities in northeastern India. Through his dedication to clinical excellence, education, and translational research, he continues to make valuable contributions toward improving cancer outcomes and healthcare delivery for patients across the region.

Dr. Rajiv Kumar Kaushal, TMH, Mumbai



Dr. Rajiv Kumar Kaushal is a distinguished oncopathologist and academician currently serving as Professor of Onco-Pathology at Tata Memorial Hospital, Mumbai, one of India's premier cancer care and research institutions. With more than two decades of experience in diagnostic pathology, cancer biomarker research, and molecular oncology, he has made significant contributions to advancing cancer diagnosis and personalized oncology care in India.

Dr. Kaushal obtained his MD in Pathology from Tata Memorial Hospital (2004–2007) and subsequently joined Tata Memorial Hospital as faculty. Over the years, he progressed through various academic positions, serving as Assistant Professor and later Clinical Professor before attaining the position of Professor in the Department of Onco-Pathology. Prior to joining Tata Memorial Hospital, he completed his residency training at the Postgraduate Institute of Medical Education and Research (PGIMER), Chandigarh.

His research interests encompass cancer pathology, molecular oncology, cancer biomarkers, immunohistochemistry, thoracic pathology, lung cancer, gastrointestinal malignancies, cytology, and digital pathology. Dr. Kaushal has authored and co-authored over 230 scientific publications, which have received thousands of citations, reflecting his substantial impact on cancer research and pathology. His work has contributed to improved understanding of tumor biology, diagnostic accuracy, and translational cancer research.

A strong advocate of technological innovation in pathology, Dr. Kaushal has been actively involved in promoting digital pathology and artificial intelligence–enabled diagnostics. He is recognized internationally for his contributions to modernizing pathology workflows and enhancing cancer diagnostics through digital transformation. He also serves in leadership roles within the digital pathology community, including his association with the Asian Society of Digital Pathology, where he has contributed to educational initiatives and professional collaborations across Asia.

Through his combined roles as clinician, researcher, educator, and mentor, Dr. Rajiv Kumar Kaushal continues to play a pivotal role in advancing oncopathology, cancer research, and precision oncology, while training the next generation of pathologists and cancer specialists in India.

Mr. Ramaswami R, Bruker, India



Ramaswami R. is a seasoned business leader and analytical sciences professional with over three decades of experience in scientific instrumentation, mass spectrometry, chromatography, and commercial operations across India and South Asia. He currently serves as Director – Commercial Operations (India and South East Asia) at Bruker Daltonics, where he leads business strategy, market development, and commercial operations for advanced analytical and mass spectrometry solutions across academia, life sciences, pharmaceuticals, clinical diagnostics, food, environmental, and industrial sectors.

Prior to joining Bruker, Ramaswami held senior leadership positions at Bruker Chemical and Applied Markets and Agilent Technologies, where he played a pivotal role in expanding analytical instrumentation markets and strengthening customer engagement across the region. His extensive expertise encompasses strategic sales, business development, market expansion, customer support, and team leadership.

A graduate in Chemistry with an MBA in Marketing from Sikkim Manipal University, Ramaswami combines strong technical knowledge with exceptional commercial acumen. Throughout his career, he has successfully built and led high-performing teams, fostered industry-academia collaborations, and driven the adoption of cutting-edge analytical technologies.

Recognized for his leadership, customer-centric approach, and commitment to scientific advancement, Ramaswami continues to contribute significantly to the growth of analytical sciences and life science research across India and Southeast Asia.

Dr. Rashmi Rana, Sir Ganga Ram Hospital (SGRH), Delhi



Dr. Rashmi Rana, Professor at the Department of Biotechnology & Research, Sir Ganga Ram Hospital (SGRH), Delhi, and an adjunct faculty and Ph.D. coordinator at MAHE, Manipal and Course Coordinator, PG Diploma in Clinical Research and Regulation at SGRH. Dr. Rana is a leading researcher in the fields of brain tumor (Glioma and Meningioma) diagnostics, dengue, sepsis, and chronic kidney disease (CKD). Since joining SGRH in 2017, Dr. Rana's research has focused on early diagnosis and therapeutic strategies for gliomas, a type of aggressive brain tumor. Her work has led to the identification of LGALS3BP as a promising biomarker for early glioma detection, enabling better prognosis and monitoring of tumor progression across glioma grades (I-IV). Dr. Rana is now pursuing innovative strategies for glioma treatment, utilizing a three-dimensional approach. She aims to silence LGALS3BP to inhibit tumor growth and progression. Additionally, Dr. Rana is employing CRISPR gene-editing technology to correct mutated genes that drive glioma. Her research also includes developing specialized machinery to cross the blood-brain barrier, delivering chemotherapy drugs directly to tumor sites for improved treatment efficacy while minimizing side effects. Alongside her glioma work, Dr. Rana is actively involved in research on dengue, sepsis, and CKD, expanding her expertise in diverse areas of biomedical science. Her ground breaking contributions have earned her numerous prestigious awards, including the ESMO, HUPO, and EMBO fellowships, the Bill & Melinda Fellowship in 2023, the HCFI Dr. K. K. Aggarwal Research Innovation Fund Award, DST Young Scientist Award, NAMS Fellow, VIHA Young Scientist Award, Part of EMBO leadership programme, NAMS task force member on vector borne diseases, Convenor in Proteomic Society of India, ASSOCHAM research excellence award and the FCR Award from Harvard. She also serves as an editor for several journals and publishing houses. She awarded S. Nundy Best Published Research Article, 2025. She has

published more than 67 articles in International and National journals. Recently, Recently She established a Multi-Omics Core Facility in SGRH, Delhi. Currently, Dr. Rana is leading five ongoing research projects and completed three project successfully, while mentoring team of scientists, doctoral, and graduate students. Her work continues to make significant strides in the fields of Brain Tumor Research and therapeutic innovations.

Abstract: Clinical Proteomics and Personalized Medicine: Shaping the Future of Healthcare

Introduction: Clinical proteomics is the large-scale study of proteins expressed in cells, tissues, and biological fluids under specific physiological or pathological conditions. Since proteins are the primary functional molecules in biological systems, proteomic analysis provides valuable insights into disease mechanisms, biomarker discovery, and therapeutic responses. The integration of clinical proteomics with personalized medicine has revolutionized healthcare by enabling patient-specific diagnosis and treatment strategies.

Methods: Clinical proteomic studies employ advanced technologies such as mass spectrometry (MS), two-dimensional gel electrophoresis (2D-GE), liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). Biological samples, including blood, urine, and tissue biopsies, are analyzed to identify and quantify protein expression patterns associated with diseases. Bioinformatics tools are then used to interpret complex proteomic datasets and identify clinically relevant biomarkers.

Results & Discussion: Clinical proteomics has significantly contributed to the identification of disease-specific protein biomarkers for cancer, cardiovascular disorders, neurodegenerative diseases, and infectious conditions. These biomarkers facilitate early diagnosis, disease monitoring, prognosis, and prediction of treatment outcomes. In oncology, proteomic profiling helps classify tumor subtypes and select targeted therapies, improving treatment efficacy while minimizing adverse effects. Furthermore, proteomic analyses reveal molecular pathways involved in disease progression, supporting the development of novel therapeutic targets. Despite challenges such as sample complexity, data standardization, and high analytical costs, continuous advancements in proteomic technologies and computational approaches are enhancing their clinical applicability. Thus, clinical proteomics serves as a cornerstone of personalized medicine, paving the way for more precise, predictive, and patient-centered healthcare in the future.

Dr. Ratnasekhar CH, CSIR-CIMAP, Lucknow



Dr. Ratnasekhar CH is a Senior Scientist and Group Leader of the Metabolomics & Cell Metabolism Laboratory at CSIR-Central Institute of Medicinal and Aromatic Plants (CSIR-CIMAP), Lucknow, India. He leads the institute's high-throughput Metabolomics Facility and has over 15 years of experience in metabolomics, lipidomics, metabolic flux analysis, analytical chemistry, chemometrics, machine learning, and mass spectrometry-based characterization of complex biological systems.

He obtained his Ph.D. in Metabolomics from CSIR-Indian Institute of Toxicology Research (IITR), India. His research integrates LC-MS, GC-MS, Orbitrap-HRMS, NIR-based metabolomic fingerprinting, and systems metabolism for applications in medicinal and aromatic plants, food authentication, natural products research, neurological disorders, circadian biology, and translational metabolomics.

Dr. Ratnasekhar has held postdoctoral research positions at the University of Cambridge, University College London, The Francis Crick Institute, Queen's University Belfast. As Principal Investigator, he has secured six competitive research grants from DST, CSIR, DBT, and ICMR totaling approximately ₹6.6 crore.

He has authored more than 65 peer-reviewed publications, invited reviews, and book chapters in leading journals, including Nature Communications, TrAC Trends in Analytical Chemistry, Food Chemistry, Talanta, Journal of Pharmaceutical Analysis, Molecular Systems Biology, and Free Radical Biology and Medicine. His publications have received over 1,600 citations, with an h-index exceeding 24.

Abstract: Metabolomics, lipidomics and 13C flux-based approches to investigate Celllular metabolism

Introduction: Metabolomics, lipidomics, and stable isotope-assisted metabolic flux analysis have emerged as powerful tools for understanding cellular metabolism in health and disease. In neurological disorders, including Parkinson's disease and related neurodegenerative conditions, metabolic dysfunction often precedes overt pathology and involves alterations in mitochondrial function, redox homeostasis, neurotransmitter metabolism, and lipid remodeling. Recent advances in Orbitrap high-resolution accurate mass spectrometry (HRAMS) have significantly enhanced our ability to comprehensively characterize these metabolic perturbations. This talk will provide an overview of LC-Orbitrap HRAMS-based analytical workflows for metabolomics, lipidomics, and fluxomics and demonstrate their applications in investigating neurological disorders using Drosophila melanogaster models.

Methods: The session will cover experimental design, sample preparation, LC-Orbitrap HRAMS data acquisition, MS/MS-based metabolite and lipid annotation, and stable isotope (^13C)-tracer approaches for metabolic flux analysis. Strategies for data processing, chemometrics, pathway analysis, machine learning-assisted interpretation, and biological integration will also be discussed.

Results and Discussion: Representative case studies from Drosophila models of neurodegeneration will illustrate how integrated metabolomics, lipidomics, and fluxomics can reveal alterations in energy metabolism, mitochondrial function, oxidative stress pathways, neurotransmitter biosynthesis, and lipid homeostasis. Particular emphasis will be placed on understanding metabolic rewiring associated with Parkinson's disease-like pathology and identifying potential metabolic biomarkers and therapeutic targets. The workshop will highlight practical considerations, analytical challenges, and emerging opportunities for combining high-resolution mass spectrometry with systems metabolism approaches to advance neurological research and translational metabolomics.

Dr. Ravi Trivedi, Zydus, Ahmedabad



Ravi Kumar Trivedi, Ph.D. in Pharmaceutical Chemistry, has 28 years of experience in Drug Discovery and Development of small and large molecules, with expertise in Drug Metabolism and Pharmacokinetics and translational research. He is currently Vice-President and Head of the BA-DMPK function at Zydus Research Centre, a leading and proven discovery/development organization for small and large molecules. Zydus has a proven track record of bringing NCEs and Biosimilars to market. His current role also involves supporting projects in Complex Generics, CGT, Animal Health, and Biotech/Large Molecules. In additional role, he leads innovation initiatives across business units. He is experienced in transitioning Discovery programs into Phase I (15), Phase II (11), and Phase III (5) clinical trials. He was part of the team that launched five Biosimilars in various markets across the globe. Earlier, he worked in various capacities with Dr Reddy's Labs, Nektar Therapeutics, Jubilant Biosys, Biocon-BMS R&D Centre, and Sun Pharma Advanced Research Centre, taking on increasing roles and responsibilities. His areas of interest are translational research, MIDD (HDP, PK-PD correlation, PBPK, PoP PK) for discovery & developmental candidates, and achieving operational excellence/team building. He is an ardent supporter of utilizing new technologies at various stages of Discovery and Development.

He is associated with various scientific forums, viz., founder member and served as the presiding chair for the APA-India chapter for the year 2023-24, as well as represented India at the Global Bioanalytical Consortium. He has published over 35 articles in peer-reviewed international journals, holds three patents, and regularly delivers scientific talks at various scientific forums. He is also an honorary Professor at Kumaon University, part of course content design for Marwadi University, Rajkot & PDEU Gandhinagar.

Abstract

Metabolomics and lipidomics describe the comprehensive analysis of endogenous metabolites and lipid species, providing insight into the biochemical state of a biological system and its response to drugs or disease. While pharmacokinetics explains what the body does to a drug, metabolomics and lipidomics (along with genomics-transcriptomics-proteomics)

elucidate what the drug does to the body by capturing dynamic changes in metabolic pathways and lipid networks, enabling a systems level understanding of therapeutic response and toxicity. These analyses are enabled by advanced mass spectrometry platforms, particularly high-resolution mass spectrometry (HRMS) and targeted LC-MS/MS approaches, which offer high sensitivity, selectivity, and broad coverage across diverse biological matrices. Accurate quantitation requires robust workflows incorporating optimized sample preparation, internal standards, data normalization, and reproducibility to ensure reliable translation from discovery to developmental stage studies under regulated environment. The applications can be demonstrated by few of the following points:

- Identification and quantitation of endogenous metabolites and lipid species as biomarkers of efficacy and toxicity,
- Characterization of perturbed metabolic pathways to understand mechanism of action and disease biology,
- Lipid profiling to investigate roles in inflammation, oncology, and metabolic disorders, and
- Integration with pharmacokinetics, proteomics, and systems pharmacology to support model-informed drug development (MIDD).

Tracking alterations in metabolite and lipid profiles across possible tissues, biofluids, and populations under healthy versus disease conditions (following treatment as well) enables biomarker discovery, supports patient stratification, and strengthens translational research. Further, incorporation of metabolomics and lipidomics data into integrative models enhances prediction of drug response, facilitates early go/no-go decisions, reduces development risk, and advances precision medicine.

Dr. Ritu Kulshrestha, VPCI, Delhi



Dr. Ritu Kulshrestha, is the Director Professor and Head, Department of Pathology, V.P. Chest Institute, University of Delhi since 2012. She established the Molecular Pathology laboratory at VPCI in 2009 and since then has been leading her research group in the field of non-communicable lung diseases including Lung fibrosis and lung cancer and the nanotherapy of these diseases. Her group has been regularly performing Genomics (EGFR, ALK-1, BRAF, KRAS, ROS, PD-L1 etc), Cell culture, nanotherapeutics for personalized therapy of lung cancer. She has authored 52 papers in National and International Journals, 17 Book chapters and edited 4 books. She has co-supervised 8 MD thesis and 3 PhD thesis. Dr Ritu Kulshrestha has received two international fellowships. She has been the Member-Secretary of Dept of Health research funded VPCI-DHR- ICMR Multidisciplinary Research Unit from 2014-2019. Since 2010 she has been the Principal Investigator of 12 extramural funded research projects (funded by DST-fast Track, SERB, ICMR- nano Task Force, DHR, VPCI-DHR-ICMR-MRU, CSIR, LSRB-DRDO).

Her areas of research include Lung fibrosis, lung cancer and nanotherapy. She has worked to elaborate the pathophysiological and proteomic basis of pulmonary fibrosis and Pulmonary artery hypertension using invitro and invivo tools viz A-549, U-937, THP-1 cell lines and Wistar Rat model after bleomycin induced lung injury and Cigarette smoke and highlighted involvement of important Signaling pathways. She has also worked on attenuation of lung and vascular remodelling by using repurposed drugs-N-acetylcysteine, Sildenafil, Bosentan, Pioglitazone. Dr Kulshrestha has prepared nanoformulation of Pirfenidone for inhalational therapy in bleomycin induced rat model of lung fibrosis. She is also assessing the efficacy of conjugation of nano-formulations with chemotherapeutic and antifibrotic agent in lung cancer cell line to prevent EMT. The results of her ICMR-Nanotask force project (2019-23) have been filed for Patent. She has research projects and collaborations with AIIMS Delhi, IIT Kanpur, INMAS DRDO, DIPAS, Jamia Milia Islamia etc. Dr Ritu Kulshrestha is the Founder Secretary of the Pulmonary Pathology Society of India which is registered with Headquarters at Department of Pathology, V.P. Chest Institute, in 2008.

Dr. Rohit Budhraja, Zydus, Ahmedabad



Dr. Rohit Budhraja possesses over 13 years of experience in mass spectrometry-based proteomics, specializing in the discovery and validation of biomarkers. He received his Ph.D. in Biochemistry under the mentorship of Dr. Lorenz Adrian at the Helmholtz Centre for Environmental Research in Leipzig, Germany. He completed his postdoctoral training at the Mayo Clinic in the USA, under the mentorship of Dr. Akhilesh Pandey and Dr. Eva Morava. At Mayo Clinic, Dr. Rohit pioneered several methodologies in quantitative proteomics and glycoproteomics to discover biomarkers and gain insights into the pathomechanisms of different cancers and congenital glycosylation disorders. Prior to Ph.D., he has associated with Centre for Cellular & Molecular Biology, Hyderabad and Lambda Therapeutic Research Ltd, Ahmedabad. Currently, he is engaged at Zydus Research Centre as a Senior Scientist, where he focuses on developing and integrating a quantitative multi-omics approach, including proteomics, glycoproteomics and metabolomics, into various drug discovery and development initiatives. He has presented his research at multiple national and international conferences and has published over 30 articles in peer-reviewed journals. He holds membership in various scientific societies, including the American Society of Mass Spectrometry (ASMS), the Society for Glycobiology (SFG) and the Proteomics Society, India (PSI).

Abstract: Exploring Post-Translational Modifications Using Mass Spectrometry

Post-translational modifications (PTMs), including phosphorylation, glycosylation, acetylation, and ubiquitination are critical regulators of protein function, enabling dynamic control of cellular processes in both normal physiology and disease. These covalent modifications alter protein conformation, interaction networks, and cell signaling, thereby regulating complex pathways. Among them, phosphorylation and glycosylation are particularly prominent, facilitating signal transduction and structural heterogeneity, respectively. Phosphoproteomics enables quantitative mapping of kinase-driven signaling dynamics, while glycoproteomics facilitates characterization of glycoforms and microheterogeneity at the glycopeptide level. Liquid chromatography–tandem mass spectrometry (LC–MS/MS) has emerged as a powerful platform for high-resolution, site-specific characterization of PTMs. In this talk, I will present LC–MS/MS-based workflows for the analysis of phosphorylation and glycosylation, focusing on experimental design, enrichment strategies, data acquisition, and interpretation of tandem mass spectra. Computational approaches for peptide identification, PTM site localization, and confidence evaluation will also be outlined, along with common analytical challenges such as low abundance, spectral complexity, and ambiguity in modification assignment. Work from my research will be presented, demonstrating how these approaches have been applied in congenital disorders of glycosylation and cancer to uncover alterations in phosphorylation and glycosylation of various cellular and secreted proteins. These studies provide insights into disease pathomechanisms and support the identification of biomarkers, therapeutic targets, and determinants of drug response. Overall, this talk will emphasize on the utility of combining complementary PTM analyses to generate deeper biological insights and enhance the translational impact of proteomics in disease research.

Dr. Saikat Das, AIIMS, Bhopal



Dr. Saikat Das is a distinguished radiation oncologist at AIIMS Bhopal,specializing in advanced cancer treatment techniques. His research focuses on optimizing radiotherapy protocols to enhance precision in radiation delivery, improving treatment outcomes while minimizing side effects. Dr. Das has been actively involved in innovative projects integrating cutting-edge imaging technologies and personalized treatment strategies in radiotherapy. His work aims to refine therapeutic approaches to ensure maximum efficacy and patient safety. A prolific researcher, he has contributed to leading oncology and radiology journals, advancing knowledge in cancer care. Beyond his clinical and research contributions, Dr. Das is dedicated to mentoring students and fostering interdisciplinary collaborations to drive progress in radiotherapy. His commitment to innovation and excellence continues to shape modern cancer treatment practices, reinforcing the role of precision medicine in oncology.

Dr. Sandipan Ray, IIT Hyderabad



Dr. Sandipan Ray is an Associate Professor and the Group Leader of the Circadian Rhythms and Disease Biology Laboratory at the IIT Hyderabad, India. Dr. Ray obtained his Ph.D. degree with an "Excellence in Ph.D. Research" award from the IIT Bombay in 2014. He is a highly dynamic, enthusiastic, and motivated scientific professional with over 15 years of experience in translational research and an outstanding track record of scientific publications (H-index of 30). Dr. Ray's research group conducts high-quality research that makes significant contributions to cutting-edge omics research on circadian rhythms, signaling networks, and human diseases. Dr. Ray is a recipient of multiple prestigious awards, including the Thermo Scientific Annual Tandem Mass Tag International Research Award (2018), the Faculty Research Excellence Award from IIT Hyderabad (2024), and the Young Scientist Award at the 11th World Congress of Chronomedicine (WCC 2025). He is associated with multiple leading scientific organizations, including the HUPO, US-HUPO, PSI. He was elected to the prestigious Royal Society of Biology, UK, in 2020. He is currently serving as the Vice President of the Indian Society for Chronobiology (InSC). He has scientific publications in top-tier international journals such as Science, Nature, and Nature Review Journals.

Abstract: Multiplexed Quantitative Proteomics for Mechanistic Insights into Circadian Rhythms and Clock-oriented Therapeutics

The circadian system defines an endogenous rhythm that governs various behavioral, physiological, and metabolic processes in a cyclic pattern of almost 24-hour periodicity. Disruptions in the circadian system increase the risk for various chronic diseases, including cancers and mental, neurological, metabolic, and cardiovascular diseases. Pharmacologically targeting components of the clock machinery is now emerging as a new therapeutic avenue. The application of next-generation quantitative proteomics approaches using ultra-sensitive mass spectrometers is beneficial for decoding the molecular mechanisms of circadian oscillations and for the pharmacological modulation of the circadian clock machinery. In recent years, several comprehensive quantitative proteomics datasets have emerged investigating the synchronization mechanism of circadian rhythms, post-transcriptional mechanisms of circadian regulation, pharmacological modulation of circadian rhythms, and oscillations in diverse metabolic pathways. We investigated the molecular targets of circadian period-modulating compounds in human osteosarcoma cells using an integrated multidimensional quantitative proteomics workflow combining global proteome, phosphoproteome, and kinome mapping, and thermal proteome profiling (TPP). We have demonstrated changes in the phosphorylation levels and activity of several proteins and kinases involved in essential signaling pathways, including MAPK, BCR, AMPK, and mTOR signaling, in response to circadian clock modulating compounds. Our results indicate that the effects of circadian rhythm–modulating compounds are not restricted to a handful of known targets but function by acting on multiple cellular targets embedded within diverse but well-defined physiological pathways. Our findings also suggest the necessity for an inclusive understanding of the circadian regulation of anticancer drugs to define their best dosing time for obtaining an improved therapeutic benefit.

Dr. Sangeeta Choudhary, Sir Ganga Ram Hospital, New Delhi



Prof. Sangeeta Choudhury, Vice Chairperson & Professor GRIPMER, Department of Biotechnology & Research, Sir ganga Ram Hospital, New Delhi is the Team leader of the 'Cancer biology and Stem Cell Therapeutics Section'. Her Post-Graduation mentor was Dr. Jagdish S Nadkarni who established 'Daudi' a Burkitt's lymphoma cell-line, at Division of Immunology, Tata Memorial Hospital, Mumbai; completed her Ph.D. Biochemistry under Prof. Rathindranath K Bhattachrya, Department of Radiation Biology, Bhabha Atomic Research Centre, Mumbai and Tata Memorial Hospital, University of Mumbai; as NIH-Research Fellow with Prof. Mark Hill, School of Medical Sciences, University of New South Wales, Sydney, Australia and later Dr. Charles E Rupprecht, Viral and Rickettsial Zoonoses Branch, Division of Viral and Rickettsial Diseases, Centers for Disease

Control and Prevention, USA as Vaccine Action Program (VAP) Fellow. On returning to India, she joined Dr. Satish Kumar Gupta's Lab / Department of Reproductive Biology, National Institute of Immunology, New Delhi, majorly working towards developing a dual vaccine for fertility and rabies. Herein she developed several animal models including mice, monkeys and dogs' models. More, recently her team's central focus has been Gastrointestinal cancers (Pancreatic Cancer and Colorectal Cancer) postulating allogeneic umbilical cord tissue-derived mesenchymal stem cells and its exosomes as one of the therapeutics.

Furthermore, her research work has resulted in development of FIVE patents [Ultrasensitive and accurate detection of Breast cancer; Completion Ref # 202011007723; mExo-siR therapy for Pancreatic cancer; Ref # 202211073830; tLent-CRISPR Exo therapy for pancreatic cancer; Ref # 202211073831, Chimeric Antigen Receptor (CAR) therapy for solid tumors']. Recently in 2024-25, she was awarded the 'BMJ SOUTH ASIA AWARD' in recognition of her Excellence in Medical Education (BMJ Awards), 'OUTSTANDING RESEARCHER' in Cancer Biology for her contribution and achievement in the discipline of Biomedical Sciences (Center for Health and Medical Sciences, Venus International Foundation), ' 'BEST SCIENTIST' (EET CRS – Faculty Awards) and 'APJ ABDUL KALAM AWARD' in recognition of her outstanding research achievements in the field of Cancer Biology (Assoc. of Researchers and Academics, India). In the past, she has been recipient of many awards, notably, Lady Tata Trust Fellowship; Department of Atomic Energy (Govt. of India) Fellowship; Union for International Cancer Control (UICC-TF); EMBO Fellowship [Mesenchymal cells in inflammation, immunity and cancer], Athens, Greece; Certification on "Ethics in Stem cell & Biomedical Research", Rutgers University, USA & Universitas Padjadjaran, Indonesia. She is also the Member Secretary of Institutional Bio-Safety Committee (DBT), Research Committee and former Secretary of Institutional Committee for Stem Cell Research (ICSCR) and Expert member at Rajiv Gandhi Cancer Institute and Research Centre and South Asia University, a SAARC endeavor. Dr. Choudhury has guided 9 PhD scholar, 4 DNB scholars and 40 Masters Students and also Examiner for Doctoral students as well as Journals / Project Reviewer & PhD coordinator, Jamia Hamdard, Delhi.

Abstract: Proteomic signature of primed Wharton's Jelly Mesenchymal Stem Cells reveals Immunomodulatory mechanism to combat Pancreatic Cancer

Background & Aim: Mesenchymal stem cells (MSCs) from umbilical cord have the potential therapeutic applications in context of injured, immune related & inflammatory diseases due to high proliferation rate, multilineage differentiation potential and immune tolerance properties. While clinical trials have clearly demonstrated strong safety records, efficacy of MSCs is still modest and inconsistent. Hypothesizing that priming MSCs prior to administration can improve their therapeutic efficacy, present study investigates the modulation of MSC behavior through cytokine priming and assesses their effectiveness in ameliorating inflammatory conditions. Proteomic analysis shows compositional changes post cytokine priming.

Method: Wharton's jelly derived from human umbilical cord (hWJMSCs) were primed with tumor necrosis factor-alpha (TNF-α; 25ng/ml) and interferon-gamma (IFN-γ; 25ng/ml), incubated for 24 hrs at 37°C/5%CO2, their morphological alterations, multi-lineage differentiation potentials (osteocytes/chondrocytes/adipocytes), immunophenotypying (CD90+73+105+44+34-45-19- HLADR-), Adhesion molecules (ICAM, VCAM, NCAM) migration capabilities were examined. Label-free quantitative LCMS (nLC/MS/MS coupled to Orbitrap fusion Tribrid massspectrometer) analysis was performed on more than 2400 proteins identified. Further, immunogenic potentials are being tested using PBMNCs from healthy human donors.

Result: hWJMSCs primed with TNF-α (hWJMSC-T)/IFN-γ (HWJMSC-I) showed >90% expression of CD90+ 73+ 105+ 44+. Microscopically morphological distinction stained with phyalloidin/DAPI observed showed hWJMSC-T as elongated and flattened cells and complement & coagulation cascade and Pro-angiogenic proteome signature in abundance, suggesting their role in innate immunity homeostasis. On the other hand, IFN-γ induction showed immune-modulating protein

signature of infection/inflammation especially, Guanylate-binding proteins. Differentially expressed protein signature points towards modulation of NOD-like receptor signaling and cell adhesion molecule pathways.

Conclusion: Data herein provides the evidences that stem cell properties of regenerative capability remain conserved and do not compromise under inflammatory conditions. Additionally, primed hWJMSCs can modulate or prevent infection most likely via cross-talk between cascades of defense systems. Thus, suggesting a potential role as alternate strategy to regulate inflammation and/or reshape inflammatory microenvironment.

Dr. Santosh Varma, GMC, Ambernath



Dr. Santosh Varma is a distinguished clinician, academician, and Dean of Government Medical College (GMC), Ambernath. His interests span clinical medicine, medical education, translational research, and public health. Dr. Varma has been actively involved in promoting evidence-based healthcare practices and fostering research-oriented medical education. He has contributed to several clinical and academic initiatives aimed at improving patient care, healthcare delivery, and disease management strategies. Through his leadership, teaching, and research activities, he continues to support the advancement of medical sciences and healthcare education in India.

Dr. Saravanan Kumar, Thermo Fisher Scientific, India



Dr. Saravanan Kumar is a scientific leader with over 17 years of experience in advanced analytical sciences, specializing in mass spectrometry, proteomics, biopharmaceutical analytics, and omics technologies. His expertise encompasses the analysis and characterization of complex biomolecules, including monoclonal antibodies (mAbs), antibody–drug conjugates (ADCs), peptide therapeutics, oligonucleotides, mRNA, glycoproteins, glycans, and small molecules. Through his work, he has played a key role in advancing analytical workflows and fostering collaborations between academia and industry to support research, development, and regulatory science.

Currently serving as Senior Manager – Biopharma & Omics at Thermo Fisher Scientific, Dr. Kumar leads scientific and application initiatives across India. His responsibilities include supporting biopharma, pharma, and omics workflows, enabling end-to-end analytical method development and characterization of biologics and therapeutic modalities, collaborating with industry and academic partners, and driving scientific engagement and application excellence across diverse customer segments.

Dr. Kumar's career reflects a unique blend of industrial leadership and research excellence. At Thermo Fisher Scientific, he has held several scientific and leadership positions focused on high-resolution mass spectrometry applications for biologics characterization, including glycoproteins, PEGylated proteins, antibody–drug conjugates, vaccine candidates, and peptide therapeutics. Prior to joining Thermo Fisher Scientific, he conducted advanced proteomics and mass spectrometry research at the International Centre for Genetic Engineering and Biotechnology (ICGEB). With support from Bruker Daltonics India, he played a pivotal role in establishing a state-of-the-art Mass Spectrometry and Omics facility at ICGEB. He began his scientific journey at the CSIR–Institute of Genomics and Integrative Biology (IGIB), where he developed expertise in proteomics, glycoproteins, structural biology, molecular biology, and protein purification.

Dr. Kumar earned his PhD in Proteomics and Mass Spectrometry from Jawaharlal Nehru University (JNU), where his research focused on mass spectrometry-based characterization of proteins, glycoproteins, antibodies, proteoglycans, parasite protein complexes, disulfide bonds, plasma glycoproteins, lectins, and protein isoforms. He also holds a postgraduate degree in Biotechnology from the University of Madras, with research conducted at CSIR-IGIB, and a bachelor's degree in Biotechnology from Vellore Institute of Technology (VIT).

An accomplished researcher, Dr. Kumar has authored and co-authored more than 25 international publications, book chapters, application notes, and technical articles in the fields of proteomics, glycoproteomics, mass spectrometry, and biopharmaceutical analytics. His publications have appeared in leading journals including *Nature Communications*, *Molecular & Cellular Proteomics*, *Journal of Proteome Research*, *Journal of Proteomics*, *Methods in Molecular Biology*, *Plant Biotechnology Journal*, *Proteome Science*, and *Biochimie*. His scientific contributions continue to advance the understanding and analytical characterization of complex biological molecules, supporting innovation in life sciences, biotechnology, and drug development.

Abstract: Breaking the Dynamic Range Barrier in Metabolomics: The eDR Principle for Enhanced Metabolome Coverage.

Despite significant advances in mass spectrometry, the reliable identification and quantitation of low-abundance ions in the presence of highly abundant species remains a major analytical challenge, particularly when analysing complex biological matrices. A fundamental limitation of modern mass spectrometers is achieving an optimal balance between maximizing ion population for sensitivity and avoiding space-charge effects that can compromise mass accuracy, resolution, and dynamic range.

One effective strategy to overcome these limitations involves segmenting the mass spectrum into discrete m/z windows and subsequently reconstructing the full spectrum through a stitching approach. By reducing ion crowding within individual mass ranges, this methodology minimizes ion overload, lowers spectral noise, and substantially extends the detectable dynamic range, thereby enabling improved detection of low-abundant analytes.

Building upon these concepts, we have developed an intelligent MS1 multiplexing strategy coupled with optimized ion injection times. This innovation has been implemented as the enhanced Dynamic Range (eDR) scanning mode on the Thermo Scientific™ Orbitrap™ Excedion™ Pro Hybrid Mass Spectrometer. The eDR approach enhances ion utilization efficiency across the mass range, improves the detection of low-intensity features without compromising the measurement of high-abundance species, and significantly increases metabolome coverage.

This session will introduce the principles underlying eDR acquisition, and highlight its applications in metabolomics workflows, demonstrating how enhanced dynamic range can drive deeper and more comprehensive metabolite profiling.

Dr. Satish Sharma, Manipal Hospital, Ranchi



Dr. Satish Sharma is a distinguished Medical Oncologist and currently serves as a Consultant in Medical Oncology at Manipal Hospitals, Ranchi. He is recognized for his expertise in the diagnosis and management of a broad spectrum of solid tumors and hematological malignancies, delivering evidence-based and personalized cancer care. He holds qualifications of MBBS, DNB (Medicine), DM (Medical Oncology) and is also a European Certified Medical Oncologist (ECMO).

Dr. Sharma has extensive experience in treating breast cancer, lung cancer, gastrointestinal cancers, gynecological cancers, head and neck cancers, urological malignancies, lymphomas, leukemias, and other hematological disorders. His clinical interests include chemotherapy, immunotherapy, targeted therapy, precision oncology, preventive oncology, and advanced cancer therapeutics.

Prior to joining Manipal Hospitals, Dr. Sharma received advanced oncology training at the Gujarat Cancer and Research Institute (GCRI), Ahmedabad, one of India’s leading cancer centers. He has actively contributed to cancer research, scientific publications, and academic activities aimed at improving cancer diagnosis and treatment outcomes.

Beyond his clinical practice, Dr. Sharma is deeply involved in cancer awareness, early detection initiatives, and patient education programs. Through his commitment to compassionate care, research, and innovation, he continues to advance oncology services in eastern India and improve the lives of patients battling cancer.

Dr. Siddhartha P Duttagupta, IIT Bombay



Dr. Siddhartha P. Duttagupta is a distinguished faculty member at the Indian Institute of Technology (IIT) Bombay and an accomplished researcher in biomedical engineering, healthcare technologies, and translational medical research. His work focuses on developing innovative diagnostic platforms, biosensors, point-of-care technologies, and digital health solutions aimed at improving healthcare accessibility and outcomes. Through interdisciplinary collaborations involving engineering, medicine, and life sciences, he has contributed significantly to the advancement of affordable healthcare technologies. Dr. Duttagupta has authored numerous scientific publications, mentored young researchers, and actively promotes innovation-driven healthcare solutions. His contributions continue to bridge the gap between engineering research and clinical applications, fostering advancements in precision diagnostics and healthcare delivery.

Dr. Soumil Vyas, Sir H.N. Reliance Foundation Hospital, Mumbai



Dr. Soumil J. Vyas, MBBS, MD, DNB, FRCS (Upper GI/HPB), MNAMS, M.Med (Surg, Singapore), FAIS, FEBS, FIAGES, FMAS, FACS, is a highly accomplished Surgical Oncologist and Hepato-Pancreato-Biliary (HPB) Surgeon with extensive expertise in gastrointestinal cancers, liver transplantation, and advanced gastrointestinal surgery.

Dr. Vyas specializes in Surgical Oncology with a focus on Gastrointestinal Oncology, Liver, Gallbladder and Pancreatic Surgery (HPB Surgery), Surgical Gastroenterology, and Liver Transplantation. He is recognized for his contributions to the management of complex gastrointestinal and hepatopancreatobiliary malignancies, combining advanced surgical techniques with multidisciplinary cancer care.

He is a Fellow of the Intercollegiate Specialty Board of the Royal College of Surgeons of Edinburgh (UK) in Upper GI and HPB Surgery, a Fellow of the European Board of Surgery (HPB Surgery), and a Fellow of the American College of Surgeons (FACS). These prestigious international fellowships reflect his commitment to excellence in surgical practice, education, and patient care.

Dr. Vyas has been actively involved in advancing cancer surgery and hepatobiliary care through clinical practice, surgical innovation, academic activities, and multidisciplinary collaboration. His expertise in complex oncological procedures and liver transplantation has established him as a leading figure in the field of gastrointestinal and HPB surgery in India.

He is a highly regarded clinician-scientist specializing in the management of solid tumors, precision oncology, and translational cancer research. With extensive training in medical oncology and cancer therapeutics, Dr. Vyas is committed to integrating cutting-edge scientific advances into patient-centered cancer care.

His clinical expertise encompasses the diagnosis and treatment of a wide range of malignancies, including breast cancer, lung cancer, gastrointestinal cancers, genitourinary cancers, and hematological malignancies. Dr. Vyas has a strong interest in personalized medicine, molecular oncology, biomarker-driven therapies, immunotherapy, and targeted treatment approaches that improve patient outcomes and quality of life.

In addition to his clinical practice, Dr. Vyas is actively involved in academic research, clinical trials, and multidisciplinary cancer care programs. He has contributed to several scientific publications and has participated in national and international oncology forums, advancing the translation of emerging discoveries into clinical practice. His work

emphasizes evidence-based medicine and the adoption of innovative treatment strategies tailored to individual patient needs.

Through his contributions to oncology, research, and medical education, Dr. Vyas continues to play an important role in advancing precision cancer care and improving healthcare outcomes for patients across India.

Dr. Srikanth Rapole, NCCS, Pune



Dr. Srikanth Rapole completed his master's degree in organic chemistry from Devi Ahilya University. He did his PhD in analytical chemistry from Indian Institute of Chemical technology (IICT), Hyderabad where he developed new mass spectrometry methods for analysing beta-carbo-peptides. He did his post-doc from University of Massachusetts (UMASS, Amherst) on metal protein interactions and protein-protein interactions to understand the mechanism of protein aggregation and amyloid formation. He worked as proteomics and mass spectrometry lab director for two years at University of Connecticut. He is currently working as a Scientist F at NCCS, Pune. Dr. Srikanth's laboratory is investigating potential biomarkers and therapeutic targets for various cancers using state-of-the-art, highly sensitive mass spectrometry-based proteomic approaches. In addition, his group is also working to identify and quantify key metabolites and lipids associated with various cancers using mass spectrometry and bioinformatics. He has headed several multi-institutional projects with bilateral collaborations with international research laboratories in Germany, Portugal and USA. He is an active member of the Indian Society for Mass Spectrometry, the American Society for Mass Spectrometry, the Indian Society of Translational Research, and the Proteomics Society, India. He is currently the Vice President of Proteomics Society, India and plays a large role in growing the society. He received the eminent mass spectrometrist award from Indian Society for Mass Spectrometry (ISMAS). He has published more than 100 publications in reputed international journals.

Abstract: Application of clinical proteomics to discover potential targets and biomarkers for Hematological malignancies

Hematological malignancies are a highly heterogeneous group of diseases that include leukemias, lymphomas, and myelomas that affect blood, bone marrow, and lymph nodes. All these are closely associated through the immune system; a disease affecting one of these will frequently affect the others as well. Understanding hematological malignancies at the protein level is important for predicting therapy response, enabling disease diagnosis, and developing targeted treatments. Our group extensively applied advanced proteomic approaches in Multiple Myeloma (MM) and Acute Myeloid Leukemia (AML) and identified several candidate biomarkers/targets. The identified candidate markers/targets will not only be useful for diagnosis and therapeutics but also provide valuable insights into the molecular mechanisms of MM and AML.

Dr. Sudhir Nair, ACTREC, Navi Mumbai



Dr. Sudhir Nair is a distinguished Head and Neck Surgical Oncologist, clinician-scientist, and academic leader at the **Advanced Centre for Treatment, Research and Education in Cancer (ACTREC), Tata Memorial Centre, Navi Mumbai**. He currently serves as **Professor and Head of Head & Neck Surgery** and **Head of the Department of Surgical Oncology**, where he leads one of India's foremost programs in head and neck cancer care, research, and education.

Dr. Nair obtained his **MBBS, MS, and MCh** degrees and further enhanced his expertise through a **Post-Doctoral Research Fellowship at Memorial Sloan Kettering Cancer Center (MSKCC), New York**, one of the world's leading cancer centers. He has over two decades of experience in the management of head and neck cancers, with particular interest in oral cancers, thyroid malignancies, complex oncologic surgery, reconstructive techniques, and translational cancer research.

An accomplished researcher, Dr. Nair has authored more than 180 peer-reviewed scientific publications and has made significant contributions to understanding the biology, prevention, management, and outcomes of head and neck cancers. His work bridges clinical practice and translational research, focusing on improving survival and quality of life for cancer patients.

In addition to his clinical and research accomplishments, Dr. Nair is a dedicated teacher and mentor who has trained numerous surgical oncologists and researchers. Through his leadership at ACTREC and Tata Memorial Centre, he continues to advance innovation in cancer surgery, multidisciplinary oncology care, and evidence-based cancer treatment in India and globally.

Dr. Suman S. Thakur, CCMB, Hyderabad



Dr. Suman Thakur's research interest involves applying Mass Spectrometry in Health and Diseases, especially finding the Early Biomarkers, understanding of Cancer Progression, Metastasis, and Drug Development. His lab uses mass spectrometry-based high throughput quantitative proteomics, natural product chemistry, cell biology, animal model, and modern biology approaches to find the target, develop new drugs, and elucidate its molecular and mechanistic details against cancer. Investigationof the efficacy of various purified/characterized natural and synthetic metabolites with minimum side effects on different cancers including childhood and aggressive cancer, using in vitro and in vivo methods areamong his major areas.

Further, his interest is to elucidate themode of action of a few selected compounds targeting cell adhesion, AKT signaling and tyrosine kinase in cancer. Currently, he is Associate Editor of the Journal of Proteome Research (JPR), Associate Editors in Frontiers in Oncology, Academic Editor in PLOS One, and Editorial board members of BBA-Protein and Proteomics, BB Report, and Scientific Reports.

Abstract: Quantitative Proteomics of Aggressive Cancer: Unlocking the Path from Biomarkers to Therapies

Mass spectrometry-based proteomics has found its applications in the field of biological sciences and medical biology including basic and translational research. Targeted and quantitative proteomics are able to find cause of the disease including narrowing down to a particular protein /gene. Our group is trying to understand the cancer progression and working to develop novel anticancer drug against various aggressive cancers including melanoma and Lung Cancer. We have quantified several thousand proteins in various aggressive cancers to elucidate the mechanism of cancer progression. Melanoma is one of the most aggressive and fatal skin cancers. The morbidity and mortality of this form of skin cancer is escalating every decade. In spite of years of intense investigation, there has been a very small development in the survival of patients with disseminated melanoma. Further, Lung cancer is a global problem and occurs in both male and female We have investigated successfully the efficiency of various novel natural and synthetic metabolites targeting oncogene and cancer suppressor gene of melanoma and lung cancer using cell culture and mouse model with the help of quantitative proteomics, molecular biology and biochemical techniques. Mode of action and targeted signaling mechanism of these novel drugs have been revealed through quantitative proteomics and biochemical techniques. Mass spectrometry results show Ras related protein RAP1A, pancreatitis associated protein 1 (PAP1) and anticarcinoma embryonic antigen light chain variable region (A2NMA3) plays an important role in melanoma progression using in vivo mouse model studies. The in vitro studies suggest, up-regulation of p53, Bax, Foxo1, cytochrome c, Caspse-8, 9, 2, 3 and cleaved PARP along with the down-regulation of Bcl2 level and p-Akt after the treatment of melanoma cells. Further, observed apoptosis was partly via mitochondria-mediated death cascade and inhibition of Akt signaling in human malignant melanoma cells. Further, in vivo proteomics study in Lung cancer shows involvement of several RAS related protein, EGFR, TALIN, and ICAM1 in cancer progression.

Mr. Sunil Kumar, ISRO, Bangalore



Mr. Sunil Kumar is an accomplished aerospace engineer and technology leader at the **Indian Space Research Organisation (ISRO), Bengaluru**, with over 15 years of experience in launch vehicle systems, human spaceflight programs, biomedical research, and astronaut training. Since joining ISRO in 2010, he has played a pivotal role in the design, development, testing, and qualification of critical mechanical systems for India's launch vehicles, contributing significantly to the nation's space exploration capabilities.

A graduate in **Mechanical Engineering from SASTRA University**, Mr. Kumar has led multidisciplinary engineering efforts encompassing system conceptualization, product design, manufacturing realization, qualification testing, vendor development, and mission-critical component delivery. His technical expertise has supported several major ISRO programs and advanced the reliability and performance of launch vehicle mechanisms.

From 2019 to 2021, he served as **Project Manager for Gaganyaan**, India's ambitious human spaceflight mission, where he contributed to spacecraft structural systems, life-support technologies, interface engineering, and program coordination. Currently, as **Lead for Biomedical Research and Astronaut Training**, he is spearheading the establishment of advanced astronaut training facilities and a Center of Excellence in Biomedical Research to support India's future human spaceflight endeavors.

Mr. Kumar's work bridges engineering innovation, human physiology, and space medicine, positioning India at the forefront of astronaut training and crewed space missions. He is also a member of the **Indian National Society for Aerospace and Related Mechanisms (INSARM)** and remains committed to advancing India's capabilities in space exploration and human spaceflight research.

Dr. Surekha Zingde, IWSA, Mumbai



Dr. Surekha Zingde is member of the Board of Trustees of the Indian Women Scientists' Association (IWSA). She was the past President of IWSA (2017-19). She was the second President of the Proteomics Society, India during 2014-16 and is presently a member of its Executive Council (2023-25). Dr. Zingde retired as Dy. Director, Cancer Research Institute, ACTREC, Tata Memorial Centre, Kharghar, Navi Mumbai, in March 2013 after 33y service with the Centre. Her expertise is in Cancer Biology, chronic myeloid leukemia, membrane proteins, signal transduction and Oral cancer proteomics.

She is Chairperson of the Indian Scientific Advisory Committee of Lady Tata Memorial Trust and the Ethics committee of ACTREC. She is actively involved in academics with multiple institutions as an advisor. She has been a reviewer for several journals and reviewer of thesis from different universities. She was Professor of Life Sciences of the HBNI. Dr. Zingde has been a visiting faculty at University of Mumbai-DAE-CEBS, a member of the Research and Recognition Committee of ICT, Mumbai and University of Mumbai and member of government project review and funding committees. She has vast experience in setting up a Research Institute. Eleven students have completed their Ph.D and 4 students their MSc under her guidance. She has 76 peer reviewed papers, several book chapters, a monograph and 4 patents.

Dr. Surya Pratap Singh, IIT Dharwad



Dr. Surya Pratap Singh is a faculty member at the **Indian Institute of Technology (IIT) Dharwad**, where he is actively engaged in teaching, research, and academic leadership in the field of biosciences and interdisciplinary biological engineering. His research integrates modern approaches in molecular biology, biotechnology, systems biology, and computational methods to address fundamental and translational challenges in life sciences.

Dr. Singh's work focuses on understanding complex biological processes and leveraging emerging technologies to develop innovative solutions for healthcare, biotechnology, and sustainable biological systems. His research interests encompass molecular mechanisms of disease, functional genomics, bioinformatics, omics-driven biology, and data-enabled approaches for biological discovery. Through multidisciplinary collaborations, he aims to bridge basic biological research with real-world applications in medicine and biotechnology.

At IIT Dharwad, Dr. Singh has contributed to the development of interdisciplinary research programs and the training of undergraduate, postgraduate, and doctoral students. He is actively involved in mentoring young researchers and fostering innovation-driven scientific inquiry. His research findings have been disseminated through publications in reputed scientific journals and presentations at national and international conferences.

Dr. Singh continues to advance modern biosciences through research excellence, academic mentorship, and collaborative scientific endeavors that address emerging challenges in biology and healthcare.

Dr. Swapnil Rohidas Shinde, IIT Bombay



Dr. Swapnil Rohidas Shinde is an Assistant Professor in the Department of Biosciences and Bioengineering at the **Indian Institute of Technology Bombay (IIT Bombay)**. He is an emerging leader in the field of cell biology, with research focused on the molecular mechanisms governing **cilia and flagella assembly, intracellular transport, and ciliary signaling pathways**. His work seeks to understand how defects in these processes contribute to human diseases known as ciliopathies.

Dr. Shinde earned his Ph.D. in Biotechnology from the **Centre for DNA Fingerprinting and Diagnostics (CDFD), Hyderabad**, where he worked on cellular signaling and membrane trafficking. He subsequently pursued postdoctoral research at the **University of California, San Francisco (UCSF)** under the mentorship of Prof. Maxence Nachury, investigating mechanisms of protein trafficking and signaling within primary cilia.

His laboratory at IIT Bombay combines cell biology, molecular genetics, microscopy, and biochemical approaches to study intracellular transport and ciliary function. Dr. Shinde has published influential research in leading journals including *Developmental Cell*, *Journal of Cell Biology*, *Nature Communications*, and *Cell Reports*.

He has received several prestigious recognitions, including the **Young Faculty Award at IIT Bombay**, the **Sandler Program Independent Research Grant at UCSF**, and the **David and Joyce Copenhagen Prize for Best Published Paper in Visual Sciences**. Through his research and mentorship, Dr. Shinde continues to advance our understanding of cellular organization, signaling, and human disease.

Dr. Swati Chitrangi, Thermo Fisher Scientific, India



Dr. Swati Chitrangi is a seasoned life sciences professional, strategic product leader, and technocommercial expert with over 17 years of experience spanning biotechnology, proteomics, genomics, cell biology, regenerative medicine, and advanced in vitro platforms. She currently serves as a Technocommercial Leader at Thermo Fisher Scientific, where she drives product strategy, innovation, go-to-market initiatives, and business growth across India and South Asia.

Dr. Chitrangi holds a Ph.D. in Biological Sciences and has further strengthened her leadership expertise through executive management training at the Indian Institute of Management (IIM) Lucknow. Throughout her career, she has successfully bridged scientific innovation with commercial execution, enabling the translation of complex life science technologies into scalable solutions for academia, biotechnology companies, pharmaceutical industries, and research institutions.

Prior to joining Thermo Fisher Scientific, Dr. Chitrangi held leadership positions in product management, drug discovery solutions, regenerative medicine, and analytical method development. She served as Head of Product Management for Drug Discovery Solutions at Krishgen Biosystems and as Head of Production at Advancells Group, where she led initiatives in cell therapy and exosome-based therapeutics. Earlier, she worked as Principal Scientist and Senior Scientist at Yashraj Biotechnology, contributing significantly to analytical development and biotechnology product innovation.

Dr. Chitrangi also pursued postdoctoral research at the Indian Institute of Technology Bombay, where her work focused on stem cell-derived exosomes and their therapeutic potential in cancer biology. Her multidisciplinary expertise encompasses induced pluripotent stem cells (iPSCs), organoids, spheroids, CRISPR technologies, exosome biology, AI-driven drug discovery, translational research, and precision medicine.

Recognized for her ability to integrate scientific rigor with strategic business leadership, Dr. Chitrangi has been instrumental in developing customer-centric solutions, fostering industry-academia collaborations, and accelerating the adoption of advanced life science technologies. Through her leadership, innovation, and commitment to advancing biomedical research, she continues to play a key role in shaping the future of precision healthcare and life science innovation in India and beyond.

Dr. Syed Hasan, ACTREC, Navi Mumbai



Dr. Syed Hasan has earned a Ph.D. and completed postdoctoral training in Hemato-oncology at the Faculty of Medicine, University of Rome Tor Vergata, Italy. Since 2017, he has been serving as the Principal Investigator at the Hasan Lab in the Advanced Centre for Treatment, Research, and Education in Cancer (ACTREC), Tata Memorial Centre. The primary focus of Dr. Hasan's laboratory at ACTREC in Mumbai is unraveling the molecular basis of resistance to targeted therapies in acute myeloid leukemia and breast cancer. Dr. Hasan has been honored with prestigious awards/recognitions, including the ICMR-DHR International Fellowship, Ramalingaswami Fellowship from the Department of Biotechnology GoI, the European Hematology Association Fellowship, Netherlands, and the Society of Hematology & Oncology, Houston, USA (India Ambassador).

Dr. Vadiraja Bhat, Sciex, India



Dr. Vadiraja (Vadi) Bhat is a distinguished proteomics expert and techno-commercial leader currently serving as Head of Market Development at SCIEX India, part of the Danaher Corporation. With nearly 30 years of global experience in life sciences, he has deep expertise in mass spectrometry, proteomics, biopharmaceutical analysis, and omics applications. He has played a pivotal role in advancing analytical technologies and driving their adoption across biopharma, academia, healthcare, and applied research markets.

A seasoned leader, Dr. Bhat brings extensive expertise in biologics, peptides, and LC-MS-based workflows, spearheading new market creation, strategic growth initiatives, and the adoption of advanced analytical solutions. His work spans protein characterization, biomarker discovery, translational research, and high-throughput omics platforms.

Dr. Bhat earned his Ph.D. in Chemical Biology from JNCASR/IISc, Bengaluru, and subsequently conducted postdoctoral research in proteomics and mass spectrometry at the Massachusetts Institute of Technology (MIT), USA.

His professional journey includes key leadership roles at Agilent Technologies, where he contributed significantly to proteomics and biopharma market development across India and globally. He also established and led a proteomics and mass spectrometry core facility at Baylor Scott & White Health/Texas A&M University, USA, and contributed to the development of innovative LC-MS workflows at Agilent's Little Falls Centre of Excellence (CoE).

In addition to his industry leadership, Dr. Bhat serves as Adjunct Faculty at the Manipal Academy of Higher Education (MAHE), where he actively mentors the next generation of scientists and researchers. Through his scientific leadership, strategic vision, and commitment to innovation, he continues to strengthen the adoption of advanced analytical technologies and drive the growth of proteomics and precision medicine in India and beyond.

Dr. Vel Murugan, Arizona State University, USA



Dr. Vel Murugan is a molecular biologist and translational researcher whose work spans diagnostic innovation, multiomics-driven biomarker discovery, vaccine immunology, and infectious disease biology. He serves as Research Professor and Director of Clinical Research at the Biodesign Center for Personalized Diagnostics and the Health Observatory at The Arizona State University. Dr. Murugan earned his PhD from Tata Institute of Fundamental Research and completed postdoctoral training at The University of Texas at Austin and Dana-Farber Cancer Institute. He also holds an MBA from Northeastern University. His research career includes significant contributions to cancer biology, vaccine development, and infectious disease research. At ASU, Dr. Murugan has led the development of advanced molecular diagnostic platforms and biomarker-based assays for radiation exposure, infectious diseases, and environmental health threats. During the COVID-19 pandemic, he established and directed the CLIA-certified, CAP-accredited ASU Biodesign Clinical Testing Laboratory, which performed over 1.6 million diagnostic tests and sequenced more than 100,000 viral genomes. Currently, he serves as Principal Investigator of a CDC-funded Influenza Vaccine Effectiveness center, advancing precision diagnostics through the integration of genomic, epigenetic, transcriptomic, and proteomic technologies to improve public health preparedness and patient care.

Abstract: Immunogenicity of Concomitant vs. Sequential COVID-19 and Influenza Vaccination

This Phase IV randomized clinical study evaluates the immunogenicity, duration of antibody response, and safety of concomitant versus sequential administration of mRNA COVID-19 and quadrivalent cell culture-based influenza vaccines in 800 participants, comprising 600 adults aged 18–64 and 200 children aged 6–11. Conducted across four U.S. sites (we are one of the four), the trial randomizes participants into three groups to receive both vaccines either on the same day or 28 days apart in varying orders to compare immune responses against circulating SARS-CoV-2 variants and influenza viruses. The primary objective is to determine baseline and post-vaccination influenza antibody titers via hemagglutination inhibition (HAI) and microneutralization (MN) assays, while exploratory measures assess SARS-CoV-2 viral neutralization, the frequencies of antigen-specific T and B cells, and the rate of antibody waning over a 180-day period. Furthermore, the study describes the reactogenicity and safety profiles of these vaccination schedules through active surveillance for acute respiratory illness and electronic surveys capturing injection site and systemic reactions. We present data from our site by analyzing specimens including sera, and plasma, we aim to provide a comprehensive immunologic assessment of co-administration strategies for two essential seasonal vaccinations.

Dr. Vineeta Rai, CDRI, Lucknow



Dr. Vineeta Rai is a distinguished scientist at the CSIR–Central Drug Research Institute (CDRI), Lucknow, one of India's premier biomedical research institutions. Her research focuses on human genetics, population genomics, molecular epidemiology, and genetic susceptibility to complex diseases, with particular emphasis on understanding how genetic variation influences human health and disease outcomes.

Dr. Rai obtained her doctoral training in human genetics and has established herself as a leading researcher in the field of genetic epidemiology. Her work integrates molecular biology, genomics, bioinformatics, and population-based approaches to investigate the genetic basis of disorders affecting diverse Indian populations. She has made significant contributions to understanding the role of genetic polymorphisms in infectious diseases, reproductive health, metabolic disorders, and other complex human traits.

Over the course of her career, Dr. Rai has authored numerous peer-reviewed publications in reputed national and international journals. Her research has contributed to advancing knowledge of population diversity, disease susceptibility, and personalized healthcare approaches in India. She has also actively mentored young researchers and collaborated with multidisciplinary teams across academic and research institutions.

Through her scientific contributions, Dr. Rai continues to strengthen the field of human genetics and genomic medicine in India. Her work supports the development of precision medicine strategies and enhances our understanding of the genetic factors that shape health, disease, and population diversity.

Dr. Wen Donq Looi, Bruker, Singapore



Dr. Wen Dong Looi is an accomplished analytical chemist and mass spectrometry specialist currently serving as an **Application Specialist for Life Science Mass Spectrometry at Bruker Daltonics, Singapore**. With a strong background in analytical chemistry, biomarker discovery, metabolomics, and advanced mass spectrometry technologies, he plays a key role in supporting cutting-edge life science and translational research applications across the Asia-Pacific region.

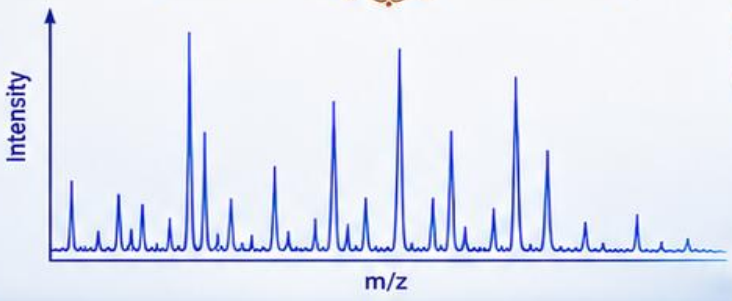
Dr. Looi earned his **Ph.D. in Analytical Chemistry from the University of Florida, USA**, where his doctoral research focused on the development of innovative mass spectrometry techniques, including electrochemistry electrospray ionization (EC-ESI) and desorption electrospray ionization (DESI) mass spectrometry. His research contributed to the advancement of analytical methodologies for studying biomolecules, metabolites, and complex biological systems. Prior to his doctoral studies, he completed his undergraduate training in Chemistry at the University of Florida.

Before joining Bruker Daltonics, Dr. Looi served as a **Principal Scientist at Nanyang Technological University (NTU), Singapore**, where he was involved in advanced scientific research and technology development. Since joining Bruker in 2018, he has worked closely with leading academic, clinical, and industry researchers, supporting applications in MALDI imaging, proteomics, metabolomics, biomarker discovery, and translational medicine.

Through his expertise in mass spectrometry instrumentation and analytical sciences, Dr. Looi continues to facilitate innovative research and technology adoption, helping scientists translate complex molecular data into meaningful biological and clinical insights.

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Invited Faculties Biography

Dr. Mukunda Gosawami, ICAR-CIFE, Mumbai



Dr. Mukunda Goswami is a distinguished scientist and academician at the **ICAR–Central Institute of Fisheries Education (CIFE), Mumbai**, a premier institution dedicated to fisheries education, research, and innovation in India. With extensive experience in molecular biology, biotechnology, genomics, and aquatic animal health, he has made significant contributions to advancing fisheries and aquaculture research by applying modern biological sciences.

Dr. Goswami's research focuses on fish genomics, molecular genetics, bioinformatics, disease diagnostics, and the development of molecular tools for sustainable aquaculture. His work integrates cutting-edge genomic and proteomic approaches to understand biological processes, improve fish health management, and enhance productivity in aquaculture systems. He has actively contributed to research on aquatic biodiversity, genetic resource conservation, and molecular marker-assisted studies aimed at supporting evidence-based fisheries management.

Throughout his career, Dr. Goswami has authored numerous scientific publications in reputed national and international journals and has successfully guided postgraduate and doctoral students. He has also been involved in several collaborative research projects funded by national agencies and has played an important role in strengthening research capacity in fisheries biotechnology.

Through his interdisciplinary research and academic leadership, Dr. Goswami continues to contribute to the advancement of aquatic sciences, biotechnology, and sustainable fisheries development, supporting India's growing blue economy and aquatic food security initiatives.

Dr. Puja Sandbhor, ACTREC, Navi Mumbai



Dr. Puja Sandbhor is a biomedical engineer and translational nanomedicine researcher specializing in immunotherapy and precision oncology. She completed her Ph.D. in Biomedical Engineering at the Indian Institute of Technology (IIT) Bombay, followed by postdoctoral research at the Johns Hopkins University, USA. She is a recipient of the Prime Minister's Early Career Research Fellowship. Dr. Sandbhor's research integrates nanotechnology, immuno-engineering, and advanced disease models to develop next-generation cancer therapeutics. Her laboratory focuses on tumor microenvironment-driven therapeutic resistance and precision treatment strategies using 3D patient-derived organoids, organ-on-chip platforms, and translational nanomedicine approaches.

Dr. Raman P. Yadav, MGMIHS, Navi Mumbai



Dr. Raman P. Yadav is distinguished microbiologist and enzymologist, explored his deep research in the area of enzymology, drug discovery, nanoscience, protein science etc. His research work is translated into number of patents including U.S. patents and publications. Evidencing thermostable lipase from *Aspergillus terreus* and development of quantum dot powered antibody-based kit for latent TB and TB antigen are distinguished achievements. His research contribution in drug sensitivity enhancement in pathogenic microbes and *Plasmodium falciparum* is remarkable. He has developed several multifunctional and advanced materials for biomedical applications. Acquired extensive research experience in working with renowned institutions like National Institute of Immunology, New Delhi and industrial laboratories. He is presently Technical Director, MGMIHS OMICS Research Center and Professor, Medical Biotechnology, MGMSBS, MGM Institute of Health Sciences (MGMIHS), Navi Mumbai.

He did Ph.D. in Microbiology from University of Delhi. He is known for several important roles including Research Leader, Enzymology, Reliance Life Sciences Pvt. Ltd, Navi Mumbai in past and Director, MGMIHS Incubation and Innovation Centre. He is well recognized and introduced in several committees. Honoured by various awards including AMI, 1998 Young Scientist and VIRA 2016 Distinguished Scientist Award.

Dr. Shubham Shrivastava, Bharati Vidyapeeth, Pune



Shubham Shrivastava, PhD, is an Associate Professor at Interactive Research School for Health Affairs (IRSHA), Bharati Vidyapeeth, Pune. Her specialization is in virology and infectious diseases, with a primary focus on the molecular mechanisms that drive viral pathogenesis and host immune responses.

Her research program addresses the molecular characterization of viruses circulating in India, including dengue, chikungunya, and SARS-CoV-2. Her work involves understanding the host-pathogen interactions to identify the key determinants of protection versus disease progression during Dengue virus infection.

Her work focuses on deciphering how platelet-derived exosomes modulate endothelial dysfunction during dengue infection. Additionally, her lab evaluates the complexities of antibody-dependent enhancement (ADE) responses in dengue patients, bridging molecular signatures with clinical severity. Her research combines fundamental molecular virology with clinical immunology to inform the development of targeted therapeutics and improve patient outcomes globally.

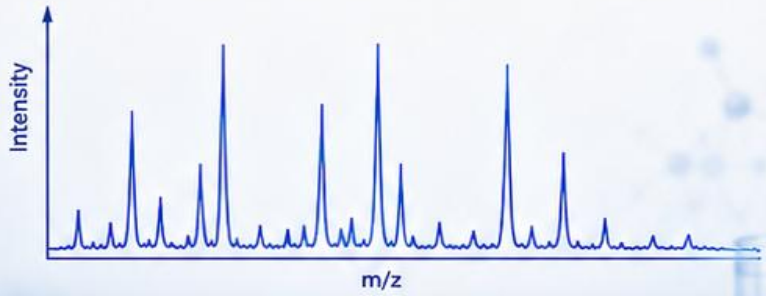
Dr. Tasleem Ahmad, NRIUMSD, Hyderabad



Dr. Tasleem Ahmad is a Research Officer (Biochemistry) at the National Research Institute of Unani Medicine for Skin Disorders (NRIUMSD), Hyderabad, under the Central Council for Research in Unani Medicine (CCRUM), Ministry of AYUSH, Government of India. With more than 18 years of research experience, his expertise spans biochemistry, molecular biology, genetics, pharmacology, biotechnology, and drug discovery. His research focuses on the scientific validation of Unani medicine through modern biochemical and molecular approaches. Dr. Ahmad has authored over 60 scientific publications and has contributed extensively to research on temperament, humoral biology, and integrative healthcare. He has also played a key role in CCRUM's flagship projects exploring the biological basis of fundamental Unani concepts.

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Panel Discussion



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PANEL DISCUSSIONS

Panel Discussion #1: Reflection of Nearly Two Decades of Proteomics: Through the Lens of Proteomics Society of India (PSI)

Proteomics has emerged as one of the most transformative scientific disciplines of the 21st century, fundamentally advancing our understanding of biological systems, disease mechanisms, biomarker discovery, and precision medicine. Over the last two decades, India has witnessed remarkable growth in proteomics research, infrastructure development, technological innovation, and human resource capacity building. The Proteomics Society of India (PSI) has played a pivotal role in fostering this growth by establishing a vibrant platform for scientific exchange, collaboration, training, and discovery.

Overview

This panel discussion aims to reflect upon the journey of proteomics in India through the perspective of PSI, highlighting major milestones, achievements, challenges, and future opportunities. The session brings together distinguished leaders, pioneers, and contributors who have shaped the proteomics landscape in the country. Through their cumulative experiences and insights, the discussion explores how proteomics has evolved from a highly specialised research domain into a critical component of modern life sciences, translational research, biotechnology, and healthcare.

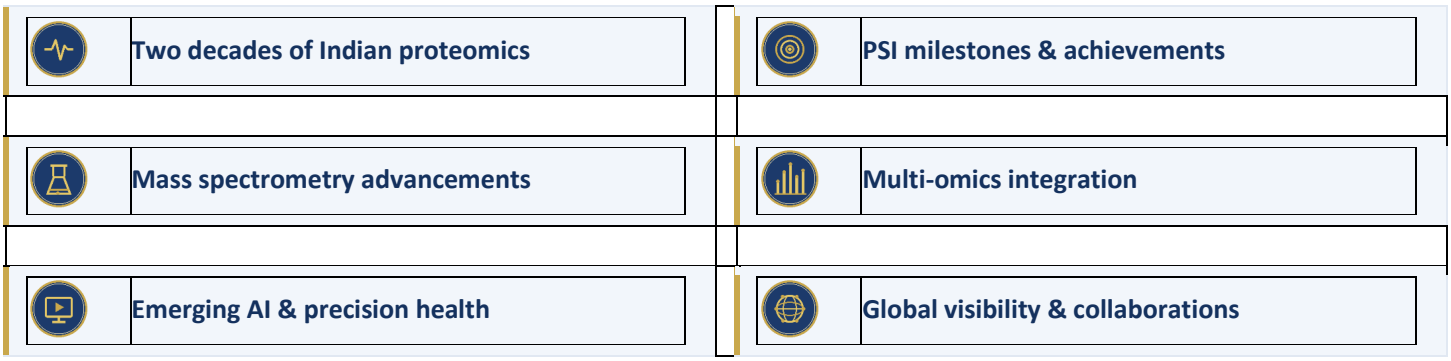
Key Themes

Key themes of the discussion include the establishment and expansion of proteomics facilities across India, the transformative impact of mass spectrometry technologies, advances in quantitative and clinical proteomics, integration of multi-omics approaches, development of skilled scientific manpower, and the role of national and international collaborations. The panel also examines how PSI has contributed to nurturing young researchers, promoting scientific excellence, and enhancing the global visibility of Indian proteomics research.

Future Directions

As the field enters a new era driven by artificial intelligence, systems biology, single-cell technologies, spatial omics, and precision health, the discussion provides valuable perspectives on emerging directions and opportunities. Panelists share their vision for advancing proteomics research, strengthening industry-academia partnerships, and translating scientific discoveries into societal and clinical impact. This reflective session not only celebrates the achievements of the past two decades but also serves as a strategic roadmap for the next generation of researchers and innovators, inspiring continued growth and global leadership of the Indian proteomics community.

Highlights at a Glance



PANEL DISCUSSIONS

Panel Discussion #2: Navigating Omics Research in India: Opportunities and Challenges for Young Investigators

The rapid advancement of omics technologies — encompassing genomics, proteomics, transcriptomics, metabolomics, lipidomics, and single-cell omics — has transformed the landscape of biological and biomedical research worldwide. In India, increasing investments in research infrastructure, national missions, collaborative networks, and translational science initiatives have created unprecedented opportunities for early-career scientists and young investigators to contribute to cutting-edge discoveries. However, alongside these opportunities, researchers face significant scientific, technical, financial, and career-related challenges while establishing independent research programmes.

Overview

This panel discussion focuses on the evolving ecosystem of omics research in India and explores pathways available for young investigators to build successful and impactful scientific careers. Bringing together accomplished researchers, mentors, funding experts, and emerging leaders in the field, the session provides practical insights into navigating the complexities of modern research environments.

Key Topics

Key topics of discussion include identifying high-impact research questions, establishing interdisciplinary collaborations, securing research funding, accessing advanced instrumentation and core facilities, managing laboratory resources, and building competitive research teams. Panelists also address strategies for publishing in high-quality journals, fostering industry-academia partnerships, translating research findings into clinical and societal applications, and leveraging international collaborations to enhance scientific visibility and impact.

Challenges and Emerging Opportunities

Particular emphasis is placed on the unique challenges faced by young investigators in India, including limited resources, the need to balance teaching and research responsibilities, securing long-term funding, and adapting to rapidly evolving, data-intensive research approaches. The discussion also highlights emerging opportunities arising from artificial intelligence, machine learning, big data analytics, precision medicine initiatives, and national omics programmes that are shaping the future of life sciences research. Beyond addressing challenges, this session aims to inspire and empower the next generation of scientists by sharing experiences, lessons learned, and success stories, while fostering mentorship, collaboration, and community building within the Indian omics ecosystem.

KEY HIGHLIGHTS

Highlights at a Glance

Funding & resource strategies	Interdisciplinary collaborations
High-impact research questions	AI, ML & big data analytics
Mentorship & community building	Precision medicine opportunities

PANEL DISCUSSIONS

Panel Discussion #3: Where Academia Meets Industry: Shaping the Future of Omics in India

The remarkable growth of omics technologies has created new opportunities to bridge fundamental scientific discovery with real-world applications in healthcare, biotechnology, agriculture, pharmaceuticals, and precision medicine. As India advances toward becoming a global innovation hub, strong partnerships between academia and industry are increasingly essential for translating research outcomes into impactful products, technologies, diagnostics, and therapeutic solutions. The convergence of these two sectors is actively shaping the future of omics research and innovation across the country.

Overview

This panel discussion explores how academia and industry can work together to accelerate scientific progress, foster innovation, and strengthen India's omics ecosystem. Bringing together leaders from academic institutions, biotechnology companies, pharmaceutical organisations, healthcare industries, start-ups, and technology providers, the session provides diverse perspectives on building effective and sustainable collaborations.

Key Themes

The discussion focuses on technology transfer, translational research, commercialisation of scientific discoveries, industry-sponsored research programmes, intellectual property management, and workforce development. Panelists examine how academic research can be aligned with industry needs while maintaining scientific rigor and creativity. Mechanisms to facilitate collaborative projects, shared infrastructure, data-driven research, and the co-development of novel omics-based solutions are also discussed.

Emerging Opportunities and Challenges

Significant emphasis is placed on emerging opportunities created by artificial intelligence, machine learning, digital health, precision medicine, and multi-omics integration — areas that require multidisciplinary expertise and collaborative frameworks combining academic creativity with industrial scalability. The panel highlights successful examples of academia-industry partnerships that have generated meaningful scientific and societal impact. The session also addresses challenges that often hinder collaboration, including funding constraints, regulatory considerations, intellectual property issues, data-sharing policies, and differences in organisational priorities, and identifies strategies to overcome these barriers.

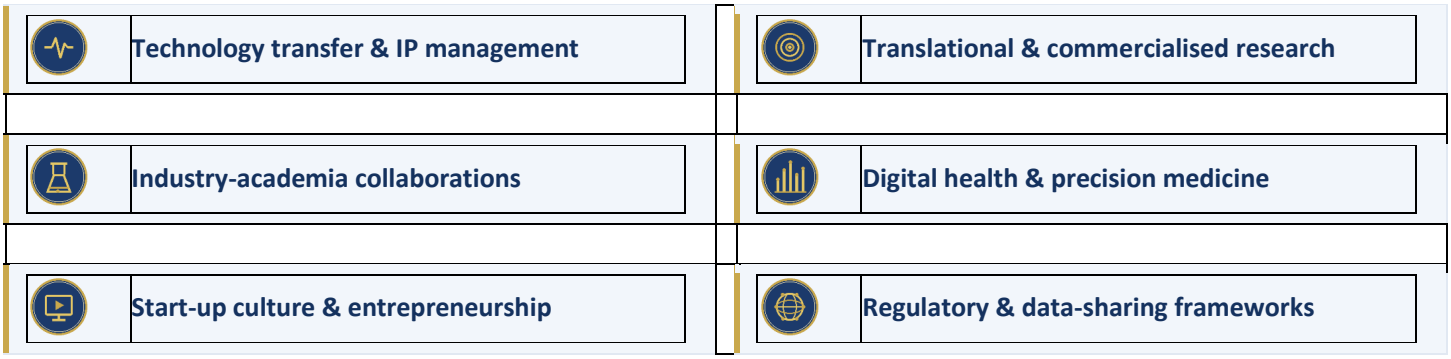
Career Pathways and Innovation

For students, researchers, entrepreneurs, and young professionals, this discussion provides valuable insights into career pathways beyond traditional academic settings and demonstrates how omics expertise can contribute to innovation and

entrepreneurship. The panel emphasises the importance of nurturing talent, fostering a start-up culture, and creating meaningful opportunities for knowledge exchange between academia and industry.

KEY HIGHLIGHTS

Highlights at a Glance



PANEL DISCUSSIONS

Panel Discussion #4: Omics in Healthcare: Opportunities and Challenges

Advances in omics technologies have revolutionised our understanding of human health and disease, opening new avenues for precision medicine, early diagnosis, disease prevention, and personalised therapeutics. By integrating information from genomics, proteomics, transcriptomics, metabolomics, lipidomics, and other emerging omics disciplines, researchers and clinicians are gaining unprecedented insights into the molecular mechanisms underlying complex diseases. These developments are transforming healthcare from a reactive model to a more predictive, preventive, personalised, and participatory approach.

Overview

This panel discussion explores the growing role of omics in modern healthcare and examines the opportunities and challenges associated with translating omics-based discoveries into clinical practice. Bringing together clinicians, researchers, healthcare professionals, industry leaders, and policy experts, the session provides a multidisciplinary perspective on the future of precision healthcare in India and beyond.

Key Themes

The discussion highlights the potential of omics technologies in improving disease diagnosis, patient stratification, biomarker discovery, therapeutic target identification, treatment monitoring, and drug development. Panelists discuss how multi-omics approaches are enabling a deeper molecular understanding of cancer, cardiovascular diseases, neurological disorders, infectious diseases, metabolic syndromes, and rare genetic conditions. The integration of omics data with artificial intelligence, machine learning, and digital health platforms is also explored as a key driver of next-generation healthcare solutions.

Challenges in Clinical Translation

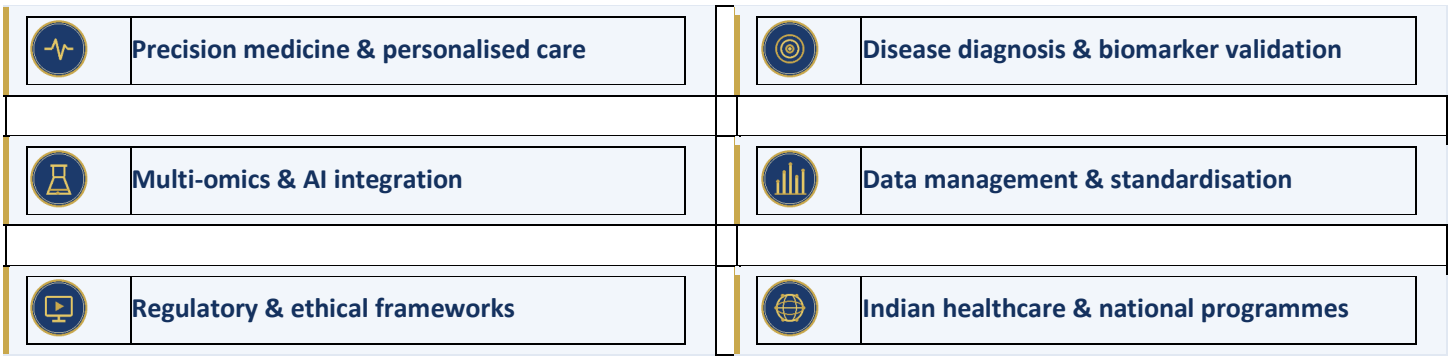
While the promise of omics-driven healthcare is immense, several challenges remain. The panel addresses critical issues such as data management and interpretation, standardisation of methodologies, validation of biomarkers, regulatory requirements, ethical considerations, patient privacy, and the high costs associated with advanced omics technologies. Discussions also focus on the need for robust clinical evidence, skilled workforce development, adequate healthcare infrastructure, and supportive policies that facilitate the adoption of omics-based approaches in routine clinical settings.

The Indian Healthcare Context

Particular attention is given to the Indian healthcare landscape, where diverse populations, unique disease burdens, and growing investments in biomedical research provide both opportunities and challenges for implementing precision medicine initiatives. Panelists share insights on national programmes, collaborative research efforts, and strategies to bridge the gap between laboratory discoveries and clinical applications, offering valuable perspectives for researchers, clinicians, students, and healthcare stakeholders.

KEY HIGHLIGHTS

Highlights at a Glance



PANEL DISCUSSIONS

Panel Discussion #5: Bridging Omics and Clinical Care: Perspectives from Clinicians and Researchers

The convergence of omics sciences and clinical medicine is transforming the way diseases are diagnosed, monitored, and treated. Advances in genomics, proteomics, metabolomics, transcriptomics, and other omics technologies have generated unprecedented insights into the molecular basis of human health and disease. However, translating these discoveries into meaningful clinical applications requires close collaboration between researchers, clinicians, healthcare providers, and technology developers. Bridging the gap between laboratory research and patient care remains one of the most critical challenges and opportunities in modern healthcare.

Overview

This panel discussion brings together leading clinicians, physician-scientists, biomedical researchers, and translational medicine experts to explore how omics technologies can be effectively integrated into clinical practice. The session fosters dialogue between those generating omics data and those utilising clinical information, emphasising the critical importance of interdisciplinary collaboration in advancing precision healthcare.

Clinical Applications of Omics

The discussion focuses on how omics-based approaches are improving disease diagnosis, patient stratification, risk prediction, treatment selection, and therapeutic monitoring. Panelists share perspectives on the clinical implementation of biomarkers, molecular diagnostics, companion diagnostics, and personalised treatment strategies across diverse disease areas, including cancer, cardiovascular disorders, neurological diseases, metabolic syndromes, infectious diseases, and rare genetic conditions.

Barriers to Translation

A key theme of the session is the challenges associated with translating omics discoveries into routine healthcare. Experts discuss barriers such as data interpretation, clinical validation, regulatory requirements, cost-effectiveness,

standardisation of analytical workflows, and integration of omics data into healthcare systems. The need for clinician education and training, and the role of artificial intelligence, machine learning, electronic health records, and digital health technologies in facilitating interpretation and clinical application of complex omics datasets, are also explored.

Opportunities in the Indian Ecosystem

Particular emphasis is placed on opportunities within the Indian healthcare ecosystem, where a large and diverse patient population offers unique possibilities for population-scale omics studies and precision medicine initiatives. Panelists discuss how collaborative research networks, biobanks, national health programmes, and translational research centres can help accelerate the adoption of omics-driven healthcare solutions in India. For clinicians, researchers, students, and healthcare professionals, this discussion provides valuable insights into building effective partnerships that connect scientific discovery with patient benefit, ultimately improving outcomes through data-driven, personalised, and evidence-based healthcare.

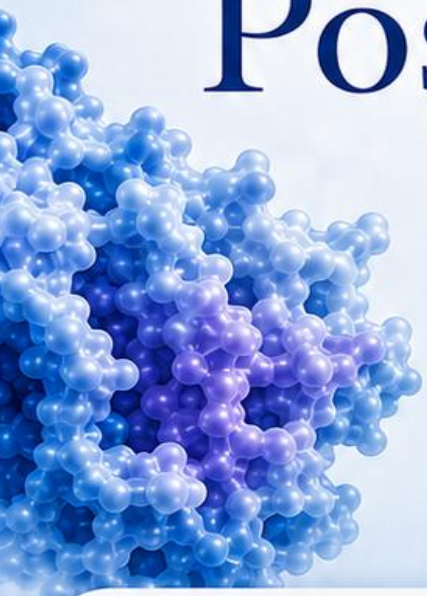
KEY HIGHLIGHTS

Highlights at a Glance

- **Clinician-researcher collaboration**
- **Molecular diagnostics & biomarkers**
- **Patient stratification & risk prediction**
- **AI & electronic health records**
- **Population-scale omics studies**
- **Translational research networks**

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Poster Abstracts







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Poster Abstracts

1. Investigating altered mouse spleen proteome upon *Plasmodium* infection using high resolution mass-spectrometry

Abrar Ahmad1, Akhila Rai2, Narahari Veeda1, Keshava Prasad2, Kamalakannan Vijayan1, Manish Kumar1*
School of Biology, Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala, India1
Centre for Omics and Systems Medicine (C-OSM) | Nitte University (Deemed to be University)2
*Corresponding author, email id: mkumar@iisertvm.ac.in

Background:
In malaria patients, spleen plays a critical role in clearance of *Plasmodium* infected RBCs,immune activation and haematopoiesis. Yet, it is unclear how the spleen proteome changes during infection. To that end, we employed mass spectrometry-based quantitative proteomics to study altered proteome of spleen in mice infected with *P. berghei* parasite.
Methods:
Spleen was isolated from *P.berghei* infected and uninfected control mice. The tissue was lysed to isolate proteins followed by trypsin digestion and TMT labelling. The samples were then analysed on high resolution Thermo Oribtrap Astral Zoom mass spectrometer for quantitative proteomic analysis.
Results:
The analysis revealed 246 murine proteins that were depleted and 27 proteins that were abundant in infected spleen. Gene ontology analysis of these differentially expressed proteins suggested their involvement in pathways like actin filament organization, heterochromatin formation, epigenetic regulation of gene expression, leukocyte cytokine production, T cell activation, inflammatory response, double stand break repair and recombinational repair.
Conclusion:
This study suggests that there is an overall dysregulation of immune signalling in the murine spleen during *P. berghei* ANKA blood stage infection. This could be due to presence of a blood-spleen barrier made up of fibroblasts (also known as barrier cells) in spleen that prevents direct contact of parasitized RBCs with immune cells, erythroblasts and reticulocytes. Also, a strong cytoskeletal disorganization is known to undergo in the spleen upon infection. This could be due to splenomegaly (enlargement of spleen), which is common in blood borne and other infections. Further experiments will be required for deeper insights into the mechanisms governing the expression of proteins identified as differentially abundant in this study.
Keywords: Spleen, Plasmodium infection, Orbitrap, Proteomics, Protein lactylation Adrija Banerjee

2. FUNCTIONAL INTERPLAY BETWEEN EISOSOMES AND THE CYSTEINE-RICH PALMITOYLATED DOMAIN (CYSPD) PROTEIN FAMILY IN YEAST.

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The cysteine-rich palmitoylated domain (CYSPD) protein family comprises small plasma membrane-associated proteins that are conserved across eukaryotes but remain poorly characterized. In Saccharomyces cerevisiae, this family includes Cpp1, Cpp2, Cpp3, and Ydl012c, all of which are targeted to the plasma membrane through palmitoylation. To gain insight into their function, we employed TurboID-based proximity labeling coupled with mass spectrometry to define the protein interaction landscape of CYSPD family members in vivo. Proteomic analysis identified a diverse set of proximal proteins associated with multiple cellular processes, including cell wall organization, endocytosis, vesicular trafficking, and plasma membrane compartmentalization. STRING network analysis revealed a particularly strong enrichment of eisosome-associated proteins, including Pil1, Lsp1, Sur7, Eis1, Seg1, Mdg1, and Ygr130c, suggesting a previously unrecognized connection between CYSPD proteins and eisosome biology. To validate this finding, we examined the localization of GFP-tagged Cpp1 in strains lacking key eisosome components. Whereas Cpp1 displayed a homogeneous plasma membrane distribution enriched toward the daughter cell in wild-type cells, deletion of PIL1, LSP1, or SUR7 caused its redistribution into punctate submembranous structures. This phenotype was specific to Cpp1, as the localization of the control plasma membrane proteins Sso1 and Ras2 remained unaffected. Moreover, a subset of Cpp1 puncta in pil1Δ cells colocalized with FM4-64-labeled early endosomes, suggesting altered endocytic trafficking in the absence of functional eisosomes. Collectively, our proximity proteomics approach identifies eisosomes as a major cellular context for CYSPD proteins and provides the first evidence that eisosome integrity contributes to their proper localization and endocytic regulation in yeast. These findings establish a foundation for understanding the biological role of this conserved but poorly characterized protein family.

3. From Spectra to Systems: Integrative Multi-omics Strategies for Translational Biomarker Characterization

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Introduction

Biological systems operate through the coordinated interplay of genes, proteins, post-translational modifications, and metabolites, each contributing distinct yet interconnected regulatory information. Decoding this molecular complexity requires integrative analytical strategies capable of translating multi-layered omics data into biologically meaningful and clinically actionable insights.

Materials and Methods

We established a standardized and end-to-end translational multi-omics protocol combining optimized experimental protocols, including ProtiFi™ S-Trap™-enabled proteomic processing, high-resolution mass spectrometry, and complementary transcriptomic analyses, to minimize technical variability while maximizing molecular coverage across biological conditions. Raw spectral outputs undergo rigorous preprocessing, including signal extraction, quality filtering, and retention time alignment, ensuring analytically robust feature selection for downstream evaluation.

Results and Discussion

Differential molecular abundance estimation is performed across experimental conditions using linear modelling frameworks with multiple hypothesis testing to control false discovery rates. Significant candidates are prioritized for multivariate analysis, while completed feature landscapes are retained for gene enrichment pathway- and network-level interrogation. Cross-platform integration is achieved using supervised and unsupervised latent factor decomposition approaches to identify shared biological axes across the transcriptomic, proteomic, phosphoproteomic, and metabolomic

datasets. These shared latent factors represent biological meaningful source of variation, such as disease progression, treatment response, or metabolic reprogramming. Co-expression and co-abundance network topology analyses further expose functionally coherent molecular modules, uncovering regulatory relationships and translational biomarker candidates that may remain undetected through single-omics approaches.

Conclusion

By bridging experimental precision with computational depth, our platform provides a seamless pipeline from biological specimen processing to advanced bioinformatics and biomarker prioritization, empowering translational discovery and accelerating precision medicine applications.

Keywords: Multi-omics; Proteomics, Metabolomics, Transcriptomics, Phosphoproteomics, Bioinformatics, Translational biomarker discovery, ProtiFi™ S-Trap™ proteomics, Systems biology, Precision medicine, Omicslink™

4. Inflammatory Proteomic Signatures Distinguish Pituitary Neuroendocrine Tumor Subtypes and Meningioma Grades Using Proximity Extension Assay

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Background: Pituitary neuroendocrine tumors (PitNETs) and meningiomas are among the most prevalent intracranial neoplasms; however, reliable circulating inflammatory markers capable of distinguishing tumor subtypes and grades remain limited. Sensitive detection of low-abundance proteins is critical for biomarker discovery, particularly for proteins that remain inaccessible to conventional mass spectrometry approaches.

Methods: This study employed proximity extension assay (PEA), a dual-antibody, oligonucleotide-based platform, to profile inflammatory proteins in serum samples from 5 healthy controls, 15 PitNET patients (acromegaly, Cushing's disease, and non-functioning pituitary adenomas), and 20 meningioma patients across different grades. PEA enables femtogram-per-milliliter sensitivity while requiring minimal sample input (1–6 µL), offering advantages over LC–MS-based methods. Differential expression and subtype- and grade-specific signatures were identified and further evaluated in the context of transcriptomic datasets.

Results: Distinct inflammatory proteomic signatures were observed across PitNET subtypes and meningioma grades. Key circulating proteins, including IL5, CXCL12, IL10, GZMH, FGF2, PTN, ADGRG1, GZMB, IL33, IL12RB1, and NO3, demonstrated subtype-specific expression patterns in PitNETs. Notably, CD83 and IL12A emerged as novel markers capable of distinguishing high-grade from low-grade meningiomas, representing previously unexplored candidates in this context. Several identified proteins also exhibited concordant trends in transcriptomics datasets, reinforcing their biological and clinical relevance.

Conclusion: This study highlights the utility of PEA for high-sensitivity profiling of circulating inflammatory proteins and identifies promising candidate biomarkers for distinguishing PitNET subtypes and meningioma grades. The integration of proteomic and transcriptomic evidence underscores the potential of these markers for improved disease stratification and minimally invasive diagnostics.

5. Identification of potential lead compounds targeting *Mycobacterium tuberculosis* shikimate kinase to combat multi-drug-resistant tuberculosis

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Background: There is an urgent need to develop new class of drug to fight against Multi-drug resistant (MDR) tuberculosis (TB). Shikimate kinase of *Mycobacterium tuberculosis* ($SK_{M.tb}$) is vital enzyme of chorismate biosynthetic pathway which provides precursor of dihydrofolate, essential aromatic amino acids, and mycobactins required for nucleotide synthesis, protein synthesis, and growth of *M.tb* inside macrophages, respectively. Gene knockout studies established that $SK_{M.tb}$ is vital for its survival and is absent in human, hence it is an attractive drug target. Its inhibitor would deliver lead compounds for the development of drugs against drug-resistant TB.
Material and Methods: Molecular docking-based screening of chemical databases was performed to identify potential inhibitors and followed by molecular dynamics (MD) simulations based refinement. Cloning, overexpression and purification of $SK_{M.tb}$ was done. Enzyme assays was followed by crystallisation experiments and MIC determination of selected compounds using Alamar assay in *M.tb*.
Results and Discussion: *In silico* screening identified 8 compounds as potential inhibitors of $SK_{M.tb}$. Inhibition assays found two compounds among them having IC_{50} in µM range which was validated using Alamar assay. Crystals were obtained with substrate but no crystal was obtained with inhibitors. Diffraction data of obtained crystals were collected at ESRF, France and solved at 1.7Å.
Conclusion: *In silico* study could help to identify inhibitors at cheap cost and rapid speed but also yields high percentage of false positives. Identified inhibitors could provide new class of lead compounds for MDR-TB.
Keywords: Tuberculosis, Shikimate kinase, Drug discovery, Crystallisation

6. Scalable Plasma Proteomics for Population-Level Aging Research: Pilot Aging Signatures from the BHARAT Study

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Population-scale plasma proteomics in low- and middle-income research settings requires workflows that are simultaneously high-throughput, low-cost, and analytically rigorous. We describe an integrated pipeline combining perchloric acid precipitation with neutralization (PCA-N) and intrinsic tryptophan fluorescence (WF) quantification, implemented on a timsTOF Pro 2 operating in diaPASEF mode, and applied to a pilot cohort from the BHARAT Study (Biomarkers of Healthy Aging, Resilience, Adversity, and Transitions): a cross-sectional aging study targeting 5,000+ participants across five age groups at the Indian Institute of Science, Bangalore.
PCA-N, originally developed as "perCA" by the Steen laboratory and extended with a neutralization step by Albrecht et al. (Mann lab, MCP 2025), uses 5 µL of EDTA plasma, perchloric acid precipitation at 4°C, and NaOH neutralization to pH 8–8.5, enabling direct in-solution trypsin digestion in 384-well format without solid-phase extraction. This eliminates a major cost and throughput bottleneck at population scale. We adapt and validate this workflow on the timsTOF Pro 2 platform under Indian field collection conditions relevant to BHARAT.
A key analytical challenge for large-scale plasma proteomics is peptide quantification prior to MS injection. We evaluate tryptophan fluorescence as a rapid, reagent-free quantification method, leveraging the conserved ~1.17% Trp residue content of the human proteome. We assess whether this conversion factor holds accurately for PCA-N-processed plasma, where abundant protein depletion and precipitation alter the peptide pool composition, using spike-in peptide standards across a range of sample types.
We apply this pipeline to a pilot cohort of 96 BHARAT participants stratified by age (young: 18–35 years; old: 60+ years) to characterize plasma proteome changes associated with aging in an Indian population. This work establishes a scalable, cost-effective foundation for the full 5,000+ sample BHARAT proteomics effort and addresses an unmet need for population-level proteomics infrastructure in South Asia.
Keywords: plasma proteomics, aging, diaPASEF, tryptophan fluorescence, population cohort, BHARAT Study, PCA-N, timsTOF

7. From Post Translational Modifications (PTMs) Analysis To Clinical Detection: FOPPR and FONLISA Technologies.

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Background: Neurodegenerative diseases such as Alzheimer's disease require highly sensitive and reliable biomarker detection methods for early diagnosis and disease monitoring. Phosphorylated tau (pTau-217) has emerged as a promising biomarker, but its low abundance in plasma demands advanced analytical technologies. Fiber Optics Particle Plasmon Resonance (FOPPR) technology enables real-time binding kinetics analysis and epitope binning under nearphysiological conditions, facilitating the selection of optimal antibody pairs. When integrated with FONLISA on the INB-D8 biomarker analyzer, this approach supports rapid, automated, and ultrasensitive detection with fg/mL sensitivity. The platform bridges PTM research and clinical diagnostics, offering a scalable solution for decentralized testing of Alzheimer's disease and other neurodegenerative biomarkers.

Methodology: A self-driven microfluidic chip integrates with uncladded optical fiber for label-free plasmonic sensing. Fiber is coated with a low-hindrance chemical layer to reduce nonspecific adsorption and enhance PTM-sensitive analysis. In FOPPR, antibodies on AuNPs interact with fiber to monitor binding kinetics and epitope binning. In FONLISA, detection antibodies capture AuNPsample complexes, generating resonance signals.

Results and Discussion: Kinetic/Affinity Analysis: FOPPR based affinity analysis (ka, kd, KD), help to understand the different Ab binding intensity on the antigen. Fig. 2(A and B), which allows to select perfect Ab pairs from the pool of Ab's for assay development. From the pool, A204;RD085 and S059;S172 Ab's were used as sandwich Ab pairs for FONLISA assay development, respectively. FONLISA Assay Development: The calibration curve of SET-1 and SET-2 Ab pair exhibit good linearity with R2 0.998 and 0.999 respectively. The recovery rate of pTau-217 in spiked plasma were within the predefined acceptance range (i.e. 80% to 120%) in different concentrations.

Conclusions: 1. The FOPPR based assay methodology selected most efficient antibody pairs and FONLISA demonstrated ultra-sensitive and rapid detection of pTau-217. 2. Assay technique is not only useful in ND diseases, also useful in other fields like immunology, infectious diseases, and cancer biology.

8. *Moringa oleifera* Lectin as a Promising Scaffold against SARS-CoV-2 Spike Glycoprotein: Protein-Protein Docking and Molecular Dynamics Simulation

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Background: The SARS-CoV-2 pandemic provoked an unprecedented global health emergency marked by widespread morbidity and mortality as well as significant disruption of socioeconomic and healthcare systems. The rapid transmission of the virus and continuous emergence of new variants highlighted the limitations of conventional therapeutic approaches and emphasized the urgent need for effective alternative interventions. *Moringa oleifera* lectins, owing to their ability to recognize and bind glycosylated viral envelope proteins, have emerged as potential inhibitors of viral attachment and fusion.

Objective: In the present study, a comprehensive *in silico* investigation was conducted to evaluate the binding potential of lectin proteins derived from *M. oleifera* against the SARS-CoV-2 spike glycoprotein.

Methods: Protein–protein docking was conducted using ClusPro, LZerD and PRODIGY online servers to generate and compare multiple docked complexes of *M. oleifera* lectin proteins (PDB ID: 5DOM, 6S3F) target against the spike glycoproteins of SARS-CoV-2 (PDB ID: 6VYB). The docked conformations were further evaluated using scoring functions (GOAP, DFire, ITScore, and RankSum) to assess interaction stability and ranking reliability.

Results: The docked complexes of *M. oleifera* lectin proteins (PDB ID: 5DOM, 6S3F) with the spike glycoproteins of SARS-CoV-2 (PDB ID: 6VYB) demonstrated the most favorable docking energies, with ClusPro center scores of −1015.7 and −1113.0 and lowest energies of −1170.4 and −1261.3, respectively. PRODIGY analysis further confirmed strong binding affinities, with ΔG values of −33.5 and −28.4 kcal/mol and corresponding Kd values in the order of 10^{-25} to 10^{-21} M.

Molecular dynamics simulation of the top-ranked complex further confirmed structural stability of the docked structure through 100 ns under near-physiological conditions using GROMACS software.

Conclusion: The results revealed that *M. oleifera* lectin exhibits strong binding affinity toward the SARS-CoV-2 spike protein and may serve as a promising antiviral scaffold for disrupting viral attachment.

9. Organelle-Specific Quantitative Proteomics Reveals System-Level Organization of Ciliary Proteins in Flagellar mutants.

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Background: Motile cilia and flagella are highly conserved microtubule-based organelles that play essential roles in cell movement and fluid transport. Their function depends on the precise assembly of axonemal protein complexes, and defects in these structures can lead to disorders such as primary ciliary dyskinesia (PCD). Although many Flagellar Associated Proteins (FAPs) have been identified, the specific functions of several remain unclear. In this study, we investigated the roles of FAP54, FAP75, FAP147, and FAP174 in flagellar structure and function using *Chlamydomonas reinhardtii* as a model organism.

Methods: Mutant strains lacking FAP54, FAP75, FAP147, or FAP174 were obtained from the Chlamydomonas Resource Center and validated through PCR, transcript analysis, and protein characterization. Isolated flagella from each mutant were analyzed by quantitative mass spectrometry to identify changes in protein composition. Proteomic findings were complemented with phenotypic analyses, including measurements of flagellar length, swimming behavior, phototaxis, adenylate kinase activity, and genetic rescue experiments where applicable.

Results: Quantitative proteomic analysis revealed that each FAP contributes to distinct aspects of axonemal organization while also sharing common functional relationships with other flagellar proteins. Loss of individual FAPs led to selective depletion of specific protein groups, suggesting roles in maintaining the stability and assembly of central pair complexes. Mutants lacking FAP54 or FAP174 showed reduced levels of central pair C1-associated proteins, accompanied by shorter flagella, impaired motility, and altered phototactic responses. The *fap147* mutant retained overall axonemal structure but exhibited loss of FAP147 protein, a modest decrease in C2a-associated proteins, and defects in directional swimming; these defects were restored by reintroduction of the wild-type gene. In contrast, the *fap75* mutant displayed depletion of central pair C2-associated and C1–C2 interface proteins, reduced adenylate kinase activity, and impaired motility, highlighting a potential link between central pair organization and energy regulation within the flagellum.

Conclusion: Our findings demonstrate that FAP54, FAP75, FAP147, and FAP174 play distinct yet interconnected roles in organizing central pair architecture and supporting efficient flagellar motility. By combining quantitative proteomics with functional analyses, this study provides new insights into the molecular basis of ciliary function and offers a framework for understanding how defects in these proteins may contribute to ciliopathies such as PCD.

Keywords: PCD, flagella mutant, *Chlamydomonas,* central pair, ciliopathies, CIB1 cassette, FAPs. organelle-specific proteomics.

10. Identification of plasma protein biomarkers for gallbladder cancer using mass spectrometry: A pilot study

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Background: Gallbladder cancer (GBC) is a rare but aggressive disease with dismal prognosis 1. Therapeutic success is limited by late diagnosis. Lack of specific symptoms or diagnostic biomarkers is a key obstacle for its early detection.

Identification of specific plasma biomarkers for GBC would enable regular screening facilitating early detection, effective disease surveillance and thereby improved patient outcome. This pilot study tests the feasibility of using a mass spectrometric approach for identifying GBC-specific plasma biomarkers.
Methods: Banked plasma samples derived from peripheral blood of 4 GBC and 6 non-malignant patients (4 with inflamed gallbladder and 2 healthy volunteers) were analysed. The top 14 abundant plasma proteins were depleted using High Select TM resin followed by protein quantification using Pierce BCA Protein Assay kit TM . Sample preparation for proteomic analysis was performed using EasyPep kit TM following manufacturer's protocol. LC-MS/MS (Eksigent Ekspert NanoLC 400; Sciex TripleTOF 6600+) was conducted in Data Independent Acquisition mode followed by protein quantification with DIANN v2.2.0. MSstats. R-based packages were used for Differential Protein Expression (DPE) and enrichment analysis.
Results: A total of 167 with an average of 161 unique proteins (~1440 precursor) were identified per sample. Principle component analysis showed non-malignant and GBC samples separated out with one exception. DPE revealed ADH1B, PZP and ACTN1 as top differentially expressed proteins in GBC plasma. An ontology enrichment analysis of the significantly upregulated proteins revealed over-representation of pathways related to cytoskeletal reorganization, cell adhesion and platelet activation.
Conclusion: Our initial findings demonstrated the possibility of distinguishing the GBC plasma from non- malignant samples. This generates the prospect for developing minimally invasive blood- based diagnostic screening, which can reduce early detection bottlenecks and improve pre-operative decision making through appropriate screening. Larger cohorts including non-GBC cancer controls are required to confirm GBC-specificity of the markers. Further validations are needed to authenticate their clinical reliability.

11. Differential Expression of Proteins in Bladder Cancer; Urine Proteomics Based Approach

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Introduction: Urinary bladder carcinoma (UBC) is one of the most common malignancies worldwide and is associated with significant morbidity and mortality. Bladder cancer is broadly classified into non-muscle invasive bladder cancer (NMIBC) and muscle-invasive bladder cancer (MIBC). Although NMIBC has a favorable prognosis, it is characterized by high recurrence and progression rates. This study aimed to identify differentially expressed urinary proteins as potential non-invasive biomarkers for bladder cancer diagnosis and surveillance.
Materials and Methods: Urine samples were collected from histologically confirmed bladder cancer patients and healthy controls. Samples were concentrated using Centricon filtration devices, and total protein concentration was determined by the Bradford assay. Proteins were subjected to in-solution trypsin digestion followed by liquid chromatography–tandem mass spectrometry (LC-MS/MS) for protein identification and relative quantification. Differential expression analysis was performed to identify candidate biomarker proteins.
Results and Discussion: LC-MS/MS analysis revealed distinct urinary proteomic profiles between bladder cancer patients and healthy controls. Several proteins were found to be differentially expressed, showing unique patterns of upregulation and downregulation in patient samples. Pathway enrichment analysis indicated the involvement of extracellular matrix remodeling, complement/coagulation cascades, and metabolic pathways associated with bladder cancer progression. Conclusion: These preliminary findings demonstrate the potential of urine proteomics for identifying non-invasive biomarkers for bladder cancer diagnosis and monitoring. Further validation in larger cohorts is required to establish clinically relevant biomarker panels. Keywords: Urine proteomics, bladder cancer, biomarkers, LC-MS/MS, non-invasive diagnosis.

12. Integrated proteomics and metabolomics investigation to understand the lymphatic nodal metastasis in oral squamous cell carcinoma

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Lymph node metastasis (LNM) is the principal determinant of poor prognosis in oral squamous cell carcinoma (OSCC), yet the molecular programs governing the transition from localized to nodally invasive disease remain poorly resolved at the level of functional effectors. Current clinical staging tools; including CT, MRI, and PET, fail to detect occult nodal disease with adequate sensitivity, creating a persistent clinical dilemma between overtreatment and undertreatment. To address this critical gap, we present a comprehensive integrated multi-omics framework, combining global data-independent acquisition (DIA) proteomics, untargeted LC-MS/MS metabolomics, and parallel reaction monitoring (PRM)-based targeted proteomics, Metabolomics/lipidomics—in matched tumor tissue and saliva specimens from pathologically-annotated LNM-positive (LNM+) and LNM-negative (LNM−) OSCC patient cohorts.

Library-based DIA proteomics of 40 tumor tissues (20 LNM+, 20 LNM−) identified 8,080 quantified proteins; 177 were significantly upregulated and 194 downregulated in LNM+ tissue ($p < 0.05$, $|FC| \geq 1.5$). The LNM+ proteomic signature was organized around a RAP1–integrin–ILK adhesion hub spanning ECM–receptor interaction, focal adhesion, adherens junction, and actin cytoskeleton pathways, with key nodes including ITGB1, ILK, VCL, ACTN4, PTK2/FAK, MMP8/9/13/14, and CDH1/CTNNB1. Concomitant elevation of oligosaccharyltransferase subunits (STT3A/B, DAD1, RPN2) and N-glycan branching enzymes (MGAT1/2/3), coupled with elevated UDP-GlcNAc and UDP-Gal from metabolomics, links post-translational N-glycan remodeling to integrin signaling stabilization. Salivary proteomics (n = 25) identified 50 DEPs and a six-protein nodal panel, ITIH1/2/4, ORM1/2, RBP4 (FC 1.72–2.20; $p < 0.05$), with 14 proteins shared across tissue and saliva datasets.

Untargeted metabolomics of tumor tissue (n = 20; 57 DEMs) and saliva (n = 29; 24 DEMs) revealed clear LNM+/− group separation by OPLS-DA, with pathway enrichment converging on sphingolipid and glycerophospholipid metabolism, alpha-linolenic/linoleic acid signaling, purine metabolism, and amino acid biosynthesis. Targeted PRM lipidomics validated four ceramide/sphingomyelin species, Cer(d19:1/41:0), Cer(d16:1/35:0), Cer(d16:1/39:0), SM(d16:1/18:3), as consistently elevated in LNM+ tissue. Pharmacological inhibition of ILK with CPD22 (IC_{50}: SCC4 ~13 µM; SCC25 ~17 µM) significantly reduced OSCC cell migration, disrupted focal adhesion architecture, and redistributed ILK from membrane-localized to diffuse cytoplasmic distribution, functionally validating the proteomic network. These findings nominate a mechanistically coherent multi-omics model, RAP1-integrin-ILK adhesion, N-glycan reinforcement, sphingolipid membrane remodelling, and a cross-matrix candidate biomarker panel for prospective non-invasive nodal stratification and pathway-informed therapeutic exploration in OSCC.

13. Deciphering the molecular basis of Vitamin D_2-induced alterations in Vitamin D_3 homeostasis: a Multi-target Docking investigation

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Introduction: Vitamin D deficiency affects nearly one billion people worldwide and remains a significant public health issue. Clinical studies have reported decreases in circulating vitamin D_3 levels after vitamin D_2 supplementation; however, the exact molecular mechanism is unclear. This study looked into how vitamin D_2 interacts with key vitamin D-metabolizing enzymes to explore a possible enzyme-driven regulatory mechanism
Materials and Methods: We obtained the protein structures of CYP2R1, CYP27B1, CYP11A1, and CYP27A1 from the Protein Data Bank (PDB) and AlphaFold databases. We performed molecular docking using Schrödinger Maestro (Release 2024-1). We analyzed binding affinities, docking poses, and protein-ligand interaction profiles to identify possible metabolic interaction hotspots.
Results and Discussion: Vitamin D_2 showed strong binding affinities for CYP2R1 (−10.694 kcal/mol), CYP27B1 (−10.671 kcal/mol), CYP11A1 (−10.720 kcal/mol), and CYP27A1 (−9.010 kcal/mol). The strongest interactions occurred with CYP2R1 and CYP27B1, two key enzymes involved in vitamin D activation. These results suggest that vitamin D_2 may occupy shared metabolic pathways and could influence vitamin D_3 processing through competition at the enzyme level.
Conclusion: This study provides computational evidence for a possible enzyme-driven interaction between vitamin D_2 and vitamin D_3 metabolism. Some enzymes appear to be potential control points for metabolism and may serve as valuable targets for future research into mechanisms and therapies. Further research is still needed to understand the mechanism
Keywords: Vitamin D_2, Vitamin D_3, Molecular Docking, CYP2R1, CYP27B1, Vitamin D Metabolism, Computational Pharmacology

14. Serum Raman Spectroscopy as a Rapid Diagnostic Modality for Oral Potentially Malignant Disorders and Oral Cancer

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Introduction: Oral cancers are frequently diagnosed at advanced stages, making early detection critical.Traditional biomarker detection involves tedious sample preparation and extensive turnaround times. Raman spectroscopy (RS) offers a rapid, highly sensitive, and non-invasive alternative requiring minimal sample preparation. Since serum reflects global biochemical changes associated with carcinogenesis, this study evaluates the efficacy of serum RS in identifying distinct molecular signatures among normal healthy controls, individuals with adverse habits but no lesions, patients with Oral Potentially Malignant Disorders (OPMDs: Leukoplakia and Oral Submucous Fibrosis), and Oral Cancer patients.
Materials and Methods: In this cross-sectional study, 3 ml of venous blood was collected from participants. After clotting and centrifugation (3000 rpm, 30 minutes), 10 µl of supernatant serum was placed on a calcium fluoride (CaF2) window. Spectral acquisition was performed using a Raman spectrograph coupled with a CCD detector, employing a 785 nm excitation laser (28 mW) and an integration time of 0.05 seconds. Data analysis was conducted using Linear Discriminant Analysis (LDA).
Results and Discussion: Serum Raman spectra successfully characterized distinct biomolecular shifts among the clinical groups. Key spectral markers distinguishing the pathologies included Phenylalanine (~1002 cm-1), Beta-carotene (~1154 cm-1 & ~1514 cm-1), DNA bases (~1340 cm-1), and Amide I (~1664 cm-1). LDA scatter plots demonstrated clear clustering and discrimination between the four groups (Normal, Habit without lesion,
OPMDs, and Oral Cancer). These molecular variations reflect underlying metabolic and structural alterations during disease progression, validating RS as an effective tool for mapping the biomolecular landscape.

Conclusion: Neoplastic transformation induces conformational and quantitative changes in serum proteins and nucleic acids before macroscopic morphological changes appear. Serum RS successfully captures these biochemical signatures, providing a low-cost, minimally invasive, and highly accurate framework for the early diagnosis and risk assessment of OPMDs and oral cancer.

Keywords: Raman Spectroscopy, Oral Cancer, OPMD, Serum Diagnostics, Proteomics, Biomarkers.

15. Structure-Based Discovery of Peptide and Substrate/Product Analog Inhibitors of Mycobacterium tuberculosis Isocitrate Lyase

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Introduction

Persistent Mycobacterium tuberculosis bacilli contribute to prolonged TB treatment. Isocitrate lyase (ICL_{Mtb}), a key glyoxylate shunt enzyme required for persistence, is an attractive target for novel anti-TB therapeutics The active site of ICL_{Mtb} is formed by residues from the C-terminal end of the barrel and active-site loop of one subunit, along with the C-terminal region of the adjacent subunit. The C-terminal region acts as a lid over the active site loop during substrate binding, making lid closure essential for catalysis. Hence, aim of this study is to identify potential inhibitors of ICL_{Mtb} among substrate and product analogs compounds and peptide-based inhibitors that could provide lead molecules to develop drugs for reducing the treatment duration of TB.

Methods

Based on this structural information, four derivative peptides were designed from the functionally critical C-terminal sequence of ICLMtb. Molecular docking was performed to compare the binding affinities of designed peptides with the native C-terminal template peptide. Molecular dynamics simulations were further carried out to evaluate the stability of peptides.

Results

Docking analysis showed that the designed peptides exhibited stronger binding affinities toward ICLMtb than the native template peptide. Molecular dynamics simulations further validated the stability of these interactions, suggesting that the designed peptides may interfere with catalytic lid closure and block enzymatic function. Since these peptides are derived from a functionally important region of ICLMtb, they mimic natural binding motifs and may act as competitive modulators of the enzyme.

Conclusion

This study proposes a peptide-based strategy to develop novel inhibitors against ICLMtb by targeting its active-site architecture and disrupting C-terminal lid closure. Further experimental validation through peptide synthesis, enzyme inhibition assays, and X-ray crystallography will be performed to confirm their inhibitory potential and binding mechanism.

Keywords

Mycobacterium tuberculosis, Isocitrate lyase, Peptide design, Inhibitors

16. Temporal proteomic profiling of murine liver identifies RDH11 downregulation associated with metabolic rewiring during MAFLD progression

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Background: Metabolic dysfunction-associated fatty liver disease (MAFLD) is characterized by excessive hepatic lipid accumulation and can progress to steatohepatitis, cirrhosis, and hepatocellular carcinoma. However, the molecular

mechanisms underlying disease-associated proteomic alterations remain poorly understood. This study employs a temporal proteomic approach to identify proteins associated with MAFLD progression.

Methods: C57BL/6 male mice were subjected to a Western diet with fructose–glucose supplementation and low carbon tetrachloride administration. Liver tissues were collected at 8, 12, 16, 20, and 24 weeks. Disease progression was evaluated using biochemical parameters (AST, ALT, triglycerides, cholesterol, insulin, body weight) and histological analyses (H&E, cytokeratin 19, desmin, PAS, α-SMA). Quantitative mass spectrometry was performed to profile global proteomic changes. Consistently regulated proteins were validated by western blotting and assessed in vitro using fatty acid-treated HepG2 cells. Human dataset validation was performed using GSE48452, TCGA-LIHC, and CPTAC, including survival analysis. Functional insights were investigated through overexpression of RDH11 followed by global proteomic analysis.

Results: Proteomic profiling revealed alterations in metabolic and structural pathways associated with MAFLD. RDH11 was identified as a consistently **downregulated** protein across disease conditions, with concordant expression patterns observed in human datasets. Overexpression of RDH11 resulted in significant modulation of pathways including steroid metabolism, fatty acid metabolism, and focal adhesion, indicating a functional role in metabolic regulation.

Conclusion: This study identifies RDH11 downregulation as a feature of MAFLD and highlights RDH11 as a potential regulator of disease-associated metabolic dysfunction and a candidate for further mechanistic investigation.

Keywords: Metabolic dysfunction-associated fatty liver disease, steatohepatitis, Western diet, Quantitative mass spectrometry, fatty acid metabolism.

17. Integration of Multi-Omics Data for Precision Agriculture: Concept of a Mobile Application – *Bhumicha Vaidya*

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Introduction

Recent progress in omics technologies have allowed for in depth studies of how plants interact with pathogens, and how they respond to stresses like drought. To fully understand these complex interactions, we need to combine data from multiple omics fields—such as genomics, transcriptomics, proteomics, metabolomics, and microbiome with agricultural databases. This project aims to introduce concept of developing a mobile application *Bhumicha Vaidya* that uses integrated multi-omics data to support precision agriculture, addressing issues like food security, adapting to climate change, sustainable farming.

Materials and Methods

The collection of multi-omics data involves using soil sensors to monitor nutrients and microbes, also drone-based imaging for assessing crop health. The integration aims to utilise statistical methods for combining multi-omics data and to keep costs low, we use simple user interfaces, collaborate with NGOs, design localized solutions, and include training modules for farmers.

Results and Discussion

The app concept will aid in efficiently gathering and analyzing multi-omics data in real-time, offering insights into plant growth, stress responses, improved nutritional content, and the development of bioenergy crops, supporting more precise recommendations for improving crops and maintaining soil health. Going beyond the limits of single-omics studies, it will provide farmers with easy-to-understand outputs.

Conclusion

The mobile application concept using integrated multi-omics data serves as a practical tool for precision agriculture, helping farmers make informed decisions to boost productivity and promote sustainability. Future improvements will include validating the app with real-world field data.

Keywords

Multi-omics, Integrative omics, Precision agriculture, Mobile app concept, Crop improvement, Drought tolerance, Sustainable farming

18. Deep Proteomic Profiling Unravels the Molecular Landscape of Psoriasis

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Background: Psoriasis is a chronic immune-system-mediated autoinflammatory skin condition, associated with the hyperproliferation of keratinocytes, resulting in the formation of skin plaques and infiltration of various immune cells, inflammatory cytokines, and myeloid dendritic cells into the skin layers. Psoriasis is of significant public health concern in India, with the prevalence rate ranging from 0.44% to 2.8% in the adult population. Despite several advances being made in understanding the immunobiology and treatment of psoriasis, the heterogeneity of the disease makes it difficult to prognosticate and predict treatment responses. By capturing the dynamic protein landscape directly within affected tissue, proteomics bridges the gap between genetic predisposition and clinical phenotype, uncovering the precise molecular networks driving psoriatic pathology.

Method: Epidermal layers from 30 paired psoriatic skin samples were isolated, digested using a PreOmics iST workflow, and analyzed via high-resolution timsTOF Pro 2 LC-MS/MS in data-independent acquisition mode. Primary processing with DIA-NN followed by statistical evaluation in Perseus identified differentially expressed proteins between lesional and non-lesional tissues.

Results: The proteomic analysis of the epidermal proteome identified 44 distinct functional modules revealing a coordinated pathological landscape. The largest signature comprising 22 proteins mapped a state of "antiviral mimicry" in the psoriatic skin, driven by the accumulation and stabilization of Type I Interferon effectors (STAT1, MX1/2, OAS2/3) and Guanylate-Binding Proteins (GBP1/2) protected by a post-translational conjugation core (ISG15, UBE2L6, DTX3L, PARP9). Synchronized lipid modules revealed an accelerated lipid biogenesis driven by the key metabolic enzymes SQLE and KYNU, providing the biochemical fuel to downstream transcriptional (JUNB/FOSL2) and mitotic (STAT3/STMN1) overdrive. Crucially, pathway analysis identified a neuro-cutaneous pruritus axis centered on the functional assembly of the Mac-1 integrin heterodimer (ITGAM/ITGB2) operating alongside the class B scavenger receptor CD36. This orchestrates the infiltration of primary neutrophil granule proteases (PRTN3, ELANE, MPO), driving localized proteolytic and extracellular amyloid-clearance stress. This localized cytotoxic burst damages dermal sensory nerve endings, providing a direct protein-level mechanism for psoriatic pruritus and characteristic plaque formation.

Conclusion: Deep proteomic profiling reveals that psoriasis is driven by a coordinated network of antiviral mimicry, accelerated lipid biogenesis, and an integrin-mediated, neutrophil-driven axis that triggers localized cytotoxicity, persistant itch and plaque formation.

19. Uremic Toxin Hippurate induces Neutrophil Dysfunction in Shock Patients: Exploring the Role of Host-Microbe Co-Metabolism and PS1145 as a Novel Therapeutic

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Background-Patients with alcohol-associated cirrhosis (AAC) face a high risk of infection-triggered sepsis progressing to septic shock (30-40% mortality). Gut dysbiosis fuels this via microbial translocation and co-metabolites, driving immune dysregulation and organ failure necessitating superior biomarkers and precise drug targets for shock diagnosis and effective treatment.

Methods-Untargeted metabolome/metaproteome analyses of plasma, stool, and neutrophils from healthy (HC), non-septic (NS), septic (SE), and septic shock (SS) patients identified hippurate as a shock-specific indicator, validated in an independent cohort and benchmarked against clinical scores. In vitro hippurate exposure of healthy neutrophils, hepatocytes, and endothelial cells with PS1145 co-treatment revealed its therapeutic blockade potential. The NIAAA alcohol mouse model further delineated hippurate's biosynthesis, excretion dynamics, and alcohol-mediated regulation.

Results: Stool metaproteome and plasma metabolome analyses revealed >278 bacterial species and >293 metabolites unique to shock. Integrated analysis identified hippurate as the best predictor of shock (FC >25, $p<0.05$, AUC>0.9). Validation in an independent cohort using traditional statistics and machine learning confirmed hippurate's superior performance (AUC>0.95, outperforming SOFA/MELD; Cox HR>3) for diagnosing shock and predicting mortality compared to current models. Stool metaproteome and metabolome analyses showed upregulation of phenylalanine-to-benzoate/hippurate conversion in the gut of shock patients (FC>1.5, $p<0.05$), with impaired hippurate clearance leading to its accumulation in circulation and within neutrophils. Hippurate at shock concentrations (>415 µM) is proinflammatory, activating neutrophils via the TLR pathway, inducing excessive ROS production and degranulation, and causing widespread organ injury. It also promotes oxidative stress and inflammation in liver and endothelial cells. PS1145, a TLR dimerization inhibitor, mitigates hippurate-induced ROS, TNF-α production, and degranulation, positioning it as a promising therapeutic candidate for shock. Therapeutic plasma exchange (TPE) also effectively reduces hippurate levels in these patients, demonstrating its utility for shock treatment.

Conclusions- In shock-associated liver cirrhosis, gut bacteria overproduce hippurate, which accumulates due to impaired kidney clearance, driving neutrophil degranulation and excessive ROS generation. Both PS1145, by curbing these proinflammatory effects, and therapeutic plasma exchange (TPE), by directly eliminating hippurate, emerge as highly promising therapeutic strategies for shock management.

Keywords: Septic shock, hippurate, clinical biomarker, PS1145, Immunoexhaution.

20. Proteomics-Driven Biomarker Identification and Validation in Oral Squamous Cell Carcinoma

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Background: In India, oral cancer ranks second in both incidence and mortality according to the Global Cancer Observatory 2022, and continues to show poor survival outcomes in patients with advanced-stage disease. Therefore, early detection is critical for improving patient outcomes. Proteomics-based approaches offer significant potential for identifying biomarkers for early diagnosis, prognosis, and therapeutic targeting.

Methods: Serum samples collected from patients with locally advanced Oral Squamous Cell Carcinoma (OSCC) at different treatment stages were enriched using organic solvents, such as acetonitrile, to deplete high-abundance proteins. The enrichment protocol was optimised and evaluated for reproducibility. The depleted serum samples were analysed by label-free quantitative proteomics using mass spectrometry (MS) for comprehensive protein profiling. Candidate proteins identified through discovery analyses will subsequently undergo targeted quantification, particularly Multiple Reaction Monitoring and antibody-based validation, such as ELISA. Protein expression levels will be correlated with clinical parameters such as tumor size and nodal metastasis, including patient survival, to evaluate their prognostic and translational relevance.

Results: Preliminary label-free Data-Dependent Acquisition analyses demonstrated efficient depletion of high-abundance proteins, thereby improving the detection of low-abundance proteins. Initial MS runs yielded reproducible peptide profiles across samples, confirming the workflow's suitability and reproducibility for downstream proteomic analyses. Additionally, several proteins associated with acute-phase response pathways and inflammatory processes were identified during the discovery phase, suggesting their potential relevance in oral cancer progression and prognosis.

Conclusion: This study aims to establish clinically relevant serum biomarkers for OSCC, with potential applications in early detection, prognosis, and translational oncology.

Keywords: Data-Dependent Acquisition, ELISA, Multiple Reaction Monitoring, OSCC, Prognosis

21. Phase Behaviour of Self-Assembled Liposomes and Cubosomes for Anti-Cancer and Anti-microbial Therapeutics

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Lipid-based drug delivery systems (DDS) have gained significant attention due to their ability to encapsulate and control the release of diverse drug molecules, including hydrophobic, hydrophilic, and amphiphilic compounds. This study focuses on the design, development, and characterization of lipid-based vesicles (liposomes) and liquid-crystalline cubic structures (cubosomes) for delivering therapeutic agents, such as anticancer and antimicrobial drugs. The primary objective is to elucidate the physicochemical and biological properties of these drug carriers, focusing on how drug properties and molecular attributes influence the interaction with lipid-based nanostructures. The study aims to investigate the phase transitions (via differential scanning calorimetry) and structural characteristics of cubosomes (via small-angle X-ray scattering) under the influence of drug encapsulation. The amount of drug that can be encapsulated in cubosomes is influenced by factors such as the type of liquid-crystalline phase, unit-cell size, and cubosome geometry. Understanding the internal structure of cubosomes and their phase behavior is critical, as these parameters directly impact cellular uptake, biodistribution, and cytotoxicity. To probe drug interactions with liposome systems, isothermal titration calorimetry (ITC) was employed. These methods enable analysis of drug-lipid interactions, including drug partitioning, release kinetics, and binding to serum proteins. Small-angle X-ray scattering (SAXS) is used to examine the crystallographic geometry and lattice parameters of cubosomes without and after drug encapsulation, providing detailed insights into the structural changes induced by drug loading.

Results: Preliminary studies with drug-liposome systems revealed that hydrophilic drugs, such as 5- fluorouracil and kanamycin, exhibit a high binding affinity to the liposome membrane, with strong interaction coefficients indicating stable binding. Drug release via diffusion was minimal, suggesting the formation of stable delivery systems that may enable

controlled and sustained drug release. In cubosome-based systems, SAXS data revealed changes in lattice parameters upon encapsulation of hydrophobic drugs with limited polar groups. CD measurements revealed that short immunogenic peptides can be encapsulated in cubosomes while preserving their functional structure. These changes indicate the influence of drug encapsulation on the cubosome's internal structure. Overall, the study provides valuable insights into the interplay between drug structure and the architecture of lipid-based delivery systems, laying the groundwork for the rational design and optimization of DDS for various therapeutic applications.

22. Identification and Characterization of Human-Associated Endogenous Viral Elements in Culicinae Mosquito Genomes

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Endogenous viral elements (EVEs) are remnants of ancient viral genomes that have been integrated into host germline DNA. These elements serve as molecular records of long-term virus-host interactions and in some cases, contribute to host genome evolution and biology. Culicinae mosquitoes constitute a valuable model for EVE research due to their ecological diversity and rich viromes. Despite this, most previous studies have focused primarily on insect-specific and other non-retroviral EVEs, while EVEs derived from human-associated viruses remain largely unexplored. The rapid expansion of publicly available mosquito genome sequences, facilitated by advances in sequencing technologies and reduced costs, now enables the investigation of outstanding questions regarding viral endogenization and host-virus evolution. This study conducted a genome-wide survey of 19 publicly available *Culicinae* mosquito genomes to identify integrations derived from human-associated retroviruses, with particular emphasis on simian foamy virus (SFV)-related EVEs. Among the 77,141 viral-like sequences identified, SFV-related elements were the most abundant group of human-associated retroviral EVEs and were detected in 11 mosquito species. Most SFV-related integrations were highly fragmented, indicating an ancient origin followed by extensive mutational decay. Phylogenetic analyses demonstrated that these elements formed distinct mosquito-associated clades, separate from contemporary primate SFVs, which supports their long-term evolutionary divergence. The presence of conserved foamy virus polymerase domains further confirmed their retroviral ancestry. Interestingly, bacterial abortive infection (Abi)-related defense domains were frequently identified in genomic regions adjacent to SFV-EVE integration sites, suggesting potential evolutionary interactions among EVEs, mobile genetic elements and host defense mechanisms. Collectively, these findings expand the known diversity of SFV-related EVEs in mosquitoes, offer new insights into retroviral evolution and long-term virus-host coevolution and underscore the value of standardized computational approaches for large-scale EVE discovery in the expanding collection of publicly available mosquito genomes.
Keywords: Endogenous viral elements (EVEs); Simian foamy viruses (SFVs); Simiispumavirus; Retroviral integrations; Culicinae mosquitoes; Paleovirology; Virus-host co-evolution

23. Exploring the Microbial Profile and Immune Proteins in Indigenous Bovine Colostrum Through Multi-Analytical Approaches

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Introduction: Bovine colostrum is a biological secretion rich in an array of microorganisms and proteins that play vital roles in neonatal development and gut microbiome colonization. Nevertheless, the relationship between microbial diversity and protein profiles in native *Bos indicus* cows remains poorly understood. The purpose of this study was to

examine the microbial profile and protein profiles using culture dependent, culture independent metagenomics and protein characterization techniques respectively.

Materials and Methods: Culture dependent analysis was conducted using selective culture media to isolate viable microorganisms. Culture independent analysis utilizing 16S rDNA sequencing was applied to assess the overall microbial diversity within the colostrum samples. Protein profile was evaluated using Bradford assay and proteins were separated by SDS-PAGE.

Results and Discussion: The results from both culture dependent and metagenomic analysis demonstrated the presence of *Limosilactobacillus fermentum*. Metagenomic analysis also identified other species including *Romboutsia timonensis* and *Macrococcus caseolyticus*. Comparative analysis revealed that colostrum samples possessed more microbial diversity than raw milk samples, suggesting their potential ability to act as a microbial inoculum. Protein analysis showed that colostrum samples contained higher protein concentrations with distinct protein bands identified through SDS PAGE technique.

Conclusion: The microorganisms present in bovine colostrum may possess probiotic potential, however further studies are required to evaluate their antibacterial and antibiofilm activities before any industrial and medicinal applications. In summary, this study provides foundational knowledge regarding the microbial diversity and protein composition of indigenous bovine colostrum.

Keywords: *Bos indicus*, 16S rDNA sequencing, Culture Dependent analysis, Culture independent analysis, Protein profiling

24. Toxic metals mixture–mediated nephrotoxicity in CKDu via 8-Hydroxydeoxyguanosine

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Background: Chronic kidney disease of unknown etiology (CKDu) is becoming a major health issue with detrimental effects like increasing loss of renal function as indicated by decrease in estimated glomerular filtration rate (eGFR), without any history of diabetes or hypertension. Environment toxicants pose a major role in driving kidney dysfunction.

Methods: This case-control study recruits 215 cases and 215 age and gender matched controls was conducted at Department of Biochemistry in colaboration with Department of Nephrology, Dr. Ram Manohar Lohia Institute Medical Sciences Lucknow, Uttar Pradesh India. Toxic metals levels were estimated in serum and urine using Perkin Elmer Nexion 1000 Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Advanced statistical analysis were employed to determine the role of metals in kidney dysfunction via DNa adduct formation.

Main results: Toxic metals like Cd, As, Hg, and Al were significantly elevated in serum and urine of CKDu patients versus controls. Multivariate regression identified independent CKDu associations: serum Cd (β = −0.382), As (β = −0.332), Hg (β = −0.250), Al (β = −0.222); a l $p<0.001$. WQS analysis ranked Cd highest (41% weight, β = 0.78), followed by As (32%, β = 0.42) and Al (17%, β = 0.32). Gaussian process and BKMR models confirmed PTE mixtures on CKDu prevalence and eGFR decline. Scatter plot and ROC curve for of 8-OhdG found threshold limit to be 9.5 µg/L with area under curve 0.690 (0.640-0.740) $p<0.001$. A regression model in association with metals and of 8-OhdG found, in multivariate analysis, only Al (β=0.104), Cd (β=0.279), and Hg (β=0.120) $p<0.05$ for al. Mediation analysis highlighted 8-OHdG's role: 11.82% (β= 0.059, $p<0.001$) for Al, 8.75% (β = -0.054) for Cd and 12.2% (β = -0.054) for Hg indicating pathway in metal-induced nephrotoxicity.

Conclusion: Chronic exposure to Cd, As, Hg, and Al, is strongly associated with CKDu and declining renal function. Elevated urinary 8-OHdG and mediation analyses indicate that oxidative DNA damage partially mediates the nephrotoxic effects of Al, Cd, and Hg. These findings suggest that environmental metal exposure and oxidative stress play key roles in CKDu pathogenesis.

Keywords: CKDu, Mercury, Toxic metals, ROC, WQS, BKMR

25. A Systems-Level Multi-Omics and Machine Learning Approach for Early and Predictive Detection of Uropathogens in Urinary Tract Infections

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Introduction: UTIs are a significant worldwide health issue and among the most common infectious diseases that impact around 150 million people each year. The increasing prevalence of multidrug-resistant (MDR) uropathogens has made clinical management a challenging issue requiring swift and accurate diagnostics and evidence-based treatment plans. To solve these issues, the present study embraces a systems-level integrative multi-omics model that integrates microbiological analysis with high-resolution proteomics and metabolomics, and reinforced with machine learning (ML)-based decision support to achieve higher diagnostic precision and predictive powers.

Materials & Methods: Midstream urine samples were collected from symptomatic (~40) and asymptomatic (~40) UTI patients where the causative pathogens were determined using the VITEK-2 automated system. Meanwhile, antimicrobial susceptibility testing (AST) was performed following the CLSI guidelines.

Results: The most common uropathogens identified in our study were *Escherichia coli* (42%) and *Klebsiella spp.* (25%), followed by *Pseudomonas spp.* (18%), *Proteus spp*. (6%), *Enterococcus spp*. (6%), and *Staphylococcus spp.* (3%). High resistance was observed to commonly used antibiotics, including ciprofloxacin, gentamicin, levofloxacin, amikacin, imipenem, and colistin, highlighting the urgent need to strengthen antibiotic stewardship.

Conclusions: Building on these results, the multi-omics data will be used to train machine learning models to identify whether a patient has a UTI and to predict antibiotic resistance patterns. Combining protein biomarkers with metabolic profiles gives a clear overall understanding of how the host and pathogen interact and how the disease progresses.

This strategy provides a potent basis of early diagnosis, individualized treatment plans, and enhanced clinical decision-making, which eventually lead to enhanced patient outcomes and effective control of antimicrobial resistance in urological infections.

Key words: Urinary Tract Infections, Multi-omics, Machine Learning, VITEK, UPEC

26. Investigating the Indian king cobra venom proteome from the western ghats in kerala incorporating de novo sequencing and multiple enzymatic digestion strategies

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Snakebite envenoming is a neglected tropical disease and reports indicates that about half of these death cases are reported in India alone. India is house to more than 60 medically important snake species. However, majority of the mortality and morbidity cases reported are due to the bites from the 'big four' snakes; *Daboia russelii, Bungarus caeruleus, Echis carinatus, and Naja naja.* Antivenom remains the mainstay treatment for snakebites and in India polyvalent antivenom is generated using venom from these 'big four' snakes. However, several studies have highlighted that antivenoms showed varying efficacies in detecting antigenic epitopes present in snake venom from different geographical locations.

In the current study, mass spectrometry-based proteomics was used to investigate the venom proteome of *O. kaalinga* through conventional bottom-up proteomics approaches incorporating de novo sequencing and multiple enzymatic digestion strategies. Functional assays and immunological cross-reactivity studies using Indian polyvalent antivenoms were also performed.

Proteomics analysis resulted in the identification of 111 proteins representing 20 different snake venom protein families and de novo analysis yielded 20 additional peptides. Similarly, chymotrypsin-based proteomics resulted in the identification of phospholipase B family, that was not determined through trypsin digestion. Notably, eight of the protein families were reported for the first time in the king cobra venom from India. Functional assays performed indicate that L-amino acid oxidase and fibrinogenolytic activities were higher in OK venom. Immunological cross-reactivity studies performed using Indian polyvalent antivenoms showed comparable end-point titration values and binding potential towards king cobra venom.

Collectively, this study provides the comprehensive proteomic characterization of O.*kaalinga* venom and depicts the significance of integrating de novo sequencing with multiple enzymatic digestion strategies in snake venomics.

Key words: Snakebite, big four, king cobra, polyvalent antivenom, proteomics.

27. An Integrative AI-ML Data- driven Pipeline for Cross-Platform Discovery of Diagnostic Gene Panels in Coronary Artery Disease and Acute Coronary Syndrome

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Introduction:

Acute Coronary Syndrome (ACS) is a leading cause of global mortality arising from plaque rupture/thrombosis. While blood based transcriptomic research has sought early genetic signatures, the field is often limited by "noise" from study variability, small heterogeneous cohorts and platform-specific bias that fail to separate acute events from chronic/stable CAD (sCAD). We built an AI/ML pipeline to identify a consensus gene panel distinguishing CAD and acute myocardial infarction (AMI) from stable disease and underlying atherosclerosis.

Material and Methods:

We harmonised 45 public human datasets: GEO transcriptomic (30 microarray, 10 RNA-seq) and PRIDE proteomic (5 LC-MS/MS) from blood, PBMCs, plasma/serum and arterial/plaque tissue spanning healthy controls, stable CAD, unstable angina (UA), AMI and recurrent AMI (Re-AMI). Differential expression used limma (microarray and LC-MS/MS) and DESeq2 (RNA-seq); effect sizes were combined by random-effects meta-analysis (metafor) and Robust Rank Aggregation across four contrasts (AMI vs control, vs stable CAD, vs UA, vs Re-AMI). Genes were tiered as core consensus (FDR<0.05, directionally concordant in ≥3/4 contrasts), AMI specific signal by removing chronic noise of sCAD, severity (vs UA) and recurrence associated (vs Re AMI), followed by Meta-GSEA. Consensus proteins were tested for concordant abundance (cross-omics validation) and the core panel is trained by multi-ensemble model, evaluated by AUC in held-out validation.

Results and Discussion:

The core tier showed AMI upregulation of ADAMDEC1, PLA2G4A, CCNA1, OLFM4, AQP9, SOCS3, TNFAIP6, CR1, S100A9 and HP, and downregulation of SNCA and SELENBP1. The AMI specific tier (vs controls and sCAD) was enriched for innate-immune/neutrophil-activation markers (AQP9, RNASE3, SOCS3, TNFAIP6, CR1, HP, OLFM4, S100A9), linked to plaque rupture and myocardial injury. Severity (AMI vs UA) and recurrence (AMI vs Re-AMI) signatures converged on SOCS3, AQP9, TNFAIP6, S100A9, CR1 and HP, with persistent innate-immune dysregulation in recurrence. Meta-GSEA revealed coordinated inflammatory-metabolic reprogramming: Interferon-Gamma Response (NES=+2.18) and Oxidative Phosphorylation (NES=+2.10) were most enriched, with TNF-alpha/NF-kB, MTORC1, Inflammatory Response and E2F/MYC activation, and downregulated Heme Metabolism and KRAS signalling were downregulated. At protein level, Haptoglobin (HP), Calprotectin (S100A8/A9) and Olfactomedin-4 (OLFM4) showed concordant differential abundance in independent LC-MS/MS cohorts, confirming cross-omics reproducibility. The multi-model ensemble classifier discriminated AMI from

healthy controls and stable CAD in held-out validation and maintained stable cross-platform performance, complementing established markers such as cardiac troponin and myoglobin.

Conclusion:

This multi-omics framework yields a tiered panel distinguishing acute infarction from chronic CAD and resolving ACS severity and recurrence, reflecting the inflammatory-metabolic reprogramming central to AMI, and offers a scalable basis for blood-based point-of-care ACS diagnostics before irreversible myocardial damage.

Keywords: Acute coronary syndromes; coronary artery disease; Biomarkers; Transcriptomics, Bioinformatics; Machine-Learning

28. Network Pharmacology-Based Host-Directed Therapeutic Targeting of *Vibrio cholerae* Reveals Multi-Pathway Inflammatory Modulation

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Introduction

Cholera, caused by *Vibrio cholerae*, continues to pose a significant public health challenge, particularly in regions with inadequate sanitation and limited healthcare infrastructure. The emergence of antimicrobial resistance (AMR) has reduced the effectiveness of conventional antibiotic-based treatments. Host-directed therapy (HDT) has gained attention as an alternative therapeutic strategy that targets host cellular pathways rather than bacterial survival, thereby reducing selective pressure for resistance development. Natural bioactive compounds possess diverse pharmacological properties and may serve as potential modulators of host immune and inflammatory responses during cholera infection.

Materials and Methods

An integrated in-silico network pharmacology approach was employed to investigate the host-directed therapeutic potential of selected natural bioactive compounds. Potential host targets were identified through target prediction databases and subjected to protein–protein interaction (PPI) network analysis. Gene Ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG) enrichment analyses were performed to elucidate biological functions and signalling pathways associated with cholera pathogenesis. Molecular docking was subsequently conducted to evaluate interactions between selected compounds and key host inflammatory targets.

Results and Discussion

Network analysis identified several hub proteins involved in immune regulation and inflammatory responses. GO and KEGG enrichment analyses revealed significant involvement of PI3K–Akt, JAK–STAT, MAPK, NF-κB, apoptosis, and oxidative stress-related signalling pathways. These pathways are crucial for cytokine production, immune activation, epithelial barrier maintenance, and regulation of host inflammatory responses during cholera infection. The multi-target interaction profile of the bioactive compounds suggested their potential to simultaneously regulate interconnected host pathways. Molecular docking demonstrated strong binding affinities between selected compounds and major host inflammatory mediators, supporting their therapeutic relevance.

Conclusion

The study highlights the potential of natural bioactive compounds as host-directed therapeutic candidates capable of modulating multiple host inflammatory and immune-regulatory pathways involved in cholera pathogenesis. These findings provide mechanistic insights into resistance-resilient therapeutic strategies and support the future development of multi-target interventions for cholera management.

Keywords

Host-directed therapy; Cholera; Network pharmacology; Molecular docking; Natural bioactive compounds; Inflammatory signalling pathways

29. Role of Conserved active site residue in Metal Coordination and Catalysis of *Mycobacterium tuberculosis* Malate Synthase

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Introduction: The Long TB treatment is due to drugs failing to kill persistent *M. tuberculosis* Malate synthase ($MS_{M.tb}$), a key enzyme of the glyoxylate shunt essential for persistence and absent in humans, is considered a promising therapeutic target. Previous structural studies have shown that the conserved residue Asp274 holds the Mg^{2+} coordinated catalytic water molecule. The water molecules has been proposed to participate in proton transfer during catalysis; however, the precise role of Asp274 remains unclear.

Materials and Methods: To investigate the functional importance of Asp274, a site-directed mutant of $MS_{M.tb}$ was generated by replacing Asp274 with Asn (Asp274Asn). The mutant protein was expressed, purified, and analyzed for enzymatic activity. Structural alterations caused by the mutation were examined using X-ray crystallography and comparative structural analysis with the wild-type enzyme.

Results and Discussion: The Asp274Asn mutant showed complete loss of enzymatic activity, indicating the essential role of Asp274 in catalysis. Crystal structure analysis revealed that the overall TIM-barrel fold of $MS_{M.tb}$ remained structurally intact despite the mutation. However, significant conformational changes were observed in the active-site region, including closure of the active-site lid, outward displacement of the CoA-binding loop, and rearrangement of the catalytic residue Asp633. Although Mg^{2+} remained present in the active site, its coordination geometry was altered and its position shifted by approximately 1.0 Å relative to the wild-type structure. In addition, loss of the native Asp274 side chain disrupted the orientation of a conserved water molecule involved in Mg^{2+} coordination, likely affecting substrate positioning and catalytic proton transfer.

Conclusion: These findings demonstrate that Asp274 plays a critical role in maintaining active-site geometry, Mg^{2+} coordination, and catalytic water organization in $MS_{M.tb}$. The study provides mechanistic insights into $MS_{M.tb}$ catalysis and may support future structure-based drug design targeting persistent *M. tuberculosis* infections.

Keywords: Mycobacterium tuberculosis, Malate Synthase, X-ray crystallography

30. Proteomic Analysis to Identify Potential Therapeutic Targets in Resistant Glioblastoma

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INTRODUCTION: Glioblastoma (GBM) is a Grade IV brain tumor with a median survival of 15 months. Despite surgical resection, temozolomide based chemotherapy, radiation therapy. TMZ resistance, mediated by MGMT, base excision repair, and mismatch repair, combined with extensive intertumoral and intratumoral heterogeneity, limits therapeutic efficacy. Identifying novel therapeutic targets of TMZ resistance remains critical for improving patient outcomes.

METHODS: Dataset obtained from Pride was analyzed using FragPipe for protein identification via Label-Free Quantification. Following quality filtering, missing values were imputed using KNN and normalized by median, log

transformation (base 10) using MetaboAnalyst. DEPs were identified at fold change threshold 2.0 and $p < 0.05$. Pathway enrichment was performed using Reactome, PPI network constructed using STRING and analyzed using Cytoscape. K-means clustering (k=3) based on integrated expression and network topology was performed using Orange. Proteins from clusters C1 and C2 with Log2FC > 2 and betweenness centrality > 0.1 were prioritized as therapeutic candidates.

RESULT & DISCUSSION: Proteomic profiling of TMZ-treated GBM samples and control revealed 286 upregulated and 269 downregulated DEPs. Pathway enrichment indicated upregulated proteins were enriched in membrane trafficking, clathrin-mediated endocytosis, while downregulated proteins were enriched in translation and ribosome-associated pathways. PPI network analysis demonstrated significant functional connectivity among upregulated proteins. K-means clustering partitioned upregulated proteins into three distinct groups based on integrated expression and network topology. Dual-threshold prioritization from clusters C1, C2 identified 7 candidate proteins: PLCG1, FTO, MYO5A, DYNLL2, DYNLT1, ITGB3, and ATP5F1C. Amongst these prior investigations implicate PLCG1, FTO, MYO5A, DYNLL2, DYNLT1, ITGB3 contribute to GBM aggressiveness. The cell surface localization of ITGB3 highlights it as a potential target for immunotherapy. ATP5F1C, a mitochondrial ATP synthase subunit with no previously established role in GBM, implicates mitochondrial energy metabolism as a potentially novel mechanism of TMZ resistance. Gene knockdown studies in TMZ-resistant GBM cell lines are warranted to validate the therapeutic relevance of these candidates.

CONCLUSION This study presents a computational proteomics study integrating differential expression, pathway enrichment, PPI network topology, and K-means clustering to identify potential therapeutic targets in TMZ resistance in GBM. Seven candidate proteins PLCG1, FTO, MYO5A, DYNLL2, DYNLT1, ITGB3, and ATP5F1C were identified. These candidates span epitranscriptomic, cytoskeletal, integrin, and mitochondrial pathways, suggesting multi-pathway resistance mechanisms as potential therapeutic targets in TMZ-resistant GBM.

Keywords: Glioblastoma, temozolomide resistance, proteomics, differential expression, protein-protein interaction network, K-means clustering, therapeutic targets

31. DECIPHERING THE ROLE OF VDAC1 IN MULTIPLE MYELOMA MALIGNANCY USING PROTEOMICS, METABOLOMICS, AND MOLECULAR APPROACHES

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Introduction: Multiple Myeloma (MM) is the second most common haematological malignancy characterized by the clonal proliferation of plasma cells. The pathophysiology of MM is complex and involves the dysregulation of cellular metabolism, apoptosis pathways, and calcium homeostasis, which collectively contribute to the survival and continued growth of myeloma cells. Despite therapeutic advancements, MM remains incurable due to complex dysregulation in cellular metabolism, apoptosis, and calcium homeostasis. Our initial label-free quantitative (LFQ) proteomics identified 222 differentially expressed proteins in patient-derived bone marrow mononuclear cells, notably highlighting the significant downregulation of Voltage-Dependent Anion Channel 1 (VDAC1) in both patient samples.

Method: To elucidate the functional role of VDAC1, we employed a multi-pronged approach involving VDAC1 overexpression in the MM cell line. We integrated LFQ proteomics and global metabolomics to map systemic cellular changes. Additionally, cell proliferation assays were conducted to assess phenotypic impact, and Immunoprecipitation-Mass Spectrometry (IP-MS) was performed to characterize the VDAC1 interactome in an MM context.

Results: VDAC1 overexpression significantly decreased MM cell proliferation. Proteomic profiling revealed that VDAC1 levels influence key signalling proteins, including STAT1, STAT3, and MAPK14, alongside critical metabolic enzymes such as PKM1, HK1, and LDHA. Parallel metabolomics analysis demonstrated that VDAC1 dysregulation disrupts pyruvate, pyrimidine, and glycolytic pathways, and the Tricarboxylic Acid (TCA) cycle. These findings suggest that VDAC1 is a central

mediator of mitochondrial function and cellular homeostasis in plasma cells. Its altered expression likely facilitates the metabolic reprogramming and survival advantage characteristic of MM clones.

Conclusion: Our study integrates molecular biology, proteomics, and metabolomics to provide a comprehensive view of VDAC1-mediated malignancy in MM. Substantial functional studies suggested VDAC1 could be a potential target for MM pathophysiology. Targeting VDAC1-mediated pathways translates into a promising strategy to improve future clinical outcomes for patients with MM.

Keywords: Multiple Myeloma, VDAC1, Metabolism, Mitochondria

32. Hyperacute Blood-Based Proteomic and Machine Learning Signatures for Stroke Subtype Differentiation: A Translational Point-of-Care Diagnostic Framework

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Background:

Quickly distinguishing between ischemic stroke, intracerebral hemorrhage, transient ischemic attack, and stroke mimics during the hyperacute phase remains a vital unmet need in stroke treatment. This issue is especially significant in settings where immediate neuroimaging is unavailable or delayed, hindering timely reperfusion and proper triage.

Objective: To validate blood-based protein biomarkers for early stroke subtype differentiation using targeted proteomics and machine learning, and to translate the most informative biomarkers into a rapid point-of-care diagnostic assay.

Methods: In this prospective, multi-center diagnostic study, patients presenting within 6 hours of symptom onset with suspected stroke (ischemic stroke, intracerebral hemorrhage), transient ischemic attack, or stroke mimics will be recruited. Serum samples will undergo multiple reaction monitoring–based targeted proteomics to quantify 22 candidate proteins identified in prior high-throughput discovery studies. Supervised machine learning models—including logistic regression, random forest, support vector machines, gradient boosting, and deep neural networks—will be trained to differentiate stroke subtypes and predict 90-day functional outcomes. Temporal profiling of top-performing biomarkers will be conducted in a predefined patient subset. The most informative biomarkers will undergo ELISA validation and be integrated into a gold nanoparticle–based multiplex point-of-care biosensor designed for prehospital and emergency department deployment.

Expected Results: We hypothesize that a multi-protein biomarker panel, combined with machine learning, will achieve high diagnostic accuracy in distinguishing ischemic stroke from hemorrhagic stroke, transient ischemic attack, and stroke mimics within 6 hours of onset. Currently, proteomics studies are underway, and the prototype for the point-of-care biosensor device is being developed through several iterations.

Keywords: Stroke, Biomarkers, Point-of-care, Proteomics, Machine Learning, Diagnostics

33. Plasma Proteomics Across Dengue, Malaria, and Non-Specific Febrile Illness Identifies Complement-Driven Signatures for Differential Diagnosis and Severity Stratification

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Introduction: Dengue virus (DENV) and Plasmodium falciparum malaria co-circulate across tropical India, producing a clinically indistinguishable febrile presentation that impedes early differential diagnosis. A subset of dengue infections progresses to severe disease — characterised by vascular leakage, thrombocytopenia, and organ impairment — yet no plasma-based tool currently enables severity prediction during the febrile phase. Published omics studies have been single-platform and cross-sectional, and none have incorporated comparative febrile cohorts to isolate dengue-specific host responses.

Materials and Methods: Plasma samples were collected from confirmed dengue fever (DF), dengue haemorrhagic fever (DHF), Plasmodium falciparum malaria, non-dengue febrile illness (NDFI), and healthy controls (HC) at L.H. Hiranandani Hospital, Mumbai. High-depth proteome profiling was performed by data-independent acquisition (DIA) mass spectrometry on an Orbitrap Fusion following perchloric acid (PCA)-based plasma fractionation, optimised across 50–300 µL input volumes. Candidate differentially expressed proteins (DEPs) were validated by parallel reaction monitoring (PRM) across dengue, NDFI, and oncological control groups. TNF-α was quantified by sandwich ELISA across all cohorts.

Results: PCA fractionation at 300 µL input resolved >1,300 protein groups per sample with high inter-run reproducibility. PLS-DA of DIA data achieved complete separation of dengue from healthy controls (Component 1, 49% variance). Pathway enrichment identified the complement cascade — classical, lectin, and alternative arms — as the most significantly dysregulated process (FDR ≤ 1×10^{-18}), alongside coagulation, acute-phase response, and lipid remodelling pathways. Key upregulated proteins included Vitronectin (VTN), Complement Factor I (CFI), LRG1, and Haptoglobin (HP). PRM confirmed quantitative dengue-specificity of the DEP panel relative to NDFI and oncological controls. Serum TNF-α was significantly elevated in dengue (1,145 pg/mL) versus NDFI (1,040 pg/mL) and HC (926 pg/mL), consistent with complement anaphylatoxin-driven macrophage activation.

Conclusion: Complement-driven proteome remodelling and downstream macrophage-cytokine activation constitute a reproducible, dengue-specific molecular axis that enables differential diagnosis from other febrile infections and tracks disease severity. Ongoing longitudinal sampling across disease phases, combined with immune cell phenotyping and in vitro ADE macrophage models, aims to consolidate this signature into a clinically deployable severity-prediction panel for dengue-endemic settings.

Keywords: dengue, plasma proteomics, DIA mass spectrometry, complement pathway, severity biomarkers, acute febrile illness, PRM, TNF-α

34. *Manihot esculenta* Ethanolic Extract and Its Green-Synthesized Gold Nanoparticles induce cell death in Hormone-Dependent and Triple-Negative Breast Cancer Cells: A proteogenomic insights into the therapeutic agent's development

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Background: Breast cancer remains one of the most prevalent malignancies and a leading cause of cancer-related deaths among women globally. Despite therapeutic advancements, challenges such as metastasis, drug resistance, and adverse effects necessitate the exploration of novel natural product-based multi-targeted therapies. This study evaluated the anti-cancer potential of ethanolic extract of *Manihot esculenta* (cassava) leaves and its green-synthesized gold nanoparticles against human breast cancer cell lines.

Objectives: This study is aimed to synthesize and characterize green-synthesized cassava leaf gold nanoparticles (CL-AuNPs), phytochemical characterization and cytotoxic effects of both crude leaf extract and CL-AuNPs, and investigate the underlying anticancer molecular mechanisms against MCF-7 and MDA-MB-231 cells.

Methods: Cassava leaves collected from Kerala were shade-dried, powdered, and extracted with 75% ethanol. The extract was analyzed using GC-MS, total phenolic content, and total flavonoid content. In vitro cytotoxicity was assessed by MTT assay. Gold nanoparticles were green-synthesized using the leaf extract and characterized by UV-Vis spectroscopy, TEM, XRD, DLS, Zeta potential, and FTIR. Mechanistic studies included ROS generation (DCFDA) and mitochondrial membrane potential (JC-1) assays. In silico studies involved molecular docking, ADME analysis, 100 ns Molecular Dynamics (MD) simulation, and proteogenomic target prediction focusing on the HER2 kinase domain.

Results: GC-MS identified 35 bioactive compounds, with major constituents being β-amyrin, phytol, and β-amyrone. The extract showed high TPC (794 µg GAE/mg) and TFC (1003 µg QE/mg). MTT assay demonstrated dose-dependent cytotoxicity with IC_{50} values of 92 µg/mL (MCF-7) and 286 µg/mL (MDA-MB-231) for the crude extract, and 184 µg/mL and 255 µg/mL for the green synthesized CL-AuNPs. Treatment significantly increased intracellular ROS (up to 1.78-fold) and caused mitochondrial depolarization. Green-synthesized AuNPs were spherical with an average size of ~29 nm. Diosgenin exhibited the highest binding affinity to HER2 kinase domain (-10.8 kcal/mol), surpassing tamoxifen. MD simulation confirmed complex stability over 100 ns. Proteogenomic analysis predicted multi-targeted modulation of kinases (including HER2/PI3K/AKT), proteases, and nuclear receptors, consistent with the observed apoptotic effects.

Conclusion: The ethanolic extract of cassava leaves and its green-synthesized gold nanoparticles exhibit potent anticancer activity against both ER-positive and triple-negative breast cancer cells through ROS-mediated apoptosis and multi-targeted proteogenomic modulation of HER2-related pathways. These findings suggest their promising potential as natural HER2-targeted therapeutic agents for breast cancer.

Keywords: Manihot esculenta, Cassava leaves, Breast cancer, Gold nanoparticles, Diosgenin, HER2, Proteogenomics, Anticancer activity

35. Biomolecular Mapping of Circulating Extracellular Vesicles to Develop AI-Driven Prognostic Panels for Early Mortality Risk Stratification in Acute Liver Failure

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Background/Aims: Acute liver failure (ALF) is a life-threatening condition with high mortality, characterized by circulating microbial and metabolic disturbances. Plasma-derived exosomes reflect systemic inflammation and provide a promising non-invasive platform to identify patients at risk of early mortality.

Method: Plasma samples from 50 ALF (25 non-survivors(ALF-NS), 25 survivors(ALF-S) patients and 20 controls were processed for extracellular vesicle isolation using protein-organic-solvent-precipitation (PRoSPR) and characterised by transmission-electron-microscopy, dynamic-light-scattering, nanoparticle-tracking-analysis, and proteomic analysis, followed by meta-proteomic and metabolomic profiling. An identified diagnostic metabolite panel was validated in a separate cohort (220 ALF; 153 ALF-NS, 67 ALF-S) using HRMS and machine learning.

Results: Plasma-derived exosomes (120–200 nm) were characterised with a concentration of $3.25 \times 10^{11} \pm 0.55$ particles/mL, zeta potential of -30.67 ± 3.6 mV, and >20 EV-specific proteins (Vesiclepedia) ($p<0.01$). Exosomal metabolomics identified over 1,000 metabolites, with more than 800 significantly altered in acute liver failure. Non-survivors showed enriched long-chain fatty acid β-oxidation and bile acid pathways, linking metabolic dysregulation to inflammation severity. Bacterial-peptide identified >15 phyla and >25 genera based alpha/beta diversity was higher in ALF-NS corresponding to increase in Bacteroidota, Actinomycetota functionally linked to energy and xenobiotic

metabolism ($p<0.05$). Higher EV levels of *Enterococcus ceocorum* and *Klebsiella pneumoniae* in ALF-NS correlated with metabolites, Clinical parameters and severity ($r^2>0.8$, $p< 0.05$). A five extracellular vesicle–derived metabolite panel showed strong prognostic value in acute liver failure (AUC = 0.98; HR = 17.58). Deoxycholic acid-3-glucuronide (8.8-fold increase) demonstrated highest importance, predicting early mortality with >95% accuracy using ANN-based machine learning. Interestingly, Upregulation of β-glucuronidase (>2-fold) and reduced ABCC3 (MRP3) impaired bile acid efflux, driving intracellular bile acid accumulation and exacerbating hyperinflammation and oxidative stress in acute liver failure non-survivors.

Conclusion: Plasma exosomal multiomics reveals an AI-validated, bile acid–centered hyperinflammatory signature that accurately predicts early mortality in acute liver failure non-survivors.

36. Phytochemical–signalling crosstalk in *H. pylori Infection*: Targeting MAPK/NF-κB–LOX-1 Axis through Medicinal Plant Extracts'.

Nfor Gael njini

Background: Nearly half of the world population is infected with *Helicobacter pylori*, a major factor implicated in several gastroduodenal disorders. Growing research highlights the therapeutic benefits of *Rosmarinus officinalis, Taraxacum officinale,* and *Eucalyptus globulus* owing to their strong antibacterial, antioxidant, and anti-inflammatory qualities. Plant metabolite profiling using analytical platforms such as MS (mass spectrometry), GC-MS (gas chromatography–mass spectrometry), and FTIR (Fourier-transform infrared spectroscopy) has revealed substantial secondary metabolites such as rosmarinic acid, eucalyptol, and quercetin. These observed benefits exert a significant protective effect through antioxidant capacity, inflammatory reduction, and prevention of programmed cell death.

Purpose: The study tries to investigate the gastroprotective potential and mechanistic role of *Rosmarinus officinalis, Taraxacum officinale,* and *Eucalyptus globulus* on *H. pylori*-induced cellular inflammation.

Method: *H. pylori*-infected gastric epithelial cells (AGS) were exposed to plant extracts, followed by evaluation of inflammatory and stress-response markers using biochemical and molecular assays. Plant profiling of secondary metabolites was performed through FTIR, MS, and GC-MS.

Results: Following treatment with plant extracts, the key inflammatory markers, including *CCL5, IL-8,* and *TNFα*, were significantly reduced in *H. pylori*-infected AGS cells. Furthermore, the protein levels of LOX-1, NF-κB, MAPK, and catalase were also considerably downregulated following plant treatment.

Conclusion: This study demonstrated notable gastroprotective properties of *Rosmarinus officinalis, Taraxacum officinale,* and *Eucalyptus globulus*. Moreover, mechanistic analysis further suggests plant extracts might reduce the activation of the LOX-1 receptor, MAPK, and NF-κB cascade. Collectively, these findings substantiate the molecular responses and support the therapeutic importance of plant-derived bioactive compounds in mitigating *H. pylori*-related gastrointestinal disorders.

Key words: *Helicobacter pylori*, medicinal plant, gastroprotection, inflammatory marker, metabolite profiling.

37. Beyond Potassium: Emerging Proteomic Markers in Vitreous Humor for Postmortem Interval Estimation.

Niharika

The most sought-after piece of information in forensic death investigations is the estimation of Post mortem interval (PMI) because the first and the most important question which arises at a crime scene is "When did the person die?". After death, body undergoes several physicochemical changes which occur in a regular sequence and therefore aid in arriving at an approximate time of death. However, conventional methods of PMI estimation are highly subjective and heavily influenced by intrinsic (sex, age, cause of death) and extrinsic environmental factors (temperature, humidity). Therefore, scientific community is continuously striving to develop more objective methods of PMI estimation.

Proteomic studies on various tissues like skeletal muscle have shown that proteins degrade in a consistent manner after death (Choi et al.,2019). However, such changes are not uniform across tissues (Beusch et al.,2025), reinforcing that

substrate selection is fundamental in PMI studies. Vitreous humor (VH) is one of the best suited candidates for PMI estimation studies because it is easy to collect, relatively inert and rarely suffers bacterial contamination. There is extensive literature demonstrating an established relationship between VH electrolytes (especially potassium) and PMI but there is a dearth of studies about the correlation between PMI and proteomics in VH. Although a promising effort was made by Boroumand et al. (2022) in the field with a pilot study which utilized top down HPLC-MS analysis to identify naturally forming peptide fragments in VH and assess their correlation with PMI. They identified 35 peptide fragments and 7 intact proteins while observing strong linear correlations of thymosin β4, vimentin fragment and polyubiquitin fragment with PMI, suggesting their potential for estimating time of death within 160 hours postmortem.
This review highlights the evidence for VH proteomics as a tool for PMI estimation and stresses for its prioritization in future forensic research.

38. OMNIMO: Moving Beyond Single-Method Bias and Expanding the Biomolecular Landscape Through Consensus-Based Feature Selection

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Background: Multi-omics integration holds considerable promise for biomarker discovery, yet existing analytical frameworks impose significant limitations: single-method dependence, restricted dataset compatibility, limited transparency of intermediate outputs, and inability to derive consensus rankings across complementary analytical paradigms. These gaps motivated the development of OMNIMO (Omnibus Modelling and N-dimensional Investigation of Multi-Omics datasets), an R-based unified analytical framework for consensus-driven differential feature selection across multi-omics datasets.
Methods: OMNIMO currently comprises five interconnected modules operating sequentially on standardised input formats. PREMO performs adaptive, diagnostics-driven preprocessing including user-specific normalisation, log2 transformation, and versioned scaling outputs, ensuring each downstream analytical method receives optimally prepared data. UNIMO implements six N-integration methods (MOFA+, MCIA, DIABLO, RGCCA, sGCCA, MEFISTO) identifying features important for cross-omics relationships. USAMO applies nine statistical tests spanning parametric, non-parametric, and omics-specialised approaches with FDR correction for differential feature detection. UCOMO employs fifteen machine learning classifiers including tree-based ensembles, regularised linear models, and support vector machines for prediction-based feature ranking. SMOFV integrates outputs from all three modules, computing within-module and cross-module consensus scores through weighted voting to generate a unified, method-agnostic feature ranking with comprehensive visualisation outputs.
Results: Applied to in-house LC-MS/MS-based plasma metabolomics and lipidomics datasets from vector-borne febrile infectious disease cohorts, OMNIMO consistently expanded the pool of Relevant Signature Features (RSFs) supported by multiple independent scientific rationales, compared to any single analytical method applied in isolation. By integrating outputs across statistical, N-integration, and classification paradigms, the consensus framework recovered biologically coherent features that individual methods would have excluded, broadening the interpretable molecular landscape of disease. Higher- consensus-tier RSFs demonstrated stronger pathway enrichment and greater cross-platform biological coherence. Benchmarking against published multi-omics datasets of equivalent disease contexts is ongoing to further validate RSF recovery against existing pipelines.
Conclusion: By systematically integrating statistical, integration-based, and classification- driven paradigms into a single consensus framework, OMNIMO expands the biomolecular landscape recoverable from multi-omics data. With user-editable parameters, minimal R programming requirements, and full transparency of intermediate outputs, it offers an accessible yet methodologically rigorous solution to the reproducibility limitations of single- method multi-omics approaches.

Keywords: R package, consensus feature selection, multi-omics N-integration, DIABLO, MOFA+, MCIA, machine learning, proteomics, metabolomics, lipidomics, differential analysis, bioinformatics, statistical analysis, OMNIMO

39. Distinct Small Molecular Imprint of Dengue Among Febrile Illnesses: Insights from Cross-Sectional Profiling and Longitudinal Dynamics Through Integrated Plasma Multi-Omics

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Background: Dengue fever presents a persistent diagnostic challenge in endemic regions due to its clinical overlap with other febrile illnesses. Most existing metabolomics studies compare dengue patients only against healthy controls, missing the clinically critical distinction from symptomatic non-dengue febrile presentations. Identifying small molecular features uniquely disrupted in dengue, distinct from both a generalised febrile response and a healthy baseline, and understanding how these signatures are temporally organised across the course of infection, are questions with direct translational relevance. Methods: This study performed LC-MS/MS-based untargeted metabolomics and lipidomics across positive and negative ionisation modes on plasma from dengue fever patients, negative febrile controls, and healthy controls, in a cross-sectional study (n=90) and a longitudinal study (n=100; 31 patients across different sample cohorts with serial fever and convalescent timepoint sampling). Consensus correlation-based integrated multi-omics analysis across metabolomics and lipidomics datasets and feature selection was performed using the in-house analytical package OMNIMO.
Results: Cross-sectional analysis revealed a coherent dengue-specific signature comprising bile acid elevation, kynurenine pathway activation with concurrent tryptophan depletion, and accumulation of aromatic amino acids and docosahexaenoic acid. A sphingolipid switch characterised by ceramide upregulation alongside sphingomyelin depletion, and systematic downregulation of triglycerides, lysophosphatidylcholines, and phosphocholine, distinguished dengue from both control groups. An intra- and inter-dataset correlation framework further recovered biologically co-regulated molecular pairs beyond conventional significance thresholds, broadening the interpretable small molecule landscape. Longitudinal analysis identified polyamine depletion as the most profound and consistent fever-state signature, with aromatic amino acid mobilisation, HPA axis activation, and selective phospholipid remodelling resolving upon recovery, confirming fever-responsive rather than constitutive alterations. Correlation network analysis revealed that the majority of metabolite co-regulatory relationships were fever-specific, indicating active restructuring of the metabolic network during infection.
Conclusion: These findings map a coherent small molecular imprint of dengue fever, capturing the biochemical features that distinguish it from other febrile illnesses and how that distinction is dynamically organised across the febrile course, providing a foundation for molecularly informed diagnostic approaches in endemic settings. Keywords: dengue fever, metabolomics, lipidomics, multi-omics integration, LC-MS/MS, febrile controls, sphingolipids, polyamines, kynurenine pathway, OMNIMO, longitudinal profiling, biomarker discovery.

40. Comparative proteomics, Functional characterization and Immunological cross reactivity studies of two medically important Vipers

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Introduction: Snakebite envenoming is a neglected tropical disease contributing to a significant number of morbidities and mortalities globally and more than 50% of snakebite deaths happens in India alone. The ‘big four’ Indian snakes responsible for majority of the envenomation are: Indian *cobra*, common krait, Russell’s viper, and saw scaled viper and

the available Indian polyvalent antivenom (PAV) are produced against these snakes. However, the PAV does not adequately address envenoming caused by other relevant species. The hump nosed pit viper (*Hypnale hypnale*; HPV) is one such example, frequently misidentified as *E. carinatus* (Saw scaled viper; SSV) due to their morphological and post-envenomation clinical features. At present there is no antivenom available for HPV bites and in some cases if PAV is administered, it results in severe adverse events in HPV envenomed victims.

Materials and Methods: Comparative venom profiling was performed using mass spectrometry-based proteomics. Different enzymatic assays like PLA_2 assay, hyaluronidase assay, LAAO assay and fibrinogenolytic assays were performed to assess the functional activity of the venom. Immunological cross-reactivity studies of Indian Polyvalent antivenom against HPV and SSV venoms were evaluated using ELISA and Immuno-blotting.

Results and Discussion: Proteomics analysis resulted in the identification of 48 proteins belonging to 19 protein families from HPV venom and 188 proteins representing 23 protein families from SSV venom.The study revealed distinct functional differences between the venoms, particularly in key enzymatic activities. HPV venom exhibited comparatively higher L-amino acid oxidase (LAAO) and fibrinogenolytic activities, whereas SSV venom demonstrated greater phospholipase A_2 (PLA_2) and hyaluronidase activities. Immunological cross-reactivity assessed by ELISA showed that SSV venom exhibited an end-point titration value of 1:72,900 with all antivenoms tested. In contrast, HPV venom displayed markedly lower end-point titration values, with Virchow antivenom showing a value of 1:900 and both PSAV and VINS antivenoms exhibiting values of 1:2,700, indicating comparatively poor recognition of HPV venom components. Immunoblotting further demonstrated differential binding and recognition of antigenic epitopes present in the two venoms by the polyvalent antivenoms. Collectively, these findings underscore the considerable variation in venom composition and antigenicity among geographically distinct snake species and highlight the consequent impact on antivenom efficacy.

Conclusion:

The venom proteomes of HPV and SSV exhibited marked differences in protein composition, enzymatic activities, and antigenic properties, which significantly influenced the efficacy of currently available Indian polyvalent antivenoms. These findings highlight the need for region-specific venom characterization and support the development of antivenoms targeting medically important venomous snake species beyond the traditional "Big Four" to improve snakebite management in India.

Keywords: Snakebite envenomation, Hump nosed pit viper, Saw scaled viper, interspecies variation, antivenom, proteomics.

41. Global trends and advances in Salivary Proteomics for early detection of Oral Squamous Cell Carcinoma (OSCC): A bibliometric analysis

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Background: Oral squamous cell carcinoma (OSCC), the sixth most common cancer worldwide, has poor 5-year survival statistics that have not improved despite sophisticated combination treatments like surgery, chemotherapy, and radiation. The necessity for noninvasive and trustworthy biomarkers is highlighted by the fact that traditional diagnostic techniques frequently fail to identify OSCC until it reaches advanced stages. Saliva is a valuable biological fluid that contains a wide range of biomarkers derived from serum, gingival crevicular fluid, and oral microorganisms and their products. Literature highlights a shift toward "salivaomics" to identify salivary biomarkers using proteomics by means of variety of molecular techniques. This bibliometric analysis aims to identify increasing trends and advances in salivary proteomics for detecting salivary biomarkers for early OSCC detection.

Methods: An electronic search performed using databases such as Elsevier's Scopus, Web of Science and Pubmed will retrieve papers till date based on the research topic. For the data analysis and its visualization, the title of the articles,

year of publication, countries, authors, journals, articles, and keywords will be analyzed using Microsoft Excel and VOSviewer software.
Results: This bibliometric analysis will evaluate the vast scientific literature addressing salivary biomarkers to identify the most prolific organizations, authors, journals, countries, and keywords used within this research domain published till 2026. Conclusion: Emerging themes highlighting the significance of salivary proteomics for biomarker identification can be found through a thorough synthesis of research studies conducted till date. This bibliometric analysis will look at recent developments in our knowledge of the worldwide patterns in salivary proteomics for early detection of OSCC. Keywords: Oral squamous cell carcinoma (OSCC), salivary biomarkers, salivaomics, proteomics, early detection, bibliometric analysis

42. Tissue Proteomics Reveals Lipid Metabolic Reprogramming as a Driver of Oral Squamous Cell Carcinoma Progression in an Indian population

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Background: Oral squamous cell carcinoma (OSCC) is a leading cause of cancer-related mortality, with India contributing over 1/3 of the global burden. OSCC progresses from normal epithelium through premalignant lesions to invasive carcinoma, yet poor prognosis persists due to late-stage diagnosis and absence of reliable biomarkers. In the Indian population, habitual exposure to betel nut, areca nut, tobacco, and alcohol imposes distinct metabolic vulnerabilities, compounding disease-associated reprogramming. Nevertheless, population-specific proteomic studies across OSCC progression stages remain scarce, underscoring the need for robust, validated biomarkers to improve early detection and clinical outcomes.

Method: To address this gap, we performed mass spectrometry (MS)-based tissue global proteomic profiling across OSCC disease stages, encompassing premalignant lesions and invasive carcinoma, to elucidate molecular mechanisms underlying disease progression and identify candidate biomarkers and targeted PRM study to validate those targets.

Result and discussion: Global proteomic analysis identified 8,660 proteins, of which a significant proportion exhibited differential expression across disease stages, with pathway enrichment analysis revealing coordinated dysregulation in metabolic and lipid signalling pathways. Fatty acid metabolism and mitochondrial β-oxidation were among the most significantly enriched altered pathways, indicating a pronounced shift in lipid catabolic flux during OSCC progression. Notably, PLPP3, FABP5, FABP4, BGAL, ACADS, and ACAA2 demonstrated consistent stage-dependent expression changes, mechanistically implicating lipid metabolic remodelling in the pathological progression of OSCC. Targeted proteomic validation of select candidates PLPP3, FABP5, and BGAL yielded expression profiles concordant with discovery-phase observations, affirming the analytical reproducibility and biological relevance of these biomarker candidates.

Keywords: Proteomics, Tissue, Oral squamous cell carcinoma, Premalignant lesions, Biomarker discovery, Disease progression, Lipid metabolism

43. Beyond In-Gel and In-Solution Digestions: ProtiFi S-Trap as a Next-Generation ample Preparation Workflow for Proteomics in Indian Laboratories

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Sample preparation remains a major source of variance in bottom-up proteomics, and across most Indian academic and research laboratories the classical workflows are still in-gel digestion from SDS-PAGE and in-solution digestion in urea, RIPA or GnHCl buffer. Both methods account for technical variability: in-gel is prone to keratin contamination, incomplete peptide recovery from the gel matrix, and band-to-band variability, while in-solution workflows are penalised by the need to remove salt or other detergents before LC-MS/MS, with clean-up steps introducing additional losses.
Filter-aided sample preparation (FASP) tolerates SDS but is slow and prone to membrane clogging on lipid-rich samples. Suspension trapping (S-Trap), introduced by Zougman, Selby and Banks (*Proteomics* 2014; PMID 24678027) and commercialised by ProtiFi LLC, captures SDS-solubilised proteins as a colloidal suspension on a sub-micron depth filter, allowing rapid detergent depletion and in-filter tryptic digestion can be achieved either overnight or in one hour. There are existing benchmarks alongside routine experience running ProtiFi S-Trap on cells, organoids, biological fluids, plasma, FFPE blocks and fresh-frozen tissue. At omicslink™, an Indian contract research provider for mass spectrometry–based proteomics, phosphoproteomics, metabolomics and transcriptomics, and the regional access point for world-class proteomics consumables across India and South Asia, we use the S-trap columns routinely.
Published head-to-head comparison studies shows that S-Trap delivers higher unique protein identifications and tighter intra-method reproducibility than FASP and in-solution digestion (Ludwig et al., *J Proteome Res* 2018, PMID 29754492; Hailemariam et al., *J Proteome Res* 2018, PMID 30114372), tolerates SDS, SDT, urea, RIPA and NP-40 lysates without dedicated detergent removal (Elinger et al., *J Proteome Res* 2019, PMID 30761899), supports FFPE archival proteomics via the HYPERsol workflow (Marchione et al., *J Proteome Res* 2020, PMID 31935107), and yields the highest plasma protein quantifications among S-Trap, SDC and SPEED in direct comparison (Sayers et al., *Int J Mol Sci* 2023, PMID 37047281). In our hands these gains translate into reduced technical variability, cleaner LC-MS chromatograms and improved cohort completion rates relative to legacy pipelines. ProtiFi ™ S-Trap ™ is a practical upgrade path for Indian laboratories modernising proteomics sample preparation without major infrastructure investment and available with omicslink.
***Keywords**: ProtiFi ™ S-Trap ™; sample preparation; bottom-up proteomics; FASP; in-solution digestion; clinical proteomics; India; omicslink™*

44. Serum Metabolomics through High-Resolution ^{1}H NMR Reveals Key Signatures for Cervical Cancer Progression

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Background: Cervical cancer (CaCx) remains a major health burden, particularly in low-resource settings where delayed diagnosis limits treatment success. Serum metabolomics offers a promising non-invasive strategy for identifying biomarkers associated with disease progression.

Methods: Serum samples from 85 histopathologically confirmed cervical squamous cell carcinoma patients and 25 normal controls were analysed using high-resolution 800 MHz ^{1}H NMR spectroscopy. 34 metabolites and key metabolic ratios were quantified using CHENOMX software. Multivariate analyses (PLS-DA/OPLS-DA), Random Forest modelling, and ROC curve analysis were performed to identify discriminatory metabolic features.

Results: Distinct metabolic profiles differentiated CaCx patients from controls. OPLS-DA demonstrated clear group separation, while Random Forest classification showed strong predictive performance (OOB error = 0.07). Histidine, acetate, citrate, glutamine, valine, and metabolic ratios including glutamine/glucose (QGR) and glutamate/acetate (EAcR)

emerged as key discriminators. Significant reductions in amino acids and TCA-cycle-related metabolites indicated disruptions in glutaminolysis, branched-chain amino acid metabolism, energy production, and mitochondrial function. ROC analysis revealed excellent diagnostic performance for several metabolites (AUROC > 0.90).

Conclusion: The present study demonstrates that serum metabolomic profiling using high-resolution ^{1}H NMR spectroscopy can effectively distinguish cervical cancer patients from healthy individuals through characteristic metabolic alterations. The identified metabolite panel reflects cancer-associated metabolic reprogramming involving amino acid utilization, mitochondrial dysfunction, and energy metabolism. The strong classification performance obtained through OPLS-DA, Random Forest, and ROC analyses underscores the diagnostic value of these metabolic signatures. Importantly, the non-invasive nature of serum-based metabolomics makes it an attractive approach for developing clinically applicable biomarkers that may complement existing screening methods. With further validation, these findings could contribute to improved early diagnosis, risk assessment, and personalized management of cervical cancer.

Keywords: Cervical Cancer; Serum Metabolomics; ^{1}H NMR Spectroscopy; Metabolic Reprogramming; Early Detection.

45. Investigating the Essential Role of Annexin A1 in Neuroinflammation Associated with Hepatic Encephalopathy in Rat

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Background: Moderate hepatic encephalopathy (MoHE) is a metabolic brain disorder secondary to chronic liver disease, characterized by cognitive and psychiatric disturbances. While Annexin A1 (AnxA1) is traditionally an anti-inflammatory protein maintaining blood-brain barrier (BBB) integrity, its role in MoHE-induced neuroinflammation remains unclear. This study investigated whether AnxA1 contributes to neurotoxicity via nuclear translocation.

Methods: MoHE was induced in male Charles Foster rats using thioacetamide (100 mg/kg, i.p.) for 10 days. Cognitive and motor functions were evaluated via NOR, Y-maze, RAM, and Rota-rod tests. Molecular analysis included Western blotting, immunofluorescence, and subcellular fractionation. BBB integrity was assessed via sodium fluorescein and tight junction protein expression (Occludin, ZO-1). Neuronal arborization and spine density quantified neurodegeneration. Future work will utilize LC–MS/MS and phosphopeptide enrichment to map translocation-linked phosphorylation sites, alongside compartment-specific Co-IP-MS to identify binding partners driving AnxA1's pro-inflammatory shift.

Results: TAA-treated rats exhibited significant motor and cognitive deficits. AnxA1 was markedly upregulated in hippocampal CA1, CA3, and DG regions. Subcellular fractionation revealed a significant shift of AnxA1 into the nucleus, correlating with nuclear NF-κB activation and a pro-inflammatory cytokine profile (high IL-6, TNF-α; low IL-10, IL-4). Furthermore, MoHE rats showed increased BBB permeability and downregulated Occludin/ZO-1. Increased GFAP expression confirmed astrogliosis, while morphological analysis showed significant shrinkage in neuronal arborization and reduced spine density.

Conclusion and Future Directions: AnxA1 transitions from a protective to a pro-inflammatory mediator in MoHE; its nuclear translocation activates the NFκB cascade, driving BBB disruption and neurodegeneration. This functional switch is likely governed by site-specific PTMs. Future LC–MS/MS-based phosphoproteomics and interactomics will be pivotal in identifying the specific post-translational modifications and molecular partners governing this translocation, potentially uncovering novel therapeutic targets for hepatic encephalopathy.

46. Metabolomic Profiling of Phage-Resistant *Escherichia coli* Reveals Metabolic Adaptations Associated with Phage Resistance

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Background: Antibiotic resistance has become a global healthcare concern, with the emergence of multidrug-resistant (MDR) pathogenic bacteria alarming and projected to cause 50 million deaths by 2050. Hence, there is an urgent need for alternative antibacterial treatment Despite various advantages, including high specificity and self-replicating, phage therapy has limitations, including a narrow host range and the emergence of phage resistance in the targeted bacteria. However, phages that coevolve with bacteria can overcome phage resistance, highlighting their therapeutic potential. Understanding the physiological and metabolic adaptations underlying phage resistance may provide valuable insights for the development of more effective phage-based therapeutics.

Methods: A laboratory coevolution experiment was performed using *Escherichia coli* MG1655 and the T4-like bacteriophage EC_YwIITB. A phage-resistant bacterial isolate was obtained. To identify genetic determinants associated with bacterial resistance and phage counter-adaptation, whole-genome sequencing (WGS) was conducted on selected bacterial isolate. Genomic DNA was sequenced on the Illumina platform, generating paired-end reads, and sequence analysis was performed using breseq (v0.38.3). For metabolomic analysis, intracellular metabolites were quenched and extracted using a methanol/ethylene glycol (45:55, v/v) protocol. Untargeted metabolomic profiling was carried out using Orbitrap-based mass spectrometry in both positive and negative electrospray ionization (ESI) modes, followed by multivariate and univariate statistical analyses to identify significantly altered metabolites.

Results: Partial resistance to EC_YwIITB phage was confirmed in the evolved *E. coli* isolate. WGS analysis revealed insertion sequence-mediated genomic rearrangements affecting the *waaO*, *clpS*, *folK*, and *ggt* genes. Comparative metabolomic analysis identified several significantly altered metabolites in the phage-resistant strain, including FMN, nicotinic acid, L-methionine sulfoxide, adenosine, adenine, spermidine, citrulline, dimethylarginine, phenylalanine, valine, urocanic acid, γ-aminobutyric acid (GABA), and pyridoxine. These metabolites indicate substantial reprogramming of central metabolic pathways in response to phage selection pressure.

Conclusion: This study highlights the metabolic adaptations associated with the evolution of phage resistance in *E. coli* and provides insights into the molecular basis of host–phage interactions. Metabolomic profiling revealed a markedly altered redox and cofactor metabolic state in the resistant mutant, characterised by perturbations in flavin and nicotinamide metabolism, nitrogen metabolism, amino acid metabolism, and methionine/S-adenosylmethionine (SAM)-associated pathways. These findings contribute to our understanding of the physiological consequences of phage resistance and may inform the design of more robust phage-based antibacterial strategies.

47. In Silico Transcriptomic Analysis of Duchenne Muscular Dystrophy: Tissue Progression Modelling and Muscle-Serum Molecular Concordance

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Background: Duchenne Muscular Dystrophy (DMD) is a severe X-linked myopathy in which fibrotic remodelling, metabolic failure, and chronic inflammation drive progression beyond the primary dystrophin defect. Linking tissue-level disease signals to accessible circulating biomarkers remains a central unresolved challenge. This study constructs a continuous tissue progression axis from bulk transcriptomic data and evaluates its concordance with publicly available serum proteomic profiles.

Methodology: Skeletal muscle microarray data (GSE38417; n = 22; GPL570) were processed following GCRMA normalisation and limma-based differential expression ($|\log_2 FC| \geq 1$, BH-FDR < 0.05). Genes were stratified into curated functional modules (Fibrosis, Inflammation, OXPHOS, Muscle Structure) and a PC1-derived disease severity axis was constructed exclusively from DMD samples to enable continuous progression modelling. Gene-wise Spearman correlations with this axis were FDR-adjusted. Serum age-association coefficients from a published SomaScan proteomics dataset (Ikelaar, Barnard, Eng et al., Nature Communications 2025; concordant across two independent cohorts at FDR < 0.05) were matched against tissue progression correlations across 1,676 overlapping genes to assess directional concordance between tissue and serum profiles.

Results: PC1 captured 50% of transcriptome-wide variance and cleanly separated DMD from control samples. Fibrosis was the strongest progression correlate (Spearman ρ = +0.63, FDR = 0.017) and OXPHOS showed the sharpest decline (ρ = -0.75, FDR = 0.003), with the inverse relationship between these two modules providing a systems-level representation of the pathological transition from regenerative maintenance toward fibrotic replacement. Tissue-serum concordance analysis across 1,676 genes revealed a weak global correlation (Pearson r = -0.08, Spearman ρ = -0.073), with directional agreement in approximately 47% of genes. This pattern is consistent with tissue transcription and circulating protein abundance reflecting distinct aspects of DMD pathology rather than capturing the same biological signal through different assays.

Conclusion: The weak global concordance between tissue and serum is interpreted as a biologically meaningful finding rather than a null result, suggesting a difference between an active disease signature captured in muscle and a functional-decline signature captured in circulation. Ongoing work extends the tissue axis to an independent GEO cohort (GSE109178) for cross-cohort validation and investigates the biological properties of concordant and discordant gene subsets. This framework provides a principled basis for understanding the relationship between tissue and blood-based signals in DMD progression.

Keywords: Duchenne Muscular Dystrophy, transcriptomics, disease progression modelling, serum proteomics, biomarker concordance, fibrosis, oxidative phosphorylation

48. Genome-Wide DNA Methylation Analysis as a Potential Biomarker for Early Detection of Oral Cancer

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Oral Squamous Cell Carcinoma (OSCC) is one of the most common malignancies affecting the oral cavity and remains a major health concern due to its high incidence and poor prognosis when diagnosed at advanced stages. The identification of molecular biomarkers capable of detecting disease-associated changes at an early stage is therefore of considerable clinical importance. Among the various epigenetic mechanisms, DNA methylation has emerged as a key regulator of gene expression and is frequently altered during cancer development.

In the present study, genome-wide DNA methylation profiling was performed to investigate epigenetic alterations associated with oral cancer. Genomic DNA isolated from healthy individuals and oral cancer patients was subjected to bisulfite conversion followed by analysis using the Illumina Infinium MethylationEPIC v2.0 BeadChip platform, enabling interrogation of more than 935,000 CpG sites across the human genome. Quality assessment, methylation profiling, differential methylation analysis, principal component analysis, hierarchical clustering, and functional annotation were carried out to identify disease-associated methylation signatures.

Distinct methylation patterns were observed between healthy and diseased samples. Principal component analysis demonstrated clear segregation of the two groups, indicating the presence of disease-specific epigenetic alterations. Several differentially methylated genes, including ABL1, TICAM1, GPER1, ARMC9, NUS1, MPDU1, and PTPRN2, were identified. Functional annotation suggested their involvement in cellular signalling, immune regulation, metabolic processes, and pathways implicated in carcinogenesis, including MAPK signalling.

The findings of this study indicate that genome-wide DNA methylation alterations are associated with oral cancer and may provide a valuable source of candidate biomarkers for early disease detection. Further validation in larger cohorts may facilitate the development of non-invasive epigenetic screening approaches for OSCC.

Keywords: Oral Squamous Cell Carcinoma, DNA Methylation, Epigenetics, Biomarkers, Illumina EPIC Array, Early Detection.

49. Proteomic Profiling of Plasma-Derived Exosomes Reveals Thrombosis- and Immune-Associated Signatures in Non-Small Cell Lung Cancer

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Background: Non-small cell lung cancer (NSCLC), accounting for nearly 85% of all lung cancer cases, remains a major cause of cancer-related mortality worldwide. Exosomes are small extracellular vesicles involved in intercellular communication and play critical roles in tumor progression, metastasis, and immune modulation. Proteomic characterization of plasma-derived exosomes may provide insights into NSCLC pathogenesis and biomarker discovery.

Methods: Plasma-derived exosomes from NSCLC samples were analyzed using label-free quantification (LFQ)-based proteomics. Protein identification and quantification were performed using MaxQuant and LFQ-Analyst. Differential expression, principal component analysis (PCA), gene ontology enrichment, and protein network analyses were conducted to evaluate biological significance. Comparison with Vesiclepedia was performed to validate exosome-associated proteins.

Results: A total of 309 proteins were identified, with LFQ intensities generated through MaxQuant analysis. Univariate and multivariate analyses revealed 16 differentially expressed proteins, predominantly immunoglobulins along with several unique proteins. PCA demonstrated two distinct sample clusters with a few outliers. Comparative analysis with Vesiclepedia identified 56 additional exosome-associated proteins. Functional enrichment and network analyses highlighted pathways associated with thrombosis, wound healing, immune responses, and extracellular vesicle-related processes. Subcellular localization analysis confirmed that most identified proteins originated from the extracellular space, supporting their exosomal nature. Key differentially expressed proteins included PF4, LPA, PZP, PIGR, and HBD.

Conclusion: This study highlights the potential role of plasma-derived exosomal proteins in NSCLC progression and thrombosis-associated pathology. The identified protein signatures may serve as promising candidates for biomarker development and therapeutic targeting in NSCLC.

50. Proteomic signature of primed Wharton's Jelly Mesenchymal Stem Cells reveals Immunomodulatory mechanism to combat Pancreatic Cancer

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Background & Aim: Mesenchymal stem cells (MSCs) from umbilical cord have the potential therapeutic applications in context of injured, immune related & inflammatory diseases due to high proliferation rate, multilineage differentiation potential and immune tolerance properties. While clinical trials have clearly demonstrated strong safety records, efficacy of MSCs is still modest and inconsistent. Hypothesizing that priming MSCs prior to administration can improve their therapeutic efficacy, present study investigates the modulation of MSC behavior through cytokine priming and assesses their effectiveness in ameliorating inflammatory conditions. Proteomic analysis shows compositional changes post cytokine priming.

Method: Wharton's jelly derived from human umbilical cord (hWJMSCs) were primed with tumor necrosis factor-alpha (TNF-α; 25ng/ml) and interferon-gamma (IFN-γ; 25ng/ml), incubated for 24 hrs at 37°C/5%CO2, their morphological alterations, multi-lineage differentiation potentials (osteocytes/chondrocytes/adipocytes), immunophenotypying (CD90+73+105+44+34-45-19- HLADR-), Adhesion molecules (ICAM, VCAM, NCAM) migration capabilities were examined. Label-free quantitative LCMS (nLC/MS/MS coupled to Orbitrap fusion Tribrid massspectrometer) analysis was performed on more than 2400 proteins identified. Further, immunogenic potentials are being tested using PBMNCs from healthy human donors.

Result: hWJMSCs primed with TNF-α (hWJMSC-T)/IFN-γ (HWJMSC-I) showed >90% expression of CD90+ 73+ 105+ 44+. Microscopically morphological distinction stained with phyalloidin/DAPI observed showed hWJMSC-T as elongated and flattened cells and complement & coagulation cascade and Pro-angiogenic proteome signature in abundance, suggesting their role in innate immunity homeostasis. On the other hand, IFN-γ induction showed immune-modulating protein signature of infection/inflammation especially, Guanylate-binding proteins. Differentially expressed protein signature points towards modulation of NOD-like receptor signaling and cell adhesion molecule pathways.

Conclusion: Data herein provides the evidences that stem cell properties of regenerative capability remain conserved and do not compromise under inflammatory conditions. Additionally, primed hWJMSCs can modulate or prevent infection most likely via cross-talk between cascades of defense systems. Thus, suggesting a potential role as alternate strategy to regulate inflammation and/or reshape inflammatory microenvironment.

Keywords: Mesenchymal stem cells, pro-inflammatory cytokines, inflammation, immunomodulation.

51. Wheat Amylase-Trypsin Inhibitor Proteins as Proteomic Biomarkers at the Interface of Food Safety, Nutrition, and Human Health

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Background: Wheat amylase-trypsin inhibitor (ATI) proteins are multifunctional cysteine-rich defense molecules that contribute to grain protection against pests and are increasingly recognized for their broader significance in food safety, nutritional quality, and human health. Recent evidence suggests that ATI proteins may influence dietary responses, food sensitivities, and grain quality, positioning them as promising translational biomarkers within modern agri-food systems. In this study, ATI proteins from the Indian bread wheat cultivar HD 3086 were comprehensively characterized using an integrated proteomic, biochemical, structural, and bioinformatic approach to evaluate their functional diversity and biomarker potential.

Methods: ATI proteins were isolated from wheat grains of cultivar HD 3086 using Sephadex G-50 gel filtration chromatography. Their enzymatic inhibitory activities against α-amylase and trypsin were evaluated to assess biological functionality. Proteomic profiling was performed using high-resolution nano LC–MS/MS to identify ATI isoforms. Bioinformatic analyses were conducted to examine conserved motifs, structural features, and physicochemical properties. Secondary structure composition was analyzed using circular dichroism (CD) spectroscopy. Additionally, UV–Near Infrared (UV–NIR) spectroscopy effectively differentiated healthy and insect-infested grains through distinct molecular signatures associated with moisture variation and biochemical degradation, underscoring ATI-linked applications in grain quality monitoring and food safety surveillance.

Results: Purified ATI proteins exhibited strong α-amylase inhibitory activity (90.6 ± 0.72%) and moderate trypsin inhibitory activity (62.9 ± 0.8%), confirming their functional bioactivity. Proteomic analysis revealed multiple ATI isoforms, including alpha-amylase inhibitor 0.28, CM16, alpha-amylase inhibitors 0.19/0.53, CMX variants, and subtilisin-chymotrypsin inhibitors, indicating high molecular diversity. Bioinformatics results showed conserved cysteine-rich motifs and stable inhibitory domains across isoforms, supporting structural robustness. CD spectroscopy revealed a predominantly β-sheet-rich structure with minimal α-helical content, consistent with high protein stability. UV–NIR spectroscopy successfully distinguished healthy and insect-infested grains through distinct spectral signatures linked to biochemical degradation and moisture variation.

Conclusion: This study demonstrates that wheat ATI proteins in cultivar HD 3086 exhibit significant structural diversity, strong enzymatic inhibitory activity, and high molecular stability. Beyond their established role in plant defense, ATIs show strong potential as proteomic biomarkers for grain quality assessment, food safety monitoring, and agricultural diagnostics. These findings establish a translational framework for integrating ATI proteins into precision agriculture, foodomics, and nutritional quality improvement strategies.

Keywords: Wheat ATI proteins, Proteomics, LC-MS/MS, Food Safety, Nutritional Quality, Human Health, Bioinformatics, Translational Research, Circular Dichroism, UV-NIR

52. Differential Plasma Contact System Activation by Wild-Type and Arctic Amyloid-beta-42 (Aβ42) Aggregates: Implications for Vascular Dysfunction in Alzheimer's Disease

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Alzheimer's disease (AD) is characterized by the accumulation of amyloid-β (Aβ) aggregates. It is increasingly recognized to involve vascular abnormalities, including blood-brain barrier dysfunction, inflammation, impaired cerebral blood flow, and cerebral amyloid angiopathy. The plasma contact system is a vascular proteolytic pathway that contributes to coagulation and inflammatory responses. The Arctic Aβ42 mutation (E22G) accelerates Aβ aggregation and causes familial AD; however, its effects on plasma contact system activation are unknown.

To address this question, wild-type (WT) Aβ42 and Arctic Aβ42 aggregates were characterized by transmission electron microscopy and incubated with normal pooled plasma. Contact system activation was assessed using clotting assays, chromogenic activity assays, and Western blotting.

Consistent with its aggregation-prone nature, Arctic Aβ42 formed abundant fibrillar aggregates. Unexpectedly, Arctic Aβ42 was a weaker activator of the plasma contact system than WT Aβ42, producing delayed plasma protease activity, prolonged clotting times, and reduced high-molecular-weight kininogen cleavage.

The dissociation between fibril formation and contact system activation was unexpected, as Arctic Aβ42 aggregated more readily than WT Aβ42. These results indicate that fibril abundance alone does not predict contact system activation. These differential effects of the plasma contact system in circulation contribute to differences in cerebrovascular pathology associated with the Arctic mutation, including vascular injury and hemorrhagic complications in AD.

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53. Enhancing Target-Site Exposure of Formononetin in Bone Marrow via Bioenhancer Assisted Phospholipid Complexation.

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Background: Formononetin (FNT), a phytoestrogen, has shown osteogenic effect in Ovariectomized (OVX) induced osteoporosis but is limited by poor bioavailability. This study aimed to compare the osteogenic potential of pure FNT and Formononetin-Piperine-Phospholipid complex (FNT-PIP-PC) in OVX-induced osteoporosis and to quantify free FNT concentration in rat bone marrow. An in vivo study was conducted using an OVX-induced osteoporosis rat model.

Methods: Adult Sprague-Dawley rats (SD) rats were ovariectomized and treated orally with FNT or FNT-PIP-PC at 5mg/kg for 12 weeks. Evaluations included body composition analysis, µCT, L5 compression, bone markers, and pharmacokinetics in bone marrow using LC-ESI-MS/MS.

Results: FNT-PIP-PC treatment significantly restored trabecular bone volume and microarchitecture in femur and tibia, improved uterine mass, increased Osteocalcin (OCN), and reduced C-terminal telopeptide of type-1 collagen (CTX) levels. These findings aligned with enhanced mRNA expression of RUNX, RANKL, BMP2, and OPG. Additionally, FNT-PIP-PC improved pharmacokinetic parameters like Cmax, AUC0-t, and AUC0-∞ of free FNT from FNT-PIP-PC compared to pure FNT.

Conclusion: To conclude Oral dosing of FNT-PIP-PC in OVX-induced osteoporosis rats significantly improved the osteogenic potential of FNT and enhanced its free concentration in bone marrow for therapeutic use with less toxicities.

Keywords: Formononetin, Osteoporosis, Pharmacokinetics, Ovariectomy, Piperine.

54. Integrated proteomics reveals subtype-specific molecular programs and shared metabolic vulnerabilities in pituitary adenomas

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Pituitary adenomas are clinically heterogeneous tumors classified into functional and non-functional subtypes, yet their underlying molecular architecture remains incompletely defined. Here, we employed data-independent acquisition

parallel accumulation–serial fragmentation (DIA-PASEF)– based proteomics to systematically characterize the proteomic landscape of acromegaly, Cushing disease, and non-functional pituitary adenomas (NFPA) compared with normal pituitary tissue. Across ~9,000 quantified proteins, we identified extensive subtype-specific and shared differential expression patterns.

Functional adenomas exhibited distinct molecular features: acromegaly showed enrichment in ribosome biogenesis and the translational machinery, consistent with increased hormone synthesis, whereas Cushing disease was characterized by extracellular matrix remodeling, platelet activation, and coagulation pathways, indicating microenvironmental and systemic alterations. In contrast, NFPA showed marked downregulation of hormone-related proteins, alongside enrichment of metabolic and mitochondrial pathways, reflecting a loss of endocrine function and metabolic adaptation. Despite these differences, a shared core signature involving oxidative phosphorylation and mitochondrial activity was observed across all subtypes.

Protein–protein interaction network analysis revealed coordinated functional modules, including mitochondrial respiration and ribosomal processes, while targeted parallel reaction monitoring validated representative differentially expressed proteins. Furthermore, integration of machine learning and spatial clustering identified subtype-specific biomarker panels with strong discriminatory potential.

Collectively, this study defines a systems-level proteomic framework for pituitary adenomas, highlighting metabolic reprogramming, translational control, and extracellular signaling as key axes of tumor biology. These findings provide mechanistic insight into subtype heterogeneity and nominate candidate biomarkers and pathways for future diagnostic and therapeutic development.

Keywords: Pituitary adenoma, Acromegaly, Cushing, NFPA, Proteomics, Mass spectrometry, dia-PASEF, biomarkers

55. Enrichment Strategies for Central Pair Apparatus and Low-Abundance Proteins in the *Chlamydomonas reinhardtii* Flagellar Proteome

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Chlamydomonas reinhardtii is a key model for studying 9+2 motile cilia, yet proteomic characterisation is hindered by overrepresentation of highly abundant axonemal proteins. The central pair apparatus (CPA) harbours proteins essential for mechanotransduction and beat regulation, but discrepancies between Phytozome and UniProt complicate annotation. This study aimed to expand the low-abundance flagellar proteome using biochemical fractionation and LC-MS/MS on an Orbitrap Fusion Lumos.

Flagellar samples were partitioned into five fractions: C1-enriched, C2-enriched, axoneme, membrane/matrix, and insoluble pellet. An ATP-based CP extrusion protocol further enriched rare CPA components. A Python pipeline cross-matched Phytozome v5.6 FASTA sequences against UniProt accessions via BLAST to address annotation gaps. Proteins were quantified using MaxQuant razor peptide intensities at 1% Benjamini-Hochberg FDR, log2-transformed, and median-normalised. Enrichment patterns were assessed using volcano plots and heatmaps.

Fractionation increased detection sensitivity relative to whole-flagella samples, identifying proteins across all fractions, including those absent in unfractionated controls. The annotation pipeline reconciled all the Phytozome entries to UniProt accessions. Volcano plots revealed distinct enrichment patterns across C1, C2, and axonemal fractions; however, the tubulin-dominated MS1 signal continued to mask rarer targets. Heatmap clustering confirmed reproducible enrichment, though dynamic range remained a limiting factor.

This work expands the annotated *C. reinhardtii* flagellar proteome and demonstrates that CPA fractionation effectively resolves distinct protein classes. Accessing low-abundance and transient proteins will require additional depletion or orthogonal fractionation strategies. This workflow establishes a reproducible foundation for comparative studies of flagellar mutants and ciliopathy models.

Keywords: Central Pair Apparatus, *Chlamydomonas reinhardtii*, Axoneme, Enrichment, Proteomics

56. Comparative Multi-Omics Analysis of *In Vitro* Dedifferentiated and Cambium Meristematic Cells of *Picrorhiza kurroa* Reveals Distinct Cellular and Metabolic Reprogramming

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Introduction: Cambium meristematic cells (CMCs) and dedifferentiated cells (DDCs) are distinct *in vitro* plant cell types that differ in their cellular organization, growth characteristics, and metabolic potential. Understanding the molecular and physiological differences between these cell lines is important for developing efficient cell culture systems for secondary metabolite production. Therefore, this study aimed to establish and comprehensively characterize CMCs and DDCs of *Picrorhiza kurroa* through integrated morphological, transcriptomic, proteomic, and metabolomic analyses.

Materials and Methods: DDCs and CMCs were established from rhizome explants under optimized culture conditions. Cellular morphology was examined using scanning electron microscopy (SEM). Comparative transcriptomic analysis was performed to identify differentially expressed genes (DEGs) and associated pathways. Proteomic profiling was conducted using a timsTOF Pro 2 mass spectrometer coupled with the diaPASEF workflow. Picrosides accumulation was quantified through UPLC-based metabolite profiling.

Results and Discussion: SEM analysis revealed distinct morphological differences between the two cell lines, where CMCs consisted of small, isodiametric, densely cytoplasmic cells with smooth surfaces, while DDCs exhibited enlarged, irregularly shaped cells with heterogeneous surface characteristics. Transcriptomic analysis identified 4,905 DEGs, including 2,127 upregulated and 2,778 downregulated genes in CMCs relative to DDCs. Among these, 1,536 genes were functionally annotated and enriched in diverse metabolic and signalling pathways, indicating extensive transcriptional reprogramming. Proteomic profiling identified 3,979 proteins in CMCs and 2,999 proteins in DDCs, revealing variation in protein abundance and cellular functions. Metabolic profiling shows higher picrosides accumulation in CMCs than in DDCs. The integrated omics datasets collectively indicated enhanced cellular activity, metabolic specialization, and biosynthetic potential in CMCs.

Conclusion: The study demonstrates that CMCs possess distinct morphological features, extensive molecular reprogramming, and superior metabolite-producing capability compared with DDCs. These findings highlight the potential of CMCs as a sustainable and efficient platform for large-scale production of picrosides.

Keywords: Dedifferentiated cells, Transcriptomic, Proteomic, Secondary metabolites

57. Micro-Raman Spectroscopic Delineation of Oral Potentially Malignant Disorders and Cancer Risk Assessment

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Introduction: There is a critical need for minimally invasive technologies to diagnose oral cancer and precancer. Raman spectroscopy (RS) detects structural and conformational biochemical changes in tissues before clinical manifestations

appear, making it a promising tool for early diagnosis and risk assessment. This study aims to stratify patients into four groups—oral cancer, oral potentially malignant disorders (OPMDs), individuals with adverse habits but no OPMDs, and healthy controls—using micro-RS of saliva and serum. Furthermore, it evaluates cancer risk and compares the diagnostic efficacy of salivary and serum profiling.

Materials and Methods: A comparative micro-Raman spectroscopic evaluation of serum and salivary samples was conducted across the four distinct clinical groups. The obtained raw spectra underwent preprocessing, including baseline correction and vector normalization, to eliminate noise. The spectral data were then analyzed using a patient-wise approach, employing unsupervised Principal Component Analysis (PCA) for initial pattern recognition, followed by supervised Linear Discriminant Analysis (LDA) with crossvalidation to build classification models.

Results and Discussion: The RS analysis revealed distinct biomolecular signatures differentiating the clinical groups. Significant intensity-related variations were observed in key biochemical constituents, specifically amino acids, Amide I, and DNA peaks, in both serum and saliva samples. Crucially, the spectral profiles not only differentiated various types of OPMDs but also successfully discriminated between OPMDs with and without dysplasia. These spectral differences underline the technique's capability to capture subtle metabolic and proteomic shifts associated with malignant transformation.

Conclusion: Micro-Raman spectroscopy serves as a rapid, accurate, and minimally invasive diagnostic tool for delineating OPMDs and assessing oral cancer risk. Both serum and saliva demonstrate significant potential as reliable biofluids for early OPMD detection and continuous risk monitoring using this spectroscopic approach.

Keywords: Micro-Raman Spectroscopy, Oral Cancer, OPMD, Serum, Saliva, Liquid Biopsy, PCA-LDA.

58. *In Silico* Evaluation of Cucurbitaceae Seed Lectins Targeting SARS-CoV-2 Spike Glycoprotein for Antiviral and Diagnostic Applications

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Background

Cucurbitaceae seed lectins (CSLs) are plant derived carbohydrate binding proteins with strong specificity toward glycosylated biomolecules. The SARS-CoV-2 spike glycoprotein exhibits dense N-linked glycans, particularly high-mannose residues that play a crucial role in viral attachment and entry. Targeting these glycosylation sites offers a promising strategy for antiviral intervention and proteomics driven therapeutic development.

Objective

To evaluate the antiviral potential of Cucurbitaceae seed lectins by analyzing their binding interactions with the receptor binding domain (RBD) of the SARS-CoV-2 spike glycoprotein using *in silico* proteomic approaches.

Methods

Lectin protein interactions were assessed using molecular docking and computational binding analysis. The binding affinity of CSLs with the spike RBD was evaluated and compared with the human ACE2 receptor using the HDOCK web server and PRODIGY binding affinity prediction tool. Structural stability and interaction dynamics were further analyzed through molecular dynamics simulations to validate docking results.

Results

CSLs demonstrated strong binding affinity and high specificity toward the RBD of the SARS-CoV-2 spike protein. Docking analysis identified top scoring lectins with favorable binding energies, forming stable hydrogen bonds and hydrophobic interactions within key active site residues. Comparative analysis indicated that CSLs exhibited higher or competitive binding affinity relative to ACE2, suggesting their potential to effectively block viral entry.

Conclusion

This study highlights the potential of Cucurbitaceae seed lectins as promising antiviral agents by targeting glycosylated regions of the SARS-CoV-2 spike protein. The strong and stable interactions observed through proteomics driven computational analysis support their application as viral entry inhibitors and candidates for future antiviral and biosensor development.

Keywords: Proteomics, Lectins, SARS-CoV-2, Glycoprotein, Molecular Docking, Antiviral Agents

59. Structural characterization of the quorum sensing regulator AbaR from *Acinetobacter baumannii* for anti-virulence drug discovery

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Introduction: Quorum sensing (QS) in *Acinetobacter baumannii,* plays a critical role in virulence and biofilm formation. This has led to a significant decline in the effectiveness of existing antimicrobial therapies against *Acinetobacter baumannii* infections. AbaR, a LuxR-type transcriptional regulator, plays a central role in regulating transcription of QS-controlled genes. This process occurs through binding of the receptor autoinducer complex to the DNA promoter region after sensing its specific autoinducer molecule. Despite its critical role, the lack of structural data has delayed the development of targeted anti-virulence strategies.

Methods: Purified protein was crystallized using sitting-drop vapor diffusion method. X-ray diffraction data were collected at 2.1 Å resolution on the XRD2 beamline, Elettra-Sincrotrone Trieste, Italy. The structure was solved by molecular replacement using an AlphaFold2-predicted model, as available LuxR family homologs shared only ~33% sequence identity with AbaR. The structure was refined through iterative cycles of Refmac5 and manual rebuilding in Coot.

Results: The structure of the AbaR-autoinducer complex was determined in the orthorhombic $C222_1$ space group. The asymmetric unit contains a monomer with autoinducer, N -(3-Oxododecanoyl)-L-homoserine lactone bound within the ligand-binding pocket. The final Rwork and Rfree values are 0.20 and 0.24, respectively. The structure revealed two distinct domains: an N-terminal autoinducer-binding domain (α-β-α sandwich fold) and a C-terminal DNA-binding domain (helix-turn-helix motif), connected through a flexible linker region. This represents the characteristic domain organization in LuxR family transcriptional regulators. The autoinducer resides within a hydrophobic cavity formed between the β-sheets and α-helices 3, 4 and 5 of the ligand-binding domains.

Conclusion: The AbaR-autoinducer complex structure provides the structural framework for rational design of quorum sensing inhibitors that can disrupt AbaR function and quench quorum signaling in *Acinetobacter baumannii*.

Keywords: Quorum sensing, Biofilm formation, antimicrobial resistance, Antivirulence therapy

60. IL-6–Thrombin Axis Drives Disseminated Intravascular Coagulation induced by Anti-PD-L1 Therapy in a pre-clinical breast cancer Model

Surabhi Raman

Immune checkpoint inhibitors (ICIs) targeting PD-1/PD-L1 have transformed cancer treatment; however, their full spectrum of adverse effects remains to be thoroughly studied. We report a tumor-specific, lethal coagulopathy resembling disseminated intravascular coagulation (DIC) following anti-PD-L1 monoclonal antibody (mAb) administration in a 4T1 breast tumor mouse model. More than 50% of 4T1-bearing Balb/c mice died within one hour of receiving a second anti-PD-L1 dose. This phenomenon was not observed in mice bearing other tumor types or treated with anti-PD-

1 mAbs. Pretreatment with antithrombin, anti-IL-6 mAb, or tissue factor pathway inhibitor prevented death, implicating a thrombin- and IL-6–dependent mechanism of action. The lethality persisted in Rag2^{-}/$^{-}$ mice, indicating T-cell-independent immune involvement. Tumor-bearing mice showed splenomegaly, and flow cytometry analysis of the spleen revealed the accumulation of CD11b^{+}Gr1^{+} myeloid-derived suppressor cells (MDSCs) in 4T1-bearing mice. These findings support a model in which anti-PD-L1 mAb stimulates MDSCs and other immune cells to secrete excessive levels of IL-6, confirmed by gene expression levels, thereby triggering pro-thrombin activation and causing DIC. This study reveals a previously unrecognized innate immune–mediated side effect of PD-L1 blockade that may parallel the rare but severe coagulopathies observed in ICI-treated patients.

Keywords: PD-L1 blockade, IL-6, Thrombin, DIC, MDSCs, 4T1 tumor model 1629/1691

61. Three-Month Mortality and Outcomes in a Multicenter Prospective Stroke Cohort from India

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Introduction: Rapid differentiation of acute ischemic stroke (AIS) from intracerebral hemorrhage (ICH) remains critical for early therapeutic intervention. Blood-based proteomic biomarkers hold promise for developing rapid and minimally invasive diagnostic tools, particularly in resource-limited settings. Establishing a clinically well-characterized stroke cohort is essential for translational proteomics and biomarker validation studies.

Methods: This ongoing prospective observational study recruits acute stroke patients presenting within 6 hours of symptom onset at two tertiary care centers in New Delhi, India. Peripheral blood samples were collected for targeted plasma proteomics. Clinical and demographic parameters including age, sex, National Institutes of Health Stroke Scale (NIHSS), and modified Rankin Scale (mRS) were documented at recruitment. Three-month outcomes included mortality and rehospitalization. Cumulative incidence proportions were calculated, and risk ratios (RR) for mortality were estimated for age ≥65 versus <65 years and by sex.

Results: Data from 470 unique patients were analyzed. The mean age was 55.8 ± 14.3 years, and 67.1% of patients were male. Three-month mortality occurred in 20 patients (20.43%), and rehospitalization occurred in 10 patients (10.21%). Mortality incidence was higher among patients aged ≥65 years (0.81%) compared with those <65 years (0.29%), corresponding to a risk ratio of 2.77. Mortality risk was similar between males (0.32%) and females (0.65%). Successful blood collection and plasma processing within the hyperacute 6-hour window was achieved in the majority of recruited participants, supporting the feasibility of high-throughput targeted plasma proteomics in acute stroke settings.

Conclusion: This multicenter prospective stroke cohort demonstrates low three-month mortality and rehospitalization rates, with older age associated with nearly threefold increased mortality risk. The integration of detailed clinical phenotyping with targeted proteomics may facilitate future identification of sensitive biomarkers for stroke subtype differentiation and prognostication.

Keywords: Stroke; cohort study; mortality; aging; outcomes; low- and middle-income countries

62. Proteomic Insights into Late Embryonic Development and Limb Morphogenesis in *Tachypleus gigas*

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Introduction: The horseshoe crab species *Tachypleus gigas* is considered a data-deficient species with limited information available despite its ecological and evolutionary importance as a living fossil. In particular, information associated with early embryonic development remains largely unexplored. The present study aimed to investigate the developmental progression and stage-specific proteomic profile of early embryonic stages.

Materials and Methods: Embryos were collected and examined through morphological and developmental observations. Whole protein extraction was performed from S13, S16, S18, and S20 embryonic stages, followed by LC-MS/MS-based proteomic analysis. Identified proteins were analyzed using STRING v12.0. Functional enrichment and pathway analysis were performed. Domain identification and protein sequence similarity studies were performed on selected proteins to understand their biological significance during development.

Results and Discussion: The study revealed dynamic changes in protein expression, indicating stage-specific regulation of developmental processes. Proteomic analysis identified 289, 592, 1025, and 340 proteins in developmental stages 13, 16, 18, and 20, respectively, demonstrating progressive changes in protein diversity during embryogenesis. Several proteins associated with cell adhesion, cytoskeletal organization, signal transduction, nervous system development, energy metabolism, stress response, and morphogenesis were identified. Around 64 proteins associated with limb morphogenesis and appendage development were selected for further investigation. Comparative sequence analysis revealed significant similarity of these proteins with homologs from other species, indicating evolutionary conservation of developmental pathways. In addition, domain and motif analyses highlighted the presence of conserved functional regions among the protein sequence.

Conclusion: This study provides one of the first comprehensive insights into the developmental proteome of *T. gigas* and expands the current understanding of molecular events associated with horseshoe crab embryogenesis. This work lays the foundation for future comparative proteomic and developmental studies in other chelicerates and understudied marine arthropods.

Keywords

Tachypleus gigas; Embryogenesis; Horseshoe crab; Proteome analysis; Development; Proteins

63. From Gastric Coinfection to Neural Dysfunction: Secretome-mediated Gut-Brain Communication in Brain organoids

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Background: Communication between gastrointestinal and central nervous system, via the gut-brain axis, is increasingly recognized as a crucial factor in maintaining neural homeostasis. External environmental cues such as pathogenic infections including *Helicobacter pylori* (*H. pylori*) and Epstein-Barr virus (EBV) in the peripheral systems such as gut have been recognized as a contributor to neuronal dysfunction, yet the molecular mediators linking these systems remain poorly defined.

Methods: Here, we investigated whether the secretome from gastric coinfection of *H. pylori* and EBV can influence neuronal signalling using an integrated proteomic, lipidomic, and organoid-based approach. We initially characterized the coinfected secretome via proteomic and lipidomic analyses and identified a key regulator that could potentially lead to neural dysfunction. The secretome-exposed brain organoids were utilized to assess synaptic alterations. We also inhibited the key protein of secretome to validate the observed outcomes of synaptic dysfunction in brain organoids.

Results: The lipidomic analysis of secretome revealed substantial remodelling in the secreted lipid cargo which was observed via enrichment of phospholipids and sphingolipids. Moreover, complementary proteomic profiling identified enrichment of redox-associated pathways, highlighting glutamate-cysteine ligase catalytic subunit (GCLC) as a key regulator of oxidative balance. Functional validation in cerebral organoids exposed to coinfected secretome showed significant upregulation of metabotropic glutamate receptor 1 (GRM1) indicative of excitatory signalling. Pharmacological inhibition of GCLC using buthionine sulfoximine (L-BSO) attenuated GRM1 expression, supporting redox-dependent mechanism linking secretome-induced oxidative signalling to glutamatergic dysregulation.

Conclusion: Collectively, these findings demonstrate that coinfection remodels gastric secretome into a bioactive signalling milieu that has the ability to alter neuronal function in a coordinated manner. This study provides a mechanistic insight into the secretome-mediated gut-brain communication and highlights redox-driven modulation of neuronal signalling as a key feature of coinfection-induced responses.

Keywords: Gut-brain axis, multi-omics, *Helicobacter pylori*, Epstein-Barr virus, brain organoids, neuroplasticity

64. Mapping the Molecular Landscape of Colorectal Cancer in the Indian Population: A Deep Quantitative Proteomic Study

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Colorectal cancer silently kills over 900,000 people each year — yet for Indian patients, who face a rapidly escalating burden of this disease, we still know remarkably little about the molecular forces driving it. Global proteomic studies have largely looked elsewhere. We decided to look here.

Using data-independent acquisition mass spectrometry (DIA-MS) on a Bruker timsTOF Pro 2 in PASEF mode, we mapped the proteome of CRC at unprecedented depth — 9,281 proteins quantified across 11 paired tumor and adjacent normal tissue samples, one of the most comprehensive CRC proteomic datasets from the Indian subcontinent. What emerged was not a list of numbers, but a story: tumor cells hijacking the cell's entire biosynthetic machinery — ramping up ribosome biogenesis, RNA processing, and replication — while simultaneously dismantling the structural scaffolding that holds normal tissue together. Extracellular matrix organization collapses. Antioxidant defenses, particularly the glutathione axis, are stripped away. 431 proteins shift significantly, and network-based clustering reveals these are not isolated events — they are coordinated, module-level rewiring of cellular identity.

Within this landscape, a striking perturbation of the retinol metabolism pathway caught our attention. Sorafenib, a known modulator of this axis, may hold relevance here — a question we are actively pursuing.

Selected candidates were orthogonally validated by Parallel Reaction Monitoring (PRM) on an Orbitrap Fusion, anchoring our discovery-phase findings in targeted analytical rigour.

The molecular portrait of CRC in Indian patients has, until now, remained largely unpainted. This work begins to change that.

65. Exhaled breath condensate (EBC) bile acid profile correlates with Plasma bile acid profile in alcohol related liver diseases

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Background Plasma bile acid levels are closely associated with alcohol-related liver disease (ARLD) and reflect hepatic dysfunction. Exhaled breath condensate (EBC) represents a novel, non-invasive matrix for metabolite assessment. We evaluated EBC for assessing identifying different bile acid fractions and compared with plasma bile acids in ARLD patients.

Methods

This study enrolled 181 healthy individuals to establish baseline breath bile acid profiles in EBC, assessing postprandial, age, sex, and weight-related variations. EBC and paired plasma bile acids were then analyzed in 120 patients with alcohol-related cirrhosis (ARC) and 120 with severe alcohol-associated hepatitis (SAH) using high-resolution mass spectrometry.

Results

Altogether, 19 bile acids were identified in plasma of which 15 were identified in the breath samples. The most abundant bile acids in both plasma and breath were glycine- and taurine-modified bile acids. Cholic acid and deoxycholic acid were

the most affected bile acids, and correlated with changes in gender, age, weight or diet respectively (FC>1.5, p<0.05). Glycochenodeoxycholic acid (FC>6.5, p<0.001), Glycoursodeoxycholic acid (FC>11,p<0.001), and Glycodeoxycholic acid (FC>9.3, p<0.001) were significantly increased in the EBC samples of SAH patients as compared to ARC or controls. Glycochenodeoxycholic acid, glycoursodeoxycholic acid, and glycodeoxycholic acid exhibited strong diagnostic performance in EBC (AUC >0.85) and plasma (AUC ≈0.82), demonstrating high concordance between breath and plasma bile acid profiles.

Conclusion: Glycochenodeoxycholic acid, Glycoursodeoxycholic acid, Glycodeoxycholic acid levels are significantly elevated in breath and plasma of SAH patients compared with alcohol cirrhosis patients, with a diagnostic efficiency of 85%. Exhaled breath condensate is a novel, non-invasive method for detailed bile acid assessment and early prognostication of poor outcome in ARLD patients.

66. A Photocrosslinkable c-di-GMP-Based Chemoproteomic Platform for Unraveling Bacterial Signaling Mechanisms

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Cyclic-di-guanylate monophosphate (c-di-GMP) is a central bacterial second messenger that regulates several aspects of bacterial physiology including motility, adhesion, virulence, and biofilm formation.[1] Consequently, targeting the c-di-GMP signaling pathways presents a promising strategy for antibacterial development.[2] To overcome this gap, we have designed and synthesized bifunctional chemoproteomic probes for c-di-GMP that incorporate a photo-crosslinkable diazirine and an alkyne handle, facilitating efficient protein enrichment. These probes were synthesized through a modular approach in nine steps, employing in-house developed guanosine 3'-phosphoramidites and O6-modified H-phosphonates. In this poster, we present our synthetic strategy and demonstrate the utility of these photoaffinity probes for quantitative chemoproteomic profiling of c-di-GMP–protein interactions in Pseudomonas aeruginosa lysates. Application of the probes recovered 33% of the known c-di-GMP interactome and revealed 60 putative binding partners. Biochemical validation of selected proteins highlights broader roles of c-di-GMP in bacterial physiology and biofilm-associated pathways. These findings underscore the potential of our probes to uncover novel c-di-GMP effectors and illustrate the power of discovery proteomics in advancing antibacterial research.

67. CD73 as a Modulator of Gemcitabine Response in Pancreatic Ductal Adenocarcinoma

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Background: Pancreatic ductal adenocarcinoma (PDAC) shows a poor clinical response to gemcitabine (GEM), largely due to the activation of resistance-associated survival pathways. The intrinsic isoform of CD73 has been reported as a mediator of chemoresistance by promoting survival signalling; however, its expression dynamics under sustained low-dose versus transient high-dose GEM exposure remain inadequately characterized. Additionally, the lack of structural information for intrinsic CD73 (i-CD73) limits the development of rational drug strategies targeting this molecule.

Aim & Objectives: This study aimed to evaluate CD73-associated signaling under continuous and transient GEM exposure in PDAC cells and to identify potential small-molecule inhibitors of i-CD73 using in-silico approaches.

Methodology: MiaPaCa-2 cells were cultured continuously with varying concentrations of GEM for 3 months, up to 250 nM, and compared with cells transiently treated with 350 nM GEM (IC_{50}) for 48 hours. Expression of CD73, Akt, and other GEM resistance–related markers was analyzed by Western blotting and RT-PCR. Apoptotic markers were assessed in

parallel. Structural prediction of i-CD73 was performed using AlphaFold and i-TASSER, followed by molecular docking against FDA-approved drugs and an indigenous compound library using AutoDock Vina.

Results: Both continuous and transient GEM exposure resulted in upregulation of CD73 and key GEM resistance signaling markers. However, apoptotic markers were significantly induced only under transient IC_{50} treatment, suggesting coexistence of resistance signaling and cell death. In silico docking identified multiple candidate compounds with favorable binding affinity for i-CD73.

Future Directions: Future studies will focus on establishing a stable GEM-resistant PDAC model, in-vitro validation of identified drug candidates, and evaluating the impact of i-CD73 targeting on GEM sensitivity.

68. Longitudinal change in the plasma metabotype indicates Therapeutic plasma exchange in Acute on chronic liver failure patients should be done every 12 hours

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Background and Aims: Therapeutic plasma exchange (TPE) has shown some benefits in ACLF patients as it reduces inflammatory cytokines, albumin/water-bound toxins and improves the survival of ACLF patients. Analogous changes in the plasma metabolic landscape post-TPE in ACLF patients are unknown and could predict non-survival or TPE requirements.

Method: In this study, TPE was performed on ACLF patients (N = 42), and plasma samples of patients were collected at pre-therapy (baseline), mid-therapy, post-therapy, and at 6hrs and 12hrs post-therapy, respectively. A total of 250 plasma samples were subjected to untargeted metabolomics using HRMS. Temporal change in the plasma metabolic profile of non-survivors was compared to survivors (30 days) using weighted metabolome correlation network analysis (WMCNA). Non-survivor-specific metabolites were identified(baseline) and subjected to clinical correlation and outcome prediction.

Result: Plasma metabolomics identified 620 features. ACLF patients, as compared to healthy, showed 142 metabolites (Up - 77; Down - 65(FC > 1.5, $p < 0.05$)). Partial Least Square-Discriminant Analysis (PLS-DA) analysis and hierarchical clustering segregated ACLF patients. ACLF patients showed dysregulated energy, nucleotide, amino acid metabolism, and others. Analysis of Post TPE compared to pre-TPE showed 130 metabolites (Up - 63; Down - 67(FC >1.5, $p < 0.05$)) differentially expressed. PLSDA and hierarchical clustering showed clear distinction in the post-therapy metabolic landscape of ACLF patients. TPE specifically remodelled Tryptophan, Carbohydrate, Urea, and bile acid metabolism. Post-therapy levels of chenodeoxycholic acid and others (FC > 76, AUC > 0.9, $p < 0.05$) were responsible for the segregation of post-therapy metabotype. WMCNA and pathway enrichment analysis revealed a temporal post-TPE decrease in the urea cycle, bile acids, and tryptophan metabolism, whereas amino acids and carbohydrate metabolism-linked metabolites were increased. Interestingly the metabolic profile of ACLF showed a reversal of metabotype in 6 hrs which got prominent by 12 hrs suggesting an urgent need for another TPE. The plasma of non-survivors was highly enriched for DAMPS/PAMPS compared to survivors. Further, single TPE very effectively clears the plasma of survivors but was found ineffective for non-survivors. Non-survivors showed a significant increase in Citric acid, Nicotinic acid, and others (FC > 10, AUC > 0.99, $p < 0.05$), which directly correlated with the severity and clinical factors (MELD, SOFA, and others, $R2 > 0.7$, $p < 0.05$) and can be used as a putative indicator for non-survival or requirement of TPE.

Conclusion: Temporal change in the metabolic phenotype of ACLF patients is predictive of TPE response, and an increase in plasma level of Citric acid, Nicotinic acid, and others by 12 hrs post TPE warrants an urgent need for another TPE in ACLF patients.

69. Serum Proteome Profiling of Pituitary Neuroendocrine Tumors Reveals Subtype-Specific Signatures Using DIA-PASEF and Targeted PRM Validation

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Background: Pituitary neuroendocrine tumors (PitNETs) account for approximately 15% of intracranial neoplasms and present significant diagnostic challenges, particularly for subtypes such as acromegaly, Cushing's disease, and non-functioning pituitary adenomas (NFPAs). The lack of minimally invasive biomarkers necessitates reliance on imaging and surgical intervention. Comprehensive serum proteomics offers a promising strategy for identifying circulating biomarkers and understanding subtype-specific biology.

Methods: A multi-platform high-resolution mass spectrometry (HRMS) approach was employed, integrating data-independent acquisition parallel accumulation–serial fragmentation (diaPASEF), machine learning, and Orbitrap-based parallel reaction monitoring (PRM). Serum samples from 77 individuals were analyzed in the discovery phase, followed by validation in an independent cohort of 60 samples. Protein identification, differential expression, and machine learning-based feature selection

were performed to identify pan- and subtype-specific signatures, with targeted peptide-level validation using PRM.

Results: A total of 1,771 proteins were identified, enabling the construction of a robust panel of candidate biomarkers. Machine learning approaches revealed shared pan-PitNET signatures, including zyxin, WD44, STYL4, FHOD1, and FYB1, which were validated at the peptide level, indicating activation of pro-tumorigenic pathways. Subtype-specific analysis demonstrated distinct molecular alterations: acromegaly was associated with post-receptor feedback adaptation, MEK–ERK pathway dysregulation, lipogenesis, and epithelial–mesenchymal transition. Cushing's disease exhibited significant upregulation of CEP104, SPARC, and DOCK3 ($p < 0.0001$), suggesting actin cytoskeleton remodeling linked to ciliary function and TGF-β signaling. NFPA was characterized by potential impairment of extracellular matrix-mediated anti-proliferative signaling and opsonization pathways. These findings highlight marked molecular heterogeneity despite a shared anatomical origin.

70. Temporal Neutrophil proteomics identifies fever-induced changes in neutrophil function and their role in inflammation and infection clearance

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Introduction: Culture-negative febrile illnesses present significant diagnostic challenges due to the absence of identifiable pathogens despite ongoing inflammation. Neutrophils are key mediators of host defense, yet the temporal molecular mechanisms underlying fever progression remain incompletely understood. This study aimed to characterize neutrophil proteomic dynamics during fever and identify potential biomarkers associated with febrile states.
Methods: Neutrophils collected across different fever and non-fever time points (0 hr, 24 hr, 48 hr, 72 hr) were subjected to high-resolution proteomic analysis. More than 10,000 proteins were identified and analyzed using hierarchical

clustering. Functional pathway enrichment, protein–protein interaction network analysis, and receiver operating characteristic (ROC) curve analysis were performed to characterize temporal protein expression patterns and evaluate biomarker potential.

Results: Hierarchical clustering identified 15 protein clusters, of which four temporally distinct clusters were selected for detailed analysis. Cluster 22663 (early fever) was enriched in immune signaling, host–pathogen interactions, and neutrophil migration pathways. Cluster 22662 (intermediate fever) demonstrated activation of MAPK, PI3K–AKT, TNF, Toll-like receptor, and NF-κB signaling pathways, reflecting intensified inflammatory responses. Cluster 22669 (sustained fever) was associated with persistent inflammatory activation, autophagy, cellular stress responses, and neutrophil extracellular trap formation. Cluster 22670 (late fever) showed enrichment of cytokine signaling, oxidative phosphorylation, lipid metabolism, and cellular adaptation pathways. Network analysis identified PIK3CA, MAPK1, and CAMK2A as major regulatory hubs. ROC analysis revealed IRF7 (AUC 0.972), VPS37B (AUC 0.944), MMD (AUC 0.917), and RHOF (AUC 0.833) as promising biomarkers for fever.

Conclusion: Neutrophil proteomics revealed distinct temporal inflammatory and metabolic programs associated with fever progression. These findings identify key molecular pathways and candidate biomarkers that may improve the diagnosis and monitoring of culture-negative febrile conditions.

71. From Glycan Code to Point-of-Care Readout: A Lectin-Based Strategy for Rapid SARS-CoV-2 Biosensing

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Background: Rapid, accurate and deployable diagnostics are essential for effective infectious disease management. Within clinical proteomics, viral glycosylation patterns represent conserved and mutation-resilient biomarkers, particularly in the SARS-CoV-2 spike glycoprotein. Lectins provide a stable and cost-effective alternative to conventional antibodies, leveraging glycan-specific recognition. In the present study, Cucurbitaceae family was selected owing to its diverse array of seed lectins with strong affinity toward mannose, galactose and N-acetylglucosamine residues characteristic of viral glycan shields, along with their stability and documented bioactivity.

Methods: A proteomics-driven "code-to-chip" strategy was employed, integrating molecular docking, glycoinformatics and proteomics-guided validation with experimental analysis. Cucurbitaceae seed lectins (CSLs) were computationally screened for binding to N-linked glycans of SARS-CoV-2 spike protein. High-affinity candidates were further validated through *in vitro* workflows including extraction, partial purification, structural characterization, glycan-binding assays and cytocompatibility evaluation. Integrated datasets guided the rational design of a lectin-functionalized lateral flow assay (LFA) biosensor.

Results: Selected CSLs exhibited strong and stable interactions with conserved glycan epitopes of the spike protein. Experimental validation confirmed their functional specificity, structural integrity and non-toxic profiles. These findings have paved the way towards eventual development of a lectin-based LFA biosensor capable of rapid, label-free detection with high sensitivity and specificity, delivering an immediate visual readout suitable for point-of-care applications.

Conclusion: This study offers a translational, clinical and proteomics-based framework for bridging molecular-level glycan recognition with device-level diagnostics. The proposed lectin-based LFA platform is expected to provide a rapid, scalable, cost-effective and mutation-resilient solution for detection of SARS-CoV-2 on one hand and potential adaptability as advanced next-generation POC diagnostics for other, newly emerging viral and parasitic pathogens, on the other.

Keywords: Clinical proteomics; Glycan targeting; Lectin biosensor; SARS-CoV-2; Point-of-care diagnostics

72. Extracellular Matrix Remodelling and Fatty-Acid-Oxidation Failure Define a Stage-Progressive Serum Proteomic Signature of Acute Kidney Injury

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Background: Acute kidney injury (AKI) affects a large fraction of hospitalised and critically ill patients and frequently progresses to chronic kidney disease (CKD). Its diagnosis still rests on serum creatinine and urine output, functional markers that rise only after substantial nephron loss, lack sensitivity in early injury, and reveal nothing about the molecular programmes driving progression or the heterogeneous etiologies underlying it. A circulating, mechanism-anchored proteomic signature could resolve both disease severity and aetiology.

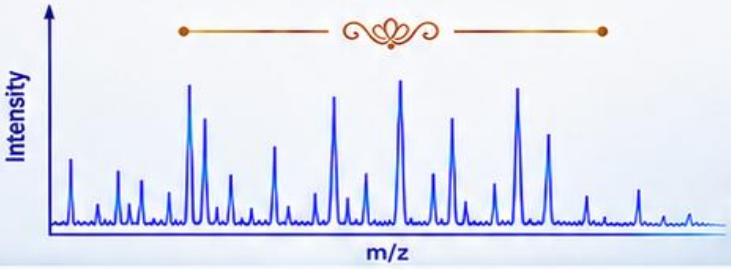
Methods: Deep serum proteomics was performed across KDIGO Stages 1–3 and healthy controls following standardisation of an in-house, high-throughput, cost-efficient perchloric-acid (PerCA) depletion workflow enabling broad low-abundance proteome coverage with minimal batch effects (pool correlation 0.998). Stage-wise differential expression, multivariate (PCA/PLS-DA/VIP) modelling, pathway and disease-association enrichment, and etiologic stratification of cancer-associated versus non-oncologic AKI were conducted.

Results: Proteomic remodelling scaled tightly with injury severity: separation from controls widened progressively across stages, with PC1 capturing 22.4% of variance at Stage-1'versus 37.2% at Stage-3. We found six fibro-inflammatory proteins: BMP1, COL1A, MMP14, SPP1, IL1RL1, and SULF2, that went up steadily as AKI got worse across the KDIGO stages (ANOVA $p \leq 1\times10^{-12}$). We saw the same proteins go up in both the cancer-associated and the non-cancer AKI patients. Functional enrichment converged consistently on extracellular-matrix (ECM) organisation, collagen-fibril assembly, and cell adhesion, while downregulated proteins implicated complement and coagulation dysregulation. Collectively, these proteins delineate a BMP1–COL1A–MMP ECM-remodelling axis that couples inflammatory and TGF-β-driven fibrotic signalling to mitochondrial fatty-acid-oxidation failure and lipotoxicity, consistent with collagen-activated DDR1 signalling reported in AKI-to-CKD transition.

Conclusion: Serum proteomics defines a stage-progressive, aetiology-aware fibrotic-lipotoxic signature mechanistically linking ECM remodelling to FAO impairment in AKI-to-CKD transition, providing a foundation for a clinically deployable precision biomarker panel

APT-2026

School Outreach Program:
AI in Healthcare



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School Outreach Program: AI in Healthcare

Overview

As part of APT-2026 (Advances in Proteomics Technologies), the **School Outreach Program on "AI in Healthcare"** has been designed to inspire and engage school students with emerging technologies that are transforming modern healthcare and biomedical research. This unique initiative aims to introduce young learners to the rapidly evolving fields of **Artificial Intelligence (AI), Machine Learning (ML), Multi-Omics, Big Data Analytics, Precision Medicine, and Digital Healthcare**, while fostering scientific curiosity and innovation among future generations.

The program combines interactive learning, expert talks, and student engagement activities to provide participants with an accessible understanding of how AI is being used to improve disease diagnosis, healthcare delivery, predictive analytics, and personalized medicine. Through real-world examples and demonstrations, students will explore how computational technologies are enabling smarter healthcare solutions and accelerating scientific discoveries.

The scientific sessions are organized into thematic modules focusing on **Career Development**, **AI/ML in Healthcare**, and **Applications of Multi-Omics, Big Data, and Artificial Intelligence in Medicine**. The program features talk by internationally renowned scientists and clinicians, including experts from academia, healthcare institutions, and industry. Sessions will highlight the role of proteomics, genomics, clinical multi-omics, and data science in addressing healthcare challenges and advancing precision medicine.

In addition to expert lectures, participating schools will have the opportunity to present their ideas and innovations through dedicated student interaction sessions. These activities are designed to encourage creativity, scientific thinking, teamwork, and communication skills among students while exposing them to contemporary developments in biomedical science and healthcare technology.

The outreach program emphasizes hands-on learning, expert interaction, and real-world applications of AI-driven healthcare solutions. By connecting school students with leading researchers and innovators, the initiative seeks to cultivate the next generation of scientists, healthcare professionals, and technology leaders. Through this multidisciplinary educational platform, APT-2026 aims to strengthen scientific awareness and inspire young minds to contribute to the future of intelligent and data-driven healthcare.

AI In Healthcare

Artificial Intelligence (AI) is becoming one of the most important technologies in modern healthcare and biomedical research. AI systems can analyze enormous amounts of data much faster than humans, helping scientists and doctors identify patterns, make predictions, and support medical decision-making. Today, AI is being used in many areas, including protein research, drug discovery, medical imaging, wearable health devices, personalized medicine and more.

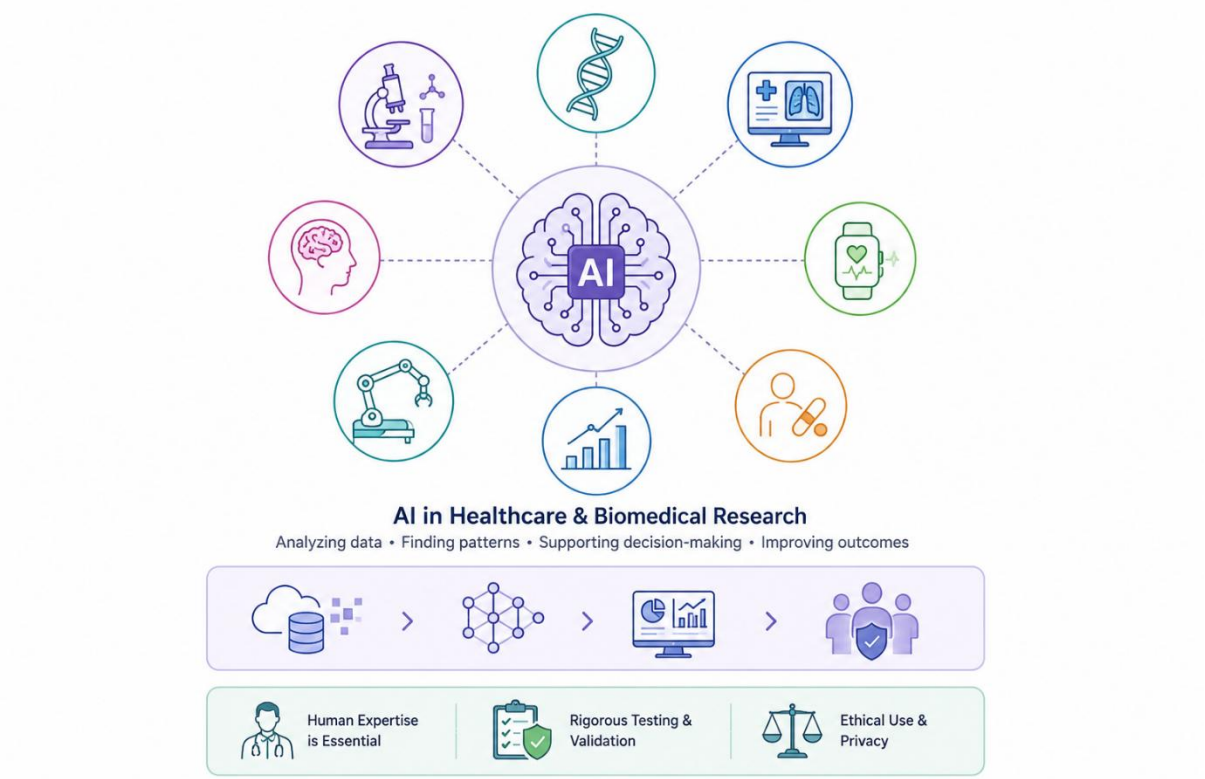


Figure 1. Artificial intelligence is transforming healthcare and biomedical research by uncovering patterns in complex data to support diagnosis, discovery, monitoring, and patient care.

One reason AI has become so important in healthcare is the enormous amount of biological and medical data generated today. Modern hospitals produce millions of medical images and patient records, while research laboratories generate huge datasets related to genes, proteins, and diseases. AI methods are especially useful for finding patterns in this data that would be difficult or extremely time-consuming for humans to analyze manually. In some cases, AI systems can process information in minutes that might otherwise require months or years of work.

Many of the examples given below show how AI is helping researchers better understand biology at the molecular level. Systems such as AlphaFold can predict protein structures with remarkable accuracy, while tools like DrugProtAI and AlphaCross-XL help scientists study proteins and identify possible drug targets more efficiently. Other examples focus on healthcare applications that directly affect patients, such as AI systems that assist doctors in reading medical scans, detecting cancers earlier, or analyzing retinal images to identify signs of disease.

AI is also changing how health is monitored outside hospitals. Wearable devices and biosensors can continuously track heart rate, glucose levels, sleep patterns, and other health signals in real time. Researchers are also exploring how AI may help in areas such as mental-health support, robotic surgery, antibiotic discovery, and brain-computer interfaces that could restore communication for people with paralysis or severe neurological conditions. Some of these technologies are already being used in hospitals and laboratories, while others are still experimental and actively being studied around the world.

Although AI can greatly improve speed and efficiency, it does not replace doctors, scientists, or laboratory experiments. Human expertise, careful testing, and ethical oversight remain extremely important. AI systems can sometimes make mistakes, especially if they are trained using incomplete or biased data. For this reason, most healthcare AI tools are designed to assist human experts rather than function independently. Understanding both the possibilities and limitations of AI is important for using these technologies responsibly in the future.

The following examples introduce some of the most important and interesting ways in which AI is being used in healthcare and biomedical research today. Together, they show how AI is influencing many different areas of science and medicine, from studying molecules inside cells to improving diagnosis, treatment, monitoring, and patient care.

1. AlphaFold: Predicting Protein Structures with AI

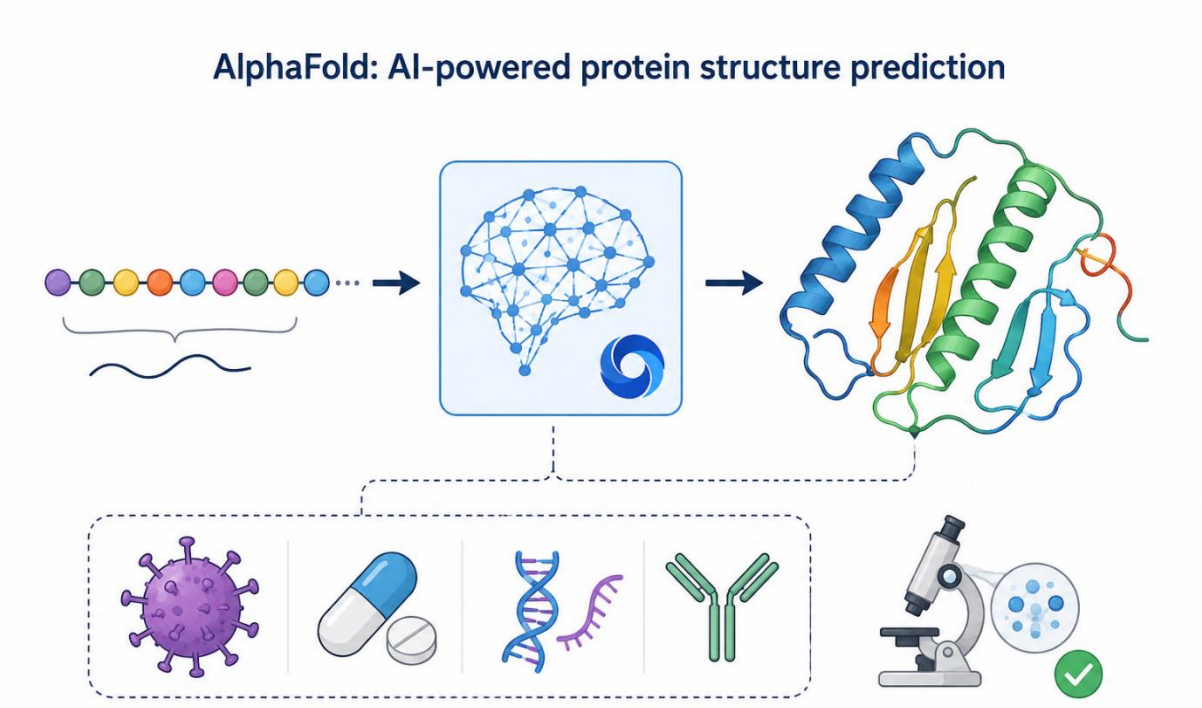


Figure 2. AlphaFold uses AI to predict protein structures from amino-acid sequences, accelerating biological research and drug discovery.

Proteins are tiny molecular machines inside living cells, and their three-dimensional shape determines what they can do in the body. For many decades, scientists had to use slow and expensive laboratory methods such as X-ray crystallography or cryo-electron microscopy to figure out protein structures.

AlphaFold, developed by Google DeepMind, uses artificial intelligence to predict protein shapes directly from amino-acid sequences. This was considered a major breakthrough because it solved a scientific challenge that researchers had

struggled with for nearly 50 years. The system can now predict structures for millions of proteins in a fraction of the time older methods required. Scientists use these predictions to study diseases, understand viruses, and design possible medicines more efficiently. Later versions such as AlphaFold 3 can also model interactions between proteins, DNA, RNA, and drug-like molecules. Researchers around the world freely access the AlphaFold database, making it one of the most widely used AI tools in biology today. However, predicted structures still need experimental verification because real biological systems are often more complex than computer models.

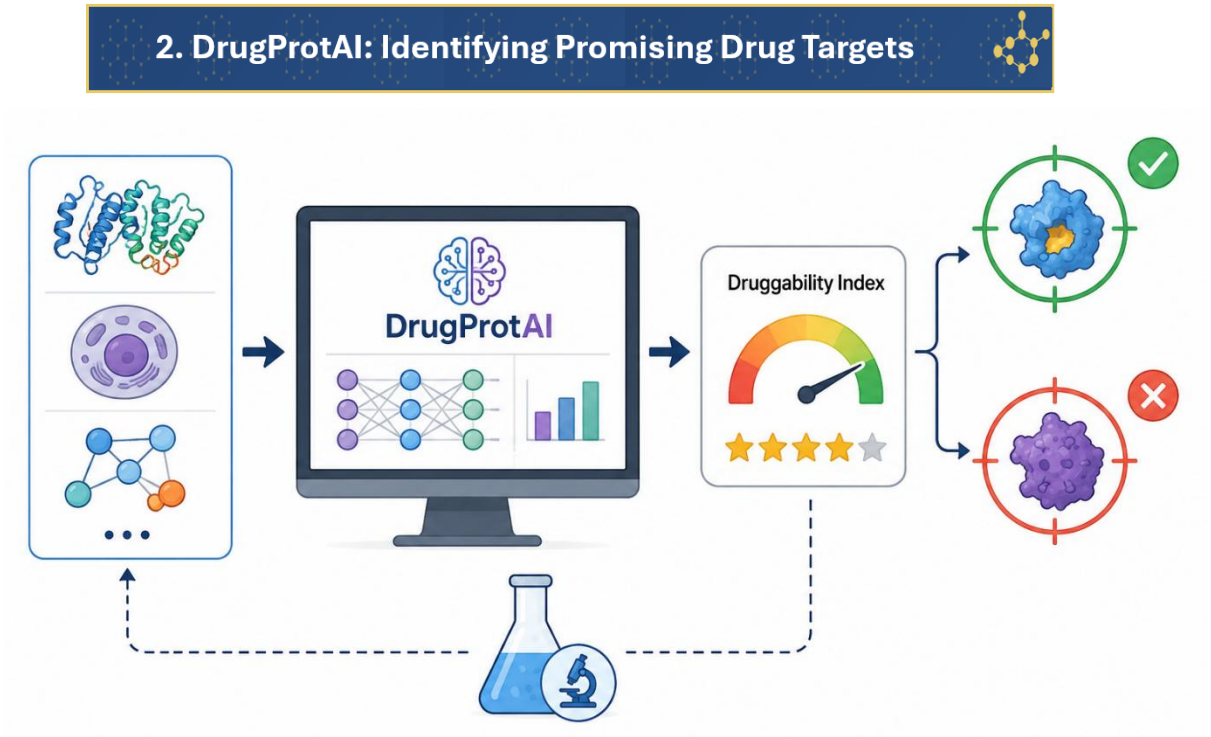


Figure 3. *DrugProtAI uses AI to identify promising drug targets, helping researchers prioritize proteins with the highest potential for medicine development.*

DrugProtAI is an AI system developed by researchers at IIT Bombay to help identify proteins that could become good targets for medicines. One of the biggest problems in drug discovery is that scientists sometimes spend years studying proteins that eventually turn out to be poor targets for treatment.

DrugProtAI attempts to solve this by calculating how “druggable” a protein is using machine-learning methods. The system studies many biological features, including protein structure, cellular location, and interactions with other proteins. It then produces a “druggability index” that estimates whether a useful medicine could realistically bind to that protein. This allows researchers to focus on the most promising targets earlier in the research process. By reducing wasted effort, AI systems like DrugProtAI may save both time and money in pharmaceutical development. The project also demonstrates how AI research in India is contributing to global biomedical science. Even so, predictions from DrugProtAI are only the beginning of the process, and laboratory experiments are still necessary before any drug can be developed.

3. AlphaCross-XL: Linking AI Predictions with Real Experiments

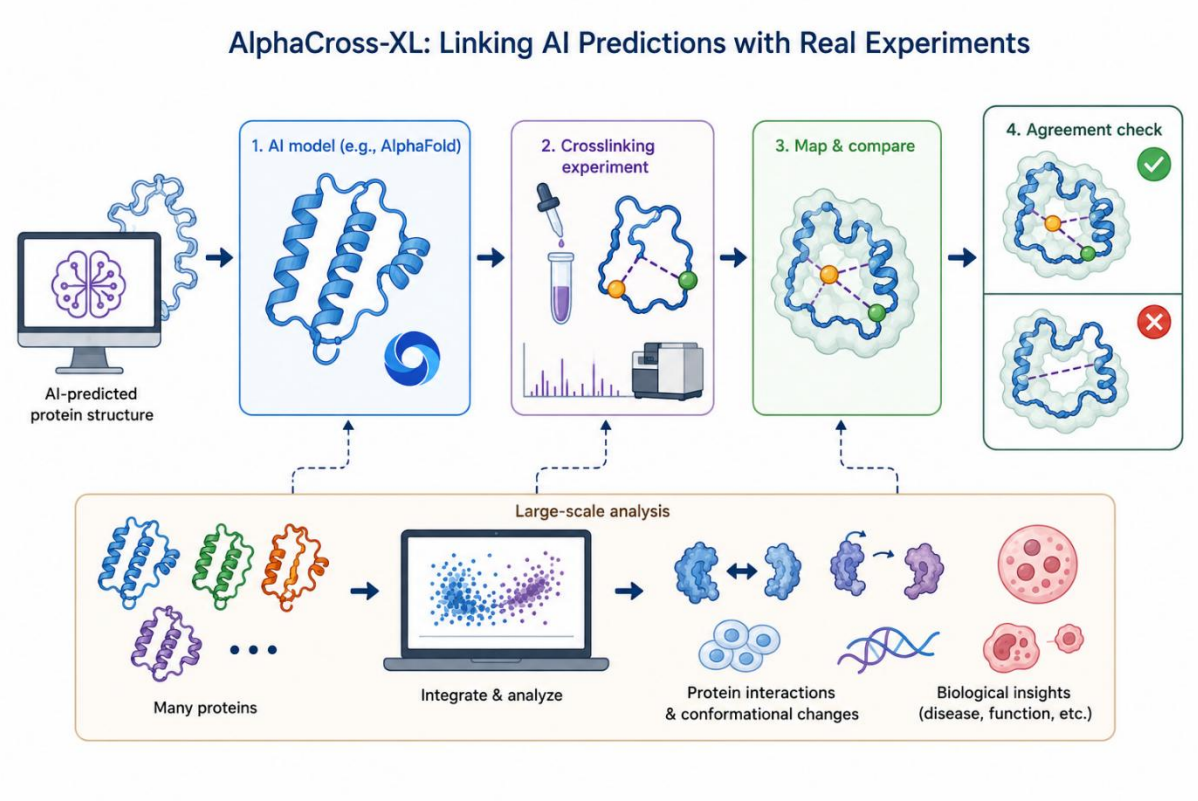


Figure 4. *AlphaCross-XL combines AI-predicted protein structures with experimental data to help scientists better understand protein behavior and biological function.*

AlphaCross-XL is a research tool that combines AI-generated protein models with real experimental biological data. While systems such as AlphaFold predict protein structures computationally, scientists still need ways to compare those predictions with how proteins behave inside living cells.

AlphaCross-XL helps researchers do this by mapping experimental “crosslinking” data onto three-dimensional protein structures. Crosslinking experiments reveal which parts of proteins are physically close together in real biological systems. The software can then compare these measurements with AI-predicted structures to see whether they match. This helps scientists study protein folding, protein interactions, and diseases caused by damaged or misfolded proteins. One important feature is that the system can work across extremely large protein datasets rather than studying only one protein at a time. Researchers also use it to investigate how proteins change shape under different biological conditions. The tool shows how AI becomes even more powerful when combined with laboratory experiments instead of replacing them completely.

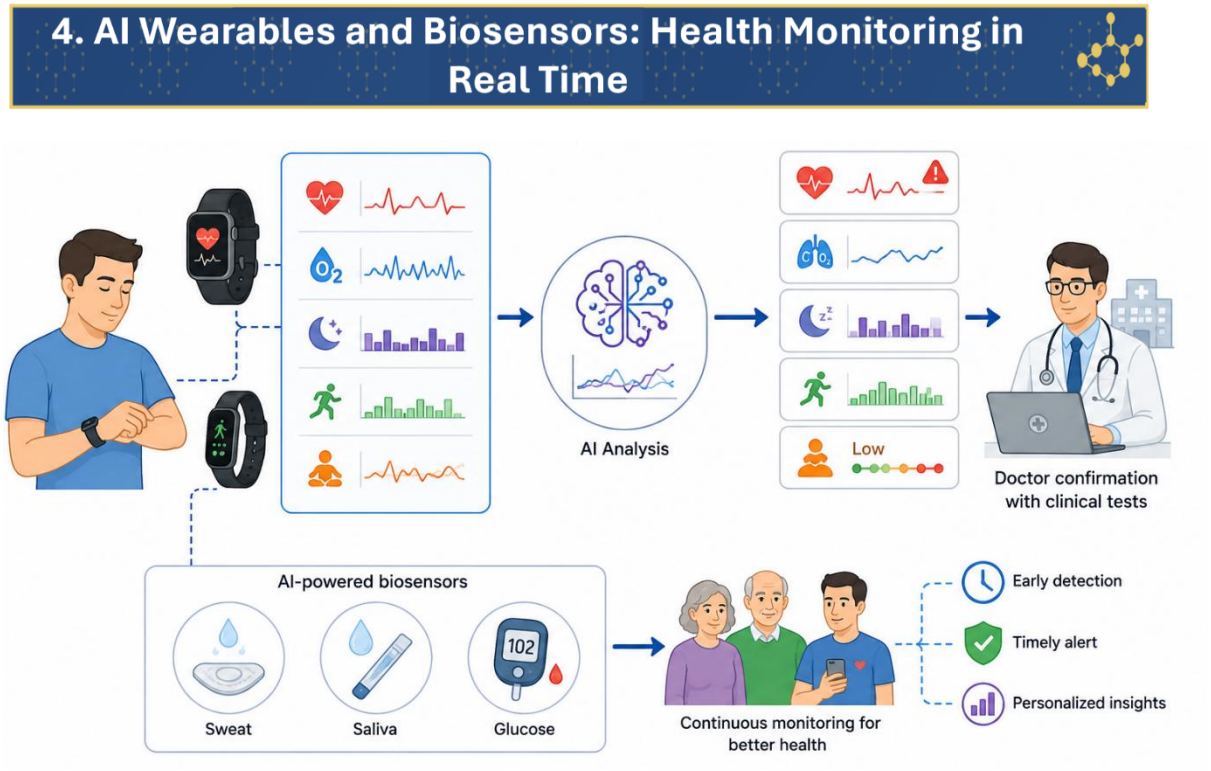


Figure 5. *AI-powered wearables and biosensors continuously monitor health signals, helping detect potential problems early while supporting more personalized healthcare.*

Modern wearable devices such as smartwatches and fitness bands are increasingly using AI to monitor health continuously. These devices can measure signals such as heart rate, blood oxygen levels, sleep quality, stress patterns, and physical activity throughout the day. AI algorithms analyze large streams of data and search for unusual patterns that humans may not notice easily. Some systems can detect irregular heart rhythms such as atrial fibrillation before patients experience obvious symptoms.

Researchers are also developing biosensors that can analyze sweat, saliva, or glucose levels in real time without repeated blood tests. Continuous monitoring is especially useful for elderly people and patients with chronic illnesses like diabetes. AI helps reduce false alarms by distinguishing between harmless variations and potentially dangerous patterns. These technologies are gradually shifting healthcare from hospital-centered monitoring to personal-device-based monitoring. However, wearable devices are not perfect medical instruments, and doctors still need to confirm important findings using clinical tests.

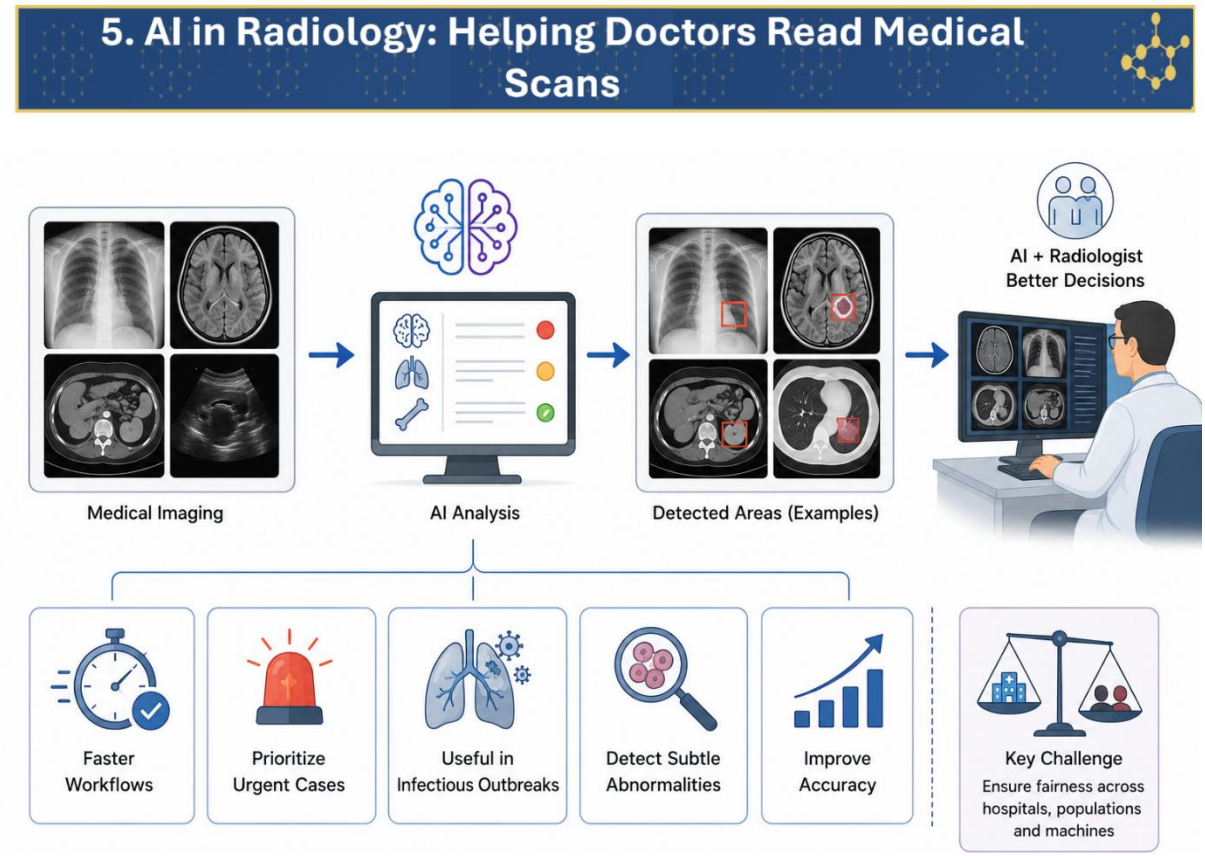


Figure 6. *AI-assisted medical imaging helps doctors analyze scans more efficiently by highlighting potential abnormalities and supporting faster, more accurate diagnoses.*

Radiology involves studying medical images such as X-rays, CT scans, MRIs, and ultrasounds to diagnose diseases and injuries. AI systems trained on large image datasets can now identify suspicious regions such as tumors, fractures, internal bleeding, or lung infections. These systems do not replace radiologists, but they can act as a powerful second set of eyes.

AI is especially useful in situations where doctors must examine thousands of images quickly and carefully. Some tools can prioritize urgent cases so that patients with serious conditions receive faster attention. During the COVID-19 pandemic, researchers also explored AI methods for rapidly analyzing chest scans. AI-based systems have shown promise in detecting early-stage cancers and subtle abnormalities that humans might overlook during busy clinical work. Hospitals worldwide are beginning to integrate imaging AI into real healthcare workflows. However, one major challenge is ensuring that these systems work fairly across different hospitals, patient populations, and imaging machines without introducing bias.

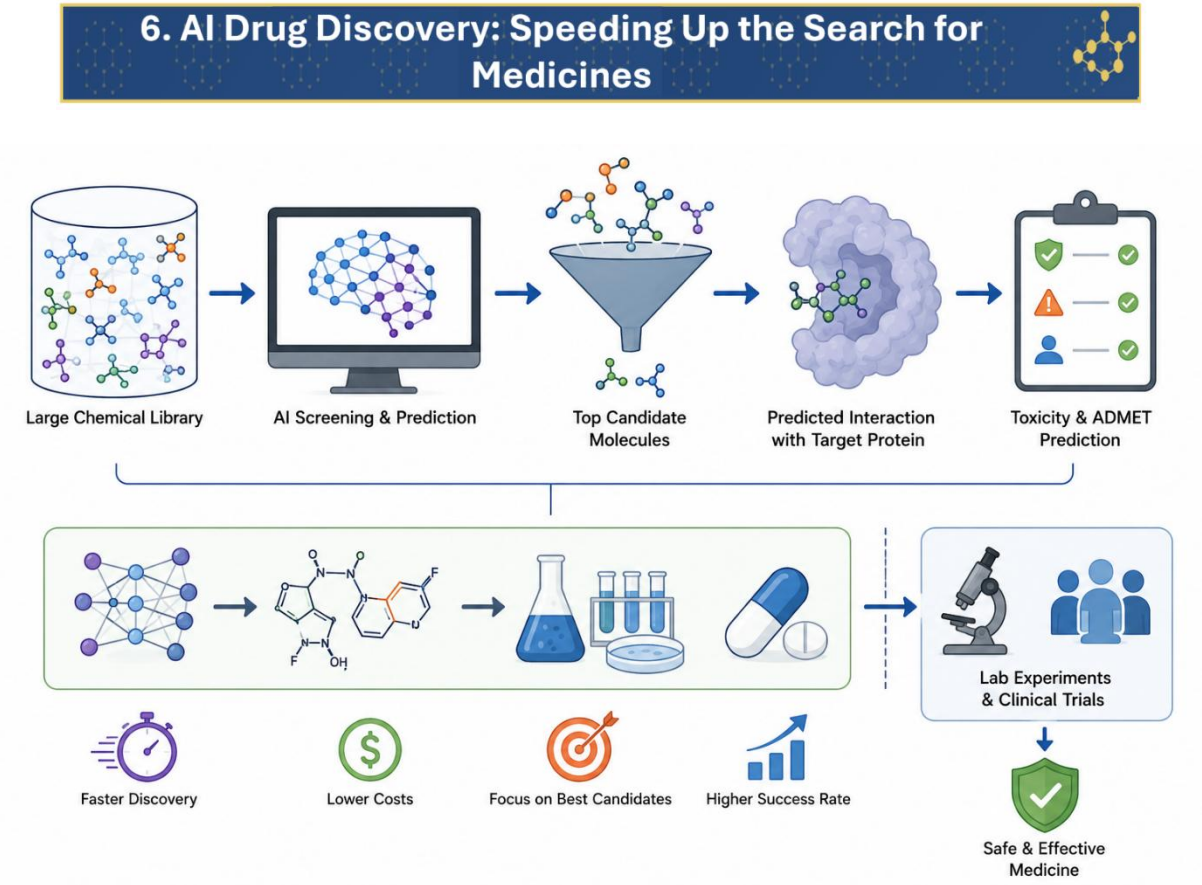


Figure 7. *AI accelerates drug discovery by identifying promising drug candidates from vast chemical libraries, helping researchers focus laboratory testing on the most likely successes.*

Developing a new medicine is extremely expensive and can take more than a decade from initial research to final approval. AI is helping scientists speed up the early stages of this process by searching through enormous chemical libraries much faster than humans can. Machine-learning models can predict which molecules are most likely to interact successfully with disease-related proteins. Instead of testing millions of compounds experimentally, researchers can narrow the search to a smaller number of promising candidates.

Pharmaceutical companies now use AI to identify possible drug molecules, estimate toxicity risks, and predict how compounds may behave inside the body. Some AI systems can even generate entirely new molecular structures that humans may never have considered. This has created major interest in AI-driven biotechnology companies around the world. Even so, AI does not eliminate the need for laboratory testing or clinical trials because many predicted drug candidates still fail during human testing. AI mainly helps researchers make better decisions earlier in the drug development process.

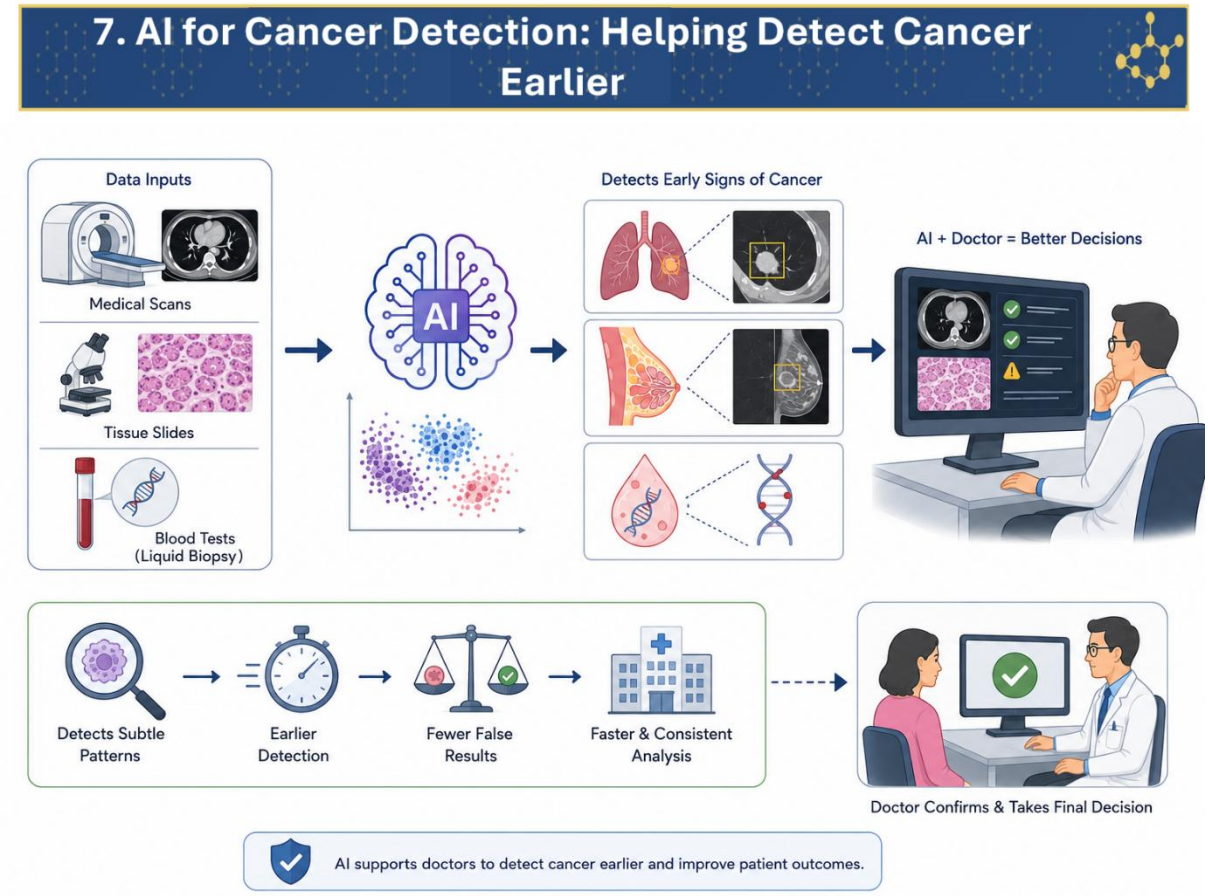


Figure 8. *AI-assisted cancer detection helps doctors identify subtle signs of disease earlier by analyzing medical scans, tissue samples, and blood-based biomarkers.*

Cancer treatment is often more successful when the disease is detected early, and AI is becoming an important tool in this area. AI systems can analyze medical scans, tissue slides, and blood-test data to search for subtle signs of cancer. Some models are trained using millions of medical examples, allowing them to identify patterns that are difficult for humans to recognize.

Researchers are also exploring “liquid biopsies,” where AI studies fragments of tumor DNA circulating in blood samples. This could someday allow cancers to be detected using simple blood tests before major symptoms appear. AI tools are already helping doctors in areas such as breast cancer screening, lung cancer imaging, and digital pathology. Certain studies have shown that AI systems can reduce false positives and false negatives when used alongside human experts. Hospitals are increasingly adopting AI-assisted diagnostic workflows for faster and more consistent analysis. However, medical decisions still depend on trained doctors because incorrect predictions could have serious consequences for patients.

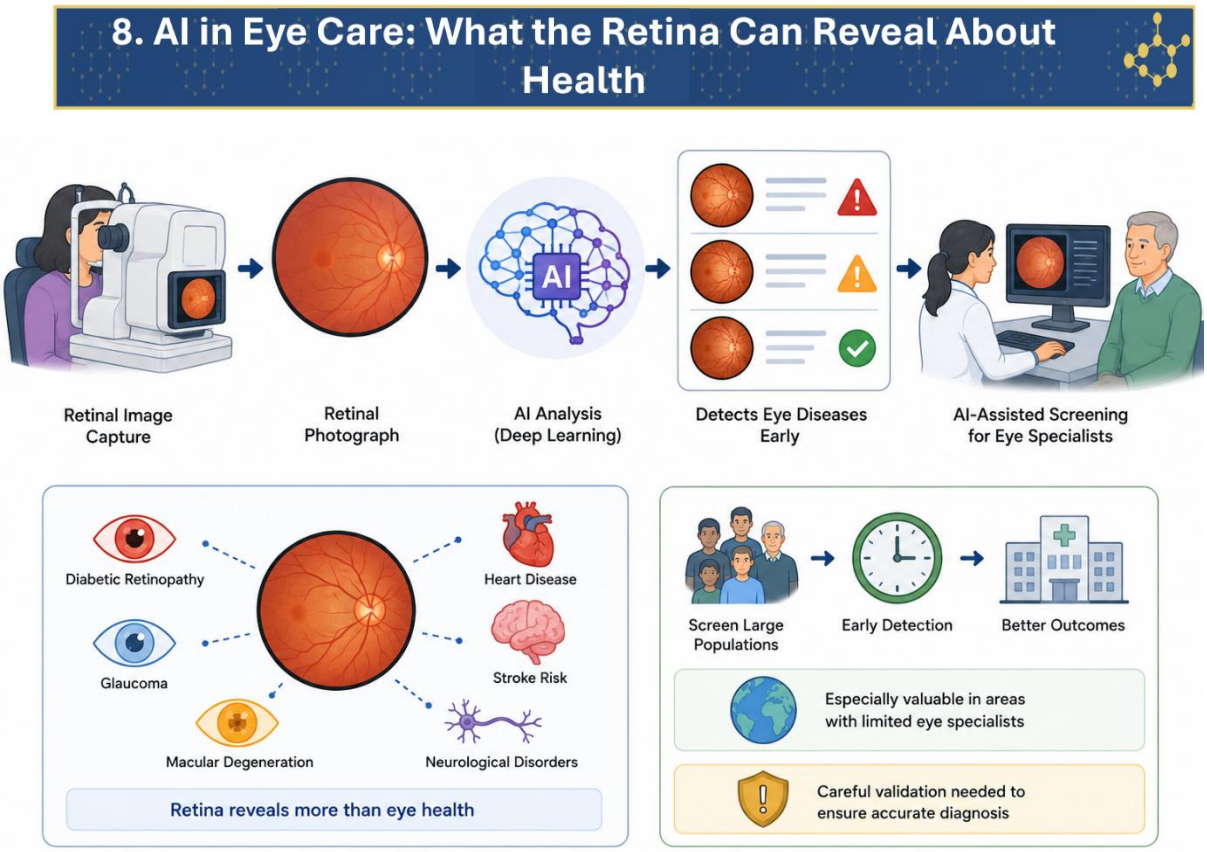


Figure 9. *AI-powered retinal imaging can detect eye diseases and reveal broader health risks, enabling earlier screening and more accessible preventive care.*

The human retina contains a dense network of blood vessels and nerve tissue, making it extremely useful for studying overall health. AI systems trained on retinal photographs can detect eye diseases such as diabetic retinopathy, glaucoma, and macular degeneration. In some clinics, AI screening tools are already used before patients meet an eye specialist.

Researchers have discovered that retinal images may also contain information about heart disease, stroke risk, and even neurological disorders. Foundation models such as RETFound were trained on millions of eye scans to recognize hidden biological patterns invisible to the human eye. These systems may help doctors identify diseases years before symptoms become obvious. AI-based eye screening is particularly important in regions where trained ophthalmologists are limited. Automated systems can help large numbers of patients receive early screening more efficiently. Nevertheless, eye-care AI still requires careful validation because incorrect diagnoses could delay necessary treatment.

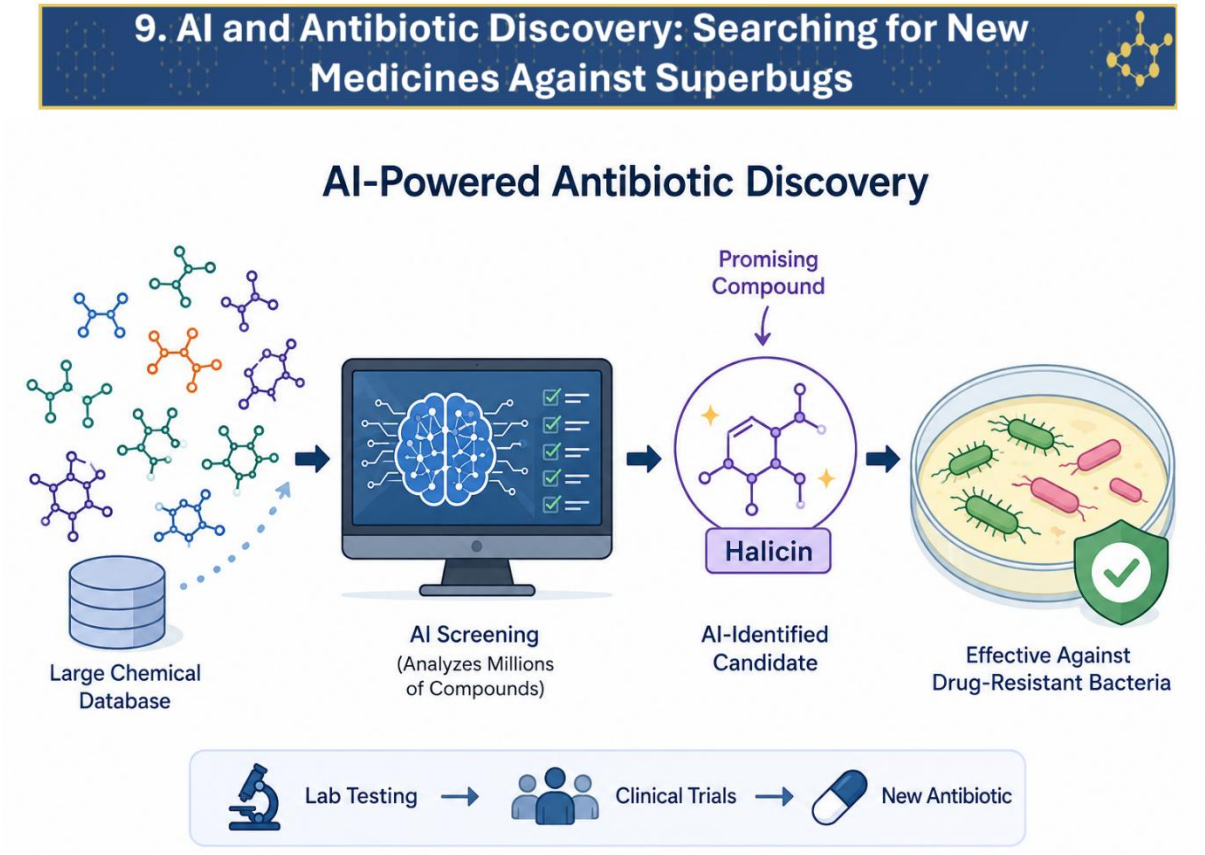


Figure 10. *AI accelerates the search for new antibiotics by identifying promising compounds against drug-resistant bacteria, helping researchers combat the growing threat of antimicrobial resistance.*

Antibiotic resistance is becoming one of the most serious public-health problems in the world. Many bacteria are evolving resistance to existing medicines, making infections harder to treat. AI is helping scientists search for entirely new antibiotic molecules by analyzing huge chemical databases rapidly.

One famous example is the discovery of “Halicin,” an antibiotic identified using AI at MIT. The AI system screened very large chemical libraries containing millions of compounds and found a molecule that looked very different from traditional antibiotics. Halicin showed strong activity against dangerous drug-resistant bacteria in laboratory studies. Researchers believe AI may help discover completely new classes of antibiotics that humans would otherwise overlook. This approach saves enormous amounts of time compared to traditional screening methods. AI-driven antibiotic research demonstrates how machine learning can contribute directly to solving global health challenges. Still, newly discovered compounds must pass years of laboratory and clinical testing before they can become approved medicines.

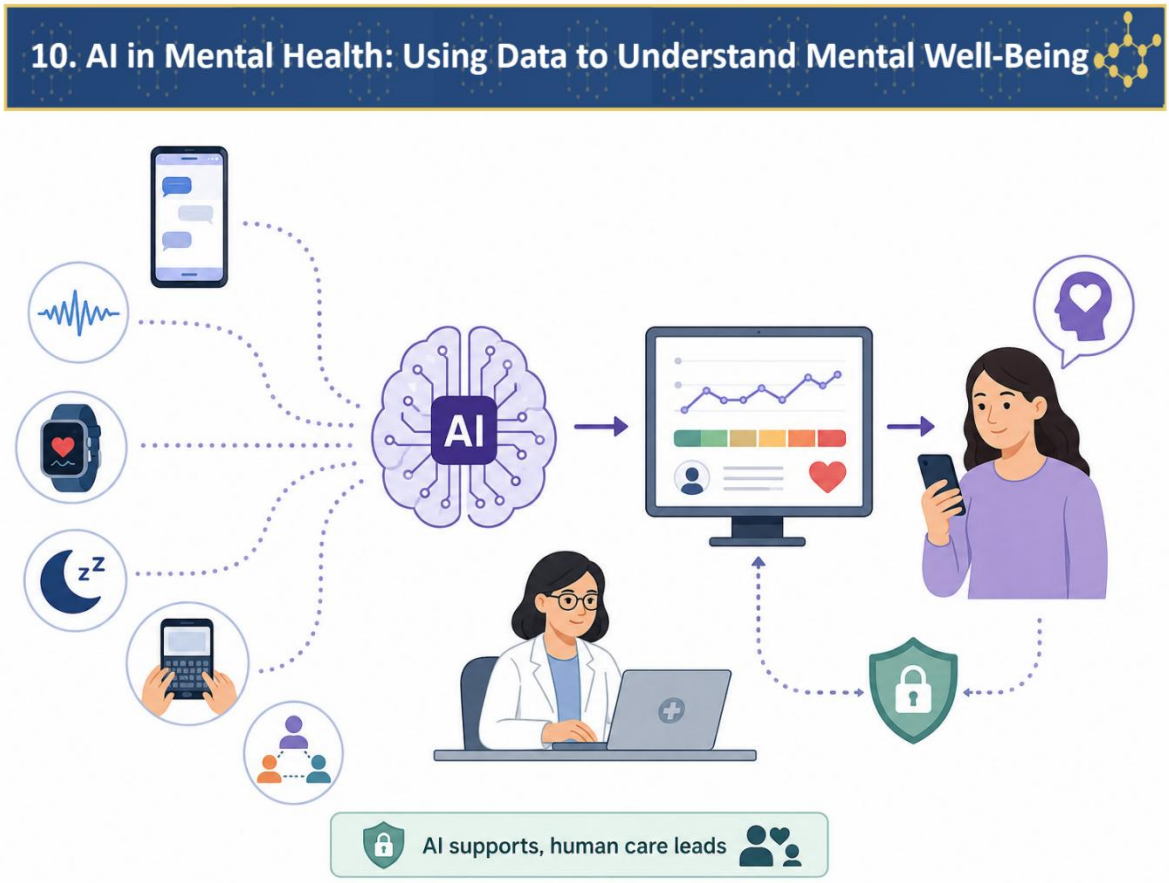


Figure 11. *AI can help identify patterns linked to mental well-being and provide early support, while human professionals remain essential for care and decision-making.*

Researchers are exploring whether AI can help identify early signs of mental-health conditions such as depression, anxiety, or cognitive decline. Some systems analyze speech patterns, sleep behavior, typing speed, social activity, or wearable-device data to detect unusual changes over time. AI chatbots are also being tested as mental-health support tools that can provide basic guidance or emotional check-ins. In certain cases, these systems may help people access support earlier than they otherwise would.

Researchers are particularly interested in how wearable devices and smartphone data can reveal behavioral changes linked to stress or emotional health. AI may eventually help doctors monitor patients continuously instead of relying only on occasional clinic visits. However, mental-health applications raise especially important concerns about privacy, consent, and reliability. Human emotions are highly complex, and AI systems can misunderstand context or produce inaccurate conclusions. Most experts agree that AI should support mental-health professionals rather than replace them.

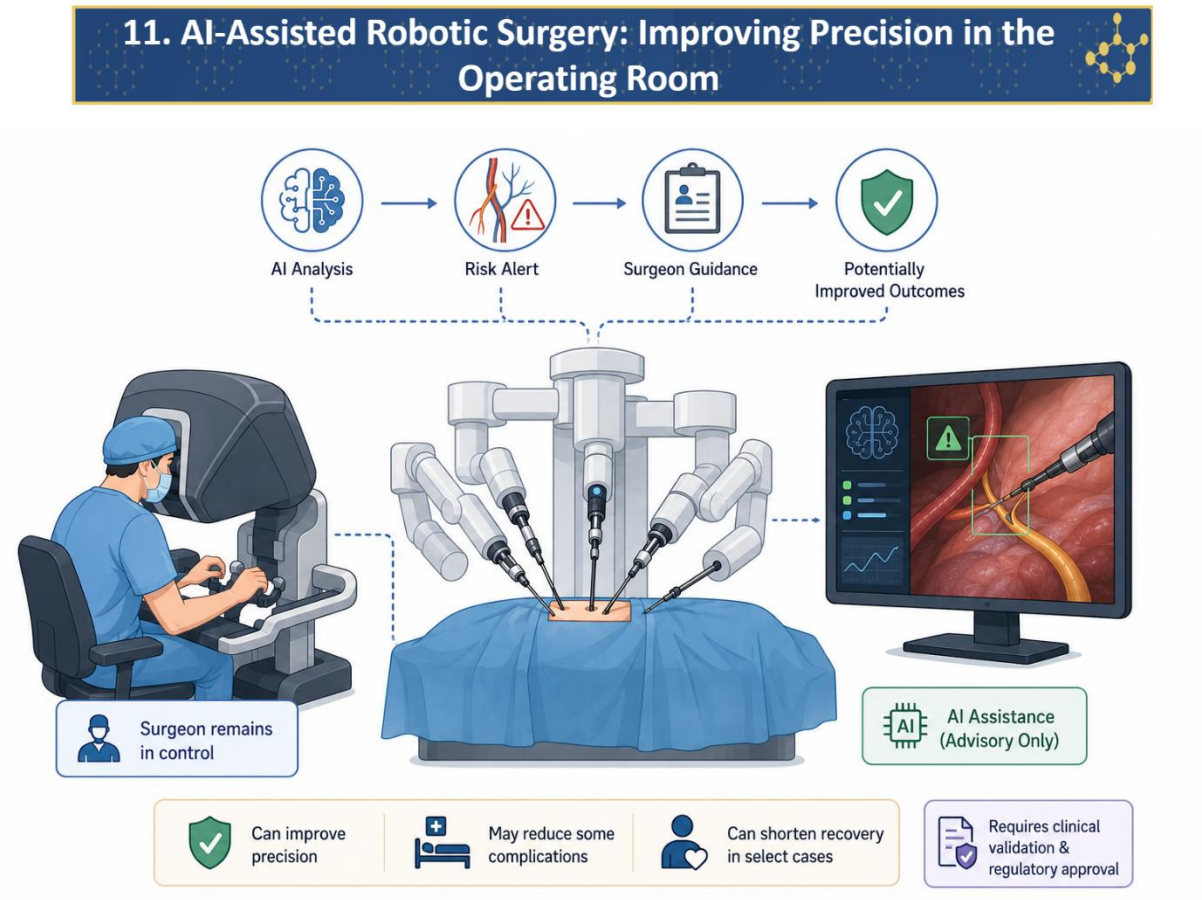


Figure 12. *AI-assisted robotic surgery supports surgeons with real-time guidance and risk alerts, helping improve precision while keeping human experts fully in control.*

Robotic surgical systems are already used in hospitals to help surgeons perform delicate operations with greater precision and stability. AI is now being added to these systems to assist with navigation, motion analysis, and risk prediction during surgery. Some AI-assisted tools can warn surgeons about nearby blood vessels or nerves that could be damaged accidentally. Advanced systems may also analyze previous surgeries to provide suggestions for improving surgical technique.

Companies such as Intuitive Surgical and Stryker are developing AI-enhanced robotic platforms for different types of procedures. Studies suggest that AI-assisted robotic surgeries may reduce complications and shorten recovery times in certain situations. Despite the advanced technology, the surgeon remains fully responsible for decisions during the operation. AI acts more like a sophisticated assistant rather than an independent operator. Because surgeries directly affect patient safety, robotic systems must undergo extremely strict testing and regulatory approval before widespread clinical use.

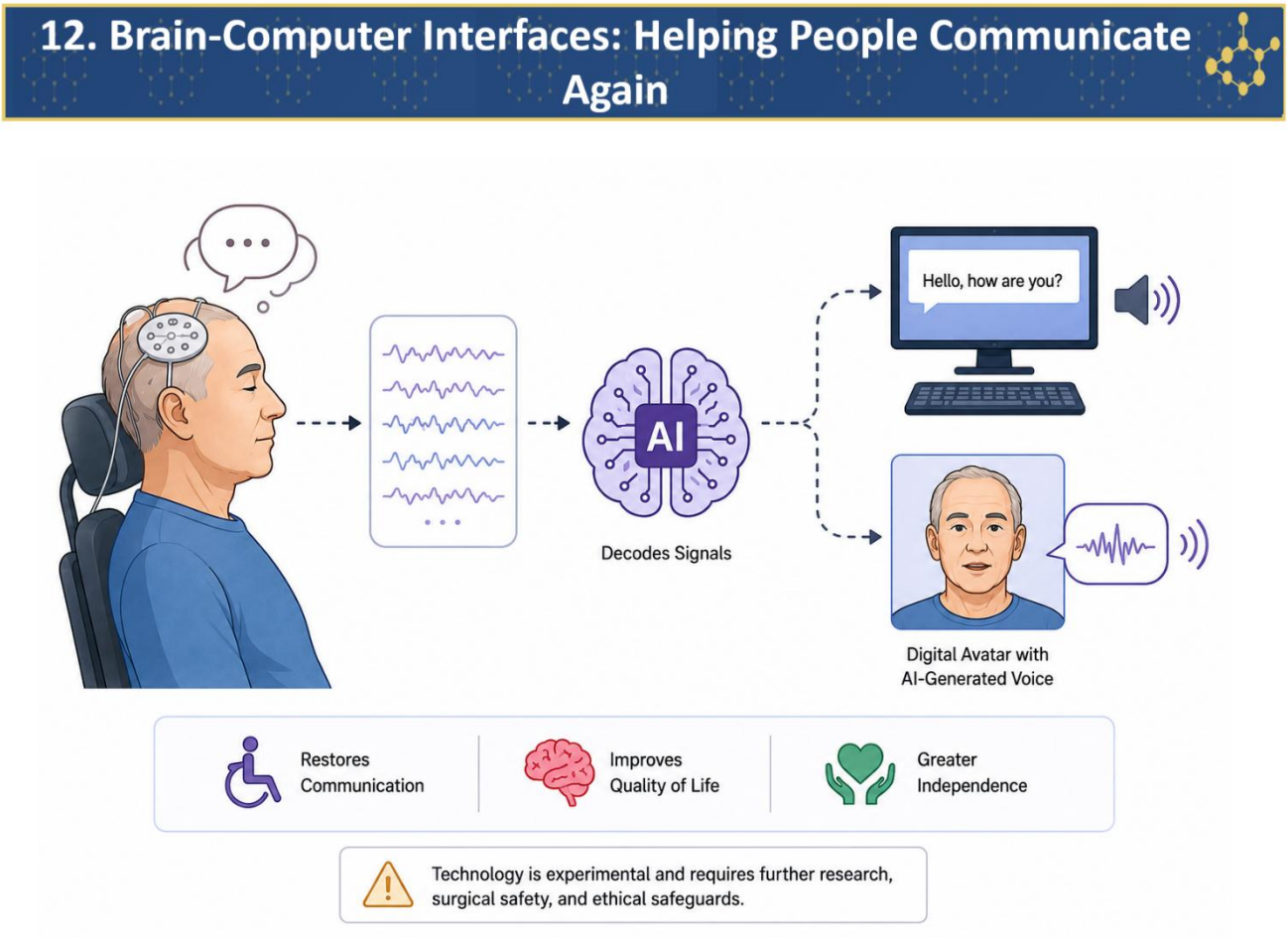


Figure 13. *AI-powered brain–computer interfaces can translate neural signals into speech or text, helping restore communication for people with severe neurological disabilities.*

Brain-computer interfaces, often called BCIs, are systems that connect brain activity directly to computers using tiny sensors. Researchers are developing these technologies to help people who cannot speak or move because of conditions such as paralysis, stroke, or ALS. AI plays a crucial role by decoding electrical signals produced when a person thinks about speaking or moving.

Recent experiments have shown that AI can translate brain signals into text or speech in near real time. In some demonstrations, patients were able to communicate using digital avatars that spoke with AI-generated versions of their own voices. These advances could dramatically improve quality of life for people with severe disabilities. Brain-computer interface research combines neuroscience, engineering, and machine learning in highly interdisciplinary ways. However, the technology is still experimental and faces challenges involving surgical safety, long-term reliability, and ethical concerns about privacy. Even so, BCIs are one of the clearest examples of how AI may eventually transform human healthcare and communication.

Important Limits of AI in Healthcare

Although AI is extremely powerful, it is not magical and cannot solve every medical problem automatically. AI systems depend heavily on the quality and diversity of the data used to train them. If training data are incomplete or biased, the system may produce unreliable or unfair results. Most AI predictions in healthcare still require validation through experiments, clinical trials, and doctor supervision. Many exciting research discoveries take years before becoming approved treatments for patients. Privacy and data security are also major concerns because medical information is highly sensitive. In addition, hospitals must ensure that AI systems work consistently across different populations and healthcare environments.

The most successful healthcare systems are likely to combine human expertise with AI tools rather than replacing doctors completely. Understanding both the possibilities and limitations of AI is important for using these technologies responsibly in the future.

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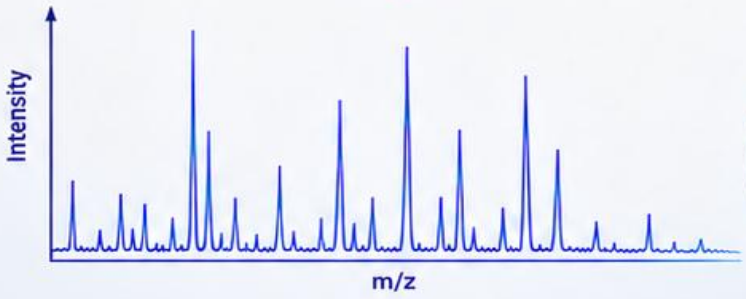
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SECTION II

APT-2026

WORKSHOPS



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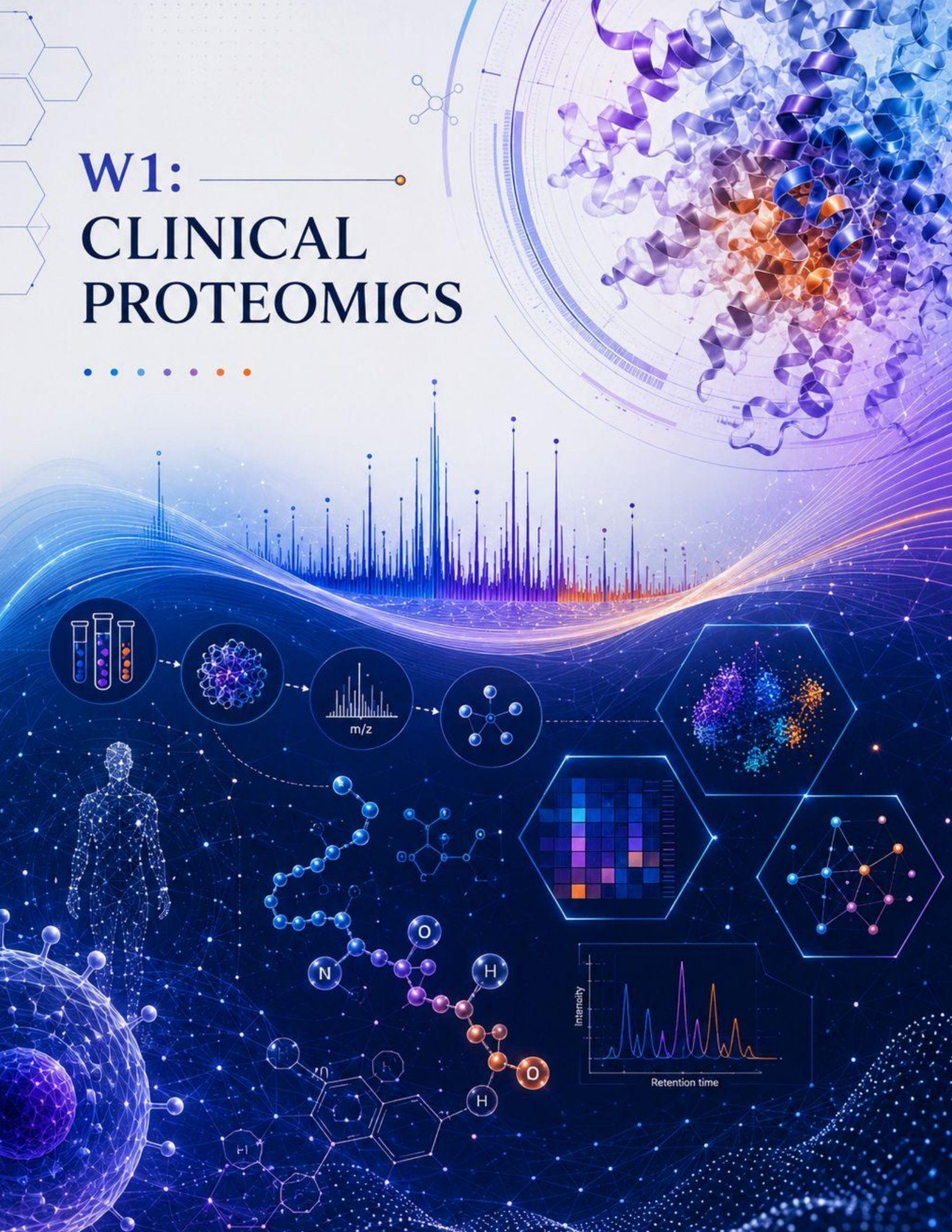
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W1: CLINICAL PROTEOMICS







DHR-ICMR Clinical Proteomics

SCIENTIFIC PROGRAMME

Overview

The DHR-ICMR-sponsored Workshop 1 at APT-2026 is dedicated to Clinical Proteomics, bringing together leading national and international experts to discuss recent advances in proteomics technologies and their applications in healthcare, translational research, and precision medicine. The workshop is designed to provide participants with both conceptual understanding and practical exposure to modern proteomics workflows used in biomedical and clinical research.

The scientific sessions will cover diverse themes, including cancer proteomics, clinical proteomics, multi-omics integration, biomarker discovery, and mass spectrometry-based applications. Renowned speakers from institutions such as UCSF, Harvard Medical School, Arizona State University, University of Manitoba, and UC San Diego will present emerging trends and innovations in proteomics-driven healthcare research.

A major component of the workshop focuses on hands-on training in proteomics sample preparation and protein quantification workflows, including cell lysis, SDS-PAGE, protein digestion, peptide quantification, and sample preparation strategies for mass spectrometry analysis. Participants will also gain practical exposure to mass spectrometry sample acquisition, instrument setup, data acquisition parameters, and evaluation of MS data through live demonstrations and application sessions conducted by experts and technical instructors.

The workshop aims to bridge the gap between advanced proteomics technologies and their real-world clinical applications. Participants will gain insights into how proteomics and multi-omics approaches are accelerating the understanding of disease, biomarker discovery, therapeutic development, and precision medicine. This workshop is designed for students, researchers, clinicians, and industry professionals. The workshop provides practical training and scientific insights into modern proteomics technologies and their clinical applications.

AT A GLANCE

Key Highlights

- Clinical & cancer proteomics
- Biomarker discovery & multi-omics
- Hands-on proteomics workflows
- Mass spectrometry data acquisition & analysis

W 1.1

Clinical Proteomics — From Discovery to Diagnosis: History, Technology, and Clinical Translation

A comprehensive guide to the history, fundamental principles, and technological evolution of clinical proteomics, with recent achievements, key papers, and pioneering scientists.

Chapter	Topics Covered
1. What is Clinical Proteomics?	Definition, scope, the proteome vs genome, why proteins matter in disease, clinical specimen types
2. Historical Development	From 2D-PAGE to SELDI-TOF to modern MS, OVA1, the first FDA-cleared proteomic test
3. Core Technologies	Sample types, MS platforms (Orbitrap, TOF, triple quadrupole), DDA vs DIA, targeted MRM/SRM/PRM
4. Biomarker Discovery and Validation Pipeline	Discovery, verification, validation phases; analytical and regulatory requirements
5. Clinical Applications by Disease Area	Oncology, cardiology, neurology, infectious disease, rare/genetic disease, newborn screening
6. Recent Achievements (2023-2026)	Population-scale plasma proteomics, DIA clinical adoption, newborn screening by MS, AI integration
7. Landmark Research Papers	9 annotated key papers spanning history to 2025
8. Pioneering Scientists	8 key researchers and their contributions
9. Historical Timeline	1975-2026 development milestones

W 1.1

What is Clinical Proteomics?

Clinical proteomics is the application of proteomic technologies, principally mass spectrometry, to the diagnosis, prognosis, monitoring, and mechanistic understanding of human disease. It bridges fundamental protein science and routine clinical laboratory medicine, translating the discovery-driven methods of research proteomics into validated, reproducible assays suitable for patient care.

1.1 Why Proteins, Not Just Genes?

The genome provides the blueprint for an organism, but it is the proteome, the complete set of expressed proteins, that executes nearly all biological functions and is directly altered by disease processes. Genomic information is largely static across a person's lifetime, whereas the proteome is highly dynamic: protein abundance, post-translational modification (phosphorylation, glycosylation, proteolytic cleavage), and protein-protein interactions change continuously with disease

state, treatment response, and physiological status. A patient's genome cannot tell a clinician whether a tumour is responding to chemotherapy today; circulating tumour-derived proteins potentially can.

Proteins are also the direct targets of the great majority of approved drugs and the most accessible class of molecule for non-invasive clinical sampling, since many disease-relevant proteins are secreted, shed, or leaked into accessible body fluids such as blood, urine, cerebrospinal fluid (CSF), and saliva. This combination, functional relevance, dynamic informativeness, and clinical accessibility, makes the proteome an exceptionally valuable diagnostic substrate.

KEY CONCEPT

Clinical proteomics is distinct from discovery proteomics. Discovery proteomics aims to identify as many proteins and modifications as possible in a research setting; clinical proteomics requires assays that are precise, reproducible, validated against regulatory standards, and deployable at scale in a hospital laboratory, often analysing only a small, carefully selected panel of proteins.

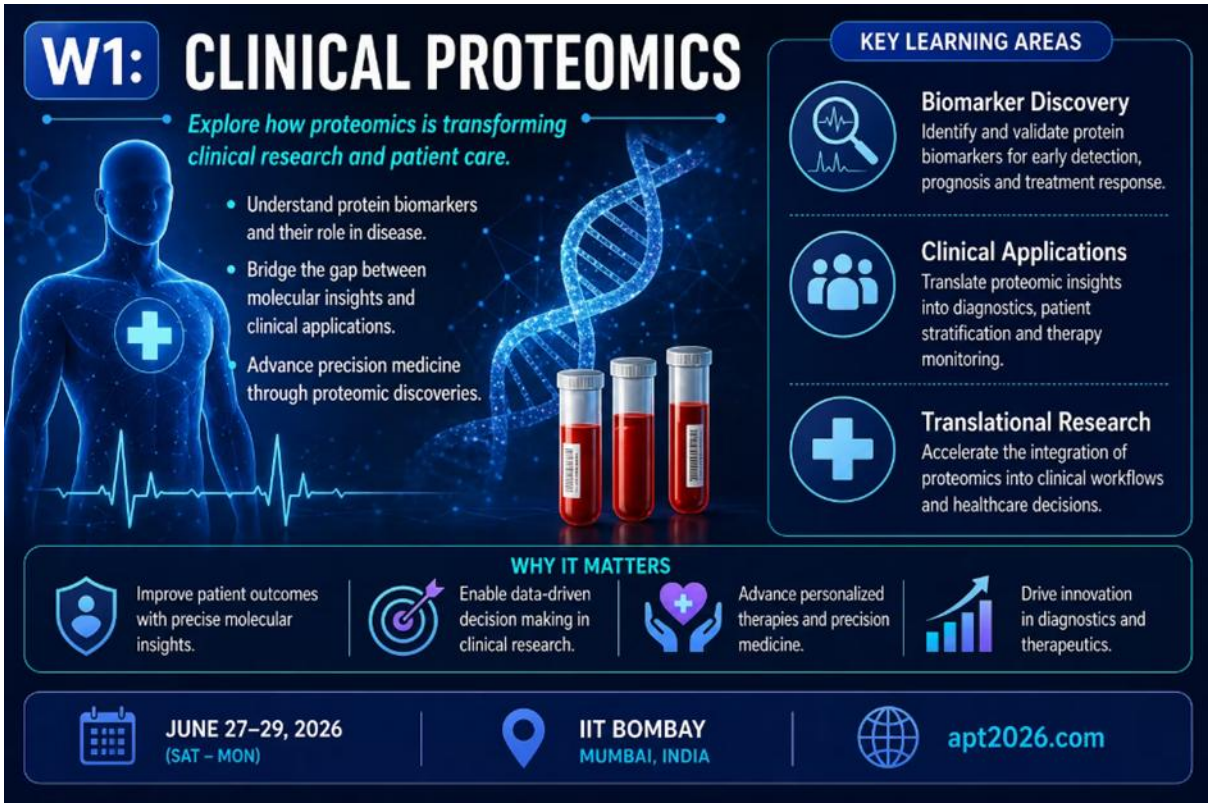


Figure W1.1. The Multi-Omics Dynamic Cascade. Hierarchical flow of biological information from the genome to the transcriptome and ultimately the proteome, illustrating how genetic information is progressively transformed into functional cellular outcomes.

1.2 Clinical Specimen Types in Proteomics

The choice of biological specimen profoundly shapes the proteomic workflow, the achievable depth of analysis, and the clinical utility of the resulting biomarkers:

Specimen	Characteristics	Clinical Utility
Plasma / Serum	Most accessible specimen; extreme dynamic range (10 orders of magnitude in protein concentration); dominated by albumin and immunoglobulins (>99% of protein mass from ~20 proteins)	Population screening, disease risk prediction, longitudinal monitoring, minimally invasive sampling

Urine	Filtered through the kidney glomerulus; reflects renal and systemic pathology; less complex matrix than plasma but more variable concentration	Renal disease, bladder and urological cancers, non-invasive monitoring
Cerebrospinal Fluid (CSF)	Direct reflection of CNS biology; lower protein concentration than plasma; invasive lumbar puncture required for collection	Neurodegenerative disease (Alzheimer's, Parkinson's), CNS infection, CNS malignancy
Dried Blood Spots (DBS)	Minimal volume (a few drops); stable at room temperature; ideal for newborn screening and remote/resource-limited settings	Newborn screening for inborn errors of metabolism and immunity, population-scale studies
Tissue Biopsy / FFPE	Direct disease tissue; formalin-fixed paraffin-embedded (FFPE) is the clinical pathology standard, widely archived in biobanks	Tumour molecular subtyping, treatment selection, retrospective biomarker validation studies
Saliva / Other Fluids	Completely non-invasive; lower protein complexity; concentration affected by oral health and collection method	Point-of-care testing, paediatric and field-deployable diagnostics

1.3 The Dynamic Range Problem in Plasma Proteomics

Human blood plasma presents the single greatest analytical challenge in clinical proteomics. The concentration of the most abundant plasma protein, albumin (35-50 g/L), exceeds that of clinically important low-abundance cytokines and tumour markers (often picograms per millilitre) by up to ten orders of magnitude. Without specific enrichment or depletion strategies, mass spectrometers preferentially detect the small number of highly abundant proteins, missing the rare proteins of greatest diagnostic interest entirely. This single problem has driven the development of immunoaffinity depletion columns, targeted enrichment strategies, and increasingly sensitive instrumentation throughout the history of the field.

W 1.2

Historical Development of Clinical Proteomics

Clinical proteomics has evolved over five decades through several distinct technological eras, each addressing the limitations of its predecessor and progressively closing the gap between research discovery and routine clinical deployment.

2.1 The Electrophoresis Era (1970s–1990s)

The earliest clinical protein profiling relied on two-dimensional gel electrophoresis (2D-PAGE), separating proteins first by isoelectric point and then by molecular weight to generate a two-dimensional protein 'fingerprint' of a biological sample. While 2D-PAGE could resolve thousands of protein spots and remains valuable for visualising global proteome changes, it was labour-intensive, poorly reproducible between laboratories, biased against low-abundance and highly hydrophobic proteins, and fundamentally limited as a clinical assay platform because of low throughput and difficulty in absolute quantification. Combined with immunochemical methods such as ELISA for individual protein quantification, this era established the conceptual foundation, that protein abundance patterns reflect disease state, without providing the scalable technology to act on it.

2.2 The SELDI-TOF Revolution and OVA1 (1990s–2000s)

Surface-Enhanced Laser Desorption/Ionisation Time-of-Flight mass spectrometry (SELDI-TOF-MS), introduced and commercialised in the 1990s, represented the first widely adopted high-throughput clinical proteomic profiling platform. Small volumes of serum or plasma were applied directly to a 'protein chip' with a defined chromatographic surface chemistry (hydrophobic, cationic, anionic, or antibody-coated), which selectively retained subsets of proteins. Bound proteins were then ionised and detected directly on the chip by time-of-flight mass spectrometry, generating a rapid mass spectral 'fingerprint' without the need for prior chromatographic separation.

SELDI-TOF profiling of serum samples from ovarian cancer patients versus controls led to the discovery of a five-protein biomarker panel (CA125, transthyretin/prealbumin, apolipoprotein A1, beta-2-microglobulin, and transferrin) that became the basis for OVA1, cleared by the US FDA in 2009 as the first and, for many years, the only FDA-cleared in vitro diagnostic multivariate index assay (IVDMIA) built upon proteomic biomarker discovery. OVA1 remains a landmark achievement and a cautionary lesson: although four of the five OVA1 markers were discovered using SELDI-TOF, the final commercial assay was implemented using traditional immunoassay technology because the analytical precision and reproducibility of SELDI itself could not be sufficiently standardised for routine clinical laboratory deployment. This experience crystallised an enduring principle in the field: the technology used for biomarker discovery is frequently not the technology used for the final clinical assay.

HISTORICAL LESSON: THE DISCOVERY-TO-CLINIC TRANSLATION GAP

A striking and persistent discrepancy exists between the enormous research effort devoted to proteomic biomarker discovery (many thousands of candidate biomarkers published over three decades) and the very small number that have achieved regulatory clearance and routine clinical use. The reasons include insufficient analytical validation, lack of independent replication across cohorts, inadequate consideration of pre-analytical variability, and failure to engage with regulatory and health-economic requirements early in the discovery process. Modern biomarker pipelines (Chapter 4) were designed specifically to address this historical translation gap.

2.3 The Shotgun and Targeted MS Era (2000s–2010s)

The 2000s saw clinical proteomics adopt the liquid chromatography-tandem mass spectrometry (LC-MS/MS) 'shotgun' approach already transforming basic proteomics research: proteins are enzymatically digested into peptides, separated by nanoflow liquid chromatography, and identified and quantified by tandem mass spectrometry. This provided dramatically greater proteome coverage than SELDI-TOF (thousands rather than dozens of proteins) but introduced new challenges in reproducibility and quantitative precision for clinical use.

In parallel, targeted MS approaches, multiple/selected/parallel reaction monitoring (MRM/SRM/PRM), emerged as the preferred strategy for clinical-grade quantification of pre-selected protein panels. Unlike shotgun discovery proteomics, targeted MS monitors only specific, pre-defined peptide transitions (precursor-to-fragment ion pairs) with heavy isotope-labelled internal standards for absolute quantification, achieving the precision, reproducibility, and multiplexing capability needed for regulated clinical assays while retaining the specificity advantage of mass spectrometry over antibody-based methods. The Clinical Proteomic Tumor Analysis Consortium (CPTAC), launched by the US National Cancer Institute, established the CPTAC Assay Portal as a public repository of well-characterised, standardised MRM assays, formalising targeted MS as a rigorous clinical translation pathway.

2.4 The High-Resolution and DIA Era (2010s–2020s)

The introduction of high-resolution, high-mass-accuracy instruments (Orbitrap analysers from Thermo Fisher Scientific, and time-of-flight analysers from Sciex, Bruker, and Agilent) combined with the maturation of data-independent acquisition (DIA, including the SWATH-MS approach pioneered by Aebersold's group) transformed clinical discovery proteomics. DIA systematically fragments all peptides within defined mass windows in every analytical cycle, providing comprehensive, highly reproducible quantitative data across hundreds of clinical samples without the missing-value

problems that plagued earlier shotgun DDA approaches. By the early 2020s, DIA-MS was recognised in the proteomics community as 'a milestone and prospect in clinical mass spectrometry-based proteomics', enabling biomarker discovery studies of unprecedented statistical power directly from large clinical cohorts.

2.5 The Affinity-Proteomics and Population-Scale Era (2020s)

Concurrent with MS-based advances, affinity-based multiplexed platforms, principally the Olink Proximity Extension Assay (PEA) and the SomaLogic SomaScan aptamer-based platform, enabled population-scale plasma proteomic profiling without mass spectrometry. These platforms use antibody pairs (Olink) or modified DNA aptamers (SomaScan) that bind specific target proteins and generate a quantifiable DNA readout via PCR or sequencing, allowing thousands of proteins to be measured simultaneously in thousands of plasma samples at a cost and throughput unattainable by MS at that time. This technology underpinned the UK Biobank Pharma Proteomics Project (UKB-PPP), profiling nearly 3,000 plasma proteins in over 54,000 participants, the largest population proteomic resource in history (detailed in Chapter 6).

W 1.3

Core Technologies in Clinical Proteomics

3.1 Mass Spectrometry Platforms

Three principal categories of mass analyser dominate clinical proteomics, each suited to different applications:

Platform	Principle and Strengths	Typical Clinical Use
Orbitrap (Thermo Fisher)	Electrostatic ion trap with ultra-high mass resolution (>100,000) and accuracy (<2 ppm); excellent for both discovery DIA and targeted PRM	Discovery biomarker studies, deep plasma proteomics, intact protein analysis
Triple Quadrupole (QQQ)	Sequential mass filtering for highly sensitive, specific MRM/SRM transitions; gold standard for absolute quantification with isotope-labelled standards	Validated clinical assays, newborn screening (steroid and amino acid panels), targeted biomarker panels
Time-of-Flight (TOF) / Q-TOF	Fast scanning, high resolution; basis of SWATH-MS DIA approach; used in SELDI-TOF and modern Bruker timsTOF platforms	High-throughput profiling, microbial identification (MALDI-TOF), DIA-based discovery
MALDI-TOF	Matrix-assisted ionisation directly from solid samples; extremely rapid (seconds per sample), minimal sample preparation	Routine clinical microbiology (bacterial/fungal species identification), now standard of care in many hospital labs

MALDI-TOF: ALREADY ROUTINE CLINICAL PRACTICE

While most clinical proteomics applications remain in development, MALDI-TOF mass spectrometry for rapid bacterial and fungal species identification (matching the protein mass spectral fingerprint of an unknown microbial isolate against a reference library) is already standard practice in thousands of clinical microbiology laboratories worldwide, replacing slower biochemical identification methods. This is the most widely deployed clinical proteomics application today and demonstrates the achievable end point for other applications now in earlier development stages.

3.2 Data Acquisition Strategies: DDA, DIA, and Targeted MS

Data-Dependent Acquisition (DDA)

The traditional shotgun proteomics approach: the instrument selects the most abundant precursor ions in each survey scan for fragmentation. DDA is unbiased and excellent for deep, exploratory discovery work but is stochastic, the same peptide may or may not be selected for fragmentation across different runs, creating substantial missing data when comparing large clinical cohorts.

Data-Independent Acquisition (DIA)

DIA systematically fragments all precursor ions within sequential, predefined mass windows in every cycle, regardless of abundance, generating comprehensive and highly reproducible quantitative data across all peptides present in a sample. DIA has become the preferred acquisition mode for large clinical cohort studies because of its low missing-data rate and excellent run-to-run reproducibility, both essential properties for population-scale biomarker discovery and validation.

Targeted MS: MRM, SRM, and PRM

For validated, regulatory-grade clinical assays measuring a defined panel of proteins, targeted approaches remain the gold standard. Multiple/Selected Reaction Monitoring (MRM/SRM, performed on triple quadrupole instruments) and Parallel Reaction Monitoring (PRM, performed on high-resolution instruments) monitor only specific, pre-validated precursor-to-fragment ion transitions for each target peptide, using stable isotope-labelled internal standard peptides spiked into every sample for absolute quantification. This approach delivers the precision, reproducibility, multiplexing capacity, and compliance with Good Laboratory Practice and Good Clinical Practice standards required for regulated diagnostic assays, and underpins applications from newborn screening to CPTAC-validated cancer biomarker panels.

3.3 Affinity-Based Multiplexed Proteomic Platforms

Olink Proximity Extension Assay (PEA)

Each target protein is recognised by a matched pair of antibodies, each conjugated to a unique DNA oligonucleotide. When both antibodies bind their target in close proximity, the attached DNA strands hybridise and are extended by DNA polymerase, generating a unique, quantifiable DNA amplicon detected by quantitative PCR or, in the newer Explore platform, by next-generation sequencing. Olink Explore panels measure up to several thousand proteins simultaneously from a few microlitres of plasma, enabling the unprecedented scale of the UK Biobank Pharma Proteomics Project.

SomaLogic SomaScan

Uses modified single-stranded DNA aptamers (SOMAmers) engineered to bind specific target proteins with high affinity and specificity, with bound protein-aptamer complexes detected and quantified via DNA microarray or sequencing readout. SomaScan offers extremely broad multiplexing (up to ~11,000 proteins in recent versions) but, like Olink, is an antibody/aptamer-based indirect measurement rather than direct mass-based protein identification, and the two platforms show only modest inter-platform correlation (median correlation around 0.33 in head-to-head comparisons), an important consideration when interpreting biomarker results across studies using different platforms.

W 1.4

The Biomarker Discovery and Validation Pipeline

Translating a candidate protein biomarker from initial discovery to routine clinical use requires a structured, multi-phase pipeline. This framework, developed in response to the historical translation failures discussed in Chapter 2, is now the accepted standard across the field.

4.1 Phase 1 — Discovery

Untargeted, hypothesis-generating proteomic profiling (typically DIA-MS or affinity-based multiplex panels) compares disease versus control samples to generate a list of candidate proteins showing statistically significant differential

abundance. Discovery studies prioritise depth of coverage over throughput and often use well-characterised, well-phenotyped but modest-sized cohorts (tens to low hundreds of samples).

4.2 Phase 2 — Verification

Candidate biomarkers from discovery are re-measured using a more targeted, higher-throughput method (commonly PRM or MRM) in an independent, larger cohort to confirm that the differential abundance observed in discovery is reproducible and not an artefact of the discovery platform or cohort-specific confounding. This phase typically reduces an initial candidate list of dozens to hundreds of proteins down to a focused panel of the most robust and biologically plausible markers.

4.3 Phase 3 — Validation

The final, focused biomarker panel undergoes rigorous analytical and clinical validation in large, independent, ideally multi-centre cohorts using a fully locked-down assay protocol. Analytical validation establishes precision (repeatability and reproducibility), trueness/accuracy, linearity, limit of detection and quantification, specificity, and resistance to interference and carryover, the core performance characteristics required by regulatory bodies. Clinical validation establishes diagnostic sensitivity, specificity, and predictive value in the intended use population, ideally compared head-to-head against existing standard-of-care diagnostics.

WHY MOST PROTEOMIC BIOMARKERS NEVER REACH THE CLINIC

The vast majority of published proteomic biomarker discoveries never progress past Phase 1. Common failure points include: inadequate statistical power in the discovery cohort; lack of an independent verification cohort; insufficient characterisation of pre-analytical variables (sample collection, handling, and storage conditions strongly affect protein stability and can introduce systematic bias); and failure to demonstrate added clinical value beyond existing, cheaper biomarkers. Researchers planning translational proteomics studies should design the verification and validation phases into the project from the outset, not as an afterthought following an exciting discovery result.

4.4 Regulatory Pathways for Clinical Proteomic Assays

In the United States, proteomic biomarker panels intended for clinical diagnostic use are most commonly regulated as In Vitro Diagnostic Multivariate Index Assays (IVDMIAs) by the FDA, requiring demonstration of analytical and clinical validity through a formal premarket submission (510(k) clearance or De Novo classification, depending on risk category and availability of predicate devices). Laboratory-developed tests (LDTs) performed entirely within a single CLIA-certified clinical laboratory have historically followed a separate regulatory pathway with lower formal evidentiary requirements, though this landscape continues to evolve. Equivalent frameworks exist internationally (CE-marking under the EU In Vitro Diagnostic Regulation, and country-specific regulatory bodies elsewhere), and prospective developers of clinical proteomic assays must engage with the relevant regulatory pathway early in assay development.

W 1.5

Clinical Applications by Disease Area

5.1 Oncology

Cancer remains the most intensively studied clinical proteomics application area. Beyond OVA1 for ovarian cancer (Chapter 2), proteomic approaches contribute to tumour molecular subtyping from FFPE tissue, identification of therapy-predictive biomarkers, monitoring of treatment response and minimal residual disease, and discovery of early detection biomarkers for cancers lacking effective screening tools (pancreatic, ovarian, and lung cancer being priority targets). The Clinical Proteomic Tumor Analysis Consortium (CPTAC) has generated comprehensive proteogenomic characterisation,

combining genomic, transcriptomic, and proteomic data, of multiple tumour types, revealing that protein-level information frequently identifies actionable biology invisible to genomic analysis alone, since genomic alterations do not reliably predict downstream protein abundance or activity.

5.2 Cardiology

Established protein biomarkers, troponin for myocardial infarction and natriuretic peptides (BNP/NT-proBNP) for heart failure, are among the most successful examples of protein biomarkers in routine clinical use, though these were developed via traditional immunoassay rather than mass spectrometry discovery pathways. More recent large-scale plasma proteomic studies (Chapter 6) using Olink and SomaScan platforms have systematically tested whether broader proteomic panels can improve cardiovascular risk prediction beyond established clinical risk scores such as SCORE2, with multiple studies showing modest but statistically significant incremental predictive value when proteins such as GDF-15, NT-proBNP, MMP-12, and TNFRSF10B/TRAIL-R2 are combined with traditional risk factors.

5.3 Neurology and Neurodegenerative Disease

CSF and, increasingly, plasma proteomics have transformed biomarker discovery in Alzheimer's disease, Parkinson's disease, and multiple sclerosis. Plasma proteomic profiling in large prospective cohorts has identified novel candidate biomarkers for future dementia risk, while CSF and plasma protein panels are increasingly used alongside or in place of amyloid PET imaging for Alzheimer's disease diagnosis and clinical trial patient stratification. Population-scale plasma proteomics in multiple sclerosis cohorts has identified novel disease-associated proteins, including downregulation of Granzyme A, with pathway enrichment analyses revealing involvement of cytokine signalling, lysosomal processing, and leukocyte migration pathways.

5.4 Infectious Disease and Clinical Microbiology

As noted in Chapter 3, MALDI-TOF-based microbial species identification is the most widely and successfully deployed clinical proteomics application in current routine practice, used daily in clinical microbiology laboratories worldwide for rapid identification of bacterial and fungal pathogens from positive cultures, dramatically reducing time-to-identification compared with traditional biochemical methods and enabling earlier targeted antimicrobial therapy.

5.5 Rare and Genetic Disease, and Newborn Screening

Targeted, multiplexed LC-MS/MS assays measuring signature peptides as surrogate markers for disease-causing proteins directly from dried blood spots are emerging as a powerful complement to traditional metabolite-based newborn screening, particularly for inborn errors of immunity (such as X-linked agammaglobulinemia, Wiskott-Aldrich syndrome, and severe combined immunodeficiency) and Wilson disease, where no specific metabolic biomarker exists but the causative protein deficiency can be measured directly. Non-targeted, DIA-based proteomic profiling of dried blood spots is being explored as a single unified platform capable of simultaneously screening for many genetic disorders without requiring separate assays for each condition (further detailed in Chapter 6).

5.6 Haemato-Oncology: Amyloidosis and Multiple Myeloma

Mass spectrometry-based proteomic typing of amyloid deposits, identifying the specific amyloidogenic protein (light chain kappa or lambda, transthyretin, serum amyloid A, and others) responsible for a patient's systemic amyloidosis, has become a clinically important diagnostic application, since accurate amyloid typing directly determines treatment selection. Combining tandem MS with two-dimensional chromatography (MudPIT-MS) enables diagnostic algorithms based on normalised abundance ratios for amyloid subtype classification, validated against immunoelectron microscopy with complete diagnostic agreement in published studies, while eliminating the need for the tissue fractionation steps required by older immunohistochemistry-based typing methods.

Recent Achievements (2023–2026)

The past three years have seen clinical proteomics move decisively from a primarily research-oriented discipline toward genuine population-scale and point-of-care clinical impact. The following developments represent the most significant recent advances in the field.

6.1 The UK Biobank Pharma Proteomics Project (UKB-PPP)

The UKB-PPP, a collaboration between UK Biobank and 14 biopharmaceutical companies, generated the largest population-scale proteomic dataset in history: nearly 3,000 plasma proteins measured using the Olink Explore 3072 platform in over 54,000 UK Biobank participants. Sun et al. (2023) used this resource to map 14,287 primary protein quantitative trait loci (pQTLs), genetic variants influencing circulating protein levels, of which approximately 81% were novel discoveries, including ancestry-specific pQTLs identified in non-European population subgroups, substantially expanding understanding of the genetic architecture of the human plasma proteome.

Subsequent analyses of this resource have repeatedly demonstrated that circulating protein levels predict incident disease with discrimination exceeding traditional risk factors and even polygenic risk scores for numerous conditions. A landmark 2024 analysis tested 1,468 Olink plasma proteins against 23 age-related disease outcomes and mortality in 47,600 participants, reporting 3,209 significant protein-disease associations across 21 incident outcomes, and developing 'ProteinScores' using penalised Cox regression that improved 10-year disease prediction beyond age, sex, and 24 established lifestyle and clinical risk factors for six major outcomes, with the ProteinScore for incident type 2 diabetes outperforming a combined polygenic risk score plus HbA1c model.

LANDMARK ACHIEVEMENT: PROTEOMIC PREDICTION ACROSS THE DISEASE SPECTRUM

Subsequent work building on UKB-PPP has reported area-under-curve (AUC) values exceeding 0.80 for incident-disease prediction across 92 distinct diseases using plasma protein panels, alongside organ-specific 'protein clocks' capable of estimating the biological age of individual organ systems (heart, kidney, liver, lung, and others) from a single blood draw, with two notable findings: for most diseases and organs, individual protein levels match or exceed the predictive power of more elaborate composite ageing clocks, and proteomic prediction appears to substantially reflect environmental and lifestyle risk exposures (such as smoking) rather than purely intrinsic biological ageing, an important consideration for interpreting and clinically applying these scores.

6.2 DIA-MS Reaches Clinical Maturity

A 2024 perspective in Molecular & Cellular Proteomics formally recognised data-independent acquisition as 'a milestone and prospect in clinical mass spectrometry-based proteomics', reflecting the technology's maturation from a research method to a clinically deployable acquisition strategy. The combination of DIA with modern high-resolution instruments (Orbitrap Astral, timsTOF Ultra) now enables reproducible quantification of several thousand plasma or tissue proteins across hundreds of clinical samples in a single study, with missing-data rates low enough to support robust biomarker discovery and verification entirely within the MS-based workflow, narrowing the historical gap between MS-based and affinity-based platform throughput.

6.3 Non-Targeted Proteomic Newborn Screening

A series of studies from 2024–2025 has demonstrated the feasibility of non-targeted DIA-LC-MS/MS proteomic profiling of dried blood spots as a unified newborn screening platform capable of simultaneously detecting multiple genetic disorders from a single assay, rather than requiring separate targeted tests for each condition. Shibata et al. (2024, Journal of Clinical Immunology) validated a non-targeted proteomics platform for inborn errors of immunity directly from neonatal dried blood spots, while a 2025 Analytical Chemistry paper (Nakajima et al.) introduced NANDA (Non-targeted

Analysis of Non-specifically DBS-Absorbed proteins), a robotic sample preparation pipeline using low-cost iron powder particles for protein extraction, addressing the cost and throughput barriers that previously limited proteomic newborn screening to research settings.

In parallel, targeted immuno-SRM multiplexed assays have moved into sustained population-scale newborn screening practice: the Washington State Department of Health Newborn Screening Laboratory has screened over 30,000 newborn dried blood spot samples between 2022 and 2024 using a validated multiplexed LC-MS/MS assay simultaneously detecting Wilson disease and three inborn errors of immunity (X-linked agammaglobulinemia, Wiskott-Aldrich syndrome, and adenosine deaminase deficiency), representing one of the largest sustained real-world deployments of proteomic newborn screening to date and a template for expansion to other state and national screening programmes.

6.4 Refined Amyloidosis and Multiple Myeloma Diagnostics

A comprehensive 2025 review (Kratka et al., Journal of Mass Spectrometry) consolidated over a decade of progress (2012–2024) in MS-based proteomic diagnosis of amyloidosis and multiple myeloma, documenting the maturation of MS-based amyloid typing into accepted clinical pathology practice at major reference centres and describing new applications combining label-free LC-MS/MS proteomics with targeted metabolomics of bone marrow and plasma to characterise extramedullary spread in multiple myeloma, identifying 225 differentially abundant proteins in bone marrow mononuclear cells associated with this aggressive disease pattern.

6.5 Artificial Intelligence Integration in Clinical Proteomics

Machine learning is now integral to nearly every stage of the clinical proteomics pipeline: gradient boosting and LASSO regression models extract optimal biomarker panels from large proteomic datasets (as in the UKB-PPP ProteinScore analyses); neural network-based tools (DIA-NN and related software) underpin modern DIA spectral library prediction and peptide identification; and deep learning models increasingly integrate proteomic data with imaging, genomic, and electronic health record data for multi-modal clinical risk prediction. This computational integration has been essential to extracting clinically actionable signal from the very large, high-dimensional datasets generated by modern proteomic platforms.

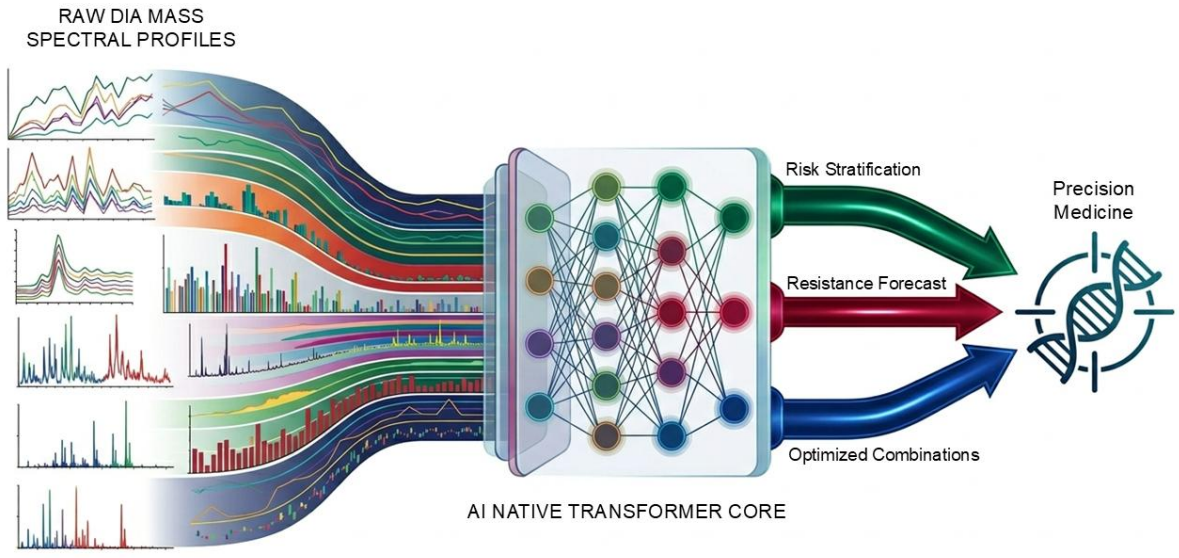


Figure 9. The AI-Native Proteomics Engine of Precision Medicine. An AI-native proteomics pipeline transforms mass spectrometry data into clinically actionable insights, enabling patient stratification, treatment-response prediction, and optimized therapeutic decision-making.

6.6 The HUPO Human Proteome Project — 2023 Status Report

The Human Proteome Organisation's Human Proteome Project (HUPO HPP) continues to provide the definitive evidence-based foundation underpinning all clinical proteomics applications, with the 2023 status report (published in the Journal of Proteome Research, 2024) confirming high-confidence experimental detection of the large majority of predicted human protein-coding genes, while highlighting the continued challenge of the 'missing proteome', a persistent set of low-abundance, tissue-restricted, or technically difficult proteins that remain undetected by current methods and represent priority targets for the next generation of clinical proteomic technology development.

W 1.7

Landmark Research Papers

The following papers span the historical foundations and the most significant recent contributions to clinical proteomics.

Petricoin EF, Ardekani AM, Hitt BA et al. | The Lancet, 2002 | DOI: 10.1016/S0140-6736(02)07746-2

Use of proteomic patterns in serum to identify ovarian cancer

The foundational SELDI-TOF serum proteomic profiling study that launched clinical proteomics as a translational discipline. Demonstrated that a pattern-recognition algorithm applied to serum mass spectra could distinguish ovarian cancer patients from healthy controls with high sensitivity and specificity, directly motivating the biomarker discovery work that eventually led to OVA1, the first FDA-cleared proteomic IVDMIA.

Gillette MA & Carr SA | Nature Methods, 2013 | DOI: 10.1038/nmeth.2309

Quantitative analysis of peptides and proteins in biomedicine by targeted mass spectrometry

A foundational methods paper establishing targeted MS (MRM/SRM/PRM) as the rigorous quantitative framework for clinical and translational proteomics, directly informing the design of the CPTAC Assay Portal and the broader adoption of targeted MS as the preferred validation-phase technology in biomarker pipelines.

Gillette MA, Satpathy S, Cao S et al. (CPTAC) | Cell, 2020 | DOI: 10.1016/j.cell.2020.06.013

Proteogenomic Characterization Reveals Therapeutic Vulnerabilities in Lung Adenocarcinoma

A landmark CPTAC proteogenomic study combining genomic, transcriptomic, and proteomic profiling of lung adenocarcinoma, demonstrating that protein and phosphoprotein-level data reveal therapeutically actionable biology, including kinase activation states, invisible to genomic sequencing alone. Established the proteogenomic integration paradigm now standard in CPTAC and similar cancer consortium studies.

Sun BB, Chiou J, Traylor M et al. | Nature, 2023 | DOI: 10.1038/s41586-023-06592-6

Plasma proteomic associations with genetics and health in the UK Biobank

The flagship UKB-PPP paper profiling nearly 3,000 plasma proteins in 54,219 UK Biobank participants using the Olink Explore 3072 platform, mapping 14,287 pQTLs (81% novel) and establishing the largest population-scale proteo-genomic resource in history. This dataset has since underpinned dozens of downstream disease-prediction and biomarker discovery studies across nearly every medical specialty.

Strathmann FG, Lorenzi PL, DeBord D | GEN Biotechnology / Clinical Mass Spectrometry, 2024-2025

Data-Independent Acquisition: A Milestone and Prospect in Clinical Mass Spectrometry-Based Proteomics

A widely cited 2024 perspective in Molecular & Cellular Proteomics (and companion commentary) formally establishing DIA-MS as a maturing, clinically deployable acquisition strategy, reviewing its advantages in reproducibility and missing-data reduction over DDA for large clinical cohort studies, and outlining the remaining barriers (standardisation, regulatory pathway clarity) to routine clinical adoption.

Shibata H, Nakajima D, Konno R et al. | Journal of Clinical Immunology, 2024 | DOI: 10.1007/s10875-024-01821-7

A Non-targeted Proteomics Newborn Screening Platform for Inborn Errors of Immunity

Demonstrated that non-targeted DIA-LC-MS/MS proteomic profiling of neonatal dried blood spots can identify and quantify disease-causing or disease-related proteins for genetic immunodeficiency disorders at the pre-symptomatic newborn stage, establishing feasibility for a unified, multi-disease proteomic newborn screening platform as an alternative to disorder-specific targeted assays.

Klippel C, Park J, Sandin S et al. | International Journal of Neonatal Screening, 2025 | DOI: 10.3390/ijns11010006

Advancing Newborn Screening in Washington State: A Novel Multiplexed LC-MS/MS Proteomic Assay for Wilson Disease and Inborn Errors of Immunity

Reports real-world clinical deployment of a validated immuno-SRM multiplexed proteomic newborn screening assay across more than 30,000 newborn dried blood spot samples in Washington State (2022-2024), one of the largest sustained population-scale clinical implementations of proteomic newborn screening achieved to date, providing a template for broader state and national programme adoption.

Kratka K, Sistik P, Olivkova I et al. | Journal of Mass Spectrometry, 2025 | DOI: 10.1002/jms.5116

Mass Spectrometry-Based Proteomics in Clinical Diagnosis of Amyloidosis and Multiple Myeloma: A Review (2012-2024)

A comprehensive decade-spanning review documenting the maturation of MS-based amyloid typing (LC-MS/MS with 2D chromatography identifying light chains, transthyretin, and serum amyloid A) into routine clinical pathology practice, alongside emerging multi-omic proteomic and metabolomic approaches for characterising high-risk multiple myeloma. Essential current reference for haemato-oncology proteomics applications.

Omenn GS, Lane L, Overall CM et al. (HUPO HPP) | Journal of Proteome Research, 2024 | DOI: 10.1021/acs.jproteome.3c00659

The 2023 Report on the Proteome from the HUPO Human Proteome Project

The authoritative annual status report of the Human Proteome Project, documenting confident experimental detection of the large majority of predicted human proteins and tracking the shrinking but persistent ‘missing proteome’. Provides the evidence-based foundation against which all clinical proteomics biomarker discovery claims should be benchmarked.

W 1.8

Pioneering Scientists in Clinical Proteomics

Scientist and Affiliation	Key Contributions
Dr. Emanuel F. Petricoin III — George Mason University; formerly FDA	Co-pioneer of SELDI-TOF serum proteomic pattern analysis for ovarian cancer detection (Lancet, 2002). His work directly catalysed the field of clinical cancer proteomics and the eventual development of OVA1, the first FDA-cleared proteomic diagnostic. Continues to advance reverse-phase protein array technology for clinical functional proteomics.

Prof. Ruedi Aebersold — ETH Zurich / University of Zurich	Pioneer of essentially all modern quantitative MS-based proteomics methodology underpinning clinical applications: developed SRM/MRM targeted quantification frameworks, co-invented SWATH-MS (the first practical DIA implementation), and co-developed Cell Surface Capture. His methodological contributions are foundational to nearly every modern clinical proteomics workflow.
Prof. Steven A. Carr — Broad Institute of MIT and Harvard	Co-led development of the targeted MS (MRM/PRM) framework for clinical biomarker verification and validation. Senior leadership role in the Clinical Proteomic Tumor Analysis Consortium (CPTAC), driving proteogenomic characterisation of multiple cancer types and establishing rigorous standards for clinical-grade targeted proteomic assays.
Prof. Matthias Mann — Max Planck Institute of Biochemistry; University of Copenhagen	Leading figure in translating high-resolution MS technology (Orbitrap-based DIA) toward clinical and population-scale plasma proteomics. Co-authored the influential 2023 perspective 'MS-Based Proteomics of Body Fluids: The End of the Beginning', articulating the path from research-grade plasma proteomics to clinical deployment.
Dr. Daniel Chan — Johns Hopkins University School of Medicine	Leading authority on the translation of proteomic cancer biomarkers from discovery to FDA-approved clinical diagnostics. Authored foundational reviews on the analytical, regulatory, and clinical validation requirements bridging biomarker discovery and routine clinical laboratory deployment, directly shaping the Phase 1-3 biomarker pipeline framework used across the field.
Prof. Osamu Ohara — Kazusa DNA Research Institute, Japan	Leading developer of non-targeted DIA-LC-MS/MS proteomic newborn screening from dried blood spots, including the NANDA robotic sample preparation pipeline. His group's work represents the most advanced effort toward a unified, multi-disease proteomic newborn screening platform as an alternative to disorder-specific targeted testing.
Prof. Benjamin B. Sun — AstraZeneca / University of Cambridge	Lead author of the flagship UK Biobank Pharma Proteomics Project paper (Nature, 2023), establishing the largest population-scale plasma proteo-genomic resource in history and mapping over 14,000 protein quantitative trait loci. His work has directly enabled dozens of subsequent disease prediction and drug target validation studies across the pharmaceutical industry and academia.
Dr. Amanda G. Paulovich — Fred Hutchinson Cancer Center	Pioneer of rigorous targeted MS assay development and the CPTAC Assay Portal, establishing community standards for analytically validated, multiplexable, and reproducible MRM-based clinical proteomic assays. Her work bridges the historically disconnected discovery and clinical translation phases of the biomarker pipeline.

W 1.9

Historical Development Timeline

Year	Milestone

1975	Two-dimensional gel electrophoresis (O'Farrell) introduced, providing the first technology capable of resolving thousands of individual cellular proteins simultaneously and establishing the conceptual foundation for global protein profiling.
1995	SELDI-TOF mass spectrometry (Hutchens & Yip) introduced, combining chromatographic protein chip surfaces with direct time-of-flight detection for rapid serum protein profiling without prior separation.
2002	Petricoin, Liotta and colleagues publish the landmark Lancet paper applying SELDI-TOF serum proteomic pattern analysis to ovarian cancer detection, launching clinical cancer proteomics as a defined translational field.
2006	Clinical Proteomic Tumor Analysis Consortium (CPTAC) established by the US National Cancer Institute to systematically generate and validate proteogenomic characterisation of human cancers.
2009	OVA1 receives FDA clearance as the first in vitro diagnostic multivariate index assay (IVDMIA) based on proteomic biomarker discovery, combining five proteins (CA125, prealbumin, apolipoprotein A1, beta-2-microglobulin, transferrin) for ovarian cancer risk assessment.
2011	Aebersold and colleagues publish the foundational SWATH-MS paper, introducing practical data-independent acquisition and transforming the reproducibility of large-scale quantitative proteomics.
2014	CPTAC Assay Portal launched as a public repository of standardised, well-characterised MRM-based targeted proteomic assays, formalising targeted MS as a rigorous clinical translation pathway.
2016	SomaLogic SomaScan aptamer-based platform and Olink Proximity Extension Assay both reach broad commercial availability, enabling affinity-based multiplexed plasma proteomic profiling at population scale.
2020	CPTAC publishes comprehensive proteogenomic characterisation of lung adenocarcinoma and other cancers, demonstrating therapeutically actionable protein-level biology invisible to genomic sequencing alone.
2021	UK Biobank Pharma Proteomics Project (UKB-PPP) pilot phase profiles plasma proteomes of the first tranche of UK Biobank participants using Olink Explore 3072.
2023	Sun et al. publish the flagship UKB-PPP Nature paper profiling nearly 3,000 proteins in 54,219 participants and mapping over 14,000 pQTLs, the largest population proteomic resource in history.
2024	DIA-MS formally recognised as a clinical milestone technology in Molecular & Cellular Proteomics. Multiple non-targeted DIA-based newborn screening proteomics platforms published. Washington State proteomic newborn screening programme surpasses 30,000 screened infants.
2025	Comprehensive decade-spanning review consolidates MS-based amyloidosis and multiple myeloma diagnostics into accepted clinical pathology practice. NANDA robotic DBS proteomics pipeline published, reducing cost barriers to population-scale newborn screening proteomics.
2026	Continued expansion of organ-specific proteomic 'ageing clocks' and disease-prediction ProteinScores toward clinical decision support integration; ongoing regulatory dialogue on pathways for population-scale proteomic risk prediction tools.


W2:
MASS SPECTROMETRY BASED PROTEOMICS
m/z
y7 y6 y5 y4 y3 y2 y1
H2N
OH
b2 b3 b4 b5 b6 b7
200 400 600 800 1000 1200 1400 1600 1800 2000
m/z





Mass Spectrometry-Based Proteomics

SCIENTIFIC PROGRAMME

Overview

This workshop provides a practical introduction to mass spectrometry (MS)-based proteomics, covering the complete workflow from biological sample preparation to data analysis and biological interpretation. Participants will gain hands-on knowledge of modern proteomics technologies used in biomedical and translational research.

The workshop will guide attendees through key steps, including sample preparation, protein digestion, MS data acquisition, protein identification, and quantitative analysis. Participants will also learn how high-resolution mass spectrometry enables large-scale protein profiling and how bioinformatics tools extract meaningful biological insights from complex datasets.

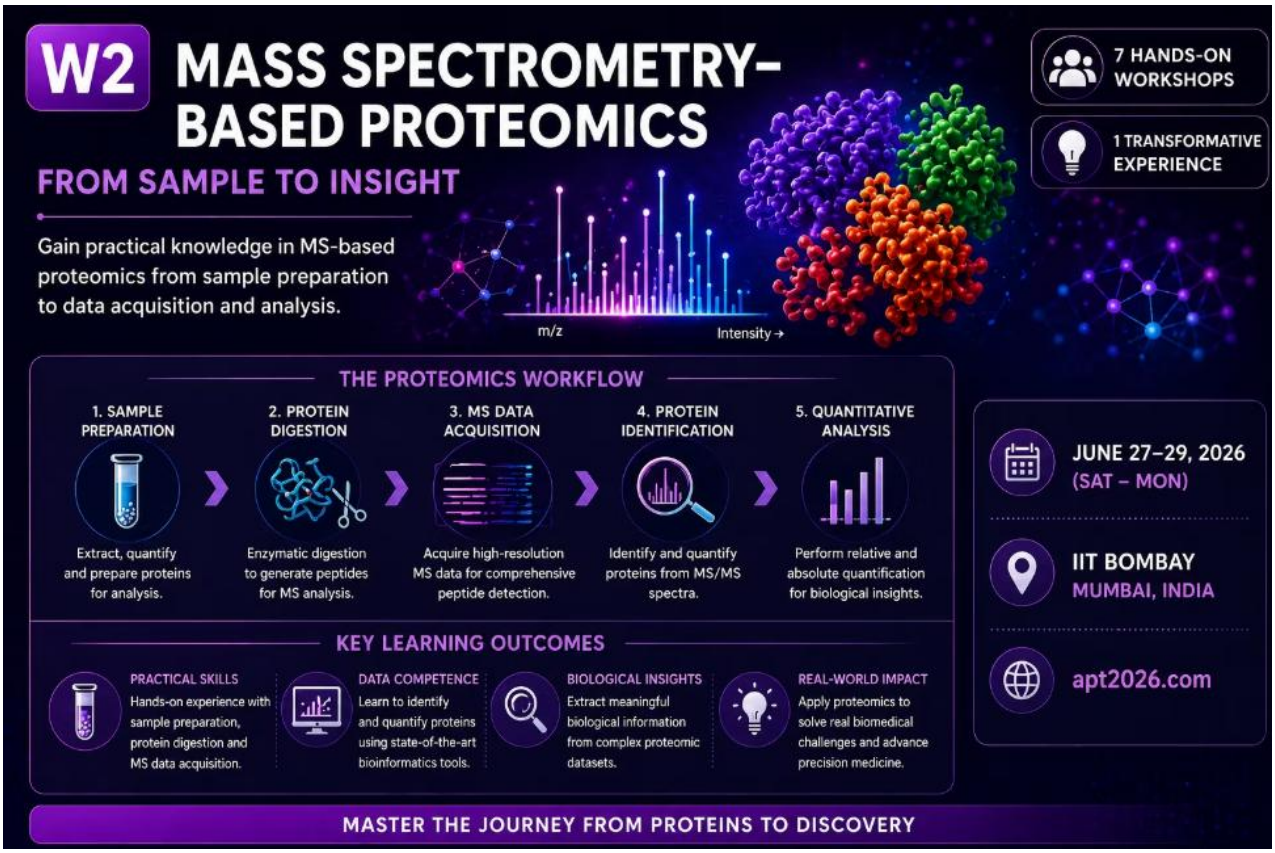
Designed for students, researchers, and early-career scientists, this workshop emphasizes both experimental workflows and data-driven analysis approaches that support biomarker discovery, systems biology, and precision medicine.

Key Learning Outcomes

- Hands-on understanding of MS-based proteomics workflows
- Knowledge of protein extraction and sample preparation techniques
- Understanding of high-resolution mass spectrometry data acquisition
- Skills in protein identification and quantitative analysis
- Introduction to Proteomics, Bioinformatics, and Data Interpretation
- Application of proteomics in biomedical and translational research

Why This Workshop Matters

- Builds strong foundational knowledge in proteomics technologies
- Enhances practical and analytical research skills
- Enables data-driven biological discoveries
- Supports applications in precision medicine and clinical research
- Provides exposure to real-world proteomics workflows and challenges



Mass Spectrometry-Based Proteomics

Principles · Instrumentation · Acquisition Strategies · Quantification · Bioinformatics · Applications

A comprehensive, in-depth guide spanning fundamental physics, instrumentation, experimental workflow, data analysis, and clinical and research applications of MS-based proteomics.

Chapter	Topics Covered
1. Foundations of Mass Spectrometry	What MS measures, ions and m/z, the three core components, why proteomics needs MS
2. Ionisation Techniques	ESI, nanoESI, MALDI; mechanism, strengths, and use cases of each
3. Mass Analysers	Quadrupole, ion trap, TOF, Orbitrap, FT-ICR, hybrid instruments, ion mobility (TIMS)
4. Tandem MS and Fragmentation	CID/HCD, ETD/EThcD, peptide fragmentation nomenclature, MS/MS and MSn
5. The Bottom-Up Proteomics Workflow	Sample prep, digestion, LC separation, MS acquisition, end-to-end protocol in detail
6. Acquisition Strategies: DDA, DIA, and Targeted MS	Principles, trade-offs, and clinical/research use of each acquisition mode
7. Quantification Strategies	Label-free, SILAC, TMT/iTRAQ, absolute quantification with isotope standards

8. Bioinformatics and Data Analysis	Database searching, FDR, software tools, spectral libraries, AI/deep learning in proteomics
9. Top-Down and Middle-Down Proteomics	Intact protein analysis, proteoforms, complementary role to bottom-up
10. Recent Technological Advances (2023-2026)	Orbitrap Astral, timsTOF Ultra/Ultra 2, PASEF/PAMAF, the $10 proteome
11. Applications for Researchers and Clinicians	Biomarker discovery, drug development, forensic science, microbiology, structural biology
12. Landmark Papers, Scientists, Timeline	Key literature, pioneering scientists, historical development

W 2.1: Foundations of Mass Spectrometry

Mass spectrometry (MS) is an analytical technique that measures the mass-to-charge ratio (m/z) of gas-phase ions. In proteomics, MS has become the dominant technology for identifying and quantifying proteins in complex biological samples, because it offers a combination of sensitivity, specificity, and throughput unmatched by any antibody-based or electrophoretic method. This chapter introduces the fundamental physical and instrumental principles that underlie every MS-based proteomics experiment, the foundation on which all subsequent chapters build.

1 What Does a Mass Spectrometer Actually Measure?

A mass spectrometer cannot weigh a molecule directly. Instead, it measures how a charged particle (an ion) behaves when accelerated through electric and/or magnetic fields, a behaviour that depends on the ratio of the ion's mass (m) to its charge (z), expressed as m/z. To be analysed, every molecule must satisfy two absolute requirements: it must exist in the gas phase, and it must carry an electrical charge. Both conditions are achieved in the ion source, the first major component of any mass spectrometer, through a process called ionisation (detailed in Chapter 2).

Once ionised, the gas-phase ions travel through a high vacuum (typically 10^{-6} to 10^{-10} torr) from the ion source, through the mass analyser (Chapter 3), to a detector. The vacuum is essential: at atmospheric pressure, ions would collide with air molecules and lose their charge or fragment uncontrollably before reaching the detector. The detector registers the arrival of ions and their relative abundance, and the resulting plot of ion abundance versus m/z is the mass spectrum, the fundamental data output of every MS experiment.

2 The Three Core Components of Every Mass Spectrometer

Component	Function	Common Examples in Proteomics
Ion Source	Converts analyte molecules into gas-phase ions without excessive fragmentation, preserving the molecular identity for downstream measurement	Electrospray Ionisation (ESI), nanoESI, Matrix-Assisted Laser Desorption/Ionisation (MALDI)
Mass Analyser	Separates ions according to their m/z ratio with a defined resolution and mass accuracy, the central determinant of an instrument's analytical power	Quadrupole, Ion Trap, Time-of-Flight (TOF), Orbitrap, FT-ICR, Trapped Ion Mobility (TIMS)
Detector	Registers the arrival of ions separated by the mass analyser and converts this into an electrical signal proportional to ion abundance	Electron multiplier, microchannel plate, image current detection (Orbitrap/FT-ICR)

3 Why Mass Spectrometry Transformed Proteomics

Before MS-based methods matured in the 1990s and 2000s, protein analysis relied predominantly on antibody-based methods (Western blotting, ELISA) and electrophoretic separation (2D-PAGE). These approaches are fundamentally limited: antibodies must be developed individually for each target protein, restricting analysis to pre-selected, hypothesis-driven panels, while 2D-PAGE, though capable of resolving thousands of protein spots, cannot directly identify the proteins it separates and offers poor quantitative reproducibility.

Mass spectrometry overcame both limitations. Coupled with the exponential growth of genome-derived protein sequence databases from the late 1990s onward, and the parallel development of sophisticated bioinformatics tools for interpreting fragmentation spectra,

MS enabled, for the first time, unbiased, high-throughput identification and quantification of thousands of proteins simultaneously from a single biological sample, without requiring any prior knowledge of which proteins might be present. This combination of unbiased discovery power and direct molecular specificity is what makes MS-based proteomics indispensable to modern biomedical research and is rapidly expanding its role in clinical diagnostics, drug discovery, and forensic science.

KEY CONCEPT: WHY MS HAS BOTH DISCOVERY AND VALIDATION ROLES

MS-based proteomics serves two distinct purposes that participants should clearly distinguish throughout this workshop. Discovery (or 'shotgun') proteomics aims for maximum, unbiased proteome coverage to generate hypotheses, identifying as many proteins as possible without preconception. Targeted proteomics measures a small, pre-defined panel of proteins with maximum precision and reproducibility, the mode required for biomarker validation and clinical assay development. The choice of ionisation source, mass analyser, fragmentation method, and acquisition strategy, covered throughout this document, is fundamentally shaped by which of these two goals a given experiment is designed to achieve.

W 2.2: Ionization Techniques

The development of 'soft' ionisation methods, techniques capable of converting large, fragile biomolecules into gas-phase ions without destroying their structure, was the single most important enabling breakthrough for MS-based proteomics. Two techniques dominate the field: Electrospray Ionisation (ESI) and Matrix-Assisted Laser Desorption/Ionisation (MALDI). Both were recognised with the 2002 Nobel Prize in Chemistry, awarded to John Fenn (ESI) and Koichi Tanaka (a precursor to MALDI), alongside Kurt Wüthrich for NMR-based protein structure determination.

1 Electrospray Ionization (ESI)

In ESI, a liquid sample (typically the eluent from a liquid chromatography column) is pumped through a narrow capillary held at high voltage (typically 1-5 kV) relative to a counter-electrode. The strong electric field at the capillary tip draws the liquid into a characteristic Taylor cone, which disperses into a fine spray of highly charged droplets. As the solvent evaporates (assisted by heated nitrogen gas and the vacuum interface), the droplets shrink and their surface charge density increases until Coulombic repulsion exceeds the surface tension holding the droplet together, causing it to undergo successive fission events (Coulomb fission) until naked, multiply charged gas-phase analyte ions are released.

Critically, ESI generates multiply charged ions for large molecules like peptides and proteins, a peptide of mass 2,000 Da might be observed at m/z 1,001 (2+ charge state), m/z 667.7 (3+ charge state), and so on. This multiple charging is what allows even very large intact proteins (hundreds of kilodaltons) to be measured within the practical m/z range of standard mass analysers, since the m/z value is reduced in proportion to the number of charges carried.

Nano-electrospray ionisation (nanoESI) is the dominant variant in modern proteomics, using extremely fine emitter capillaries (internal diameter of a few micrometres) operating at very low flow rates (20-500 nanolitres per minute). The smaller initial droplet size in nanoESI dramatically improves ionisation efficiency and sensitivity while reducing the sample volume required, properties that have made nanoESI coupled to nanoflow liquid chromatography (nanoLC-MS/MS) the standard configuration for modern bottom-up proteomics, particularly for the smaller, more precious sample amounts typical of clinical specimens and low-input biological material.

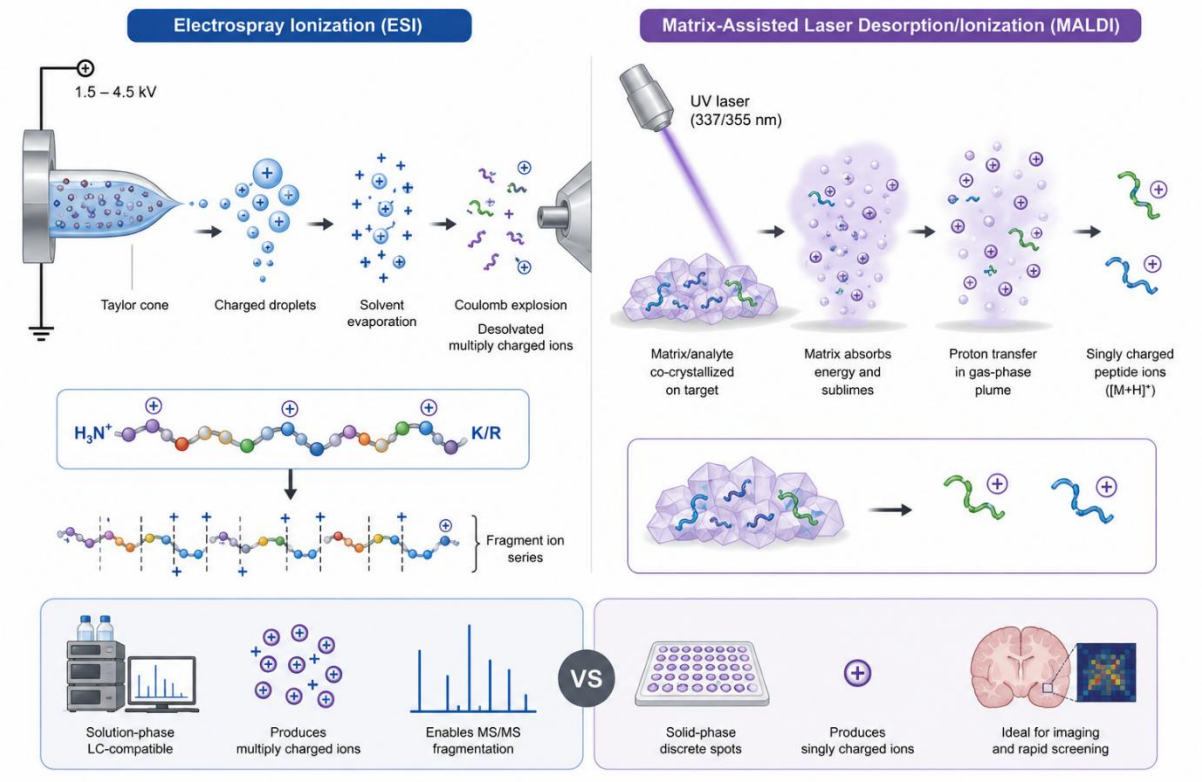


Figure 2.1. Comparison of ESI and MALDI ionization methods used in mass spectrometry-based proteomics.

2 Matrix-Assisted Laser Desorption/Ionization (MALDI)

In MALDI, the analyte is co-crystallised on a metal target plate with a large excess of a small organic 'matrix' molecule (commonly alpha-cyano-4-hydroxycinnamic acid, sinapinic acid, or 2,5-dihydroxybenzoic acid) that strongly absorbs energy at the wavelength of a pulsed laser (typically a nitrogen or Nd:YAG laser, 337 or 355 nm). When the laser pulse strikes the sample, the matrix absorbs the energy and rapidly vaporises, carrying intact analyte molecules into the gas phase along with it (desorption) while simultaneously transferring protons to the analyte (ionisation), generating predominantly singly charged ions, unlike the multiply charged ions typical of ESI.

MALDI is exceptionally fast (a single spectrum can be acquired in seconds), tolerant of moderately impure samples, and well suited to direct surface analysis. Its single major clinical success to date is rapid microbial species identification: an unknown bacterial or fungal colony from a patient sample is smeared directly onto a MALDI target plate, ionised, and the resulting protein mass spectral fingerprint (dominated by abundant ribosomal proteins) is matched against a reference library, providing species-level identification within minutes rather than the 24-48 hours required by traditional biochemical culture methods, a transformation now standard practice in clinical microbiology laboratories worldwide.

Property	ESI / nanoESI	MALDI
Sample state	Liquid (LC eluent)	Dried, co-crystallised solid
Charge states	Multiply charged ions (2+ to 50+ for proteins)	Predominantly singly charged ions
LC compatibility	Direct online coupling (LC-MS/MS)	Offline; samples spotted onto plate
Speed	Continuous, scales with LC gradient length	Very fast (seconds per spot)
Typical proteomics use	Bottom-up shotgun and targeted LC-MS/MS	Rapid microbial ID, tissue imaging (MALDI-IMS), high-throughput screening

W 2.3: Mass Analysers

The mass analyser determines an instrument's resolution (the ability to distinguish two ions of very similar m/z), mass accuracy (how close the measured mass is to the true mass), scan speed, and dynamic range. Modern proteomics instruments are almost always hybrid designs, combining two or more analyser types to leverage the complementary strengths of each.

1 Quadrupole

A quadrupole consists of four parallel metal rods to which oscillating radiofrequency (RF) and direct current (DC) voltages are applied. Only ions of a specific, selected m/z range achieve a stable trajectory through the device and reach the detector; all others collide with the rods and are lost. Quadrupoles offer relatively modest resolution but excellent speed, robustness, and quantitative precision, making them the analyser of choice for the precursor and fragment ion selection stages of triple quadrupole (QQQ) instruments used in targeted MRM/SRM quantification, and as the precursor-isolation component (Q1) in many hybrid instruments.

2 Ion Trap (Linear and 3D)

Ion traps confine ions within a defined spatial region using RF fields, either a 3D quadrupole ion trap or a linear (2D) ion trap. Trapped ions can be selectively ejected to the detector in order of increasing m/z, and critically, ion traps can perform multiple sequential rounds of fragmentation on a single trapped ion population (MS^n, multi-stage tandem MS), generating progressively more detailed structural information, valuable for de novo peptide sequencing, PTM site localisation, and complex small-molecule structural elucidation. Modern linear ion traps also serve as a fast, sensitive fragment-ion detector within hybrid Orbitrap instruments (the Orbitrap Tribrid series).

3 Time-of-Flight (TOF)

In a TOF analyser, ions are accelerated by a fixed electric field pulse and then travel through a field-free flight tube of known length toward the detector. Since all ions receive the same kinetic energy, lighter ions (lower m/z) travel faster and arrive at the detector sooner than heavier ions, and the precisely measured time-of-flight is directly related to the ion's m/z. TOF analysers offer very high scan speed (essential for the rapid, comprehensive fragmentation demanded by DIA acquisition, Chapter 6) and, in modern instruments, excellent resolution and mass accuracy, achieved partly through the use of an electrostatic 'reflectron' that compensates for small variations in ion kinetic energy. TOF is the analyser used in the Bruker timsTOF series and in MALDI-TOF microbial identification systems.

4 The Orbitrap

The Orbitrap, commercialised by Thermo Fisher Scientific from the mid-2000s and now the dominant high-resolution platform in proteomics, traps ions in stable orbits around a central spindle-shaped electrode using a combination of electrostatic attraction and the ions' own orbital angular momentum. Trapped ions oscillate axially along the spindle at a frequency precisely related to their m/z, and this oscillation induces a detectable image current in surrounding outer electrodes. Fourier transformation of this image current signal converts the time-domain oscillation data into the frequency domain and, from there, into a high-resolution mass spectrum.

Orbitrap analysers achieve extremely high mass resolution (commonly 60,000-500,000, defined as $m/\Delta m$ at a specified m/z) and mass accuracy typically better than 2-5 parts per million, properties that dramatically improve confident peptide identification, particularly in highly complex samples, and enable precise discrimination of isobaric or near-isobaric species, an essential capability for accurate isotope-labelled quantification methods such as TMT (Chapter 7).

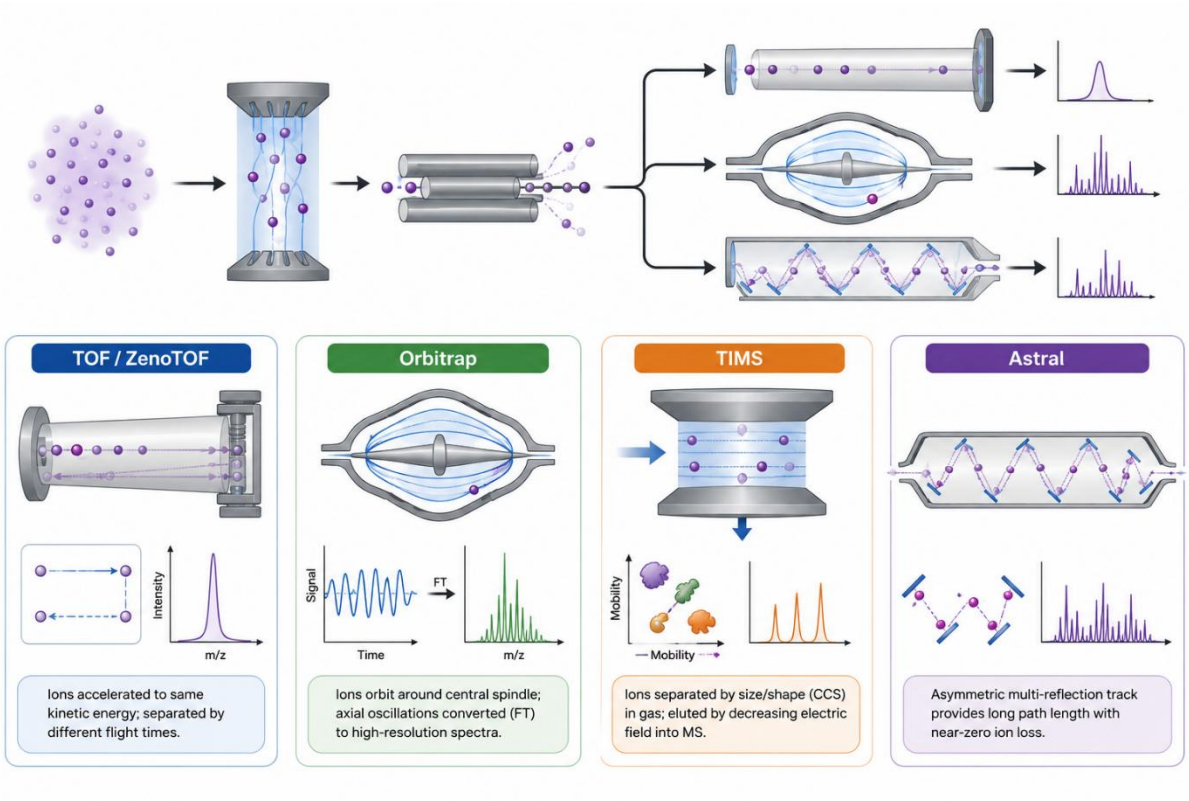


Figure 2.2. Schematic overview of major mass analyzers used in modern proteomics, including TOF, Orbitrap, TIMS, and Astral

5 Fourier Transform Ion Cyclotron Resonance (FT-ICR)

FT-ICR traps ions in a strong magnetic field (typically generated by a superconducting magnet, commonly 7-21 Tesla), where they orbit in circular cyclotron motion at a frequency inversely proportional to their m/z. As with the Orbitrap, this motion generates a detectable image current, Fourier-transformed into a mass spectrum. FT-ICR delivers the highest mass resolution and accuracy of any current mass analyser (resolution exceeding 1,000,000 is achievable), but the substantial capital cost, size, and slower scan speed of the superconducting magnet have limited its routine adoption in proteomics relative to the more practical Orbitrap, though it remains valuable for the most demanding applications in intact protein and top-down proteomics (Chapter 9).

6 Trapped Ion Mobility Spectrometry (TIMS): A Fourth Separation Dimension

Ion mobility spectrometry adds an entirely separate, gas-phase physical separation dimension to conventional MS, separating ions not by mass but by their collision cross section (CCS), their effective three-dimensional shape and size as they migrate through a buffer gas under the influence of an electric field. In Bruker's Trapped Ion Mobility Spectrometry (TIMS) implementation, ions are held stationary against an opposing gas flow by a ramped electric field, then released sequentially according to their mobility (and therefore their CCS) as the field strength is reduced. Because peptides with very similar or even identical m/z frequently differ in shape, ion mobility provides additional separation that resolves co-eluting isobaric or near-isobaric interferences before mass analysis, substantially improving both sensitivity and specificity, particularly valuable in highly complex samples and low-input applications such as single-cell and spatial proteomics.

The Parallel Accumulation-Serial Fragmentation (PASEF) method exploits TIMS by synchronising precursor ion accumulation with the TOF fragmentation duty cycle, achieving near-100% utilisation of all ions generated, a substantial sensitivity gain over conventional, largely wasteful duty cycles. The diaPASEF variant applies this principle within a DIA acquisition framework, systematically cycling through pre-defined isolation windows synchronised with ion mobility elution, the combination underlying the Bruker timsTOF SCP and timsTOF Ultra/Ultra 2 instrument families discussed in Chapter 10.

Property	Quadrupole	TOF	Orbitrap	FT-ICR
Typical resolution	~1,000-4,000	20,000-80,000	60,000-500,000	up to 1,000,000+
Mass accuracy	Low (unit mass)	<5 ppm	<2-5 ppm	<1 ppm
Scan speed	Very fast	Very fast	Moderate-fast (newer gens. faster)	Slow

Best suited for	Targeted MRM/SRM precursor/fragment selection	Fast DIA, MALDI-TOF, ion mobility coupling	Deep discovery DIA/DDA, accurate quantification	Ultra-high-resolution intact protein/top-down work

W 2.4: Tandem Mass Spectrometry and Peptide Fragmentation

Measuring the intact mass of a peptide (the MS1, or precursor ion, scan) is rarely sufficient to confidently identify which protein it originated from, since many different peptide sequences can share the same or very similar mass. The defining capability of modern proteomics, tandem mass spectrometry (MS/MS or MS2), isolates a specific precursor ion, deliberately fragments it into smaller pieces, and measures the masses of the resulting fragment ions. Because peptide bonds break at predictable positions and the masses of the 20 standard amino acids are precisely known, the pattern of fragment masses can be used to deduce the amino acid sequence of the original peptide with high confidence, the central principle underlying all modern protein identification by MS.

1 Peptide Fragmentation Nomenclature

By convention (the Roepstorff-Biemann nomenclature), when a peptide backbone fragments, the resulting ion is named according to which bond broke and which terminus of the peptide it retains. Fragments retaining the N-terminus are labelled a, b, or c ions; fragments retaining the C-terminus are labelled x, y, or z ions, with the letter indicating which of the three possible backbone bond types (Cα-C, C-N, or N-Cα) was cleaved. The specific fragment ion types observed depend entirely on the fragmentation method used, since different methods preferentially cleave different backbone bonds.

2 Collision-Induced Dissociation (CID) and Higher-Energy Collisional Dissociation (HCD)

Collision-Induced Dissociation (CID) accelerates the precursor ion and allows it to undergo multiple low-energy collisions with an inert collision gas (commonly helium or nitrogen), progressively converting kinetic energy into internal vibrational energy until the weakest bonds, predominantly the amide (peptide) backbone bonds, break. CID predominantly generates b and y ions and is efficiently performed within ion trap and quadrupole-based collision cells.

Higher-energy Collisional Dissociation (HCD) is a beam-type variant of CID performed in a dedicated collision cell (rather than within the ion trap itself), using higher collision energies that produce more complete and informative fragmentation spectra, including useful low-m/z fragment ions and a higher proportion of y-ions, while also enabling efficient simultaneous release of isobaric tag reporter ions (essential for TMT quantification, Chapter 7). HCD has become the dominant fragmentation method in modern proteomics due to its speed, compatibility with high-resolution Orbitrap detection of fragment ions, and excellent performance across both unmodified peptides and many post-translationally modified peptide classes, including glycopeptides.

3 Electron Transfer Dissociation (ETD) and EThcD

Electron Transfer Dissociation (ETD) fragments peptide precursor ions through a fundamentally different chemical mechanism: transfer of an electron from a radical anion reagent to the multiply charged peptide cation triggers rapid, radical-driven cleavage of the N-Cα backbone bond, generating predominantly c and z ions rather than the b/y ions typical of CID/HCD. Critically, ETD cleaves the peptide backbone while leaving labile post-translational modifications, particularly phosphorylation and O-linked glycosylation, intact and attached to the fragment ions, whereas CID/HCD frequently causes premature loss of these labile modifications before useful sequence information is obtained. This makes ETD (and its hybrid variant EThcD, which supplements ETD with a subsequent HCD activation step to improve fragmentation efficiency for lower charge-state ions) the method of choice for confident, site-specific localisation of phosphorylation sites and characterisation of intact glycopeptides.

4 MS^n: Multi-Stage Tandem MS

Ion trap-based instruments can perform sequential rounds of isolation and fragmentation on the products of a previous fragmentation step (MS3, MS4, and so on, collectively MS^n), generating progressively more detailed structural information about a specific fragment of interest. MS3 has also found an important quantitative application: in TMT-based multiplexed quantification, performing an additional fragmentation step that isolates only the reporter-ion-containing fragment before quantification (real-time-search-triggered MS3) substantially reduces the ratio compression artefact that otherwise distorts quantitative accuracy when reporter ions are measured directly from a co-isolated, interference-prone MS2 spectrum.

PRACTICAL NOTE FOR WORKSHOP PARTICIPANTS

When designing an MS/MS experiment, the choice of fragmentation method should be matched to the analytical goal: HCD for standard unmodified peptide identification and TMT-based quantification (the default for the large majority of discovery proteomics experiments); ETD/EThcD when confident, site-specific localisation of phosphorylation or glycosylation is the primary objective; and CID when working with

older or specialised ion-trap-centric instrument configurations. Many modern instruments allow rapid switching between fragmentation methods within a single LC-MS/MS run, enabling hybrid strategies tailored to specific peptide classes.

W 2.5: The Bottom-Up Proteomics Workflow, Step by Step

The vast majority of MS-based proteomics experiments use the bottom-up (or 'shotgun') strategy: intact proteins are enzymatically digested into peptides before MS analysis, and the identified peptides are computationally mapped back to their parent proteins. This chapter walks through the complete experimental pipeline in detail.

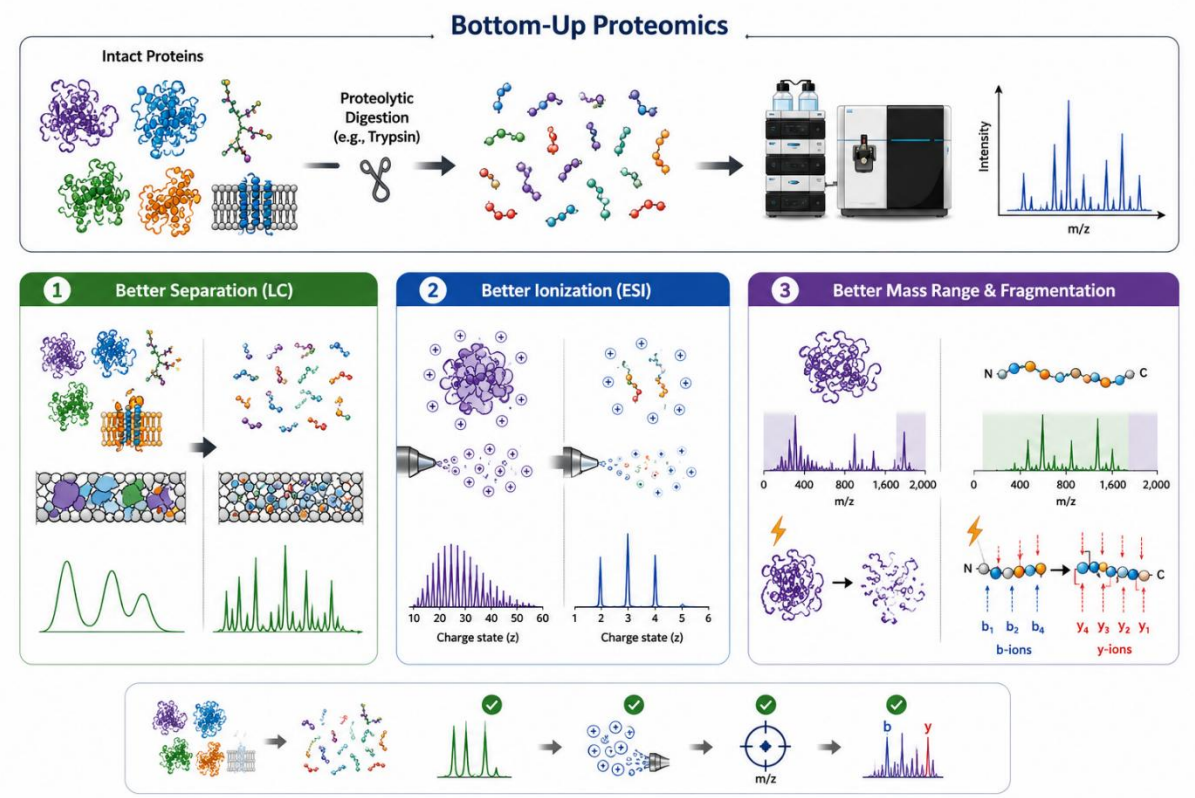


Figure 2.3. Bottom-up proteomics converts proteins into peptides for efficient separation, ionization, and mass spectrometric analysis.

Step 1: Sample Collection and Protein Extraction

Biological material (cultured cells, tissue, biofluid) is lysed to release proteins, typically using a buffer containing a strong denaturing detergent (SDS, urea, or guanidine hydrochloride) or, increasingly, chaotropic-free methods compatible with downstream mass spectrometry, combined with protease and phosphatase inhibitors to prevent unwanted protein degradation or modification loss during processing. Protein concentration is then quantified (BCA or Bradford assay) to ensure equal protein input across all samples being compared, a critical step for valid quantitative comparison.

Step 2: Reduction and Alkylation of Cysteines

Disulfide bonds between cysteine residues are reduced using dithiothreitol (DTT) or tris(2-carboxyethyl)phosphine (TCEP), unfolding the protein's tertiary structure and exposing internal regions to subsequent enzymatic digestion. The resulting free thiol groups are then alkylated, most commonly with iodoacetamide, to form a stable carbamidomethyl modification that prevents disulfide bonds from re-forming and ensures consistent, reproducible cysteine behaviour during downstream MS analysis.

Step 3: Proteolytic Digestion

Proteins are enzymatically cleaved into peptides, almost universally using trypsin, which cleaves specifically C-terminal to lysine (K) and arginine (R) residues (except when followed by proline). Trypsin is favoured because its high specificity generates peptides of an ideal average length (around 8-25 amino acids) for confident MS/MS sequencing, and because the resulting peptides carry a strongly basic residue at the C-terminus, promoting efficient, predictable multiple charging during ESI. Alternative or complementary

proteases, including Lys-C (cleaves only after lysine), chymotrypsin (cleaves after aromatic residues), and Glu-C, are used to improve sequence coverage of specific regions or proteins poorly covered by tryptic digestion alone. Digestion typically proceeds at 37 degrees C for 4-16 hours.

Step 4: Sample Cleanup and Desalting

Following digestion, samples are desalted and concentrated, most commonly using reversed-phase C18 solid-phase extraction (StageTips or 96-well plate formats), removing salts, detergents, and other contaminants that would otherwise suppress ionisation efficiency or contaminate the LC-MS system. This step is also where samples may be split for fractionation, or where isobaric labelling reagents (TMT, Chapter 7) are introduced and combined into a single multiplexed sample.

Step 5: Liquid Chromatographic Separation

Peptide mixtures are far too complex to be directly and comprehensively analysed by MS alone, even the most modern instruments cannot adequately resolve and fragment the tens of thousands of distinct peptides present in a typical proteomic sample without prior separation. Reversed-phase nanoflow liquid chromatography (nanoLC), using C18-functionalised silica or polymer particles packed into narrow-bore columns (50-150 micrometre internal diameter), separates peptides based on hydrophobicity over a gradient of increasing organic solvent (typically acetonitrile) concentration, spreading peptide elution over a window of typically 20-180 minutes and dramatically reducing the number of distinct peptide species the mass spectrometer must contend with at any given moment, directly improving both identification depth and quantitative accuracy.

Step 6: Online ESI-MS/MS Acquisition

The LC column effluent is directly electrosprayed into the mass spectrometer (Chapter 2) as it elutes. The instrument continuously acquires MS1 survey scans recording the intact mass of all eluting precursor ions, interspersed with MS2 fragmentation scans of selected precursors (Chapter 4), according to the chosen acquisition strategy (DDA, DIA, or targeted, Chapter 6). This entire acquisition process, fully automated, typically takes between 10 minutes (high-throughput, low-input applications) and several hours (deep, comprehensive discovery proteomics) per sample.

Step 7: Database Searching and Protein Identification

The raw mass spectral data is computationally matched against a reference protein sequence database (commonly UniProt, digested in silico according to the same enzyme specificity used experimentally) using a database search engine, to identify which peptide sequence most plausibly explains each observed fragmentation spectrum. This critical bioinformatics step is described in full detail in Chapter 8.

SAMPLE PREPARATION INNOVATION: SINGLE-POT WORKFLOWS

A major recent advance in sample preparation is the adoption of single-pot, solid-phase-enhanced sample preparation (SP3) and related bead-based workflows (Hughes et al., Nature Protocols, 2019), which use paramagnetic beads to capture, wash, and process proteins through reduction, alkylation, and digestion entirely within a single reaction vessel without intermediate transfer steps. These approaches dramatically reduce sample loss, are readily automatable for high-throughput studies, and have become the standard preparation method underlying both clinical-scale cohort studies and low-input applications including single-cell and spatial proteomics.

W 2.6: Acquisition Strategies: DDA, DIA, and Targeted MS

1 Data-Dependent Acquisition (DDA)

In DDA, the traditional and still widely used 'shotgun' approach, the instrument performs an MS1 survey scan, automatically ranks the detected precursor ions by abundance, and selects the most intense ions (commonly the top 10-40, 'Top-N' DDA) for sequential MS2 fragmentation before returning to acquire the next MS1 survey scan. A dynamic exclusion list temporarily prevents the same precursor from being repeatedly re-selected, allowing lower-abundance co-eluting ions their turn at fragmentation. DDA is conceptually simple, computationally straightforward to analyse (each MS2 spectrum is matched independently to a database), and remains an excellent choice for deep, comprehensive discovery experiments and for building the spectral libraries used by some DIA analysis workflows.

However, DDA's stochastic, abundance-ranked precursor selection means that lower-abundance peptides may be selected for fragmentation in one analytical run but missed entirely in a technical replicate, generating substantial missing values when comparing

many samples, a significant limitation for large-cohort clinical and population studies where consistent quantification of the same proteins across hundreds of samples is essential.

2 Data-Independent Acquisition (DIA)

DIA was developed specifically to solve DDA's missing-value problem. Rather than selecting individual precursors, the instrument systematically and repeatedly fragments all precursor ions within a series of predefined, sequential mass windows (for example, 400-425 m/z, then 425-450 m/z, and so on) spanning the full mass range of interest, in every single acquisition cycle, regardless of precursor abundance. Because every peptide present in the sample is fragmented in every analytical run, DIA generates comprehensive, highly reproducible quantitative data with dramatically lower missing-value rates than DDA, the property that has made DIA the preferred acquisition mode for large clinical cohort and population-scale proteomic studies (as discussed extensively in the companion Clinical Proteomics workshop material).

The trade-off is data complexity: because multiple precursors are co-fragmented within each wide isolation window, the resulting MS2 spectra are highly convoluted mixtures of fragment ions from many different peptides simultaneously, requiring specialised computational deconvolution against a spectral library (either experimentally generated or computationally predicted) rather than the straightforward one-spectrum-one-peptide matching used in DDA. SWATH-MS (Sequential Window Acquisition of all Theoretical fragment ion spectra Mass spectra), pioneered by Aebersold's group in 2012, was the first widely adopted practical implementation of this DIA principle and remains foundational terminology in the field.

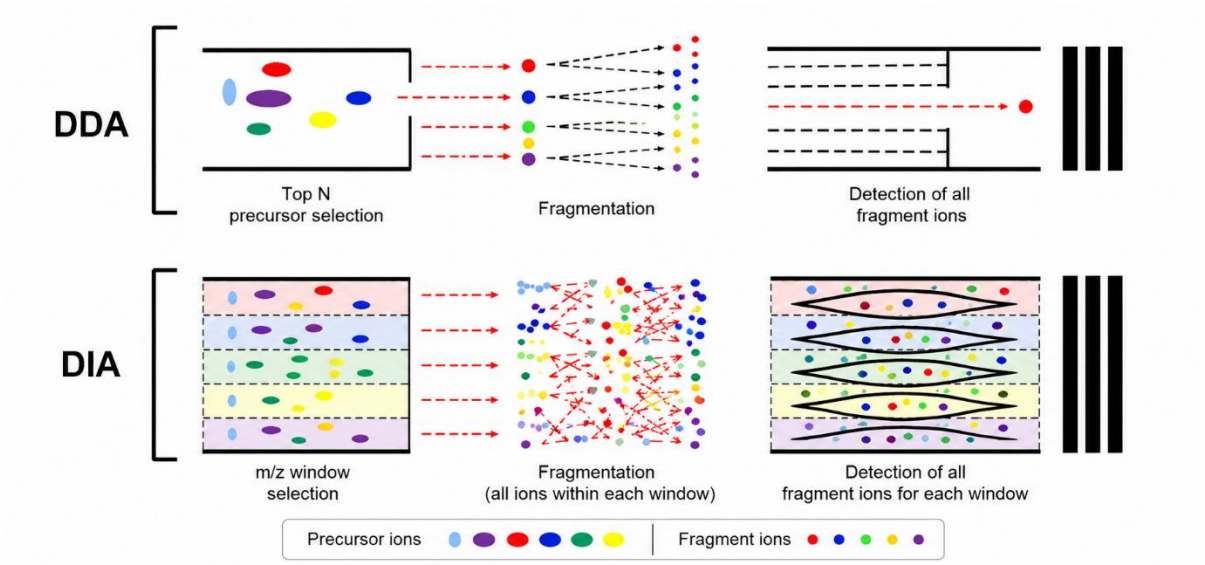


Figure 2.4. Comparison of DDA and DIA acquisition strategies for peptide identification and quantification in proteomics.

3 Targeted MS: MRM, SRM, and PRM

For applications requiring the highest possible precision and reproducibility on a small, pre-selected panel of proteins, rather than broad discovery coverage, targeted MS is the gold standard. Multiple/Selected Reaction Monitoring (MRM/SRM), performed on triple quadrupole instruments, continuously monitors a defined list of specific precursor-to-fragment ion transitions throughout the LC gradient, while Parallel Reaction Monitoring (PRM), performed on high-resolution instruments such as Orbitraps, monitors the complete high-resolution fragment ion spectrum for each targeted precursor rather than just one or two transitions. Both approaches typically incorporate stable isotope-labelled synthetic peptide standards, spiked into every sample at a known concentration, enabling rigorous absolute quantification by comparing the response of the labelled standard to the unlabelled endogenous peptide.

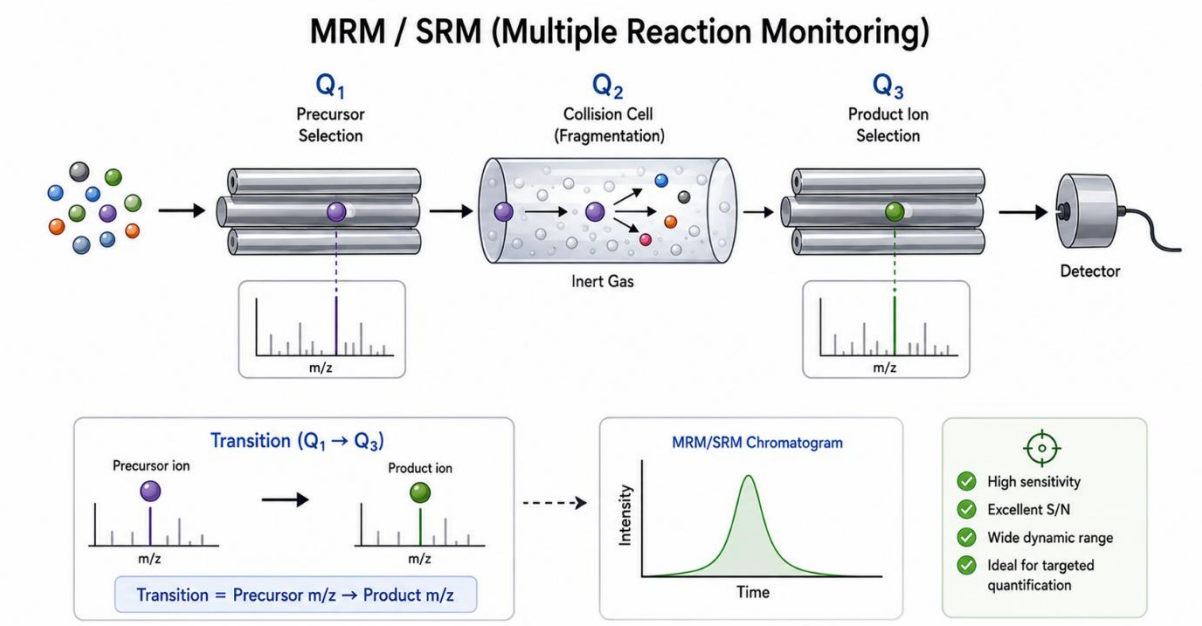


Figure 2.5. MRM/SRM selectively monitors predefined precursor-to-fragment ion transitions for highly sensitive targeted quantification.

Property	DDA	DIA	Targeted (MRM/PRM)
Precursor selection	Abundance-ranked, stochastic	All precursors, systematic	Pre-defined target list only
Proteome coverage	Broad, unbiased discovery	Broad, unbiased discovery	Narrow, defined panel only
Missing values	Higher (run-to-run variable)	Low (comprehensive every cycle)	Minimal (targeted, optimised)
Quantitative precision	Moderate	Good	Excellent (gold standard)
Data analysis complexity	Lower (1 spectrum = 1 ID)	Higher (requires spectral library/deconvolution)	Lower (pre-defined transitions)
Best use case	Deep discovery, spectral library building	Large cohort studies, reproducible quantification	Biomarker validation, regulated clinical assays

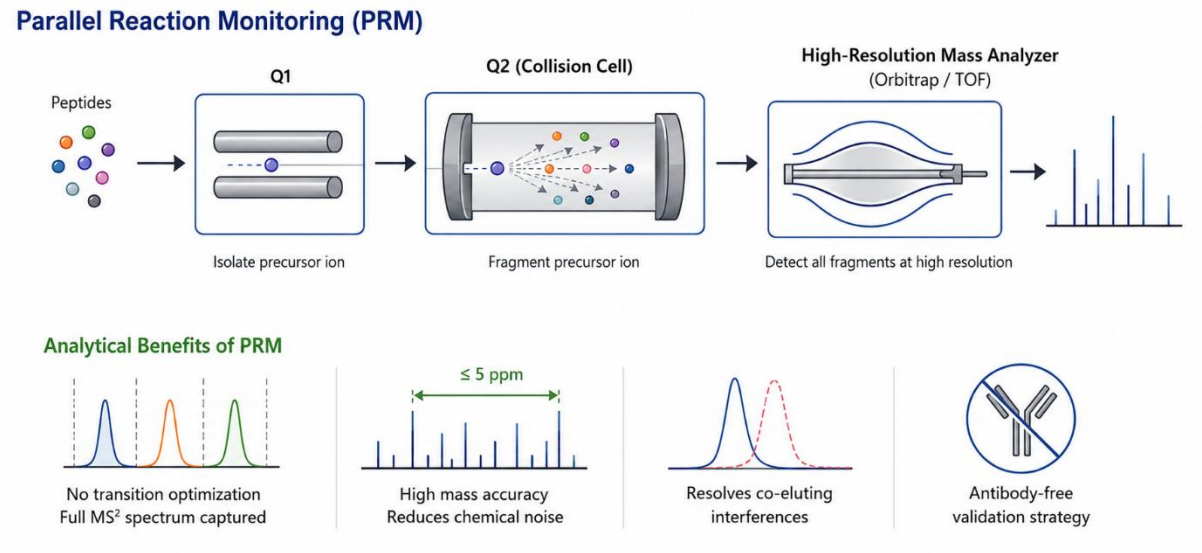


Figure 2.6. PRM enables targeted peptide quantification by capturing complete high-resolution fragment ion spectra.

W 2.7: Quantification Strategies

1 Label-Free Quantification (LFQ)

Label-free quantification compares the MS1 precursor ion signal intensity (peak area or peak height, extracted ion chromatogram, XIC) of the same peptide across separately acquired LC-MS/MS runs, without any chemical or metabolic labelling. The MaxLFQ algorithm (Cox et al., 2014) is the most widely used implementation, normalising and aggregating peptide-level intensities into robust protein-level quantitative values across an arbitrary number of samples. LFQ is the simplest, cheapest, and most flexible quantification strategy, requiring no additional reagents or sample preparation steps, and scales readily to very large sample numbers, but achieves somewhat lower precision than labelled methods because each sample is measured in a fully independent LC-MS/MS run, introducing run-to-run technical variability that labelled multiplexing approaches avoid.

2 Metabolic Labelling: SILAC

Stable Isotope Labelling by Amino acids in Cell culture (SILAC) introduces quantitative isotope labels metabolically, by culturing cells in medium containing 'heavy' isotope-substituted essential amino acids (commonly 13C/15N-labelled lysine and arginine) versus normal 'light' amino acids. After several cell divisions, newly synthesised proteins fully incorporate the heavy or light label according to which medium the cells were grown in. Differentially labelled cell populations (e.g., treated versus untreated) are then combined at the protein level before any further processing, ensuring that both conditions experience absolutely identical sample preparation, digestion, and LC-MS/MS analysis, eliminating nearly all technical variability between the compared conditions, since they are physically the same sample from the point of mixing onward. SILAC's principal limitation is that it requires actively dividing cells in culture and cannot be applied directly to primary clinical tissue, biofluids, or non-dividing cell populations.

3 Chemical Isobaric Labelling: TMT and iTRAQ

Tandem Mass Tag (TMT) and Isobaric Tag for Relative and Absolute Quantification (iTRAQ) reagents are chemical labels applied after protein digestion, reacting with free amines (peptide N-termini and lysine side chains) to covalently attach an isobaric tag, multiple differently labelled samples share an identical total mass at the MS1 level (hence 'isobaric') but, upon HCD fragmentation, each tag releases a distinct, quantifiable low-mass reporter ion (commonly in the m/z 126-135 range for TMT). This allows up to 18 samples (TMTpro 18-plex) to be combined and analysed together in a single LC-MS/MS run, with relative quantification derived directly from the reporter ion intensities in each MS2 spectrum.

TMT's principal advantage is dramatically increased throughput, since all samples in a multiplexed set undergo essentially identical LC-MS/MS analysis simultaneously, alongside excellent data completeness (every peptide identified is quantified across all channels). Its principal limitation is ratio compression: co-isolated, interfering peptides from other proteins contribute additional reporter ion signal at the MS2 level, systematically compressing measured fold-changes toward 1 and reducing quantitative accuracy. This artefact can be substantially mitigated using narrower precursor isolation windows, additional gas-phase ion mobility separation, or real-time-search-triggered MS3 quantification, which fragments only the isolated reporter-ion-bearing fragment from MS2, removing the interfering co-isolated species before reporter ion measurement.

4 Absolute Quantification with Isotope-Labelled Standards

For applications requiring true absolute protein concentration (rather than relative fold-change between samples), most notably clinical biomarker assays, synthetic, stable isotope-labelled peptide standards corresponding to specific target peptides are synthesised at known purity and spiked into every sample at a precisely known concentration before or during sample preparation. Because the labelled standard and the endogenous unlabelled peptide are chemically identical except for a small, well-defined mass shift, they co-elute and ionise identically, but can be distinguished and separately quantified by MS. Comparing the measured signal ratio of endogenous-to-labelled-standard peptide directly yields the absolute concentration of the target protein in the original sample, the quantitative rigour required for regulatory-grade clinical assay validation (as detailed in the Clinical Proteomics workshop material).

CHOOSING A QUANTIFICATION STRATEGY

Label-free (LFQ): best for flexible, low-cost, large-cohort discovery studies where absolute throughput and simplicity matter most. SILAC: best for cell culture-based mechanistic studies demanding the highest achievable quantitative precision. TMT/iTRAQ: best for multiplexed comparison of many conditions or samples in tissue or clinical specimens not amenable to metabolic labelling, prioritising throughput. Isotope-labelled standards with targeted MS: mandatory for absolute, regulatory-grade clinical biomarker quantification.

W 2.8: Bioinformatics and Data Analysis

1 Database Searching: How Spectra Become Protein Identifications

Database search engines (including SEQUEST, Mascot, Andromeda within MaxQuant, and MSFragger within FragPipe) computationally digest a reference protein sequence database in silico using the same enzyme specificity applied experimentally, predict the theoretical fragment ion masses for every resulting candidate peptide, and score how well each candidate peptide's predicted fragmentation pattern matches each experimentally observed MS2 spectrum. The candidate with the best-scoring match is reported as the peptide identification for that spectrum, and identified peptides are subsequently mapped back to their parent proteins.

2 False Discovery Rate (FDR) Control: The Target-Decoy Approach

Because database searching inevitably generates some incorrect matches purely by chance, particularly given the very large number of candidate peptides being compared against each spectrum, rigorous statistical control of the false discovery rate is essential. The near-universal solution is the target-decoy strategy: alongside the genuine ('target') protein database, a decoy database is searched simultaneously, typically generated by reversing or randomly scrambling each target protein sequence, generating peptides that share the same length and amino acid composition statistics as real peptides but that cannot represent genuine biological sequences. Because decoy matches arise purely from random chance, the number of decoy hits at a given score threshold directly estimates the number of incorrect target hits expected at that same threshold, allowing a score cutoff to be set that achieves a defined, acceptable FDR, conventionally 1% at the peptide and protein level for publication-quality proteomics data.

3 DIA-Specific Analysis: Spectral Libraries and Library-Free Search

Because DIA MS2 spectra contain co-fragmented signal from multiple precursors simultaneously, DIA data analysis software (including Spectronaut, DIA-NN, and Skyline) matches the complex DIA spectra against a spectral library, a reference catalogue of the expected retention time, precursor mass, and characteristic fragment ion pattern for every peptide of interest. Spectral libraries can be generated experimentally (running representative samples in DDA mode first to empirically characterise the proteome) or, increasingly, predicted entirely in silico using deep learning models (such as those underlying DIA-NN) trained on large compendia of previously observed peptide spectra, eliminating the need for time-consuming experimental library generation and enabling fully 'library-free' DIA analysis directly from the DIA data itself.

4 Machine Learning and Deep Learning in Modern Proteomics Software

Machine learning is now deeply integrated throughout the proteomics computational pipeline. Deep neural networks predict peptide retention time, fragment ion intensity patterns, and collision cross section purely from amino acid sequence (tools including Prosit and AlphaPeptDeep), substantially improving both spectral library prediction accuracy for DIA analysis and confidence scoring for peptide identification. A 2024 Journal of Proteome Research study demonstrated that deep learning models can predict protein identity directly from precursor MS1 information alone, illustrating the continued rapid pace of computational innovation in the field. Machine learning classifiers (commonly gradient boosting and random forest models implemented in tools such as Percolator) also routinely re-score and refine initial database search results, extracting substantially more confident identifications from the same underlying raw spectral data than the original search engine score alone would support.

5 Essential Software Tools for Proteomics Data Analysis

Tool	Primary Function	Notes
MaxQuant	DDA and DIA database search, quantification (MaxLFQ)	Free, widely adopted academic standard; Andromeda search engine built in
FragPipe (MSFragger)	Ultra-fast, open database search engine for DDA and DIA	Exceptional speed; strong support for PTM and open searching
Spectronaut	Commercial DIA analysis platform	Industry-standard for clinical and pharma DIA workflows
DIA-NN	Free, deep learning-powered DIA analysis	State-of-the-art library-free DIA search; widely cited in 2023-2025 literature
Skyline	Targeted MS data processing (MRM/PRM/DIA)	Free, widely used for targeted assay development and clinical validation
Perseus	Downstream statistical analysis and visualisation	Companion tool to MaxQuant for differential expression and pathway analysis

W2.9: Top-Down and Middle-Down Proteomics

While bottom-up proteomics (Chapter 5) dominates the field due to its scalability and throughput, it has an important inherent limitation: by digesting proteins into short peptides before analysis, information about which specific combination of modifications and sequence variants co-occurred on the same original intact protein molecule, the proteoform, is lost. A single gene can give rise to many distinct proteoforms through alternative splicing, sequence variation, and combinatorial post-translational modification, and two proteoforms that differ functionally may generate an identical set of tryptic peptides, making them indistinguishable by standard bottom-up analysis.

Top-down proteomics addresses this limitation by analysing intact, undigested proteins directly by MS, preserving complete proteoform-level information. Intact proteins are ionised (typically by ESI, generating extensively multiply charged ions, particularly valuable since charge reduction simplifies the resulting complex spectra), and fragmented using specialised methods, predominantly ETD or ultraviolet photodissociation (UVPD), that can effectively cleave large, intact protein backbones. Top-down analysis demands exceptionally high mass resolution and accuracy (commonly provided by Orbitrap or FT-ICR analysers) to resolve the very closely spaced isotope peaks and charge states characteristic of large intact protein spectra, and remains technically more challenging, lower-throughput, and generally restricted to less complex samples (purified proteins or simpler mixtures) than bottom-up analysis.

Middle-down proteomics occupies an intermediate position, using highly specific proteases or limited digestion to generate larger peptide fragments (typically 3-20 kDa, substantially larger than standard tryptic peptides but smaller than intact proteins), balancing some of the proteoform-level information retention of top-down analysis against improved throughput and reduced spectral complexity relative to full intact protein analysis, an approach particularly valuable for characterising combinatorial histone modifications and antibody proteoforms.

W2.10: Recent Technological Advances (2023-2026)

Mass spectrometry-based proteomics is approximately 35 years old as a discipline, but the pace of technological progress has accelerated dramatically over the past two to three years, with new instrument generations delivering step-change improvements in depth, sensitivity, and throughput that are actively reshaping what is analytically achievable for both research and clinical applications.

1 The Orbitrap Astral

The Orbitrap Astral mass spectrometer, introduced by Thermo Fisher Scientific, combines a conventional Orbitrap mass analyser with a novel Asymmetric Track Lossless (Astral) analyser for fragment ion detection, dramatically increasing MS2 scan speed (enabling far narrower, more specific DIA isolation windows without sacrificing throughput) while retaining high resolution. Independent benchmarking published in the Journal of Proteome Research (2026) reported that the Orbitrap Astral quantified over 225,000 peptides and approximately 13,000 proteins from complex tissue samples, representing roughly an 800% increase in proteome depth compared to a conventional Orbitrap Exploris 480 operating in DDA mode. For TMT-based multiplexed quantification specifically, the Orbitrap Astral has demonstrated a 50% sensitivity improvement at the peptide level and 20% at the protein level relative to previous-generation Orbitrap Tribrid platforms, while quantifying over 10,000 human proteins per sample within a single hour of analysis time.

2 timsTOF Ultra and timsTOF Ultra 2

Bruker's timsTOF Ultra and second-generation timsTOF Ultra 2 instruments combine enhanced TIMS ion mobility separation (Chapter 3.6) with improved TOF detection and the diaPASEF acquisition method, achieving proteome depth and sensitivity directly competitive with the Orbitrap Astral. The same 2026 Journal of Proteome Research benchmarking study reported that timsTOF Ultra delivered approximately 300% greater proteome depth than conventional DDA, with strong sample-wise quantitative correlation (Pearson r approximately 0.87) between the two next-generation platforms (Orbitrap Astral and timsTOF Ultra), indicating that both instrument families now deliver broadly comparable, complementary analytical capability at the current technological frontier, with method and software-specific differences in peptide and protein identification, rather than fundamentally different quantitative information.

3 PAMAF: A New Acquisition Paradigm

Recent innovations in ion mobility-enabled acquisition, exemplified by the PAMAF (Parallel Accumulation with Multiple Activation and Fragmentation) mode of operation, exploit high-resolution ion mobility separation to achieve fragmentation rates exceeding 1,000 Hz, delivering the data completeness traditionally associated with DIA acquisition while retaining the high-quality, less convoluted fragmentation spectra traditionally associated with DDA. This convergence of previously distinct acquisition paradigms reflects a broader trend: the historical sharp distinction between DDA and DIA is progressively blurring as instrument speed and resolving power continue to increase, with newer acquisition modes selectively combining the complementary advantages of each.

4 Toward the $10 Proteome: Cost and Throughput Innovations

A 2025 study from Ryan Kelly's group at Brigham Young University (bioRxiv, 2025) systematically demonstrated that combining simplified, originally single-cell-proteomics-derived sample preparation methods (effective down to approximately 50 nanograms of

protein, equivalent to a few hundred cells), a standardised, limited menu of LC-MS acquisition settings (eliminating time-consuming per-study optimisation), the latest-generation high-performance instruments (Orbitrap Astral or timsTOF Ultra/Ultra 2) operated with short, approximately 10-minute run times, and fully automated data processing, can reduce the practical per-sample cost of deep, quantitative proteome profiling to approximately ten US dollars, a roughly tenfold to fortyfold reduction compared to typical historical per-sample costs of hundreds of dollars. This cost reduction directly enables proteomic analysis at the sample numbers required for genuinely population-scale clinical and epidemiological studies, an essential prerequisite for the kind of large-cohort plasma proteomics described in the companion Clinical Proteomics workshop material.

IMPLICATION FOR THE FIELD

The combination of next-generation instrumentation (Orbitrap Astral, timsTOF Ultra 2), simplified low-input sample preparation, and streamlined, automated acquisition and analysis pipelines is rapidly collapsing the historical trade-off between proteome depth and sample throughput. Experiments that required hours of acquisition time and hundreds of dollars per sample only three to four years ago can now frequently be achieved in approximately ten minutes for approximately ten dollars per sample, while achieving substantially greater proteome depth. This shift is the single most important recent technological development underpinning the expansion of MS-based proteomics into genuinely large-scale clinical, population, and single-cell applications.

W 2.11: Applications for Researchers and Clinicians

1 Biomarker Discovery and Clinical Diagnostics

MS-based proteomics underpins the entire modern biomarker discovery-to-clinic pipeline, detailed extensively in the companion Clinical Proteomics workshop material, spanning discovery-phase DIA profiling of clinical cohorts, verification using targeted PRM panels, and validation-phase absolute quantification with isotope-labelled standards for regulatory submission. Applications span oncology (CPTAC proteogenomic cancer characterisation), cardiology, neurology, rare and genetic disease screening, and infectious disease, with MALDI-TOF microbial identification already standard practice in clinical microbiology.

2 Drug Discovery and Pharmaceutical Research

MS-based chemoproteomics and activity-based protein profiling identify the direct protein targets and off-target binding partners of candidate drug molecules, essential for understanding mechanism of action and predicting toxicity early in development. Thermal proteome profiling and related techniques measure drug-induced changes in protein thermal stability across the proteome to map target engagement directly in cells or tissue. TMT-based multiplexed quantification (Chapter 7) is particularly valuable in this context, enabling dozens of drug concentrations, time points, or candidate compounds to be compared within a single, internally consistent experiment.

3 Forensic Science

MS-based proteomics is an emerging molecular tool for forensic biological evidence analysis, offering advantages over traditional DNA-based methods in specific contexts, including the analysis of highly degraded samples (proteins can be more chemically stable than DNA under certain environmental conditions), tissue and body fluid identification through tissue-specific protein markers, and species identification from biological trace evidence, with growing application particularly where genetic material is absent, degraded, or uninformative.

4 Structural Biology

Beyond conventional sequence identification, MS-based structural proteomics methods, including cross-linking mass spectrometry (XL-MS), hydrogen-deuterium exchange MS (HDX-MS), and native MS of intact protein complexes, provide structural and conformational information about proteins and protein assemblies, complementing traditional structural techniques (X-ray crystallography, cryo-EM, NMR) and offering particular advantages for studying large, dynamic, or heterogeneous protein complexes that resist conventional structural methods.

5 Microbiology and Infectious Disease

As detailed in Chapter 2, MALDI-TOF-based microbial species identification is the most widely deployed routine clinical application of MS-based proteomics today. Beyond species identification, MS-based proteomics is increasingly applied to antimicrobial resistance

detection (identifying resistance-conferring enzymes or structural protein modifications directly from clinical isolates) and to host-pathogen interaction studies characterising the protein-level immune response to infection.

W2.12: Landmark Research Papers

The following papers span the historical foundations and the most significant recent technical contributions to MS-based proteomics.

Fenn JB, Mann M, Meng CK, Wong SF & Whitehouse CM | Science, 1989 | DOI: 10.1126/science.2675315

Electrospray Ionization for Mass Spectrometry of Large Biomolecules

The foundational paper establishing electrospray ionisation as a practical method for generating gas-phase ions from large, fragile biomolecules including proteins and peptides. Fenn was awarded the 2002 Nobel Prize in Chemistry for this work, which together with MALDI made modern protein mass spectrometry possible.

Aebersold R & Mann M | Nature, 2003 (updated 2016) | DOI: 10.1038/nature01511

Mass spectrometry-based proteomics

The most highly cited review establishing the conceptual and technical framework of modern MS-based proteomics, covering ionisation, fragmentation, database searching, and quantification. An essential foundational reference for the entire field, regularly updated to reflect the discipline's continued evolution.

Cox J & Mann M | Nature Biotechnology, 2008 | DOI: 10.1038/nbt.1511

MaxQuant enables high peptide identification rates, individualized p.p.b.-range mass accuracies and proteome-wide protein quantification

Introduced MaxQuant, the most widely adopted free academic software platform for proteomics data analysis, alongside the Andromeda search engine and the MaxLFQ label-free quantification algorithm. Fundamentally democratised access to rigorous, high-quality proteomics data analysis for laboratories worldwide.

Gillet LC, Navarro P, Tate S et al. | Molecular & Cellular Proteomics, 2012 | DOI: 10.1074/mcp.O111.016717

Targeted Data Extraction of the MS/MS Spectra Generated by Data-Independent Acquisition: A New Concept for Consistent and Accurate Proteome Analysis

Introduced SWATH-MS, the first widely adopted practical implementation of data-independent acquisition, fundamentally establishing DIA as a viable, reproducible alternative to DDA for large-scale, consistent quantitative proteomics and directly enabling the large clinical cohort studies that followed over the subsequent decade.

Hughes CS, Moggridge S, Muller T, Sorensen PH, Morin GB & Krijgsveld J | Nature Protocols, 2019 | DOI: 10.1038/s41596-018-0082-x

Single-pot, solid-phase-enhanced sample preparation for proteomics experiments

Established the SP3 (single-pot, solid-phase-enhanced sample preparation) bead-based workflow, now the standard sample preparation approach underlying high-throughput, low-input, and automated proteomics across clinical, population-scale, and single-cell applications.

Demichev V, Messner CB, Vernardis SI, Lilley KS & Ralser M | Nature Methods, 2020 | DOI: 10.1038/s41592-019-0638-x

DIA-NN: neural networks and interference correction enable deep proteome coverage in high throughput

Introduced DIA-NN, the deep learning-powered DIA analysis software now central to modern library-free DIA proteomics, enabling deep, reproducible proteome coverage directly from DIA data without requiring prior experimental spectral library generation.

Davis S, Scott F, Oyler J & Praissman J | Journal of Proteome Research, 2025 | DOI: 10.1021/acsmeasuresciau.3c00068

Comprehensive Overview of Bottom-Up Proteomics Using Mass Spectrometry

A comprehensive 2024-2025 overview consolidating modern bottom-up proteomics methodology, sample preparation, acquisition strategies, and data analysis into a single authoritative reference, reflecting the current technical state of the field for both newcomers and established practitioners.

Lopes FBT, Schlatzer D, Sudhadevi T et al. | Journal of Proteome Research, 2026 | DOI: 10.1021/acs.jproteome.5c01007

What Does Next-Generation Mass Spectrometry Offer for Proteomics? A Comprehensive Platform Comparison

A rigorous head-to-head benchmarking study comparing Orbitrap Astral, timsTOF Ultra, and conventional Orbitrap Exploris 480 platforms, demonstrating 300-800% greater proteome depth and substantially improved subcellular and pathway coverage with next-generation instrumentation. The definitive current reference for understanding the practical impact of the newest instrument generation.

Huang S, Wang C, Lin HJL & Kelly RT | bioRxiv, 2025 | DOI: 10.1101/2025.07.29.667408

The $10 proteome: low-cost, deep and quantitative proteome profiling of limited sample amounts using the Orbitrap Astral and timsTOF Ultra 2 mass spectrometers

Demonstrated a practical pathway to approximately ten US dollars per sample for deep, quantitative proteome profiling by combining simplified low-input sample preparation, standardised acquisition settings, next-generation instrumentation, and short run times, directly enabling genuinely population-scale proteomic studies.

W2.13: Pioneering Scientists in MS-Based Proteomics

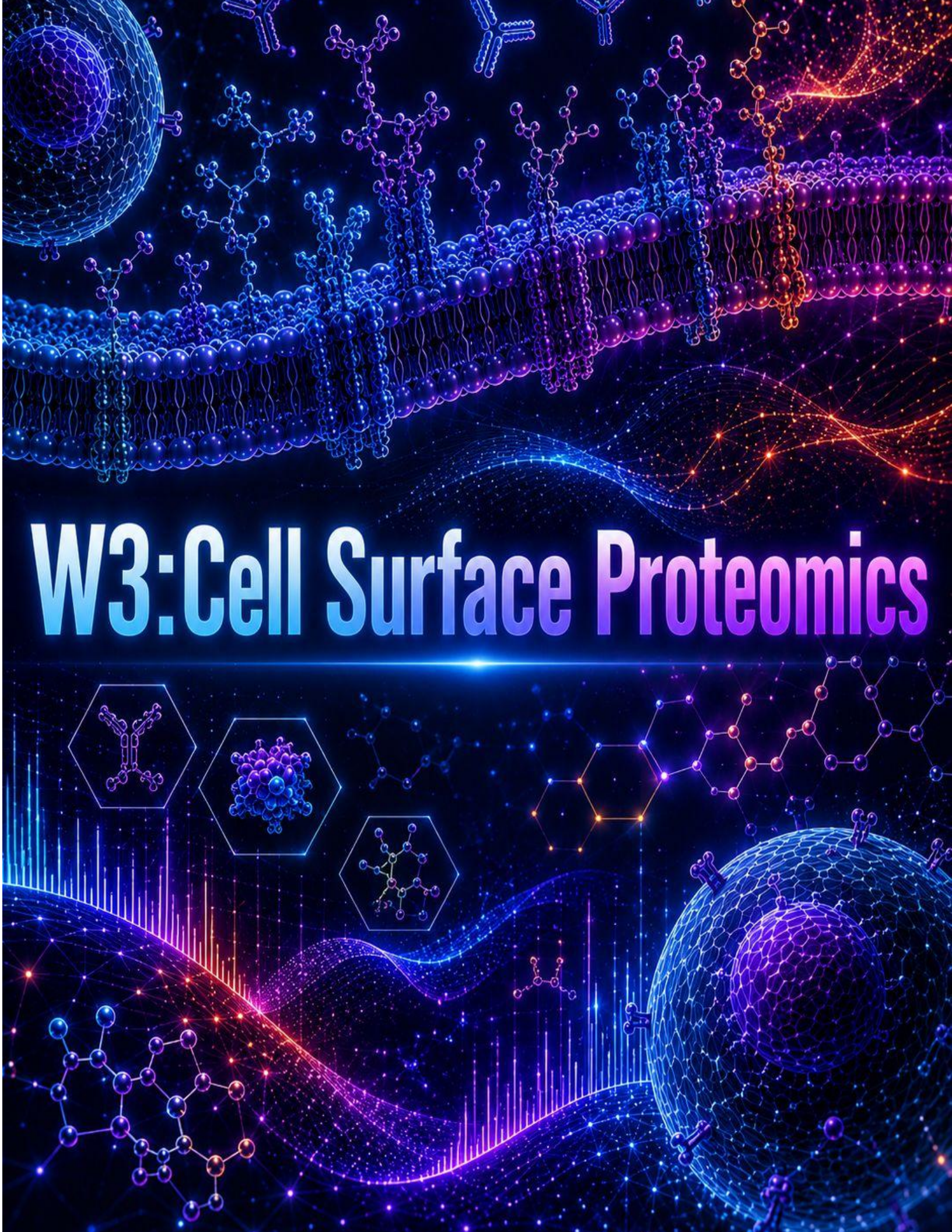
Scientist and Affiliation	Key Contributions
Prof. John B. Fenn (1917-2010) Yale University / Virginia Commonwealth University	Developed electrospray ionisation for the analysis of large biomolecules, the soft ionisation breakthrough that made it possible to study intact proteins and peptides by mass spectrometry for the first time. Awarded the 2002 Nobel Prize in Chemistry for this foundational contribution.
Dr. Koichi Tanaka Shimadzu Corporation, Japan	Developed the soft laser desorption technique that directly preceded and informed the development of MALDI, sharing the 2002 Nobel Prize in Chemistry for enabling soft ionisation of large biomolecules by laser-based methods.
Prof. Matthias Mann Max Planck Institute of Biochemistry; University of Copenhagen	One of the most influential figures in modern proteomics, co-developer of MaxQuant and the MaxLFQ quantification algorithm, pioneer of high-resolution Orbitrap-based proteomics, SILAC quantification, and numerous foundational reviews establishing the field's conceptual framework. His laboratory continues to drive instrumentation and methodology at the cutting edge of the discipline.
Prof. Ruedi Aebersold ETH Zurich / University of Zurich	Co-author of the foundational Nature review establishing modern MS-based proteomics, inventor of SWATH-MS (the first practical DIA implementation), and pioneer of targeted SRM/MRM quantification frameworks. His methodological contributions underpin essentially every modern clinical and discovery proteomics workflow.
Prof. Joshua J. Coon University of Wisconsin-Madison	Pioneer of Electron Transfer Dissociation (ETD) fragmentation and leading developer and evaluator of new-generation Orbitrap instrumentation (Orbitrap Ascend, Orbitrap Astral). His laboratory's rigorous, independent instrument benchmarking studies are foundational references for the proteomics community.
Prof. Jesper V. Olsen Novo Nordisk Foundation Center for Protein Research, University of Copenhagen	Leading authority on phosphoproteomics and post-translational modification analysis by MS, pioneer of high-sensitivity Orbitrap-based methods including ion pre-accumulation strategies, and developer of protein aggregation capture (PAC) sample preparation for multipurpose proteomics workflows.

Prof. Ryan T. Kelly Brigham Young University, Provo, Utah	Pioneer of ultra-low-input sample preparation technology (nanoPOTS) originally developed for single-cell proteomics, now central to achieving the dramatically reduced sample input requirements and per-sample costs (the '$10 proteome') driving expansion of MS-based proteomics into population-scale applications.
Prof. Albert J.R. Heck Utrecht University	Leading authority on native mass spectrometry and structural proteomics, pioneering the analysis of intact protein complexes and their non-covalent interactions by MS, extending the discipline beyond sequence identification into direct structural and stoichiometric characterisation of macromolecular assemblies.

W 2.14: Historical Development Timeline

Year	Milestone
1989	Fenn and colleagues publish the foundational electrospray ionisation paper in Science, demonstrating soft ionisation of large biomolecules including intact proteins.
1991	Tanaka and colleagues publish the soft laser desorption technique directly preceding MALDI, enabling laser-based soft ionisation of large biomolecules.
1994	Trypsin-based bottom-up shotgun proteomics methodology, combined with emerging genome sequence databases, begins to establish the modern peptide-centric proteomics workflow.
1999	The Orbitrap mass analyser concept is introduced by Alexander Makarov, eventually commercialised by Thermo Fisher Scientific in the mid-2000s.
2002	John Fenn and Koichi Tanaka share the Nobel Prize in Chemistry (with Kurt Wuthrich) for the development of soft ionisation methods for mass spectrometric analysis of biological macromolecules.
2003	Aebersold and Mann publish the landmark Nature review 'Mass spectrometry-based proteomics', establishing the conceptual framework still used to teach and organise the field today.
2008	Cox and Mann publish MaxQuant in Nature Biotechnology, providing the field's first widely adopted, free, comprehensive proteomics data analysis software platform.
2011	Electron Transfer Dissociation (ETD) becomes widely available on commercial hybrid instruments, transforming confident site-specific localisation of labile post-translational modifications including phosphorylation.
2012	Gillet, Aebersold and colleagues publish SWATH-MS in Molecular & Cellular Proteomics, introducing the first widely adopted practical implementation of data-independent acquisition.
2014	Cox and colleagues publish the MaxLFQ label-free quantification algorithm, establishing a robust, widely used standard for label-free protein quantification.
2019	Hughes and colleagues publish the SP3 single-pot sample preparation protocol in Nature Protocols, establishing the bead-based workflow now standard for high-throughput and low-input proteomics sample preparation.
2020	Demichev and colleagues publish DIA-NN in Nature Methods, introducing deep learning-powered, library-free DIA analysis and transforming the practicality of DIA-based proteomics.
2023	Thermo Fisher Scientific commercially releases the Orbitrap Astral mass spectrometer, combining Orbitrap and Astral analysers for dramatically increased MS2 scan speed and proteome depth.
2024-2025	Bruker releases the timsTOF Ultra 2 instrument family; independent benchmarking studies confirm 300-800% proteome depth improvements with next-generation Orbitrap Astral and timsTOF Ultra platforms over conventional instrumentation.
2025	Kelly and colleagues publish the '$10 proteome' study, demonstrating a practical pathway to dramatically reduced per-sample cost for deep, quantitative proteome profiling using next-generation instrumentation and simplified workflows.

2026	PAMAF and related high-speed ion mobility-enabled acquisition modes begin to blur the traditional distinction between DDA and DIA, exceeding 1,000 Hz MS2 fragmentation rates while retaining high-quality, comprehensive spectral data.


W3:Cell Surface Proteomics

Workshop 3

Cell Surface Proteomics

WORKSHOP . ENRICHMENT, QUANTIFICATION & BIOMARKER DISCOVERY

Cell Surface Proteomics

SCIENTIFIC PROGRAMME

Overview

Workshop 3 at APT-2026 focuses on the rapidly advancing field of Cell Surface Proteomics, providing participants with insights into the technologies and strategies for studying cell-surface proteins. Cell surface proteins play essential roles in cellular communication, signaling, adhesion, immune recognition, and disease progression, making them critical targets for biomarker discovery and therapeutic development.

This workshop will introduce participants to methods for the enrichment, capture, detection, and quantitative profiling of cell surface proteins. Attendees will gain an understanding of antibody-based strategies and advanced proteomics workflows for characterizing membrane-associated proteins and studying their functional roles in biological systems.

The workshop will also emphasize quantitative analysis and data interpretation approaches to uncover mechanisms underlying cellular signaling, adhesion, pathogenesis, and disease progression. Participants will explore how cell surface proteomics contributes to translational research, precision medicine, and therapeutic target identification.

Designed for students, researchers, and professionals in the life sciences and biomedical research, the workshop combines conceptual understanding with practical applications to prepare participants for emerging opportunities in surface proteomics.

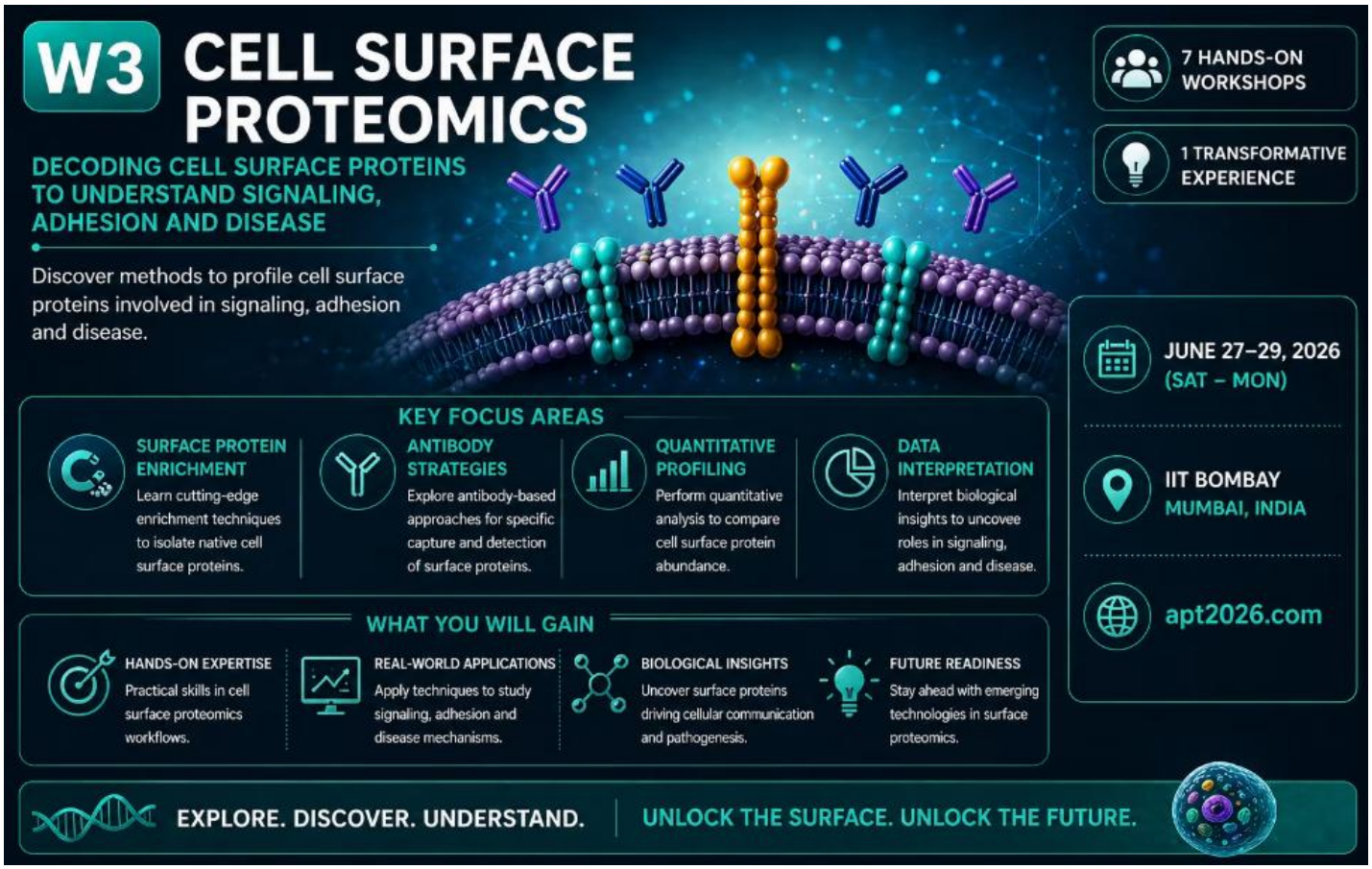
AT A GLANCE

Key Highlights

- **Surface protein enrichment techniques**
- **Antibody-based capture & detection strategies**
- **Quantitative profiling of cell surface proteins**
- **Proteomics data interpretation & biological insights**
- **Applications in signaling, adhesion & disease research**
- **Emerging technologies in surface proteomics**

Section	Topic	Topics Covered
W 3.1	**Introduction to the Surfaceome**	Definition of the surfaceome, plasma membrane landscape, pharmacological relevance, and clinical discovery value
W 3.2	**Major Analytical Bottlenecks**	Low abundance, extreme hydrophobicity, dynamic trafficking, and heterogeneous glycosylation challenges

W 3.3	**Core Enrichment Strategies**	Cell Surface Capture, Sulfo-NHS-Biotin labeling, Lectin Affinity, Proximity-Dependent Labeling, Subcellular Fractionation
W 3.4	**Standard Working Protocol: Biotin-Based Surface Proteomics**	Live-cell labeling, detergent lysis, streptavidin affinity capture, and on-bead tryptic digestion
W 3.5	**Contamination Mitigation & Quality Control**	Unlabeled negative controls, experimental workflow controls
W 3.6	**Computational Quality Control Pipelines**	GO-based annotation filtering, surface marker ratio analysis, SURFY and CSPA database cross-referencing
W 3.7	**Applications, Quantitative Workflows & Emerging Trends**	TMT multiplexing, DIA-PASEF, PRM validation strategies for surface biomarker panels
W 3.8	**Broad Experimental Applications**	Oncology & CAR-T, host-pathogen interfaces, liquid biopsy via extracellular vesicles
W 3.9	**Emerging Frontiers**	Single-cell surface proteomics, spatial surfaceomics, multi-omics system integration



ADVANCED CELL SURFACE PROTEOMICS

W 3.1 Introduction to the Surfaceome

The plasma membrane serves as the ultimate functional checkpoint and communication hub of the living cell. The entire complement of proteins stably associated with, structurally embedded within, or transiently localized to the extracellular face of this lipid bilayer is collectively defined as the surfaceome. This complex landscape encompasses classical multi-pass transmembrane receptors, peripheral membrane-associated scaffolding elements, and tightly controlled lipid-anchored (e.g., GPI-anchored) signaling complexes.

While standard global shotgun proteomics architectures catalog the gross protein expression profile across an entire cell lysate, they inherently fail to capture highly localized spatial dynamics. Investigating the unique composition of the surfaceome holds exceptional biomedical, therapeutic, and clinical discovery value due to several fundamental paradigms:

- **Pharmacological Dominance:** Over 60% of all clinically approved small-molecule drugs and therapeutics explicitly target membrane-associated or cell surface protein classes.
- **Biologics Targets:** The vast majority of modern biologics, including monoclonal antibodies (mAbs), Antibody-Drug Conjugates (ADCs), and CAR-T immunotherapies, are engineered to recognize targets exposed on the extracellular domains of surface receptors.
- **Dynamic Response Sentinels:** Dynamic structural shifts in the surfaceome landscape (via rapid endocytosis, recycling loops, targeted shedding, or exosome packaging) frequently precede alterations in global gene transcription, serving as highly sensitive early-warning sentinels of functional cell-state transitions.

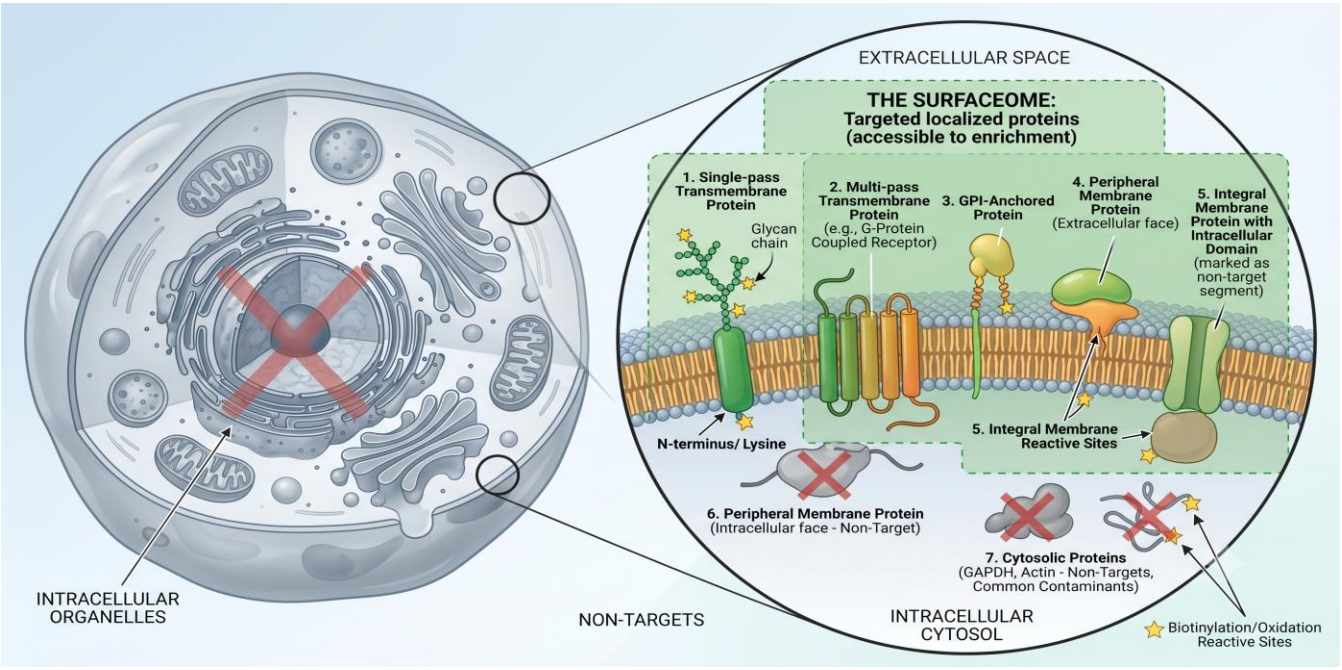


Figure W3.1: *Schematic representation of the cell surface proteome (surfaceome), highlighting accessible extracellular membrane proteins targeted for enrichment and analysis, while intracellular and cytosolic proteins are excluded as non-target contaminants.*

W 3.2: Major Analytical Bottlenecks

Characterizing the mammalian cell surfaceome using classical bottom-up liquid chromatography-tandem mass spectrometry (LC-MS/MS) methodologies presents a series of intense biochemical and biophysical hurdles:

- **Low Relative Abundance:** Plasma membrane components constitute a structurally minor percentage of the total integrated cellular protein mass. In crude whole-cell homogenates, they are easily masked by highly abundant cytosolic, structural, and mitochondrial proteins.

- **Extreme Hydrophobicity:** Transmembrane domains (TMDs) consist of hydrophobic α-helices or closely packed β-barrels. These architectures are highly insoluble in classical aqueous matrices and exceptionally resistant to enzymatic proteolytic cleavage.
- **High Dynamic Trafficking:** The surfaceome is highly fluid and metabolically reactive. Fast-acting biological events such as receptor internalization, continuous endocytosis, shedding, and exosomal export loops require experimental steps that strictly freeze molecular trafficking.
- **Heterogeneous Glycosylation:** More than 90% of validated cell surface proteins undergo significant co- and post-translational glycosylation. Heavy carbohydrate chains sterically hinder standard trypsin access, producing bulky glycopeptides that complicate standard database matching algorithms.

CORE ENRICHMENT STRATEGIES

W 3.3: Core Enrichment Strategies

To achieve deep coverage of the low-abundance surfaceome, researchers must employ selective isolation strategies on intact, viable cells before mass spectrometric measurement. The main strategies utilized in modern workflows are outlined in the table below:

Strategy	Chemical Principle	Major Advantages	Key Limitations
Cell Surface Capture (CSC) (Figure 2)	Mild sodium periodate oxidation of cell-surface sialic acids/cis-diols, covalent coupling to hydrazide-biotin linkers, and targeted enzymatic release of glycopeptides via PNGase F.	Exceptional specificity for true plasma membrane components; directly maps N-glycosylation sites; eliminates intracellular backgrounds.	Demands large starting cell inputs (>10^7 cells); entirely blind to non-glycosylated proteins; labor-intensive multistep handling.
Sulfo-NHS-Biotin Labeling (Figure 2)	Covalent modification of primary amines (ε-amino groups of Lysine residues and unblocked N-termini) utilizing membrane-impermeable active esters.	Extremely rapid, highly cost-effective, easily scalable, and provides deep, broad coverage across all structural protein classes.	High risk of internal labeling if cell membrane integrity fails slightly (>5% cell death); background binding during streptavidin cleanups.
Lectin Affinity Chromatography	Non-covalent, high-affinity capture of native glycoproteins utilizing immobilized, carbohydrate-specific lectin resins (e.g., WGA, ConA, SNA).	Isolates completely intact, biologically active structures; ideal for focused glycoform profiling and structural analysis.	Strong glycan-structure bias; co-purifies intracellular glycoproteins moving through the endoplasmic reticulum (ER) and Golgi networks.
Proximity-Dependent Labeling	Genetically targeted or functionalized enzymes (APEX2, HRP, TurboID) catalyze ultra-short bursts of reactive biotin-phenoxyl/biotin-AMP	Captures transient interactors and weak architectural networks; provides excellent temporal resolution; compatible with low inputs (<5x10^5 cells).	Demands complex prior genetic engineering or specialized execution steps; highly sensitive to radical quenching and reaction timing.

	radicals to tag neighboring complexes.		
Subcellular Fractionation	Physical disruption followed by isolation based on density, mass, or hydrophobicity using differential or density gradient ultracentrifugation.	Completely unbiased by chemical tags or chemical modifications; recovers fully active, multi-protein complexes for functional studies.	Poor resolution between actual plasma membranes and structurally similar internal organelles (ER, lysosomes, endosomes).

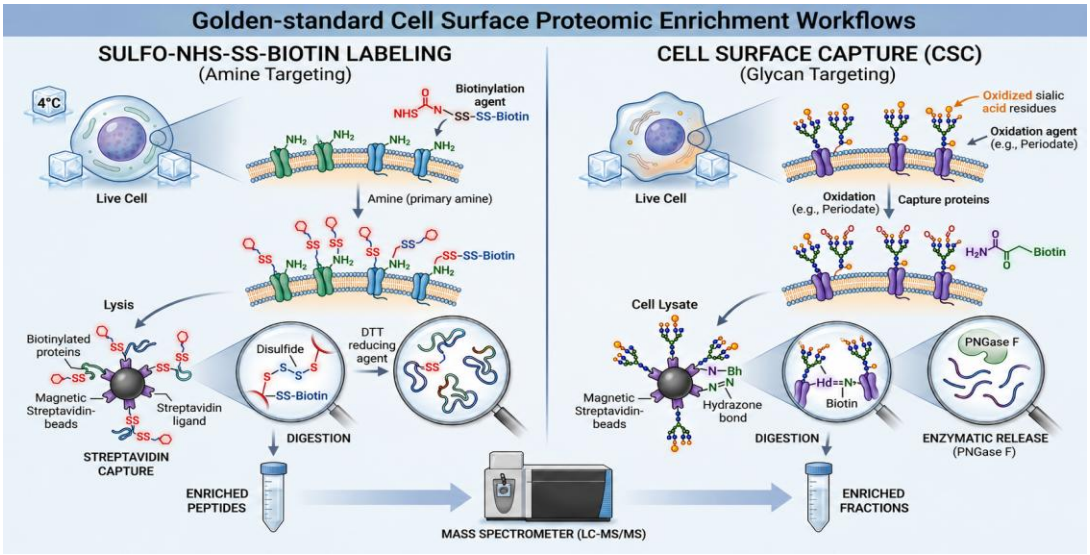


Figure W3.2: *Schematic overview of Sulfo-NHS-SS-biotin labeling and Cell Surface Capture (CSC) workflows for cell surface proteomic enrichment followed by LC-MS/MS analysis.*

STANDARD WORKING PROTOCOL

W 3.4: Standard Working Protocol: Biotin-Based Surface Proteomics

This protocol details chemical biotinylation utilizing cleavable Sulfo-NHS-SS-Biotin on living, intact monolayer or suspension cell cultures, followed by high-stringency affinity capture and downstream on-bead tryptic digestion.

Phase I: Live-Cell Surface Labeling

- **Cultivation and Viability Verification:** Cultivate target cell populations to approximately 80% confluence under standard incubator conditions. Immediately prior to chemical modification, precisely assess cell viability utilizing high-accuracy Trypan Blue exclusion or automated flow cytometry.

> ⚠ **CRITICAL OPERATIONAL WARNING:** *If the calculated cell viability falls below 95%, abort the experiment immediately. Dead or dying cell populations with compromised membrane architectures allow the membrane-impermeable Sulfo-NHS-Biotin reagent to rapidly flood the interior cytosol. This results in the heavy biotinylation of high-abundance intracellular components (e.g., GAPDH, Actins, Histones), completely invalidating the surface specificity of the downstream MS dataset.*

- **Pre-Cooling and Washing:** Transfer culture vessels directly onto a flat ice-water bed. Wash the intact cells exactly three times with ice-cold, pH-buffered Phosphate Buffered Saline supplemented with 0.1 mM CaCl2 and 1.0 mM MgCl2 (PBS++ at pH 8.0). Maintaining a strict 4°C operational window is necessary to freeze fluid-mosaic lipid dynamics and completely arrest active endocytosis.

- **Biotinylation Reaction:** Introduce freshly dissolved, ice-cold Sulfo-NHS-SS-Biotin in PBS++ (pH 8.0) to achieve a final working concentration of 0.25 to 0.5 mg/mL. Incubate the treatment vessels at 4°C for exactly 30 minutes under slow, gentle horizontal agitation.
- **Reaction Quenching:** Terminate the labeling process by adding an excess of primary amine-containing quenching buffer (e.g., 25 to 50 mM Tris-HCl or Glycine in PBS) and incubate at 4°C for an additional 10 minutes. Wash the cell layer three times with ice-cold PBS++ to remove all remaining unreacted biotin molecules.

Phase II: Detergent Lysis and Affinity Capture

- **Chaotropic Cell Lysis:** Harvest cells by scraping directly into a high-stringency chaotropic lysis buffer (50 mM Tris-HCl pH 7.4, 150 mM NaCl, 1% Triton X-100, 0.1% SDS) freshly supplemented with a 1x Protease and Phosphatase Inhibitor Cocktail.
- **Mechanical Disruption:** Subject the crude cell homogenate to brief, low-amplitude probe sonication (3 bursts of 5 seconds at 20% amplitude) to shear long genomic DNA chains and reduce sample viscosity. Clarify the raw lysate by high-speed centrifugation at 16,000 x g for 15 minutes at 4°C.
- **Streptavidin Affinity Isolation:** Determine absolute protein concentrations using a detergent-compatible BCA assay. Equalize total protein masses across samples and incubate with pre-equilibrated, high-capacity Streptavidin Agarose or magnetic affinity beads overnight at 4°C.
- **High-Stringency Sequential Washing:** Wash the bead matrix sequentially with lysis buffer, high-salt buffer (1 M NaCl in PBS), urea wash buffer (2 to 4 M Urea in 50 mM ABC), and MS-compatible buffer (50 mM Ammonium Bicarbonate or TEAB pH 8.0; 4 complete washes) to eliminate all traces of MS-suppressive detergents.

Phase III: Proteolytic Digestion and Mass Spectrometry

- **On-Bead Proteolysis Execution:** Resuspend the clean, washed bead matrix in 100 µL of 50 mM Ammonium Bicarbonate containing 1 µg of sequencing-grade Trypsin/Lys-C enzyme mixture. Incubate at 37°C overnight with continuous rapid shaking.
- **Peptide Recovery and Clean-up:** Pellet the beads, harvest the peptide-rich supernatant, and immediately stop digestion by acidifying to 0.5 to 1.0% Trifluoroacetic Acid (TFA). Clean and desalt using micro-scale C18 StageTips. Elute in 60% Acetonitrile / 0.1% Formic Acid, concentrate via vacuum centrifugation, and resuspend in 0.1% Formic Acid.
- **High-Resolution Nano-LC-MS/MS Analysis:** Inject the clean, desalted peptides onto a nano-flow ultra-high pressure liquid chromatography system online coupled to an advanced mass spectrometer. For maximum discovery depth, run a Data-Independent Acquisition Parallel Accumulation–Serial Fragmentation (DIA-PASEF) method on a trapped ion mobility mass spectrometer (e.g., Bruker timsTOF platform).

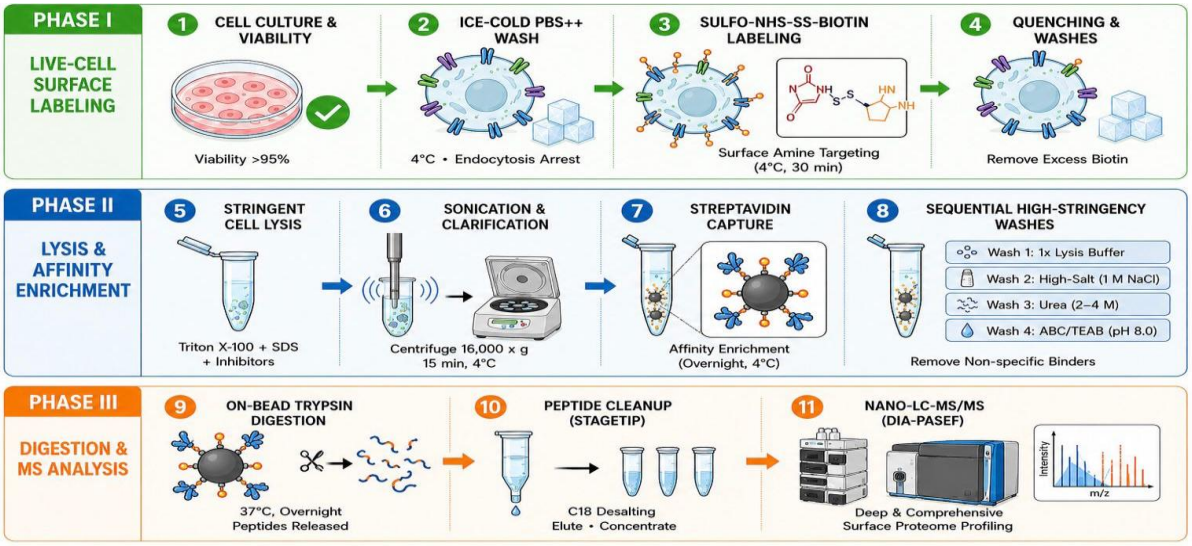


Figure W3.3: *Step-by-step workflow for live-cell surface biotinylation, streptavidin-based affinity enrichment, on-bead digestion, peptide cleanup, and downstream nano-LC-MS/MS surface proteome analysis.*

W 3.5: Contamination Mitigation & Quality Control (QC)

A critical phase of any surface proteomics experiment occurs post-acquisition: computationally proving that the identified analytes are true cell-surface entities rather than intracellular contaminants.

W 3.5: Experimental Workflow Controls

- **The Unlabeled Negative Control:** Always process a parallel control sample of identical cells that undergoes the entire sequence of washes, lysis, and digestion steps without the addition of the active biotinylation or chemical capture tags. Processing this unlabeled negative control exposes background binders and sticky, high-abundance proteins.

W 3.6: Computational Quality Control Pipelines

Following raw data processing through modern software engines (e.g., DIA-NN, FragPipe, Perseus, or Skyline), apply this two-step bioinformatic validation workflow before performing biological interpretation:

Abundance Ratio Analysis of Classical Protein Markers

Calculate the integrated MS intensity metrics of well-characterized surface molecules against highly abundant cytosolic or nuclear structural landmarks. Successful enrichment displays a high surface-to-intracellular marker ratio:

True Cell Surface Markers (Enrichment Expected)	Intracellular Contaminant Markers (Depletion Expected)
EGFR (Epidermal Growth Factor Receptor)	Histone Core Proteins (H2A, H3, H4)
Integrin Complexes (α and β structural chains)	GAPDH (Glyceraldehyde 3-phosphate dehydrogenase)
Cluster of Differentiation (CD) Antigens (CD44, CD45)	Structural Tubulins (α/β-Tubulin) and Actins
Receptor Tyrosine Kinases (RTKs)	Ribosomal Components (RPL11) & Mitochondrial Matrix Markers (COX4)

Bioinformatic Annotation Filtering

Import the final protein identifier list into automated enrichment suites or specialized surface repositories to evaluate structural annotations. Gene Ontology (GO) breakdown: Map identifications to 'Cellular Component'. Successful protocols routinely yield datasets where >70% of all identified entities are annotated under 'Plasma Membrane' [GO:0005886], 'Cell Surface' [GO:0009986], or 'Extracellular Region' [GO:0005576]. High enrichment values for 'Nucleus' [GO:0005634] or 'Mitochondrion' [GO:0005739] indicate severe experimental contamination.

Database Cross-Referencing: Filter your protein lists against validated surfaceome repositories like SURFY (the in silico predicted human surfaceome pipeline) or the Cell Surface Protein Atlas (CSPA) to confirm structural features like signal peptides and transmembrane domains.

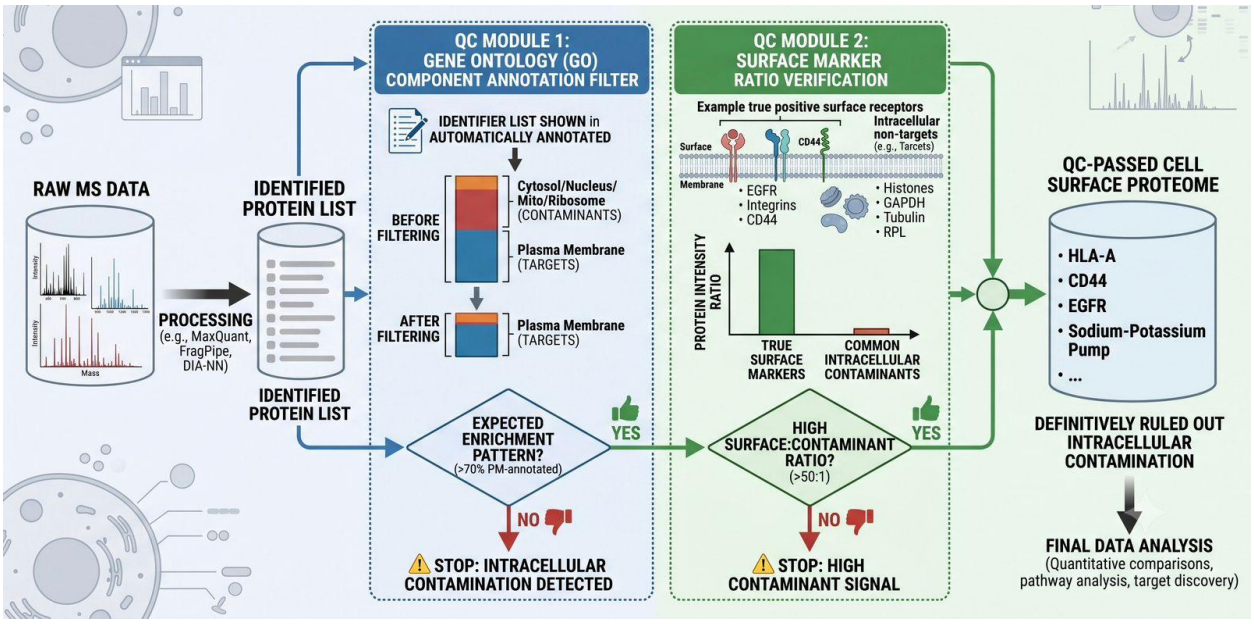


Figure W3.4: *Schematic overview of the post-MS computational quality control (QC) pipeline for cell surface proteomics, including GO-based annotation filtering and surface marker ratio verification to assess enrichment specificity and eliminate intracellular contamination prior to downstream analysis.*

APPLICATIONS & EMERGING TRENDS

W 3.7: Applications, Quantitative Workflows & Emerging Trends

Quantitative MS Integration Strategies

To track relative surfaceome shifts across differential disease states or therapeutic courses, the enrichment workflow must be integrated with robust quantitative mass spectrometry workflows:

- **TMT (Tandem Mass Tagging):** Enables precise chemical multiplexing of up to 16 or 18 individual biological samples within a single consolidated LC-MS execution loop. Enriched peptides are tagged with isobaric mass labels post-digestion, minimizing run-to-run retention time shifts and instrument drift.
- **DIA-PASEF:** Combines data-independent acquisition with trapped ion mobility spectrometry. This creates a reproducible, gap-free digital archive of the enriched sample, making it ideal for deep discovery workflows.
- **PRM (Parallel Reaction Monitoring):** The targeted MS/MS method of choice for validating a selective panel of discovered surface biomarkers across large patient or therapeutic screening cohorts, avoiding the need for western blots where high-quality antibodies are unavailable.

W 3.8: Broad Experimental Applications

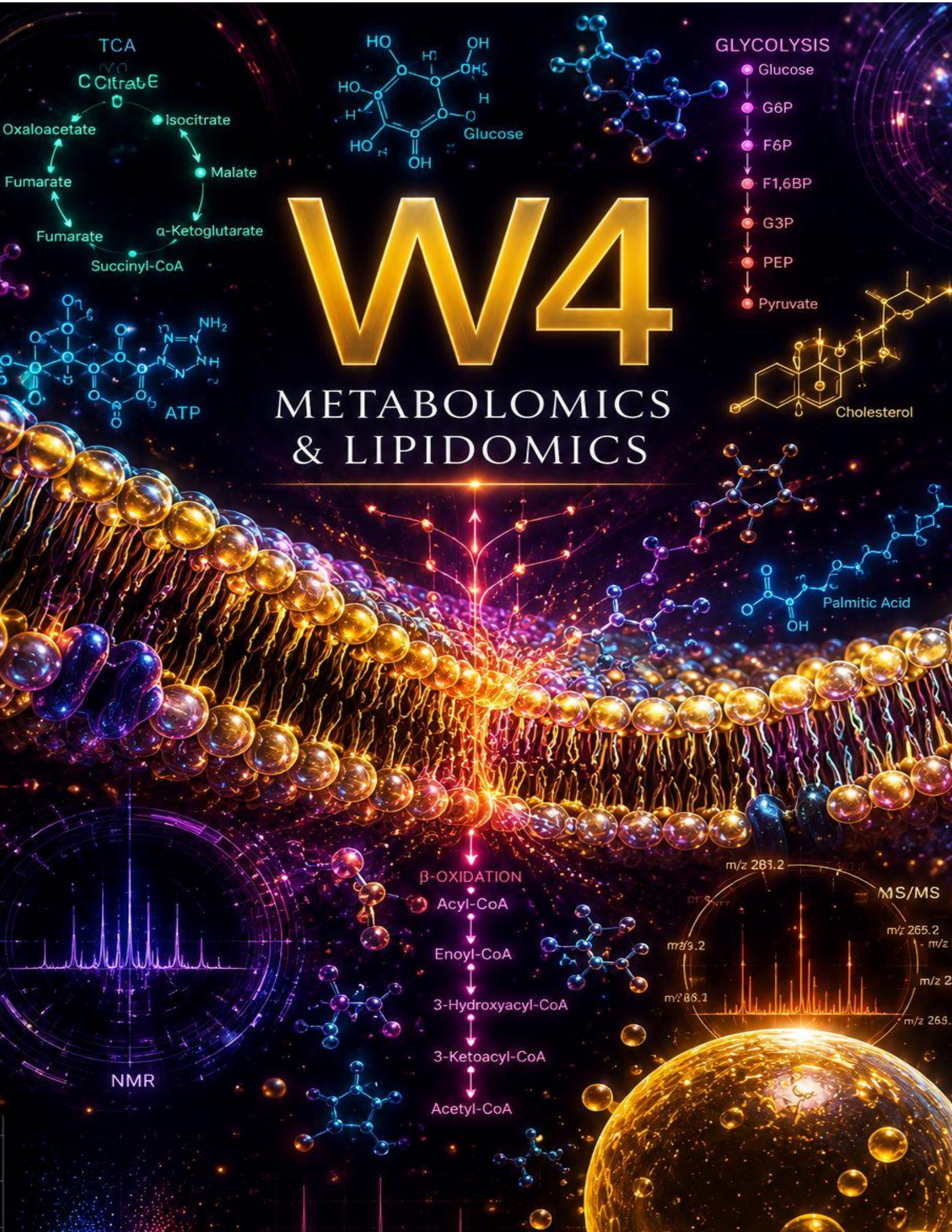
Cell surface proteomics serves as a foundational discovery layer across translational medicine disciplines:

- **Oncology and Translational Immunotherapy:** Mapping tumor surfaceomes enables the discovery of line-restricted antigens and novel neoantigens for constructing precision CAR-T cell platforms and engineered ADCs (e.g., tracking BCMA or SLAMF7 shifts in multiple myeloma models).
- **Host-Pathogen Interfaces:** Identifying specific host cell surface receptors co-opted by emerging viral or bacterial adhesion factors to block pathogen entry pathways.
- **Liquid Biopsies via Extracellular Vehicles (EVs):** Isolating and profiling the surfaceome of circulating tumor-derived exosomes from liquid biopsies (blood, plasma) to diagnose early-stage disease without invasive tissue biopsies.

W 3.9: Emerging Frontiers

The field is moving beyond bulk cell populations toward ultra-sensitive and high-dimensional spaces:

- **Single-Cell Surface Proteomics:** Merging specialized microfluidic handling platforms with heavy-isotope tagged antibody panels to catalog cell surface expression variance at single-cell resolution.
- **Spatial Surfaceomics:** Mapping the exact topological distribution and spatial density of surface receptors directly within intact, cross-linked tissue architectures.
- **Multi-Omics System Integration:** Merging deep discovery surface proteomic layers with single-cell transcriptomic (scRNA-seq) datasets to understand the correlation between transcription and surface translation.


TCA
Citrate
Isocitrate
α-Ketoglutarate
Succinyl-CoA
Fumarate
Fumarate
Malate
Oxaloacetate
Glucose
GLYCOLYSIS
Glucose
G6P
F6P
F1,6BP
G3P
PEP
Pyruvate
ATP
W4
METABOLOMICS
& LIPIDOMICS
Cholesterol
Palmitic Acid
β-OXIDATION
Acyl-CoA
Enoyl-CoA
3-Hydroxyacyl-CoA
3-Ketoacyl-CoA
Acetyl-CoA
NMR
MS/MS
m/z 263.2
m/z 265.2

Workshop 4

Metabolomics & Lipidomics

WORKSHOP . HANDS-ON METABOLOMICS & LIPIDOMICS SESSIONS

Metabolomics & Lipidomics

SCIENTIFIC PROGRAMME

Overview

Workshop 4 at APT-2026 introduces participants to the dynamic fields of Metabolomics and Lipidomics, focusing on the comprehensive analysis of metabolites and lipids to better understand biological systems, disease mechanisms, and precision medicine. These rapidly evolving omics technologies provide powerful insights into cellular pathways, metabolic regulation, and biomarker discovery.

This workshop will cover the complete metabolomics and lipidomics workflow, including sample preparation, LC-MS/MS data acquisition, data processing, metabolite and lipid identification, quantification, and biological interpretation. Participants will gain exposure to modern analytical strategies and computational approaches for analyzing complex metabolic datasets.

The sessions will emphasize the role of metabolomics and lipidomics in identifying disease-associated biomarkers, understanding metabolic pathways, and exploring systems biology approaches in health and disease research. Participants will also learn how these technologies contribute to translational research, therapeutic monitoring, and precision healthcare applications.

Designed for students, researchers, and professionals in life sciences and biomedical sciences, the workshop combines practical concepts with real-world applications to provide a strong foundation in metabolomics and lipidomics research.

AT A GLANCE

Key Highlights

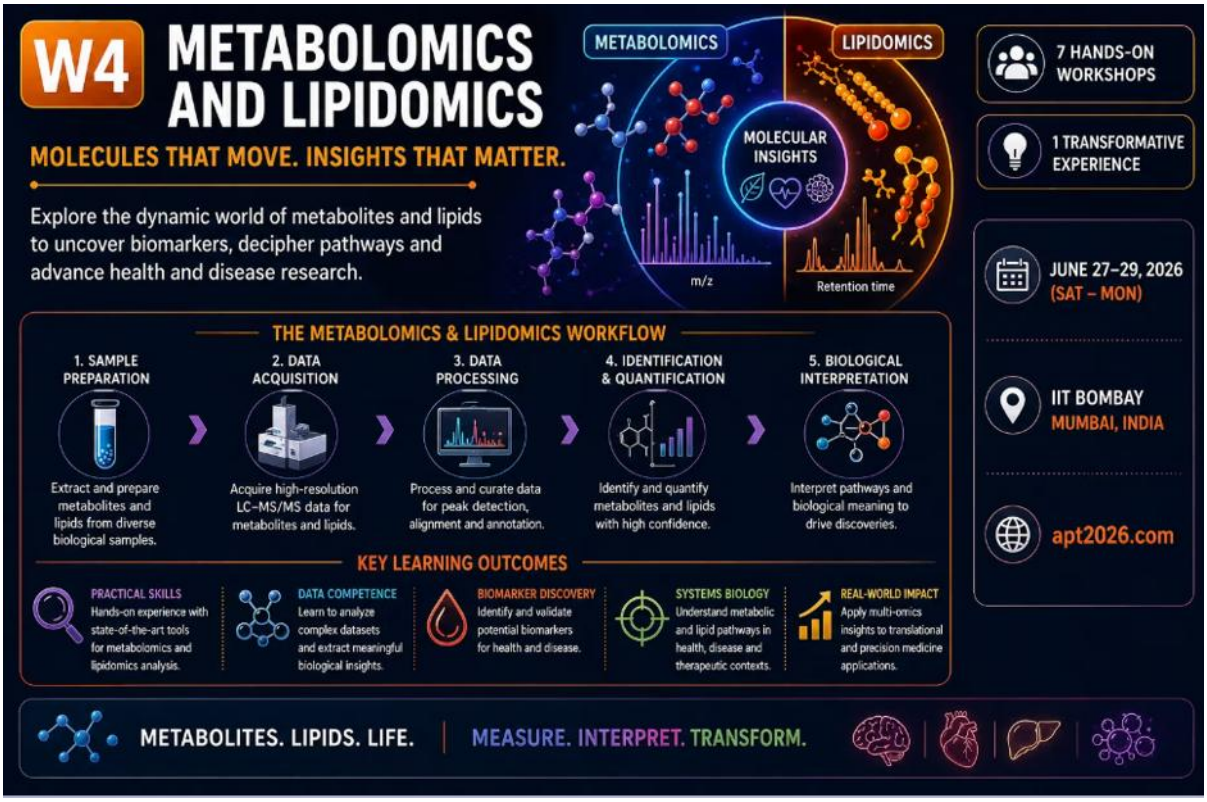
- Metabolomics & Lipidomics workflows
- LC-MS/MS data acquisition & analysis
- Sample preparation protocols
- Quality control & data processing

CONTENTS

What You Will Learn

Chapter	Topics Covered
W 4.1. Introduction to Metabolomics and Lipidomics	Definition, scope, the metabolome vs genome; lipids as specialized metabolites
W 4.2. Historical Development	From Thomson's first MS (1910) to modern single-cell metabolomics and hallmarks of cancer (2022)
W 4.3. Targeted vs. Untargeted Workflows	Untargeted discovery, targeted quantification, pseudotargeted MRM approaches
W 4.4. Chromatographic Separation Modes	RPLC for non-polar lipids; HILIC for polar metabolites; log P-based selection
W 4.5. Electrospray Ionization & Ion Modes	ESI+ and ESI− adduct types; polarity switching strategies
W 4.6. Mass Spectrometry Detection Principles	Triple quadrupole MRM; HRMS Orbitrap/Q-TOF; DDA vs DIA acquisition
W 4.7. Orbitrap Mass Analyzer	Working principle, FT image current, Q Exactive configuration, polarity switching
W 4.8. Applications of HRMS vs QqQ	Untargeted vs targeted instrument selection; biomarker discovery use cases
W 4.9–4.18. Pre-Analytical Considerations & QC	Metabolic quenching; tissue/cell/biofluid handling; consumable contamination; blank controls
W 4.19–4.20. Protocol: Polar Metabolite Extraction	80% methanol extraction from tissues, biofluids, FFPE, and adherent cell lines
W 4.21–4.23. Protocol: Lipid Extraction	MTBE-based and chloroform:methanol lipid extraction; sample types and recovery
W 4.24–4.31. Quality Control in Metabolomics & Lipidomics	Pooled QC samples, method blanks, batch drift, outlier detection, data acceptance criteria
W 4.32–4.33. Duplicate Features & Data Processing Guidelines	Fragmentation heterogeneity, analytical duplicates, feature merging and re-alignment
W 4.34–4.38. Data Analysis Workflow	LipidSearch, MS-DIAL, XCMS, MetaboAnalyst; identification grades; key QqQ settings

W 4.39–4.43. Clinical & Research Applications	Cancer diagnostics, disease pathophysiology, pharmaco-metabolomics, precision medicine



TECHNICAL CONTENT

Metabolomics & Lipidomics: Technical Principles, Clinical Applications, and Standard Extraction Protocols

W 4.1: Introduction to Metabolomics and Lipidomics

Metabolomics is the systematic, high-throughput study of low-molecular-weight molecules, generally defined as compounds with molecular masses below 1500 Daltons (Da), collectively known as metabolites. These molecules are present within biological matrices such as cells, tissues, and biofluids, including plasma, urine, and saliva, and are analyzed under specific physiological or pathological conditions.

Within the hierarchy of biological “omes,” the metabolome occupies a particularly important position. While the genome, transcriptome, and proteome provide information about the genetic potential and regulatory processes of a cell, the metabolome reflects the biochemical consequences of those processes. Because metabolites are direct products and intermediates of cellular activity, the metabolome represents the molecular state most closely associated with the observable phenotype. As a result, it provides a real-time snapshot of ongoing cellular processes and physiological status.

Lipidomics is a specialized branch of metabolomics dedicated to the comprehensive characterization and quantification of lipid species within biological systems. Although lipids are part of the metabolome, they are frequently studied separately because of their distinct physicochemical properties and the unique analytical challenges associated with their measurement. They play critical roles in biological systems, including maintaining cellular membrane integrity, acting as key signaling molecules, and serving as primary energy reservoirs. Lipids are primarily defined by their solubility in organic solvents rather than in water, which influences both extraction strategies and analytical workflows.

W 4.2: Historical Development of Metabolomics and Lipidomics

Metabolomics and lipidomics have evolved through major advances in analytical technologies such as mass spectrometry (MS), nuclear magnetic resonance (NMR), chromatography, and extraction techniques. The field progressed from the study of individual metabolites to comprehensive, system-wide molecular profiling.

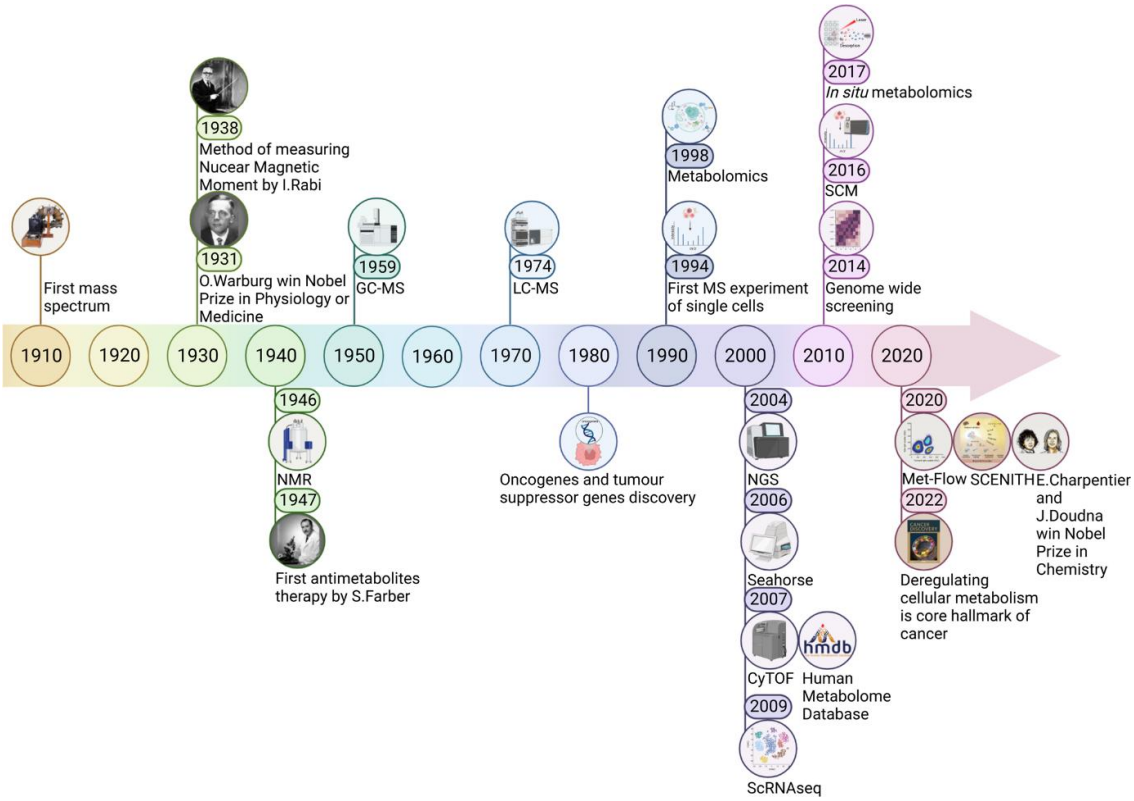


Figure 1. Timeline of the milestone events for cancer metabolism (Danzi et al. (2023))

Key developments include Joseph J. Thomson's first mass spectrum in 1910, Otto Warburg's discovery of altered glucose metabolism in cancer cells during the 1920s, and Isidor Rabi's discovery of NMR in 1938. In 1957, Folch and colleagues introduced the chloroform-methanol extraction method for lipid isolation, while the development of GC-MS and LC-MS between 1959 and 1974 greatly expanded metabolite and lipid analysis.

The term metabolomics was coined by Steven Oliver in 1998, and the launch of the Human Metabolome Database (HMDB) in 2007 provided a valuable resource for metabolite identification. Further advances between 2006 and 2008 introduced standardized quality-control practices and the MTBE extraction method. Since the 2010s, innovations in high-resolution mass spectrometry, single-cell and in situ metabolomics, and multi-omics integration have significantly improved the study of metabolism. In 2022, deregulated cellular metabolism was officially recognized as a hallmark of cancer, underscoring the growing importance of metabolomics and lipidomics in research, diagnostics, biomarker discovery, precision medicine, and systems biology.

W 4.3: Targeted vs. Untargeted Workflows

Depending on the objective of the study, mass spectrometry (MS)-based assays are split into two primary methodologies:

Untargeted Methods

These explore all detectable signals in a sample to capture a broad molecular snapshot. They are primarily used for novel biomarker discovery and hypothesis-generating studies. While they provide deep coverage, they yield semi-quantitative data (reported as peak areas or heights in arbitrary units) and face challenges regarding lower data reproducibility, false-positive peaks, and complex raw-file data processing.

Targeted Methods

These focus strictly on a predefined, structurally characterized panel of metabolites for hypothesis-driven validation. They deliver absolute quantitative metrics (reported in exact molar concentrations). Targeted profiling boasts superior quantitative accuracy, linear calibration ranges, robust limits of quantification, and high reproducibility, making it the bedrock for clinical diagnostics and translation into precision medicine.

Pseudotargeted Methods

This hybrid approach combines full-scan feature selection from pooled samples (untargeted) with the high reproducibility and precision of Multiple Reaction Monitoring (MRM) using triple-quadrupole instruments, without requiring authentic chemical standards for every single analyte.

Metabolomics	
Untargeted	**Targeted**
Discovery strategy (hypothesis generating)	Validation strategy (hypothesis driven)
Global and comprehensive analysis	Subset analysis
High number of metabolites studied	Small number of metabolites
Correlated to database/libraries	Correlated to reference standards
Qualitative identification	Identification of metabolites known a priori
Relative quantification	Absolute quantification
Challenging data interpretation	Easy data analysis and interpretation
Samples preparation requires a global metabolites extraction	Samples preparation is metabolite-specific
Biomarker discovery	Biomarker validation
Global/untargeted screening	Pathway mapping targeted metabolomic profiling

Table 1. Features of untargeted and targeted metabolomics approaches (Danzi et al. (2023))

W 4.4: Chromatographic Separation Modes

No single column can isolate the entire polarity breadth of the metabolome or lipidome. Therefore, distinct stationary phases are deployed based on the partition coefficient (log P) or chemical structure of the target group:

Separation Mode	Stationary Phase Dynamics	Target Analytes & Compound Classes
Reversed-Phase (RPLC)	Non-polar phases (C18, C8, C30). Separates based on hydrophobic interactions using organic gradients (MeOH, IPA).	Mid-polar to highly non-polar species: Free Fatty Acids (FA), Acylcarnitines (>C12), Phospholipids, Triacylglycerols (TG), Cholesteryl Esters (CE).
Hydrophilic Interaction (HILIC)	Polar stationary phase (silica, amide, zwitterionic). Starts with high organic phase; water/ACN gradient elutes polar analytes.	Water-soluble polar entities: Sugars, Amino Acids, Nucleotides, short-chain Acylcarnitines (<C10) that lack retention in RPLC.

W 4.5: Electrospray Ionization (ESI) and Ion Modes

Once separated, the column eluent enters an ESI probe, a soft ionization technique that applies a high electric voltage to transform liquid droplets into gas-phase ions while minimizing structural fragmentation. ESI switches between two ionization polarities:

Positive Ion Mode (ESI+)

Readily generates protonated molecular ions [M + H]+, ammonium adducts [M + NH4]+ (highly common for neutral lipids like triacylglycerols and cholesteryl esters when ammonium modifiers are present in the mobile phase), sodium adducts [M + Na]+ or potassium adducts [M + K]+.

Negative Ion Mode (ESI−)

Favors deprotonated molecules [M − H]−, formate adducts [M + HCOO]− or acetate adducts [M + OAc]− for lipid subclasses like phosphatidylcholines, free fatty acids, and ceramides.

W 4.6: Mass Spectrometry Detection Principles

Low-Resolution Tandem MS (Triple Quadrupole / QqQ & QLIT)

The gold standard for targeted assay systems operating in Multiple Reaction Monitoring (MRM) mode. Quadrupole 1 (Q1) isolates a specific precursor ion, Q2 acts as a collision cell using inert gas to induce fragmentation, and Q3 isolates a characteristic product fragment ion. This dual-filter process provides narrow dynamic linearity, exceptional repeatability, and high chemical specificity.

High-Resolution MS (HRMS – Orbitrap & Q-TOF)

Deployed in untargeted exploration, generating high resolving power (10,000 to 500,000 FWHM) to calculate exact structural formula masses up to parts-per-million (ppm) accuracy. HRMS uses Data-Dependent Acquisition (DDA) or Data-Independent Acquisition (DIA) fragments to isolate structural isobars and compounds with identical nominal mass.

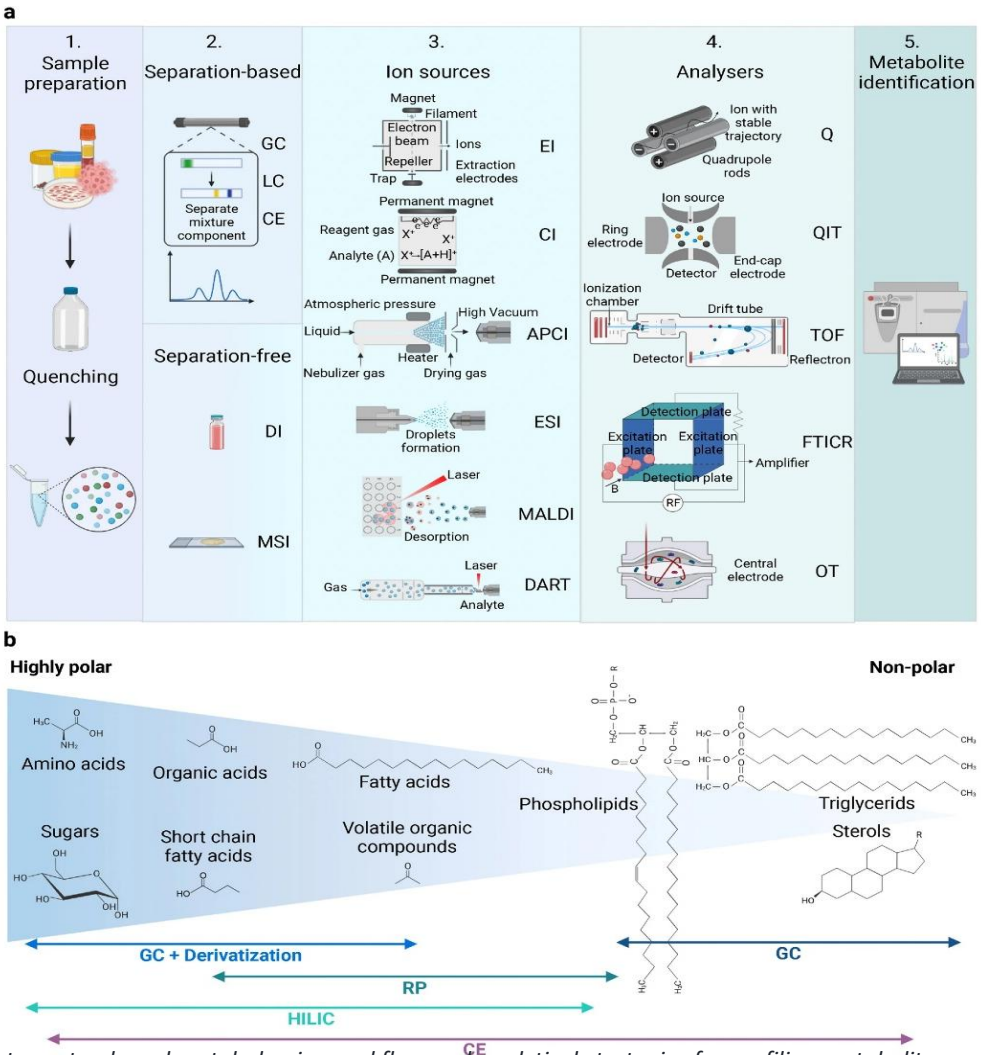


Figure W 4.2. Mass spectrometry–based metabolomics workflow and analytical strategies for profiling metabolites across a broad polarity range (Danzi et al. (2023)). Mass spectrometry (MS)-metabolomic workflow: 1. Sample preparation consists of metabolism quenching and metabolite extraction. 2. Metabolites may need a separation step with Gas chromatography (GC), Liquid chromatography (LC), Capillary electrophoresis (CE) or can be directly ionized in Direct infusion (DI) and Mass spectrometry imaging (MSI). 3. Different ionization techniques can be employed including ESI, MALDI, APCI, and DART. 4. Single (MS) or tandem (MS/MS) mass analysers can be alternatively employed. 5. Data processing includes conversion of m/z values, detection, filtering, normalization and identification.

W 4.7: Orbitrap Mass Analyzer: Principle and Configuration

The Orbitrap is a high-resolution mass analyzer widely used in metabolomics and lipidomics. It provides high resolving power and excellent mass accuracy, enabling reliable determination of exact masses and molecular formulas.

Working Principle

The Orbitrap functions as an electrostatic ion trap. Ions orbit a central electrode while oscillating along its longitudinal axis. The oscillation frequency is directly related to the ion's mass-to-charge (m/z) ratio. These oscillations generate an image current that is converted into a mass spectrum using Fourier Transform (FT) analysis.

Instrument Configuration

Modern Orbitrap instruments, such as the Q Exactive series, combine a quadrupole mass filter with the Orbitrap analyzer, allowing precursor ion selection followed by high-resolution mass detection.

Data Acquisition Modes

- **Data-Dependent Acquisition (DDA):** The most intense precursor ions from an MS1 scan are selected for fragmentation and MS/MS analysis.
- **Data-Independent Acquisition (DIA):** All ions within predefined mass windows are fragmented, providing broader metabolite coverage.

Polarity Switching

Orbitrap systems can rapidly switch between positive and negative ionization modes within a single LC-MS run, allowing efficient analysis of metabolites and lipid classes that ionize differently.

W 4.8: Applications

Compared to Triple Quadrupole (QqQ) instruments, which are primarily used for targeted quantification, Orbitrap instruments provide high-resolution full-scan data and can distinguish compounds with very similar masses. This makes them particularly valuable for untargeted metabolomics, lipidomics, and biomarker discovery studies.

W 4.9: Pre-Analytical Considerations

The pre-analytical phase is one of the largest sources of variability in metabolomics and lipidomics studies. Since biological samples remain metabolically active after collection, enzymatic and chemical reactions must be halted immediately to preserve the true in vivo metabolic state. Failure to follow standardized sample collection and handling procedures can introduce significant artifacts and compromise data quality.

W 4.10: Metabolic Quenching

Metabolic quenching refers to the rapid termination of cellular and enzymatic activity to preserve endogenous metabolite levels at the time of sample collection.

W 4.11: Tissue Samples

- Immediately after excision, tissues should be flash-frozen using liquid nitrogen, dry ice, or freeze-clamping techniques.
- During transport and processing, samples should be maintained on dry ice or chilled metal blocks to prevent metabolic degradation.
- Long-term storage should be at −80°C until extraction and analysis.

W 4.12: Cell Culture Samples

- For adherent and suspension cells, metabolism is typically quenched by rapidly removing the culture medium.
- A pre-cooled extraction solvent, such as ice-cold methanol or acetonitrile:methanol mixtures, is added directly to the cells to simultaneously stop metabolic activity and initiate extraction.
- Following quenching, samples should be stored at −80°C until further processing.

W 4.13: Timing and Nutritional Status

Biological factors such as feeding status and circadian rhythms can substantially influence metabolite levels and should be carefully accounted for in study design.

W 4.14: Circadian Effects

- Circadian regulation can influence up to 40% of the active metabolome.
- Sample collection should therefore be performed at consistent times across all study participants or experimental groups.

W 4.15: Nutritional Status

- Fasting samples are generally preferred because recent food intake can significantly alter metabolite profiles.
- Consistent dietary conditions should be maintained whenever possible.

W 4.16: Cell Culture Standardization

- For in vitro experiments, culture medium should be replaced approximately 2 hours before sample collection.
- This helps ensure that cells are harvested under comparable growth conditions and are not affected by nutrient depletion.

W 4.17: Evaluation of Consumables and Background Contamination

Leachable Contaminants

- Conventional plastic microcentrifuge tubes may release compounds such as palmitate, stearate, phthalate plasticizers, and antioxidant additives including butylated hydroxytoluene (BHT).
- These contaminants can interfere with metabolite and lipid detection.

Adsorption Effects

- Lipids can adsorb onto plastic surfaces, leading to analyte loss and reduced recovery.
- For MTBE-based lipid extraction protocols, glass vials are preferred because they minimize both lipid adsorption and contamination from plastic-derived compounds.

W 4.18: Blank Controls and Monitoring

- Every study should include reagent blanks and method blanks prepared by replacing the biological sample with water.
- Blank samples should be analyzed alongside experimental samples to identify background contaminants and remove non-biological signals during data processing.

PROTOCOLS

Extraction Protocols

W 4.19: Protocol: Metabolomics

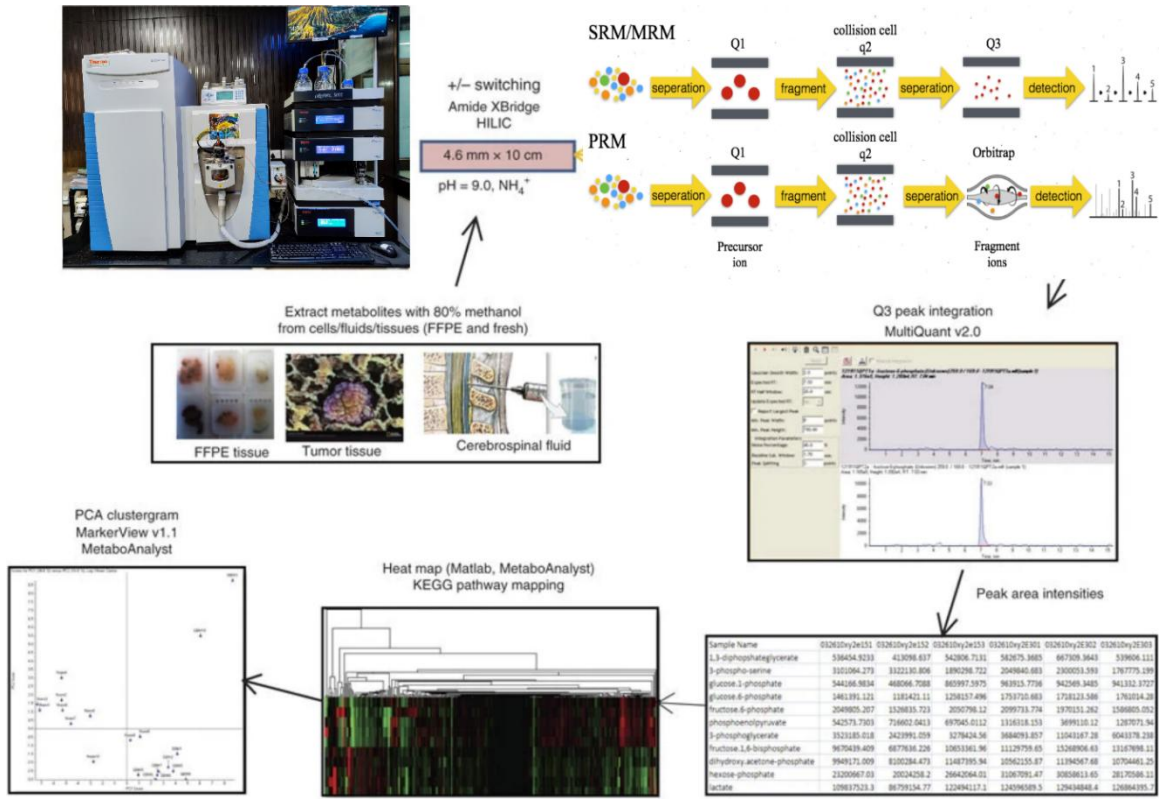


Figure W 4.3. Overview of the targeted LC-MS/MS experiment for polar metabolite profiling via SRM, using positive/negative switching from a single 15-min HILIC column run while targeting more than 250 compounds.

W 4.20: Sample Preparation: Polar Metabolite Extraction

Perform extraction from bodily tissues, bodily fluids or FFPE tissues by following the steps in options A, B or C, respectively. This protocol is also compatible with metabolite extractions from cultured cells. An example procedure for metabolite extraction from adherent cells is shown in option D.

(A) Extraction from Bodily Tissues (tumors/liver/brain/fat)

- Add 500 µl of 80% (vol/vol) HPLC-grade methanol (cooled to −80°C) to fresh or frozen tissue piece(s) in a 1.5-ml or 2.0-ml microcentrifuge tube.
- Smash/grind for 1–2 min with small pestle/tissue grinder on dry ice in the tube, vortex for 1 min at 4–8°C and incubate for 4 h at −80°C.
- Centrifuge at 14,000g (or the highest speed) for 10 min using a refrigerated centrifuge (4–8°C).
- Transfer the supernatant to a new 1.5-ml microcentrifuge tube; store at −80°C until Step 1A(viii).
- Add 400 µl of 80% (vol/vol) methanol (cooled to −80°C) to the precipitate; vortex for 1 min at 4–8°C, then incubate for 30 min at −80°C.
- Centrifuge at 14,000g for 10 min (4–8°C). Transfer and combine the supernatant from both extractions.
- Centrifuge again at 14,000g for 10 min (4–8°C). Transfer the supernatant to a new tube.
- SpeedVac/lyophilize to a pellet using no heat.

(B) Extraction from Bodily Fluids (serum/urine/CSF)

- Centrifuge at 14,000g for 10 min in a cold room (4–8°C). Transfer the supernatant to a new tube.
- Add enough methanol (cooled to −80°C) to make a final 80% (vol/vol) methanol solution.
- Gently shake to mix and incubate for 6–8 h at −80°C.
- Centrifuge at 14,000g for 10 min (4–8°C). Transfer the supernatant to a new tube.

- SpeedVac/lyophilize to a pellet using no heat.

(C) Extraction from FFPE Tissue

- Place curled FFPE slices or cores in a 1.5-ml microcentrifuge tube.
- Add approximately 1–1.5 ml of 80% (vol/vol) methanol and place at 70°C for 30–45 min.
- Remove from heat and put tube in ice to congeal the wax for 15 min.
- Centrifuge at 14,000g for 10 min (4–8°C). Transfer supernatant; chill on ice for 10 min.
- Centrifuge again at 14,000g for 5 min (cold). Transfer to a new tube and SpeedVac/lyophilize to dryness.

(D) Extraction from Adherent Cell Lines

- Change the medium of the cell plate(s) 2 h before metabolite extraction.
- Aspirate the medium completely. Put the plates on dry ice and add 4 ml of 80% (vol/vol) methanol (cooled to −80°C).
- Incubate the plates at −80°C for 20 min. Scrape the plates on dry ice with cell scraper.
- Transfer the cell lysate/methanol mixture to a 15-ml conical tube on dry ice.
- Centrifuge at 14,000g for 5 min at 4–8°C to pellet cell debris. Transfer metabolite-containing supernatant.
- Add 500 µl 80% (vol/vol) methanol (−80°C) to the pellet; vortex for 1 min, spin at 14,000g for 5 min.
- Divide and transfer 4.5 ml total extraction buffer into three 1.5-ml microcentrifuge tubes (1.5 ml each).
- SpeedVac/lyophilize to a pellet using no heat. Dried metabolite samples can be stored at −80°C for several weeks.

W 4.21: Protocol: Lipidomics

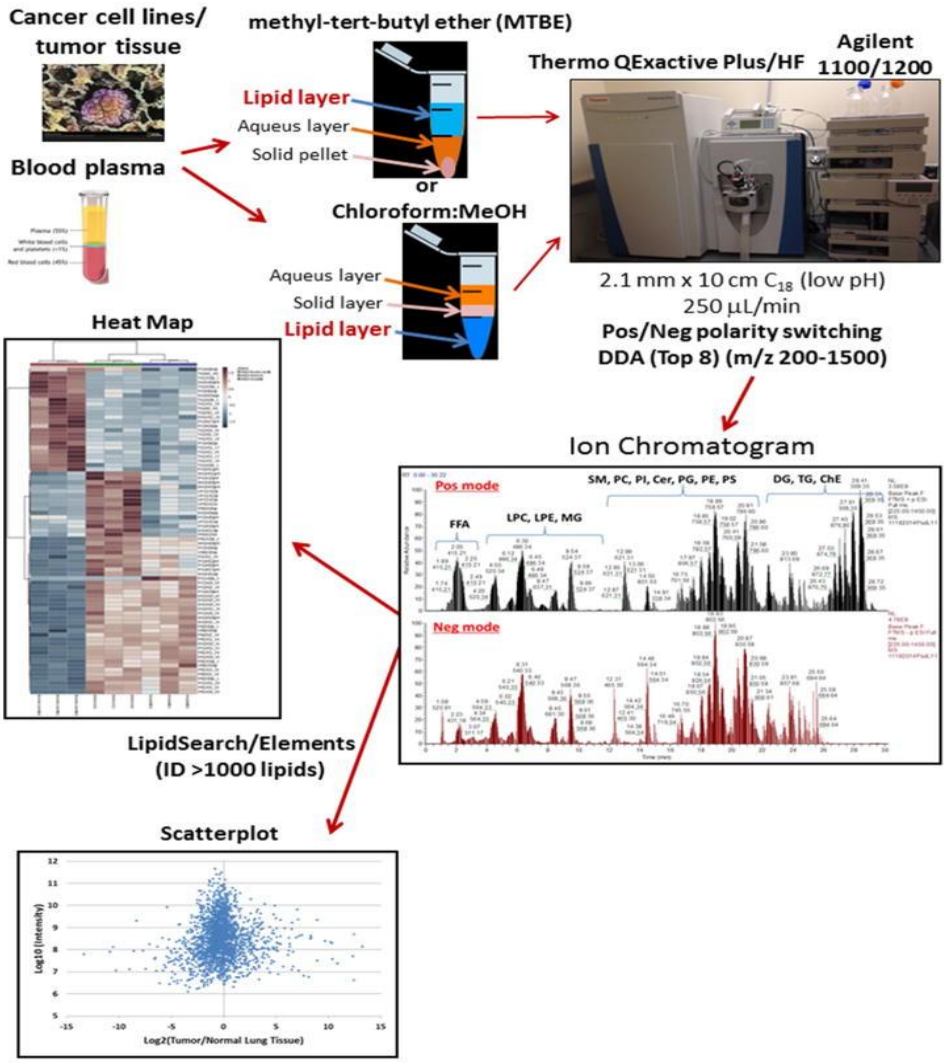


Figure W 4.4. Lipidomics platform schematic (Breitkopf et al., 2017). Overview of the untargeted LC-MS/MS experiment for lipid metabolite profiling via data-dependent acquisition (DDA) using positive/negative switching from a single 28-min reversed-phase column run while routinely identifying and quantifying more than 1000 compounds.

W 4.22: Sample Preparation: Non-Polar Lipid Extraction

Perform extraction from biological tissues, biological fluids, or cultured cells by following the steps in Options A, B, or C, respectively.

Option A: Extraction from Biological Tissues

- Snap freeze tissue and smash/grind for 1–2 min in tube with small pestle/tissue grinder on dry ice.
- Add 200 µL of 1X PBS (RT) to fresh pulverized or ground frozen tissue piece(s) in a 12 mL glass vial.
- Add 1.5 mL HPLC grade methanol and vortex for 1 min. Add 5 mL of MTBE and rock for 1 h at RT.
- Add 1.2 mL of water and vortex again for 1 min. Spin for 10 min at 1,000g (RT).
- Collect the upper MTBE liquid phase containing the non-polar lipids.
- Re-extract the lower liquid phase with 2 volume parts of MTBE/methanol/water (10/3/2.5, v/v/v) by repeating steps v–vi.
- Dry the combined MTBE phases in a SpeedVac or under a nitrogen stream.

Option B: Extraction from Biological Fluids (serum/urine/CSF)

- Centrifuge at 14,000g for 10 min at room temp to pellet solid particulates.
- Transfer 200 µL of the supernatant to 15 mL conical tube (if less fluid, add 1X PBS to total 200 µL).
- Repeat steps iii–viii (Option A). If higher volume is desired, adjust all steps so that the ratios stay the same (sample/methanol/MTBE/water: 1/7.5/25/6, v/v/v/v).

Option C: Extraction from Adherent or Suspension Cell Lines

- Change media of the 10 cm cell plate(s) 2 h prior to lipid extraction.
- Harvest cells from plates at RT and transfer to 12 mL glass vial. Spin for 5 min at 1,000g and remove supernatant.
- Add 200 µL of 1X PBS to the vial. Repeat steps iii–viii (Option A).

W 4.23: Chloroform:Methanol Lipid Extraction Procedure

- Collect tissue, cell pellet, or biological fluid prepared according to the steps above.
- Add chloroform:methanol (2:1 ratio) to a final volume 20 times the volume of the biological sample (100 mg or 100 µL in 2 mL of solvent mixture) in a 12 mL glass vial.
- Agitate the mixture for 30 min in an orbital shaker at RT.
- Add 0.2 volume parts of water (400 µL for 2 mL) and vortex for 1 min.
- Let stand for 10 min and centrifuge at low speed (1000g) to separate into three phases.
- Remove the upper aqueous phase (keep optionally for polar metabolite analysis). The middle layer contains protein, DNA and polar large molecules.
- Remove the lower phase containing non-polar lipids.
- Evaporate under vacuum using a SpeedVac or under a nitrogen stream. Dried lipid samples can be stored at −80°C for several weeks.

QUALITY CONTROL

Quality Control in Metabolomics and Lipidomics

Quality control is essential in metabolomics and lipidomics to minimize analytical variability, detect systematic errors, and ensure reliable and reproducible data.

W 4.24: Quality Control in Metabolomics and Lipidomics

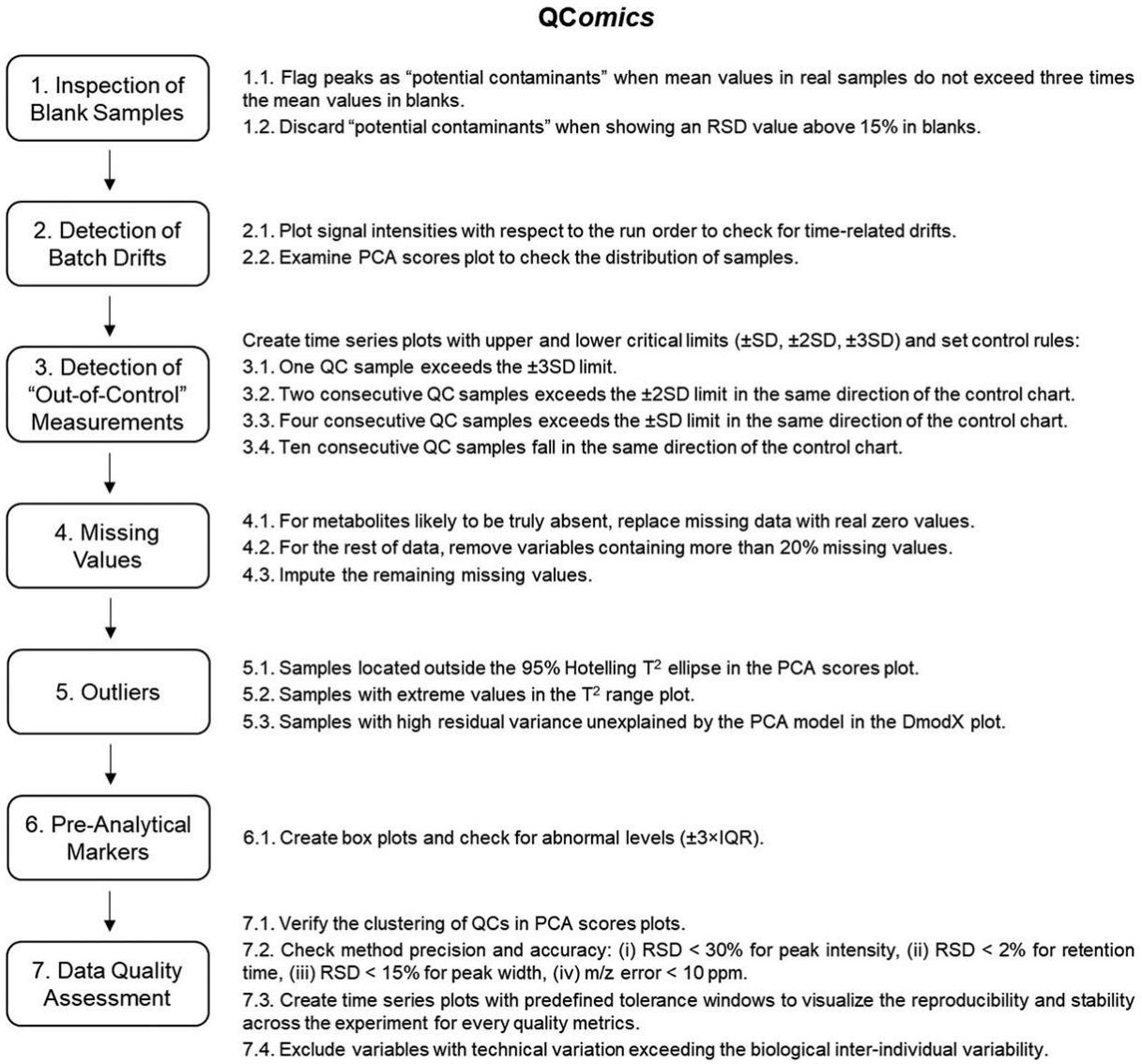


Figure 5. Overview of the QComics workflow (González-Domínguez et al. (2024))

W 4.25: Pooled Quality Control (QC) Samples

Pooled QC samples are considered the gold standard for monitoring system performance.

- Prepare a QC pool by combining equal aliquots from all biological samples.
- Inject the QC pool 5–10 times at the beginning of the run to equilibrate the system.
- Analyze one QC sample after every 10–20 study samples to monitor signal drift and instrument stability.
- Use a serial dilution series of the QC pool (1, 1/2, 1/4, 1/8, 1/16) to assess analytical linearity, with an expected $R^2 \geq 0.8$.

W 4.26: Method Blanks

Method blanks help identify contamination and background signals.

- Replace the biological sample with ultra-pure water and process it using the same extraction and analytical workflow.
- Detect contaminants arising from solvents, reagents, plasticware, or instrument carryover.
- Features with sample intensities less than three times those observed in blanks are considered potential contaminants and may be removed.

W 4.27: Batch Drift and Out-of-Control Detection

Signal drift can occur due to column degradation or reduced instrument sensitivity.

- Monitor QC sample performance throughout the batch.
- In PCA score plots, QC samples should cluster tightly together.

Westgard rules are commonly used to identify out-of-control batches, such as:

- One QC exceeding ±3 SD
- Two consecutive QCs exceeding ±2 SD in the same direction
- Ten consecutive QCs occurring on the same side of the mean

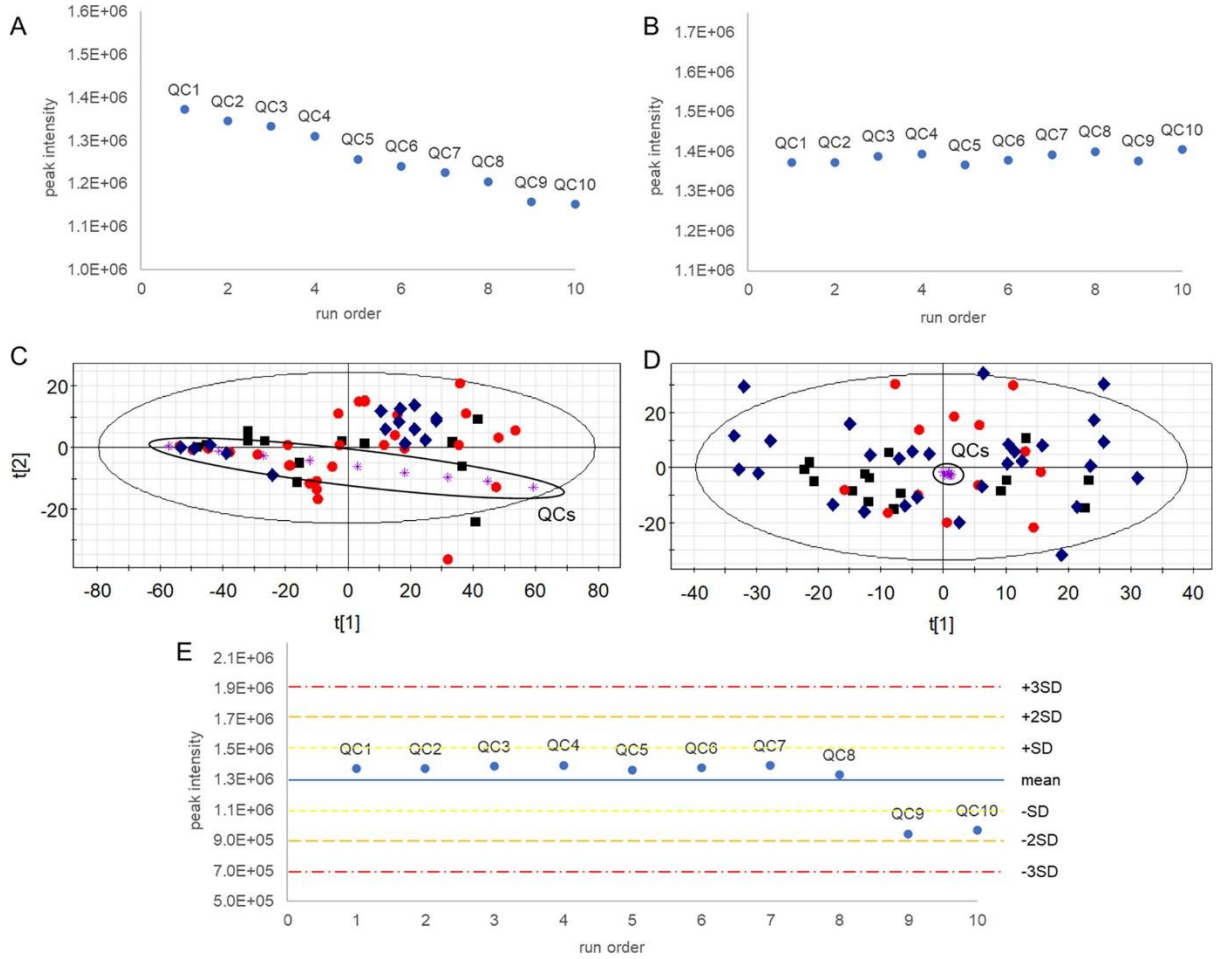
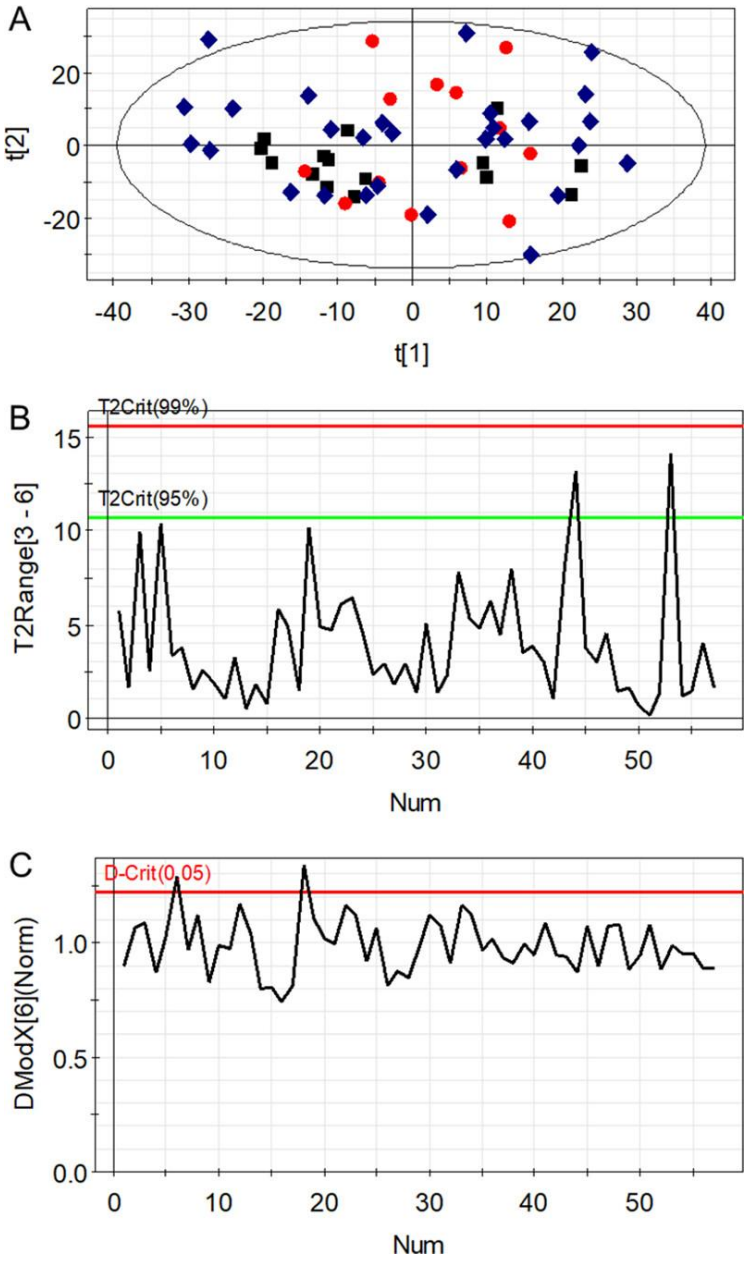


Figure 6. Detection of batch drifts and "out-of-control" measurements (González-Domínguez et al., 2024). (A) Time series plot showing signal drift in quality control samples; (B) time series plot showing stable signal in quality control samples; (C) principal component analysis scores plot showing signal drift in quality control samples; (D) principal component analysis scores plot showing stable signal in quality control samples; (E) Shewhart control chart for detecting "out-of-control" measurements.

W 4.28: Missing Values and Outliers

- Features with >70% missing values are generally considered truly absent and replaced with zeros or removed, depending on the study design.
- Features with low levels of missingness can be imputed using methods such as kNN or Random Forest.
- Potential outliers can be identified using PCA-based approaches such as Hotelling's T^2 and should only be removed after verifying analytical errors in the raw data.



- Principal component analysis scores plot with 95% Hotelling T^2 ellipse; (B) T^2 range plot; (C) DmodX plot.

Figure 7. Detection of Outliers (González-Domínguez et al. (2024)). (A) Principal component analysis scores plot with 95% Hotelling T^2 ellipse; (B) T^2 range plot; (C) DmodX plot.

W 4.29: Pre-Analytical Quality Markers

Certain metabolites can indicate improper sample handling or storage:

- **Enzymatic activity:** Increased Hypoxanthine, Sphingosine-1-phosphate
- **Oxidation:** Decreased Ascorbic acid, Dopamine
- **Anaerobic metabolism:** Increased Lactic acid and Pyruvic acid, decreased D-Glucose
- **Bacterial growth (urine):** Increased Creatine, Acetic acid, and Succinic acid

W 4.30: Sequence Injection Blueprint

To maximize experimental integrity, arrange sequence injections according to the following baseline structure:

- **Solvent Blanks:** Detect system carryover and identify baseline impurities.
- **Method Blanks:** Identify background chemical contaminants originating from extraction tubes and reagents.
- **QC Pool Conditioning:** Inject 5–10 times initially to equilibrate the column matrix.

- **QC Serial Dilution Series:** Inject a dilution curve (e.g., 1, 1/2, 1/4, 1/8, 1/16, 0) of the QC pool to establish detection linearity ($R^2 \geq 0.8$) across the compound array.
- **Randomized Biological Samples:** Always randomize individual samples within the queue to prevent instrumental injection-order bias from turning into false biological discoveries.
- **Regular QC Interleaves & Final QC:** Continuous drift correction and system evaluation.

W 4.31: Data Acceptance Criteria

Common quality thresholds include:

- QC pooled sample RSD ≤ 30% for peak intensity
- Retention time RSD < 2%
- Peak width RSD < 15%
- Mass accuracy < 10 ppm for HRMS instruments
- Signal-to-noise ratio (sample vs. blank) ≥ 10

Only datasets meeting these criteria should proceed to statistical analysis and biological interpretation.

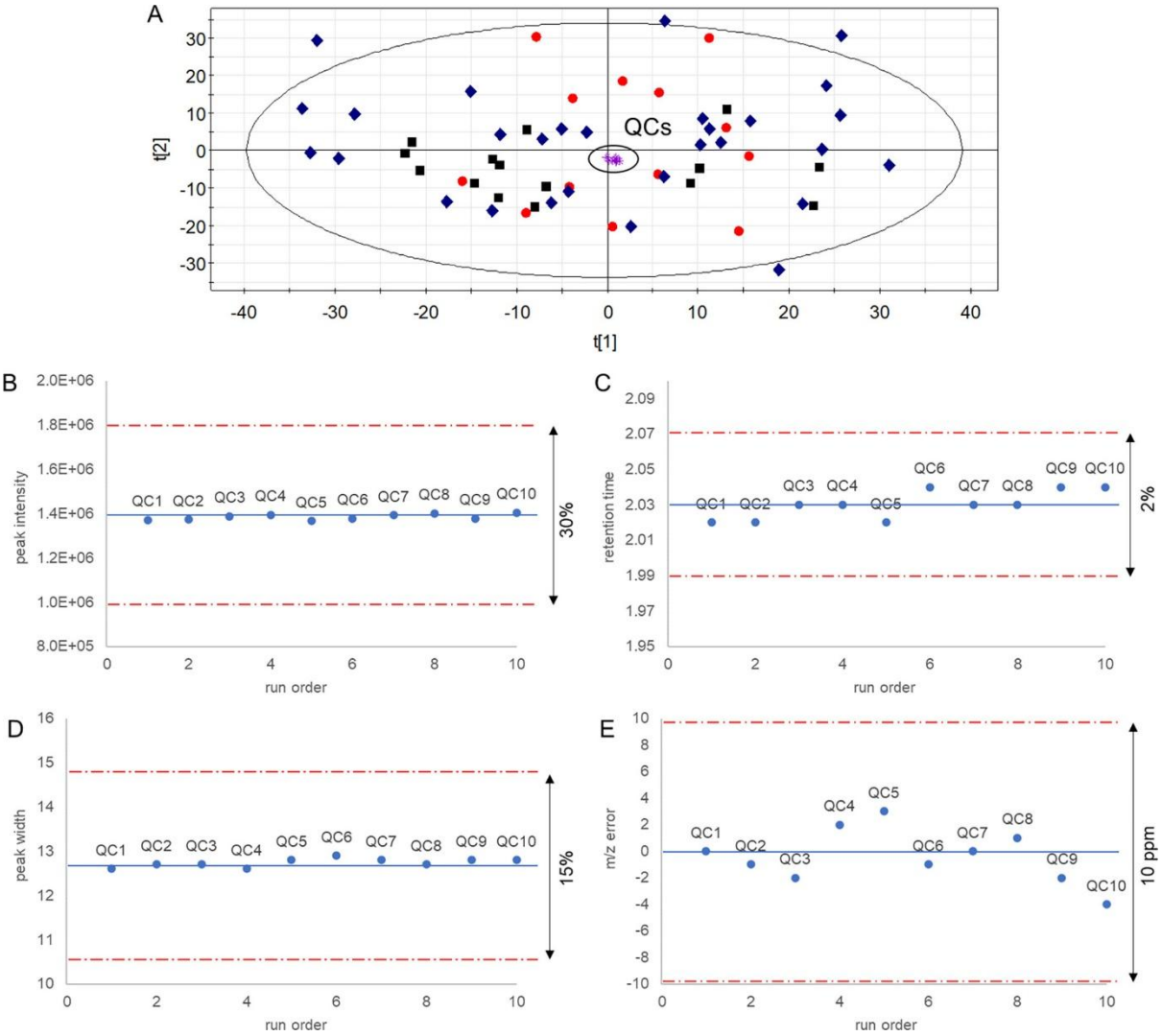


Figure 8. Data Quality Assessment (González-Domínguez et al. (2024)). (A) Principal component analysis scores plot showing tight clustering of quality control samples; (B) time series plot with predefined tolerance windows for peak intensity; (C) time series plot with predefined tolerance windows for retention time; (D) time series plot with predefined tolerance windows for peak width; (E) time series plot with predefined tolerance windows for m/z error.

W 4.32: Duplicate Features in Metabolomics and Lipidomics

Duplicate entries can arise from both molecular fragmentation behaviour and data-processing artifacts.

Molecular Heterogeneity

Identical precursor ions do not always fragment in exactly the same way. Differences in internal energy and protonation sites (protomers) can lead to multiple fragmentation pathways. Although the fragmentation of individual ions is stochastic, the collective behavior of millions of ions yields reproducible MS/MS spectra used for identification.

Competing Fragmentation Pathways

Molecular fragmentation generally occurs through two major mechanisms:

- **Charge Retention Fragmentation (CRF):** The charge remains at its original location while fragmentation occurs elsewhere in the molecule.
- **Charge Migration Fragmentation (CMF):** The charge migrates during fragmentation through proton transfer or inductive cleavage processes.

Analytical Duplicates

The same molecule may be reported multiple times due to data-processing and peak-detection issues, including narrow retention-time alignment windows that split a single peak into multiple features, broad or shoulder peaks detected as separate compounds, or detection of the same molecule in different ionization modes or as different adducts (e.g., $[M+H]^+$ and $[M+NH_4]^+$).

W 4.33: Data Processing Guidelines

To remove duplicate entries:

- Confirm that the features represent the same molecule by checking m/z, charge state, polarity, and structural information.
- Merge duplicate features by summing their intensities or retaining the most representative peak.
- Re-align datasets using a broader retention-time window when alignment errors are suspected.

W 4.34: Data Analysis Workflow

The data analysis workflow converts raw mass spectrometry data into biologically meaningful information through feature extraction, compound identification, and statistical analysis.

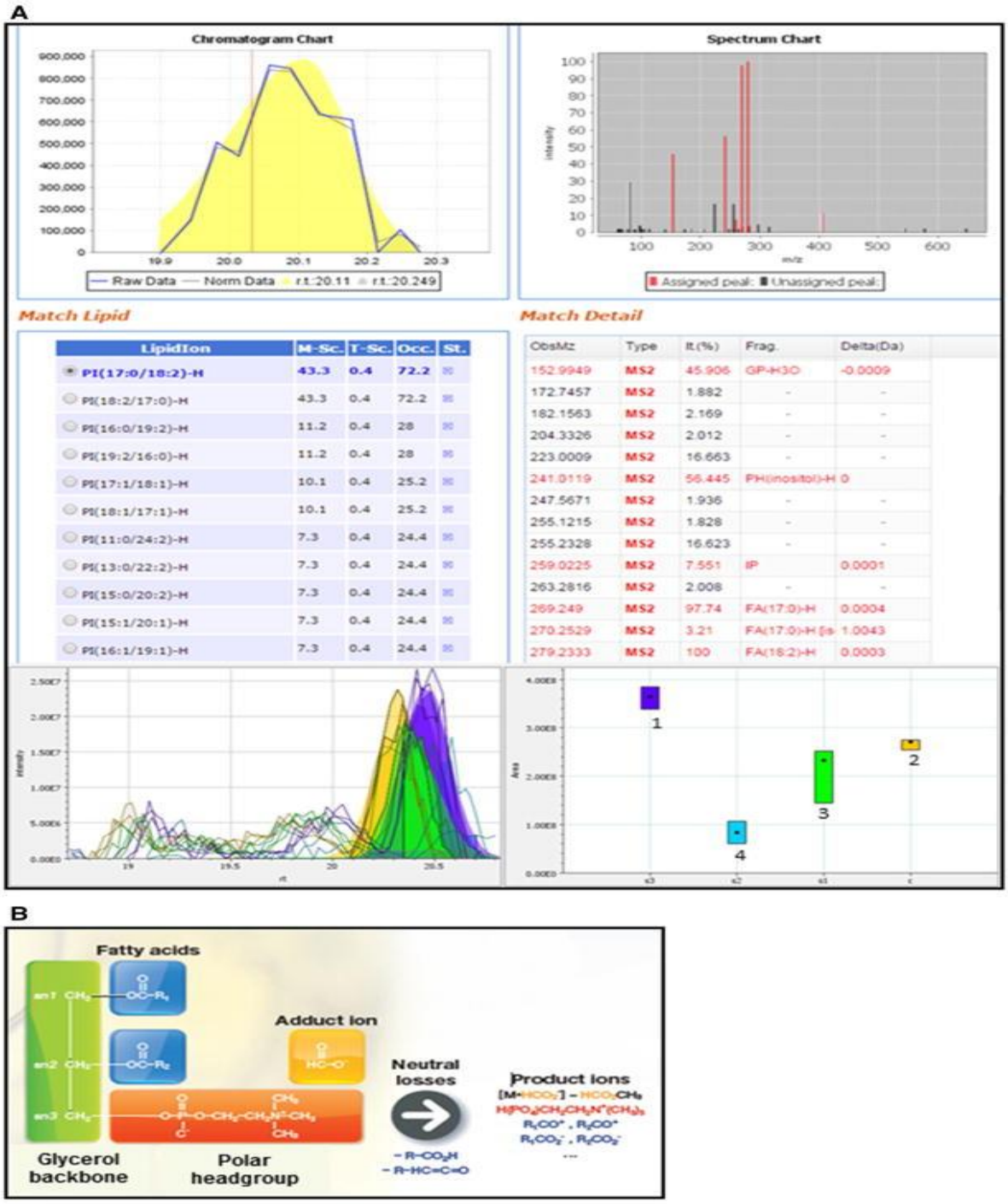


Figure 9. LipidSearch software workflow (Breitkopf et al., 2017). Raw data files from the high-resolution QExactive Plus are loaded into the LipidSearch software, which integrates the MS1 peak areas and proceeds to interpret the MS2 fragment ions for lipid ion identification based on an internal database query. Lipid molecules are then scored and rated using a quality assessment of A–D. During the peak alignment step, the lipid ion peak areas are compared across the sample set, and relative quantification is performed. Lipids are identified based on the major structural units including the lipid backbone, head group, fatty acid chain composition, and adduct ions within each polarity mode.

W 4.35: Data Processing

- Raw instrument files are converted into compatible formats using tools such as MSConvert.
- Features are detected, aligned, and deconvoluted using software such as MS-DIAL, XCMS, Compound Discoverer (CD), LipidSearch or MZmine.

W 4.36: Compound Identification

- Metabolites and lipids are identified by matching MS/MS spectra against reference libraries and databases.
- Common resources include HMDB, KEGG, LipidMaps.

W 4.37: Statistical Analysis and Quality Control

- Data normalization, quality assessment, multivariate analysis (e.g., PCA), biomarker discovery, and pathway analysis are commonly performed using MetaboAnalyst, R, and related statistical tools.

W 4.38: Key Identification Parameters

Typical LipidSearch settings include:

- Precursor mass tolerance: 5–7 ppm
- Product ion tolerance: 7–10 ppm
- Retention time tolerance: 0.25–0.8 min
- Accepted identification grades: A–C (Grade D identifications are typically excluded)

Common adducts:

- Positive mode: (+H), ($+NH_4$)
- Negative mode: (−H), (+HCOO)

CLINICAL & RESEARCH APPLICATIONS

Clinical and Research Applications of Metabolomics & Lipidomics

W 4.39: Clinical and Research Applications

Metabolomics and lipidomics provide direct insights into cellular physiology and disease-associated metabolic alterations.

Table 2. Pros, cons, and sample types of the main metabolomic technologies for the analysis of cancer metabolism (Danzi et al., 2023)

Method	Pros	Cons	Sample types
Gas chromatography-Mass spectrometry (GC-MS)	• High sensitivity for volatile metabolites • High-resolution separation • Analysis of different groups of metabolites simultaneously • Large linear range	• Long sample preparation (derivatization step for non-volatile metabolites) • Thermolabile compounds cannot be analyzed • Slow dynamic range speed • Slow analysis	• Cultured cells • Supernatant • Biofluids • Tissues • Organoids
Liquid chromatography-Mass spectrometry (LC-MS)	• Simple and fast sample preparation (derivatization not usually required) • Wide coverage of metabolites • Thermolabile compounds can be analyzed • High sensitivity • Soft ionization	• Ion suppression • Expensive • Slow analysis	• Cultured cells • Supernatant • Biofluids • Tissues • Organoids
Direct infusion-Mass spectrometry (DI-MS)	• High-throughput • Simple data processing	• Do not distinguish the isomers	• Supernatant • Biofluids

Method	Pros	Cons	Sample types
Matrix-assisted laser desorption ionization-Mass spectrometry (MALDI-MS)	• Low sample volume • Fast analysis • High tolerance towards salts • Suitable for high MW metabolites • Non-destructive	• Low reproducibility • Hard identification due to a complex matrix	• Cultured cells • Supernatant • Biofluids • Tissues • Organoids
Nuclear magnetic resonance (NMR)	• No separation • Structural information • High reproducibility • Fast sample preparation • Non-destructive	• Low sensitivity • Expensive instrument • Some chemical classes are not detected	• Cultured cells • Supernatant • Biofluids • Tissues • Organoids
Single-cell metabolomics (SCM)	• Low cell number • High resolution • High-throughput	• Challenge of combining single-cell sorting and metabolism quenching • Need for a highly sensitive and throughput analytical platform	• Cultured cells • Tissues • Organoids

W 4.40: Biomarker Screening & Cancer Diagnostics

Integrated plasma metabolomics and lipidomics excel at diagnosing early-stage pathological alterations. For example, combined profiling can differentiate Early Hepatocellular Carcinoma (HCC) from chronic Hepatitis C virus (HCV) liver disease with high sensitivity, identifying specific biomarker targets such as asymmetric dimethylarginine (ADMA), short- and long-chain acylcarnitines, and systemic depletion of circulating lysophosphatidylcholines (LPCs).

W 4.41: Deciphering Disease Pathophysiology

Pathway enrichment models bridge clinical measurements and biochemical mechanisms, highlighting dysregulated metabolic axes, such as mitochondrial beta-oxidation of saturated fatty acids or global structural phospholipid remodeling, in oncology and neurodegenerative disorders.

W 4.42: Pharmaco-metabolomics and Companion Diagnostics

Quantifying individual baseline metabolic states enables evaluation of personal pharmacokinetic clearance profiles, variations in therapeutic response, and susceptibility to adverse drug events.

W 4.43: Advancing Healthcare through the Study of Small Molecules

Metabolomics and lipidomics have become indispensable tools for understanding human health and disease because they provide a direct view of ongoing biological processes. As the downstream products of gene expression, protein activity, environmental exposures, diet, lifestyle, and interactions with the microbiome, metabolites and lipids offer a comprehensive snapshot of an individual's physiological state. Their importance is reflected in modern healthcare, where the majority of clinical diagnostic tests measure metabolites and most therapeutic drugs are themselves small molecules.

The clinical impact of these approaches is already evident across multiple areas of medicine. From newborn screening for inherited metabolic disorders to routine assessment of kidney function, cardiovascular risk, and cancer-associated biomarkers, metabolite measurements play a central role in diagnosis and disease monitoring. Advances in metabolomics

and lipidomics are also enabling more precise patient stratification, helping clinicians identify distinct disease subtypes and predict individual responses to therapy.

Beyond diagnostics, small-molecule profiling is transforming drug discovery and development. By revealing how therapies alter metabolic pathways, metabolomics and lipidomics help confirm target engagement, clarify mechanisms of action, and identify early signs of toxicity or treatment resistance. These insights improve decision-making during drug development and contribute to the delivery of safer and more effective therapies.

As these technologies continue to integrate with genomics, microbiomics, and other omics disciplines, they are expected to play an increasingly important role in predictive and preventive healthcare. The ability to detect metabolic alterations years before clinical symptoms appear opens new opportunities for early intervention and disease prevention. Ultimately, the study of small molecules provides a powerful framework for understanding disease biology, discovering new therapeutic targets, and improving patient care through more informed and individualized medical decisions.


GENOMICS
TRANSCRIPTOMICS
PROTEOMICS
METABOLOMICS
FERTILIZATION
EMBRYONIC
FETAL
YOUNG
ADULT
AGING
DISEASE
TIME
timsTOF
timsTOF
ION MOBILITY
m/z
CCS
W5
4D Omics
CHROMATOGRAM
INTENSITY
EXPRESSION MATRIX
GENES





4D OMICS

SCIENTIFIC PROGRAMME

Overview

Workshop 5 at APT-2026 will focus on 4D Omics and advanced proteomics workflows using Bruker's state-of-the-art timsTOF Pro 2 platform. This workshop is designed to provide participants with a practical and conceptual understanding of next-generation mass spectrometry technologies that enable highly sensitive, high-speed, and deep proteome analysis.

The workshop will introduce the principles of 4D proteomics, integrating retention time, mass-to-charge ratio (m/z), ion mobility, and intensity for comprehensive molecular characterization. Participants will gain insights into how the timsTOF Pro 2 system, powered by TIMS (Trapped Ion Mobility Spectrometry) and PASEF (Parallel Accumulation–Serial Fragmentation) technologies, is transforming proteomics research through enhanced sensitivity, speed, and proteome coverage.

Sessions will cover key workflows including sample preparation, LC-MS/MS data acquisition, peptide and protein identification, quantitative proteomics, and biological data interpretation. The workshop will also highlight applications of timsTOF-based proteomics in biomarker discovery, clinical proteomics, translational research, and multi-omics integration.

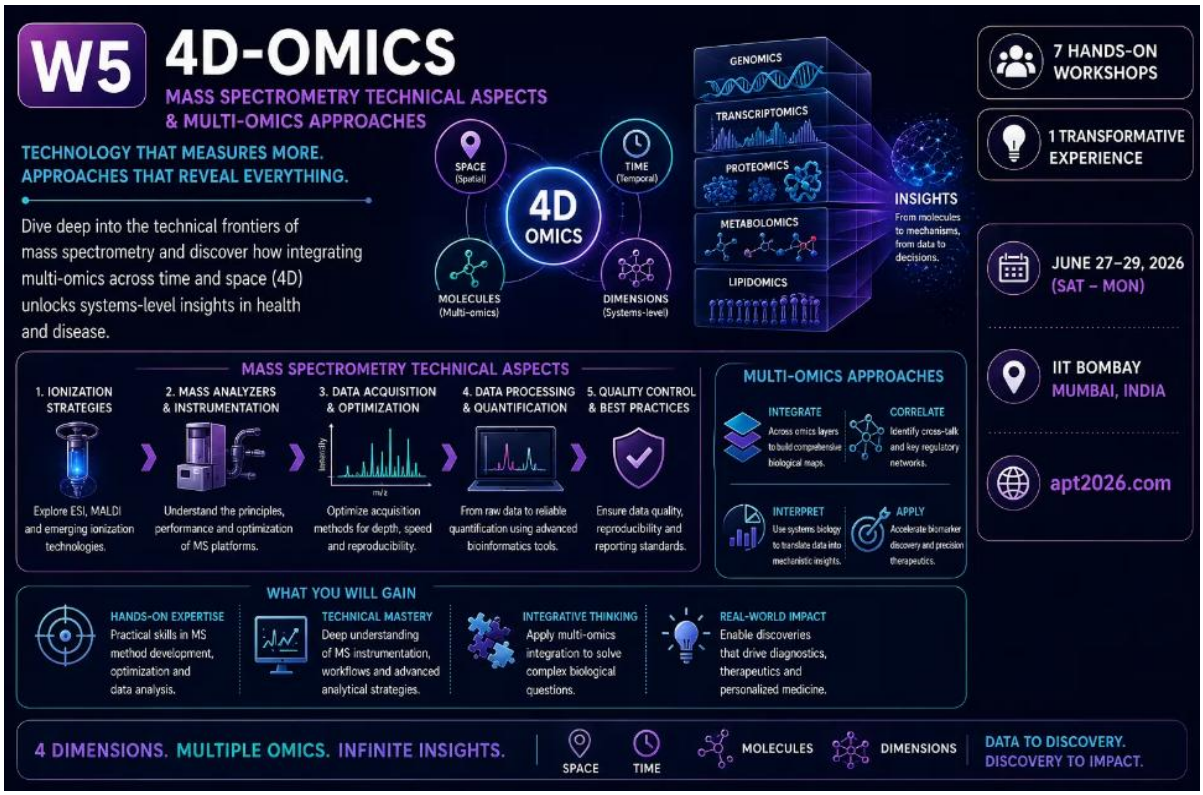
Designed for students, researchers, clinicians, and industry professionals, this workshop aims to bridge advanced instrumentation with real-world biological and clinical applications. Participants will gain exposure to cutting-edge proteomics strategies that support precision medicine, systems biology, and translational healthcare research.

Key Learning Areas

- Fundamentals of 4D proteomics
- TIMS and PASEF technologies
- timsTOF Pro 2 workflows and applications
- High-resolution quantitative proteomics
- Multi-omics and translational research applications
- Proteomics data analysis and interpretation

What Participants Will Gain

- Understanding of next-generation proteomics technologies
- Exposure to advanced mass spectrometry workflows
- Insights into high-throughput and high-sensitivity proteomics
- Knowledge of clinical and translational proteomics applications
- Practical understanding of 4D omics data generation and analysis



ADVANCEMENTS IN 4D PROTEOMICS

Advancements in 4D Proteomics

What is 4D Proteomics?

W 5.1: Definition and Core Concept

4D Proteomics refers to the large-scale analysis of proteins using four simultaneous analytical dimensions to characterize peptides and proteins with unprecedented depth, speed, and accuracy. By adding a fourth dimension — ion mobility separation — to the three classical dimensions of liquid chromatography retention time, precursor mass, and fragment mass, this approach resolves the enormous complexity of proteomics samples in a way that was previously unachievable in a single analytical run.

> **Key Definition** 4D Proteomics = Liquid Chromatography (Dimension 1) + Ion Mobility Separation (Dimension 2) + Precursor Mass (Dimension 3) + Fragment Mass (Dimension 4). The addition of ion mobility as an orthogonal separation dimension is the defining feature that distinguishes 4D proteomics from conventional LC-MS/MS workflows.

The result is a dramatic increase in the number of identifiable peptides and proteins, reduced chemical noise, and the ability to distinguish peptides of nearly identical mass — all within a single, unfractionated sample injection. 4D Proteomics is not merely an incremental improvement over existing methods; it represents a conceptual shift in how proteomics data is acquired and interpreted.

W 5.2: The Evolution from 1D to 4D

To appreciate the significance of the fourth dimension, it is useful to trace how proteomics analytical strategies have evolved:

Era	Dimensions Used	What Was Measured	Key Limitation

1D (Gel era)	Molecular weight (gel)	Protein bands separated by size	Low throughput; not quantitative
2D (LC-MS)	LC retention time + precursor mass	Peptide masses after LC separation	Co-eluting peptides create spectral interference
3D (LC-MS/MS)	LC + precursor mass + fragment mass	Peptide sequence via fragmentation spectra	Undersampling of complex mixtures; chimeric spectra
4D (LC-IMS-MS/MS)	**LC + ion mobility + precursor + fragment**	**Peptide sequence AND shape/charge state resolved**	**Larger data volumes; requires specialized software**

W 5.2: Why the Fourth Dimension Matters

In any complex proteomics sample — whether plasma, tissue, or microbiome — thousands of peptides co-elute from the LC column at any given moment. These co-eluting peptides generate overlapping signals in the mass spectrometer, creating chimeric or mixed spectra that confound identification algorithms and reduce both sensitivity and specificity.

Ion mobility separation occurs in the gas phase, after ionization but before mass analysis, and takes place on a millisecond timescale — orders of magnitude faster than LC separation (minutes) but slower than MS acquisition (microseconds). This places it perfectly in the analytical hierarchy to act as an additional filter, separating ions that would otherwise overlap in the mass spectrum.

> **The Core Advantage** Ion mobility separates ions based on their size, shape, and charge — their collisional cross section (CCS) in a gas-filled drift region. Two peptides with identical mass but different three-dimensional structures will have different CCS values and will therefore be resolved in the ion mobility dimension even when they cannot be separated by LC or distinguished by mass alone.

W 5.3: Principles of 4D Proteomics

Ion Mobility Separation — The Fourth Dimension

What is Ion Mobility?

Ion mobility spectrometry (IMS) is a gas-phase separation technique that measures how quickly ions travel through a buffer gas under the influence of an electric field. Larger, less compact ions experience more collisions with gas molecules and travel more slowly; smaller, more compact ions travel faster. The key measured parameter is the Collisional Cross Section (CCS), which encodes information about an ion's three-dimensional shape and charge state.

CCS is a fundamental molecular property — as reproducible and characteristic as mass or retention time — and provides a fourth coordinate for confident peptide identification. A peptide identified in one laboratory on one day will yield thsame CCS value when measured under identical conditions in another laboratory on another day, making CCS a powerful quality-control and cross-study-matching parameter.

Trapped Ion Mobility Spectrometry (TIMS)

The most advanced implementation of ion mobility for proteomics is Trapped Ion Mobility Spectrometry (TIMS). Unlike earlier drift-tube or travelling-wave IMS approaches, TIMS uses an electric field to trap and hold ions against a gas flow, then releases them in order of increasing mobility by gradually reducing the trapping electric field. This approach offers several critical advantages:

- 100% ion utilization: All ions entering the TIMS device are trapped and analyzed, eliminating the ion losses inherent in pulsed IMS methods. This provides a significant sensitivity advantage.
- High resolving power: TIMS achieves ion mobility resolving power of up to 250 or higher, sufficient to separate closely related peptide species including isomers.
- Rapid acquisition: A full TIMS separation cycle occurs in tens of milliseconds, fast enough to be fully compatible with LC peak widths of seconds to minutes.
- Precise CCS measurement: TIMS provides highly accurate CCS values (typically <1% deviation) that can serve as an additional identification coordinate (Figure 1).
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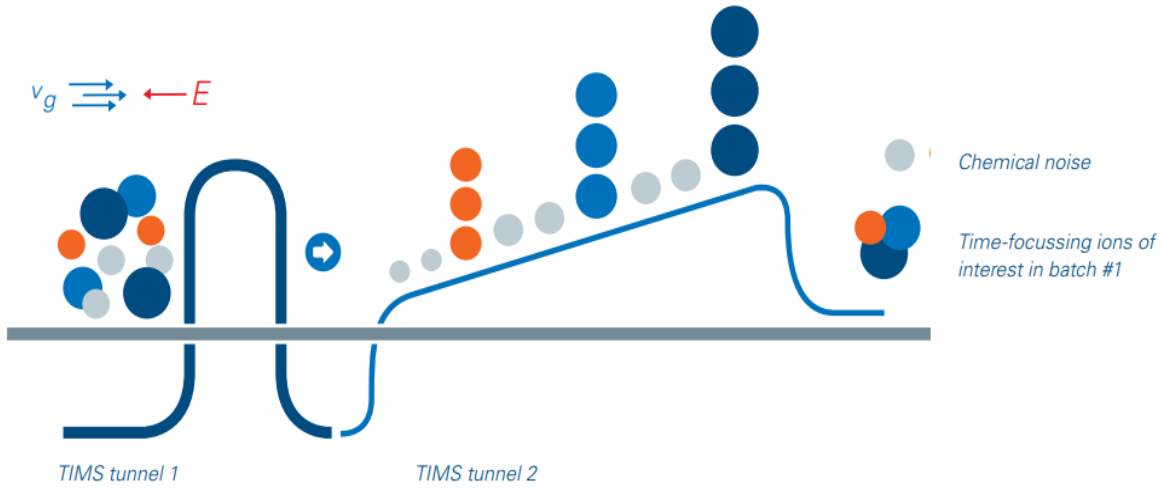
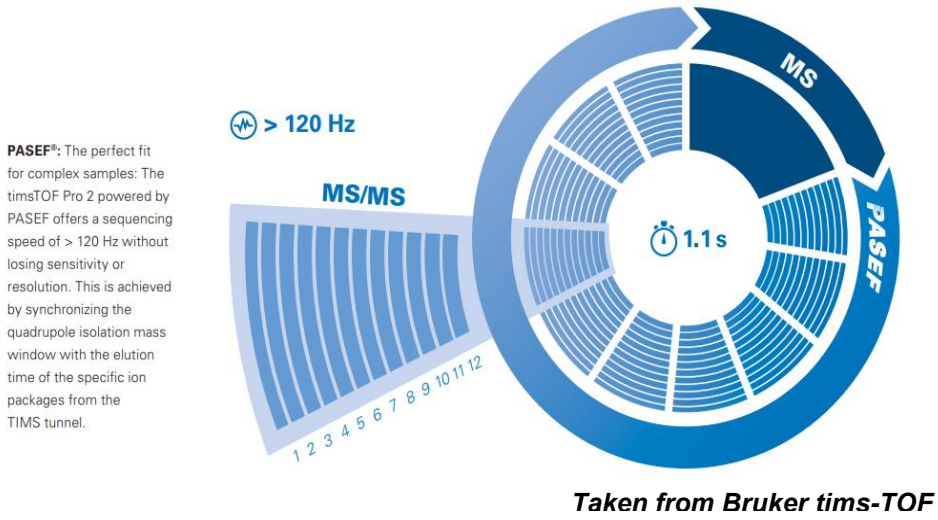


Figure W 5.14: *Schematic of the dual-TIMS analyzer showing parallel ion accumulation and serial elution. While ions of interest are time-focused and sequentially released from TIMS tunnel 2, the next batch is simultaneously accumulated in TIMS tunnel 1, achieving a near-100 % duty cycle. Chemical noise ions are separated from peptide ions of interest based on their differential mobility.*

PASEF — Parallel Accumulation Serial Fragmentation

TIMS alone would represent only an incremental improvement without a revolutionary acquisition strategy. PASEF (Parallel Accumulation Serial Fragmentation) is the data acquisition mode that unlocks the full analytical power of TIMS-based 4D proteomics.

> **The PASEF Concept** While one group of ions is being analyzed in the TIMS analyzer, the next group is simultaneously being accumulated and trapped. This parallel operation means the instrument never 'wastes time' waiting — ions are continuously accumulated while the previous set is analyzed. The result is a near 100% duty cycle and a sequencing speed of over 100 Hz (more than 100 MS/MS spectra per second), compared to ~10-20 Hz for conventional DDA instruments.



Taken from Bruker tims-TOF

Figure W 5.2: The PASEF scan function operates at a sequencing speed of >120 Hz. Within each 1.1-second TIMS elution cycle, the quadrupole rapidly shifts between precursor ions (numbered 1-12) as they elute from the TIMS device in order of their ion mobility, generating MS/MS spectra for each without any loss of acquisition time.

In a PASEF acquisition, precursor ions are selected for fragmentation not only by their mass-to-charge ratio but also by their position in the ion mobility dimension. The instrument follows a 'PASEF scan function' that steps through the mobility space during the elution of ions from the TIMS device, triggering fragmentation events at the precise moment each target

ion is released. Because mobility is correlated with charge state — higher charge states have smaller CCS values and elute earlier from TIMS — the instrument can intelligently prioritize multiply-charged peptide ions for fragmentation while avoiding singly-charged background ions (Figure 2).

Collisional Cross Section (CCS) as a Molecular Descriptor

The CCS value measured by TIMS is more than a by-product of ion mobility separation — it is a genuinely informative molecular property. For proteomics applications, CCS values provide:

CCS Application	Description and Value
Peptide identification	CCS acts as a fourth identification filter alongside RT, precursor m/z, and fragment spectrum. False identifications that pass all three MS-based filters are much less likely to also match the expected CCS value.
Isomer discrimination	Peptide isomers with identical mass and nearly identical fragmentation (e.g., leucine/isoleucine, deamidation products) can be resolved in the CCS dimension.
PTM localization	Post-translational modifications alter the three-dimensional structure of a peptide, producing a measurable shift in CCS. This aids in localizing modification sites.
Cross-study matching	CCS values are highly reproducible and instrument-independent (when calibrated), enabling confident matching of peptides across experiments, laboratories, and time points.
Spectral library building	4D spectral libraries include CCS as an entry parameter, dramatically improving the specificity of library matching in DIA workflows compared to 3D libraries.

W 5.4: Data Acquisition Modes in 4D Proteomics

PASEF-DDA (Data-Dependent Acquisition)

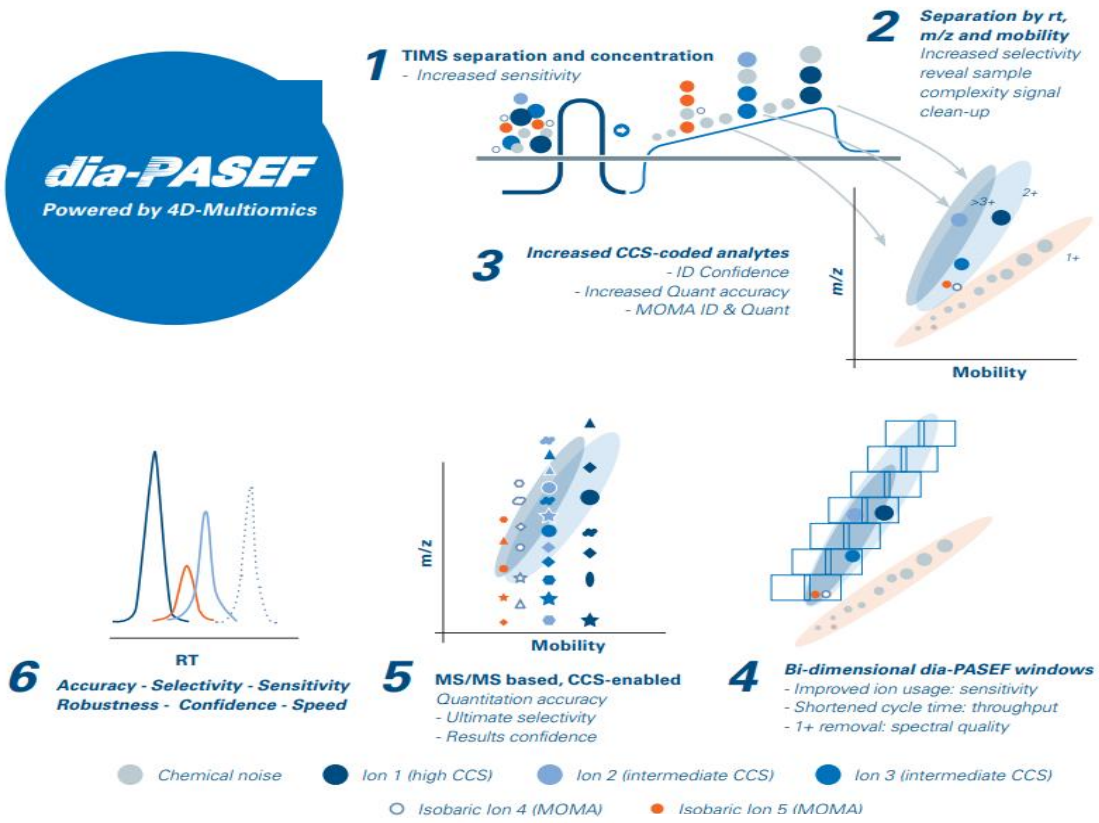
In PASEF-DDA mode, the instrument selects precursor ions for fragmentation based on a combination of their intensities, m/z values, and ion-mobility positions. The key innovations over classical DDA include:

- Charge-state based filtering: Singly-charged background ions (detergents, lipids, polymer contaminants) are excluded from fragmentation scheduling using their characteristic high CCS values. This dramatically reduces the number of wasted MS/MS events on non-peptide ions.
- Multiplexed PASEF scans: Multiple precursors at different m/z values but the same mobility range can be co-isolated and fragmented together, then deconvoluted computationally — increasing the number of MS/MS spectra per unit time.
- Dynamic exclusion with 4D coordinates: Previously fragmented precursors are excluded using all four dimensions (RT window, m/z window, charge state, AND CCS), minimizing redundant sampling.

diaPASEF (Data-Independent Acquisition with PASEF)

diaPASEF is the 4D implementation of data-independent acquisition and represents the most powerful quantitative proteomics workflow currently available. In diaPASEF:

- Isolation windows are defined in two-dimensional space: both m/z AND ion mobility. Instead of a single-wide m/z window (as in conventional DIA), diaPASEF uses narrow, diagonal windows that track the correlation between m/z and ion mobility for multiply charged peptides.
- The diagonal window design means each isolation window contains far fewer co-isolated precursors than a comparable conventional DIA window, producing cleaner MS/MS spectra and dramatically simplifying computational deconvolution.
- Proteome depth: diaPASEF routinely identifies 5,000–9,000 proteins from a single 60-minute LC run of a cell lysate — matching or exceeding what conventional DIA achieves in several hours of instrument time.
- Quantitative accuracy: The clean spectra produced by diaPASEF windows yield highly accurate peptide quantification, with coefficients of variation (CV) routinely below 10% across technical replicates (Figure 3).



Taken from Bruker tims-TOF manual

Figure W 5.3: The six key features of the diaPASEF acquisition strategy. (1) TIMS separation and ion concentration increase sensitivity. (2) Simultaneous separation in RT, m/z, and mobility dimensions reveals sample complexity. (3) CCS-coded analyte information adds identification confidence and quantification accuracy, including MOMA identification. (4) Bi-dimensional diagonal isolation windows improve ion usage and reduce cycle time while removing singly-charged background ions. (5) MS/MS-based CCS-enabled quantification provides ultimate selectivity. (6) Combined accuracy, selectivity, sensitivity, robustness, confidence, and speed.

diaPASEF vs Conventional DIA In conventional DIA, a 25 m/z isolation window at a typical peptide m/z of 700 Da might contain 30-50 co-isolated precursors. The corresponding diaPASEF diagonal window, which is narrow in m/z but scans across ion mobility, typically contains only 5-10 precursors — a 5-10 fold reduction in spectral complexity that translates directly into more confident identifications and better quantification.

W 5.5: The Role of Accumulated Spectra and Sensitivity

A unique feature of TIMS-based acquisition is the ability to accumulate signal across multiple PASEF cycles for the same precursor ion. Because ions with the same m/z and mobility are released from the TIMS device at the same time in each cycle, their signals can be co-added across cycles during data analysis. This signal accumulation increases the signal-to-noise ratio proportional to the square root of the number of accumulated cycles — providing a path to detecting very low-abundance proteins without sacrificing acquisition speed.

W 5.6: The Four Dimensions — A Detailed Look

Understanding how each dimension contributes to the overall analytical power of 4D proteomics is essential for experimental design, troubleshooting, and data interpretation.

#	Dimension	Physical Basis	Timescale	Information Content

1	**LC Retention Time**	Hydrophobicity / chemical interaction with stationary phase	Minutes to hours	Chemical class, hydrophobicity; enables prediction models
2	**Ion Mobility (CCS)**	Gas-phase size, shape, and charge of the ion	Milliseconds	Molecular shape, charge state, structural isomers, PTM-induced conformational changes
3	**Precursor Mass (MS1)**	Mass-to-charge ratio of intact peptide ion	Microseconds	Peptide mass; charge state; isotope envelope for quantification
4	**Fragment Mass (MS2)**	Mass-to-charge ratio of peptide fragment ions (b/y series)	Microseconds	Amino acid sequence; PTM localization; protein identification

Dimension 1: Liquid Chromatography Retention Time

Reversed-phase nano-flow HPLC (nanoHPLC) with C18 columns remains the primary separation step in 4D proteomics, performing the same role as in conventional LC-MS/MS. Peptides are separated over gradients of 20–120 minutes depending on sample complexity and desired proteome depth. The LC dimension reduces the complexity of the mixture entering the ion source at any given moment, but alone is insufficient to resolve the enormous chemical diversity of a proteome digest.

In 4D proteomics workflows, LC gradient optimization becomes even more important because the ion mobility and PASEF dimensions operate on a fixed timescale. The LC peak width must be sufficiently broad (typically >10 seconds) to ensure that multiple PASEF cycles accumulate for each eluting peptide, enabling signal averaging and improving quantification precision.

Dimension 2: Ion Mobility — The Defining Innovation

Ion mobility is the dimension that fundamentally distinguishes 4D proteomics. In the gas phase, after electrospray ionization, peptide ions are introduced into the ion mobility device, where they are separated based on their collisional cross section. The CCS value is determined by:

- Molecular size: Larger peptides and proteins have larger CCS values
- Molecular shape: Extended/unfolded conformations have larger CCS than compact/globular forms
- Charge state: Higher charge states generally produce smaller CCS values due to charge-induced structural compaction
- Amino acid composition: Certain residues (proline, aromatic residues) influence CCS through their effect on peptide backbone conformation

For tryptic peptides — the most common analytes in bottom-up proteomics — CCS values are highly predictable from sequence alone using machine learning models. This predictability enables the creation of in-silico 4D spectral libraries covering entire proteomes, which are essential for diaPASEF data analysis.

Dimension 3: Precursor Mass (MS1)

Following ion mobility separation, ions enter a high-resolution mass analyzer (a quadrupole time-of-flight, Q-TOF, in TIMS-based instruments) where their mass-to-charge ratio is measured with high accuracy (typically <5 ppm). This dimension provides the peptide's molecular mass, charge state, and isotope distribution. In 4D proteomics, the MS1 scan benefits directly from the prior ion mobility separation — because co-eluting ions have been partially resolved in the mobility dimension before entering the mass analyzer, the MS1 spectrum is cleaner and less congested than in conventional LC-MS/MS.

Dimension 4: Fragment Mass (MS2)

Peptide fragmentation (most commonly collision-induced dissociation, CID) produces sequence-specific b- and y-ion series that together define the peptide's amino acid sequence. In PASEF-based acquisition, fragmentation spectra benefit from the pre-separation of precursors by ion mobility, meaning each MS2 spectrum contains fragments from fewer co-isolated precursors than in conventional DDA or DIA. This reduces spectral chimera rates and improves sequence coverage, particularly for low-abundance peptides where chimeric contamination would otherwise prevent confident identification.

W 5.7: 4D Proteomics Workflow: Step-by-Step Protocol

A 4D proteomics experiment follows the same broad sample-preparation workflow as conventional shotgun proteomics, with critical differences in instrument setup, data-acquisition strategy, and computational analysis. The additional analytical power of ion mobility does not require changes to upstream sample preparation.

Step	Phase	Key Activities and 4D-Specific Considerations
1	**Sample Preparation**	Standard proteomics sample prep: cell lysis, protein extraction, reduction, alkylation, tryptic digestion, desalting. No special modifications required for 4D compatibility.
2	**LC Setup and Optimization**	Gradient optimization for peak width compatibility with PASEF cycle time; typically, 60–120 min gradients; nano-flow or micro-flow options.
3	**Instrument Calibration**	TIMS calibration using reference compounds of known CCS; mass calibration; tune source parameters for optimal ion transmission.
4	**PASEF Method Setup**	Define PASEF scan functions: set the number of PASEF scans per topN method; configure charge-state-based filtering; set dynamic exclusion parameters.
5	**Data Acquisition**	Acquire raw data in PASEF-DDA or diaPASEF mode; monitor real-time quality indicators; inject QC standards at regular intervals.
6	**Data Processing**	Convert raw data; perform TIMS demultiplexing; search against 4D spectral library or database; apply 4D FDR filtering; extract quantitative values.
7	**Downstream Analysis**	Statistical analysis; biological interpretation; pathway analysis; cross-dataset CCS-based matching.

W 5.8: Sample Preparation

4D proteomics is fully compatible with all standard proteomics sample preparation workflows. The power of the fourth dimension lies entirely in the instrument and data analysis — not in the need for special reagents or modified protocols. Standard workflows include:

- Cell and tissue lysis: Mechanical (bead beating, ultrasonication) or chemical (SDS, urea) lysis, depending on sample type
- Protein cleanup: FASP, S-Trap, SP3, or TCA precipitation to remove detergents, lipids, and other interfering compounds
- Reduction and alkylation: DTT/TCEP reduction followed by iodoacetamide or chloroacetamide alkylation
- Tryptic digestion: Standard overnight digestion at 37°C; Lys-C pre-digestion recommended for complex samples
- Desalting: C18 solid-phase extraction or StageTips to remove salts and contaminants before LC injection

> **Sample Amount Recommendation** 4D proteomics with PASEF acquisition is highly sensitive due to near-100% ion utilization. As little as 10-50 ng of total peptide digest is sufficient for comprehensive proteome coverage of simple samples. Standard loading amounts of 200-500 ng are used for complex samples requiring deep proteome coverage. This sensitivity advantage reduces sample requirements compared to conventional DDA approaches.

W 5.9: Liquid Chromatography Setup

Column and Flow Rate

The choice of the LC column and flow rate directly impacts the quality of 4D data. Key considerations:

- Column type: Reversed-phase C18, particle sizes 1.5-1.9 µm for nano-flow or 1.7-3.0 µm for micro-flow
- Column length: 15-50 cm analytical columns; longer columns improve peak capacity but require higher operating pressures
- Flow rates: Nano-flow (200-400 nL/min) provides maximum sensitivity; micro-flow (1-10 µL/min) offers improved robustness and throughput with modest sensitivity reduction

- Temperature: Column heating to 40-60°C improves peak shape and reproducibility

Gradient Design for PASEF Compatibility

PASEF acquisition benefits from LC peaks with sufficient width to accumulate multiple PASEF cycles. Critical parameters:

- Peak width target: Full-width at half-maximum (FWHM) of at least 15-20 seconds to ensure 5-10 PASEF cycles per peptide peak
- Gradient slope: Optimize the rate of organic solvent increase to spread peptide elution; overly steep gradients compress peaks and reduce PASEF accumulation
- Recommended gradient lengths: 20 min (fast proteomics, ~2,000-3,000 proteins), 60 min (standard, ~5,000-7,000 proteins), 120 min (deep proteomics, >8,000 proteins)
- Equilibration time: Allow 10-15 min column re-equilibration between injections for consistent retention times

W 5.10: Instrument Calibration

TIMS Calibration

Accurate CCS measurement requires calibration of the TIMS device using reference compounds with well-characterized CCS values. The calibration procedure:

- Standard compounds: Peptide calibrants (e.g., the Agilent ESI tuning mix, or calibrant peptide mixtures) with known CCS values covering the m/z and mobility range of interest are injected
- Calibration curve: A linear relationship between the inverse reduced mobility ($1/K_o$) and CCS is established using the Mason-Schamp equation
- Frequency: TIMS calibration should be performed at the beginning of each acquisition day and verified with QC peptides throughout the run
- Accuracy: Well-calibrated TIMS instruments achieve CCS accuracy of <1-2%, sufficient for confident cross-study matching and database searching

Mass Calibration

High-accuracy mass measurement (<5 ppm) is required for reliable peptide identification and is maintained through:

- Periodic recalibration using internal or external mass calibrants
- Automated calibration verification between sample injections
- Temperature-stabilized ion optics and mass analyzer to minimize mass drift

W 5.11: PASEF Method Configuration

PASEF-DDA Method Parameters

Setting up a PASEF-DDA method requires configuring the following key parameters:

Parameter	Typical Value	Rationale
Number of PASEF scans per MS1 cycle	8-10 scans	Balances sequencing speed with MS1 sampling rate; higher numbers increase MS/MS throughput
Target intensity for MS/MS triggering	2,500 counts	Ensures sufficient signal for quality fragmentation spectra; lower threshold increases coverage but may include noisy spectra
Charge state filter (exclude)	Charge state 1	Singly-charged ions are predominantly contaminants (lipids, polymers); excluding them dramatically increases peptide MS/MS efficiency
Dynamic exclusion duration	0.4-1.0 min	Prevents re-sequencing the same peptide; set relative to LC peak width
Collision energy	Stepped: 20-45 eV	Stepped collision energy improves sequence coverage across diverse peptide sizes and charge states
TIMS ramp time	100 ms	Duration of one TIMS elution; longer ramp improves mobility resolving power but reduces overall duty cycle

diaPASEF Method Design

diaPASEF method design requires defining isolation windows in two-dimensional m/z vs. ion mobility space:

- Window shape: Diagonal windows that follow the correlation between peptide m/z and ion mobility for doubly and triply charged ions. This correlation is predictable and relatively narrow, meaning diagonal windows can achieve high selectivity.
- Window coverage: Typical diaPASEF methods cover m/z 400-1200 Da across the full ion mobility range, divided into 8-32 windows depending on the desired scan speed and resolution.
- Cycle time: A full diaPASEF cycle (all windows) takes 0.5-2.0 seconds, providing 5-20 sampling points across a typical 10-second LC peak.
- Optimization: diaPASEF window schemes can be optimized using preliminary DDA data from the same sample type to position windows where peptide density is highest.

W 5.12: Quality Control

Rigorous QC is essential for 4D proteomics, with the additional dimension of CCS providing new QC opportunities:

- CCS drift monitoring: Track CCS values of QC peptides across a run series; drift >2% indicates TIMS calibration issues
- Retention time stability: Monitor RT of standard peptides; CV <1% expected for stable LC systems
- Protein group count tracking: Monitor number of identified protein groups per QC injection; declining counts indicate instrument degradation
- Intensity-based QC: Track signal intensity of QC peptides; drops >30% suggest source fouling or LC issues
- Missed cleavage rate: Should typically be <20% for well-prepared samples; high missed cleavage rates indicate digestion problems

W 5.13: Data Analysis in 4D Proteomics

The 4D Spectral Library

The cornerstone of 4D proteomics data analysis — particularly for diaPASEF — is the four-dimensional spectral library. Unlike conventional 3D libraries that index peptides by retention time, precursor m/z, and fragment ions, a 4D spectral library adds CCS as a fourth coordinate. The creation and use of 4D spectral libraries follows one of three strategies:

Experimental library generation: Deep PASEF-DDA data from the same or similar sample type, analyzed with a protein sequence database search. The resulting PSMs, along with their RT, m/z, CCS, and fragment spectra, form the 4D library entries. This approach is the most accurate but requires additional instrument time.

- In-silico library prediction: Machine learning models (notably Prosit-IMS, MS2ML, and DeepMobility) predict fragment ion spectra, retention times, AND CCS values from peptide sequences alone. Predicted 4D libraries now achieve accuracy comparable to experimental libraries for most standard proteomics applications and can cover entire proteomes without any prior measurements.
- Hybrid approach: Combine experimentally measured RT and CCS with predicted fragment spectra, or vice versa. This is particularly useful for studying novel organisms or non-standard sample types where experimental coverage is limited.

> **Why CCS Prediction Works** CCS values for tryptic peptides are highly predictable from sequence because the gas-phase conformation of these peptides is largely determined by their amino acid composition and sequence. Machine learning models trained on large experimental CCS datasets achieve prediction accuracies of 1-3% median absolute error — sufficient for confident use as a filtering coordinate in library searching.

Data Analysis Software for 4D Proteomics

Software	Mode	Key Features and 4D Capabilities
PEAKS Studio	*DDA/DIA*	De novo sequencing with IMS support; PTM discovery; 4D spectral library search; commercial with academic pricing

DIA-NN	*DIA/diaPASEF*	Leading open-source tool for diaPASEF analysis; deep learning-based; generates 4D spectral libraries in silico; exceptional speed and sensitivity
Spectronaut	*DIA/diaPASEF*	Commercial; robust diaPASEF analysis; dynamic retention time and CCS correction; excellent quantification accuracy
MaxQuant / TIMS version	*DDA*	PASEF-DDA analysis with CCS-based feature detection; label-free quantification; widely adopted in academic proteomics
FragPipe / MSFragger	*DDA/DIA*	Open-source; MSFragger ultrafast search engine; IonQuant for LFQ; open search for PTM discovery; strong community support
Mascot / Proteome Discoverer	*DDA*	Commercial; established workflows; Proteome Discoverer has PASEF-DDA node for Bruker raw files
AlphaTims	*Raw data*	Open-source Python tool for fast indexing and extraction of TIMS raw data; enabling custom analysis workflows

The 4D Search and Identification Pipeline

Feature Detection

4D proteomics raw data contains millions of data points across four dimensions. The first computational step is feature detection — identifying coherent signals that represent real peptide ions across all four dimensions. In 4D space, a feature is defined by its centroid position in RT, CCS, m/z, and intensity. Feature detection algorithms must:

- Distinguish peptide signals from chemical noise using all four dimensions simultaneously
- Group isotope peaks from the same peptide across the m/z dimension
- Handle the complex ion mobility peak shapes that can result from conformational heterogeneity
- Process the large data volumes (typically 10-50 GB per raw file) efficiently

Library Matching and Scoring

In diaPASEF analysis, detected features are matched against entries in the 4D spectral library. The matching score incorporates all four dimensions:

- RT match: Predicted vs. observed retention time, corrected for run-specific RT drift using alignment algorithms
- CCS match: Predicted vs. observed CCS; a window of typically ±2-4% is used; peptides outside this window are penalized or excluded
- Precursor m/z match: Mass accuracy filter, typically <10-20 ppm
- Fragment ion match: Dot product or normalized cross-correlation between observed and predicted fragment spectra

The combined 4D score achieves substantially lower false discovery rates than 3D scores alone, particularly for low-abundance peptides where any one dimension may provide marginal discrimination.

FDR Control in 4D Space

False discovery rate estimation in 4D proteomics uses the same target-decoy strategy as conventional proteomics, but with the CCS dimension providing an additional layer of confidence. A peptide identification that passes all four-dimensional filters is far less likely to be a false positive than one that passes only three. Studies have shown that incorporating CCS into FDR scoring reduces the false positive rate at any given sensitivity level by 2-5-fold compared to 3D scoring alone.

Quantification in 4D Proteomics

4D proteomics supports all standard quantification approaches used in conventional proteomics, with additional advantages from the ion mobility dimension:

- Label-free quantification (LFQ): MS1 peak areas extracted using 4D feature coordinates are more accurate than in 3D workflows due to reduced interference from co-eluting isobaric species resolved in the mobility dimension.
- TMT/iTRAQ multiplexing: PASEF acquisition is fully compatible with isobaric labeling; the clean MS2 spectra from PASEF-DDA reduce ratio compression artifacts compared to conventional instruments.

- SILAC: Standard SILAC workflows are directly compatible; the improved spectral purity of PASEF MS/MS spectra improves SILAC ratio accuracy.
- Direct CCS-based quantification: In development — CCS values can, in principle, be used to distinguish labeled and unlabeled peptides when mass differences are insufficient.

W 5.14: Applications of 4D Proteomics

Deep Proteome Profiling

The most immediate application of 4D proteomics is the depth and throughput of proteome profiling. Key benchmarks achieved with current 4D platforms:

Sample Type	Proteins Identified	Gradient Length	Key Achievement
HeLa cell lysate	>9,000	120 min	Near-complete cellular proteome coverage
HeLa cell lysate (fast)	>5,000	20 min	High-throughput clinical screening feasibility
Human plasma (depleted)	>1,000	60 min	Deep plasma proteome for biomarker discovery
Single cell (1 cell)	>1,000	30 min	Single-cell proteomics without pre-amplification
FFPE tissue	>4,000	60 min	Archival clinical sample proteomics

Clinical and Biomarker Applications

Plasma Proteomics

Human blood plasma contains proteins spanning more than 10 orders of magnitude in concentration — from albumin at mg/mL levels to cytokines at pg/mL. The dynamic range challenge of plasma proteomics makes it one of the most demanding applications in the field. 4D proteomics addresses this challenge through:

- Ion mobility-based noise reduction: Background chemical noise from lipids, glycans, and small molecules has distinct CCS profiles from tryptic peptides, enabling effective filtering that improves the detection limit for low-abundance proteins.
- Improved spectral purity: Fewer chimeric spectra mean that low-abundance peptides are not masked by interfering fragments from high-abundance co-eluting species.
- CCS as a biomarker coordinate: Changes in protein CCS values can indicate post-translational modifications or conformational changes associated with disease states, adding a new layer of biological information beyond protein abundance.

Clinical Cohort Studies

The throughput and reproducibility of 4D proteomics make it particularly suited for large clinical cohort studies. The ability to acquire 5,000+ protein quantifications per sample in a 60-minute run means that cohorts of hundreds to thousands of patients are analytically tractable. diaPASEF provides the consistent quantification (CV <10%) required to detect subtle differences in abundance across diverse patient samples.

Post-Translational Modification (PTM) Proteomics

PTM analysis benefits enormously from the fourth dimension because:

- PTMs change CCS: Phosphorylation, glycosylation, acetylation, and ubiquitination all alter the three-dimensional structure of a peptide, producing measurable CCS shifts of 1-10%. This shift can be used to confirm the presence and localization of PTMs independently of mass.
- Isomer resolution: Phosphopeptide isomers with the phosphate on different residues often have distinct CCS values, enabling localization of the modification site without ambiguity in the fragment spectrum.

- Glycoproteomics: The large glycan moieties attached to glycopeptides produce characteristic CCS values that help distinguish glycoforms, a notoriously difficult problem in conventional proteomics.
- Open search enrichment: PASEF-DDA with open search (allowing any mass modification) benefits from CCS filtering that reduces false positives among the enormous search space of modified peptides.

Targeted Proteomics (prm-PASEF)

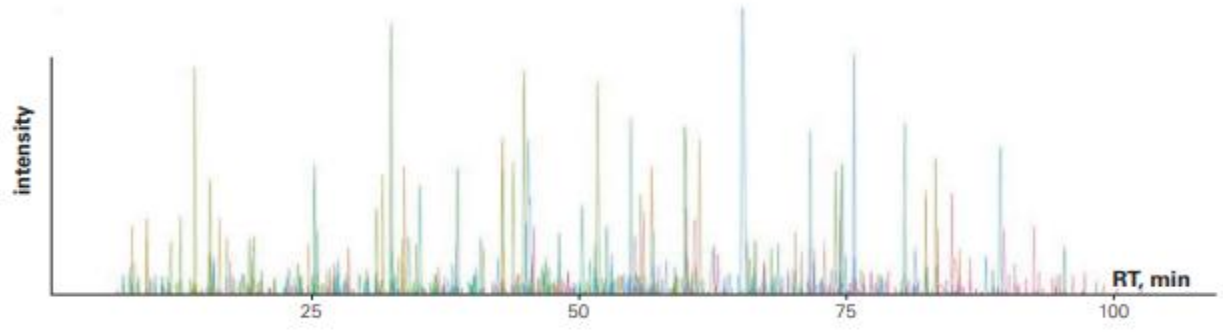


Figure W 5.4: Targeted proteomics analysis using prm-PASEF acquisition showing intensity traces for 1565 heavy and light precursors from 565 proteins across a 100-minute LC gradient. The ion mobility dimension provides an additional layer of selectivity over conventional parallel reaction monitoring, enabling confident quantification of low-abundance targets in complex plasma matrices.

For verification of biomarker candidates in large cohorts, targeted acquisition using the prm-PASEF mode enables hundreds of precursors to be monitored simultaneously with TIMS-enhanced selectivity. In a single acquisition, several hundred precursors can be targeted without compromising sensitivity.

Single-Cell Proteomics

Single-cell proteomics — quantifying proteins from individual cells — is an emerging frontier where 4D proteomics provides critical advantages. A single mammalian cell contains approximately 0.1-0.5 ng of total protein, requiring exceptional sensitivity. The near-100% ion utilization of TIMS-based instruments, combined with the noise reduction from ion mobility filtering, enables identification of 1,000-3,000 protein groups from a single cell without sample amplification or carrier proteome strategies, representing a major advance over conventional approaches.

Structural and Conformational Proteomics

The CCS dimension opens entirely new biological questions that cannot be addressed by conventional proteomics:

- Conformational changes: Proteins that undergo conformational changes (e.g., upon ligand binding, oxidative stress, or during protein folding diseases) may show CCS shifts detectable at the peptide level after controlled denaturation and renaturation.
- Cross-linking mass spectrometry (XL-MS): Cross-linked peptides have distinctive CCS values compared to non-cross-linked counterparts, aiding in the identification of cross-linked pairs within the large search space of XL-MS experiments.
- Native mass spectrometry: TIMS can be applied to non-denatured (native) protein complexes, providing CCS values for intact protein assemblies that report on quaternary structure and stoichiometry.

Metaproteomics and Environmental Proteomics

4D proteomics is increasingly being applied to metaproteomics — the study of proteins from complex microbial communities. The benefits are analogous to those in clinical proteomics: reduced spectral complexity through ion mobility, improved identification rates for low-abundance microbial proteins, and the ability to distinguish peptides from closely related organisms that may differ by only a single amino acid (and thus have similar masses but potentially different CCS values). Early studies applying PASEF acquisition to gut microbiome and ocean metaproteomics samples have demonstrated 2–3-fold increases in the number of identified microbial proteins compared to conventional DDA.

W 5.15: Advantages, Challenges, and Future Directions

Key Advantages of 4D Proteomics

Advantage	Explanation

Near-100% duty cycle	PASEF parallel accumulation means essentially no ions are wasted. Every ion that enters the source contributes to the analysis, providing a 5-10x increase in sensitivity over conventional DDA.
Dramatically reduced chimeric spectra	Ion mobility pre-separation reduces co-isolation of unrelated precursors, producing cleaner MS/MS spectra and higher identification rates, especially for low-abundance peptides.
Proteome depth without fractionation	diaPASEF routinely achieves >7,000 protein identifications from a single unfractionated injection — rivaling what once required extensive offline fractionation.
Charge-state filtering	Singly-charged contaminating ions are excluded from PASEF scheduling based on their distinct CCS signatures, thereby improving peptide MS/MS efficiency by 50-70%.
CCS as a fourth ID coordinate	The additional filtering power of CCS reduces false-positive identification rates by 2-5-fold at equivalent sensitivity levels.
Exceptional quantitative precision	The clean spectra produced by PASEF-DIA enable quantification CVs of <5-10% across technical replicates — among the best achievable in proteomics.
Unique structural information	CCS reports on molecular shape and charge distribution, providing biological information inaccessible to conventional mass-only measurements.

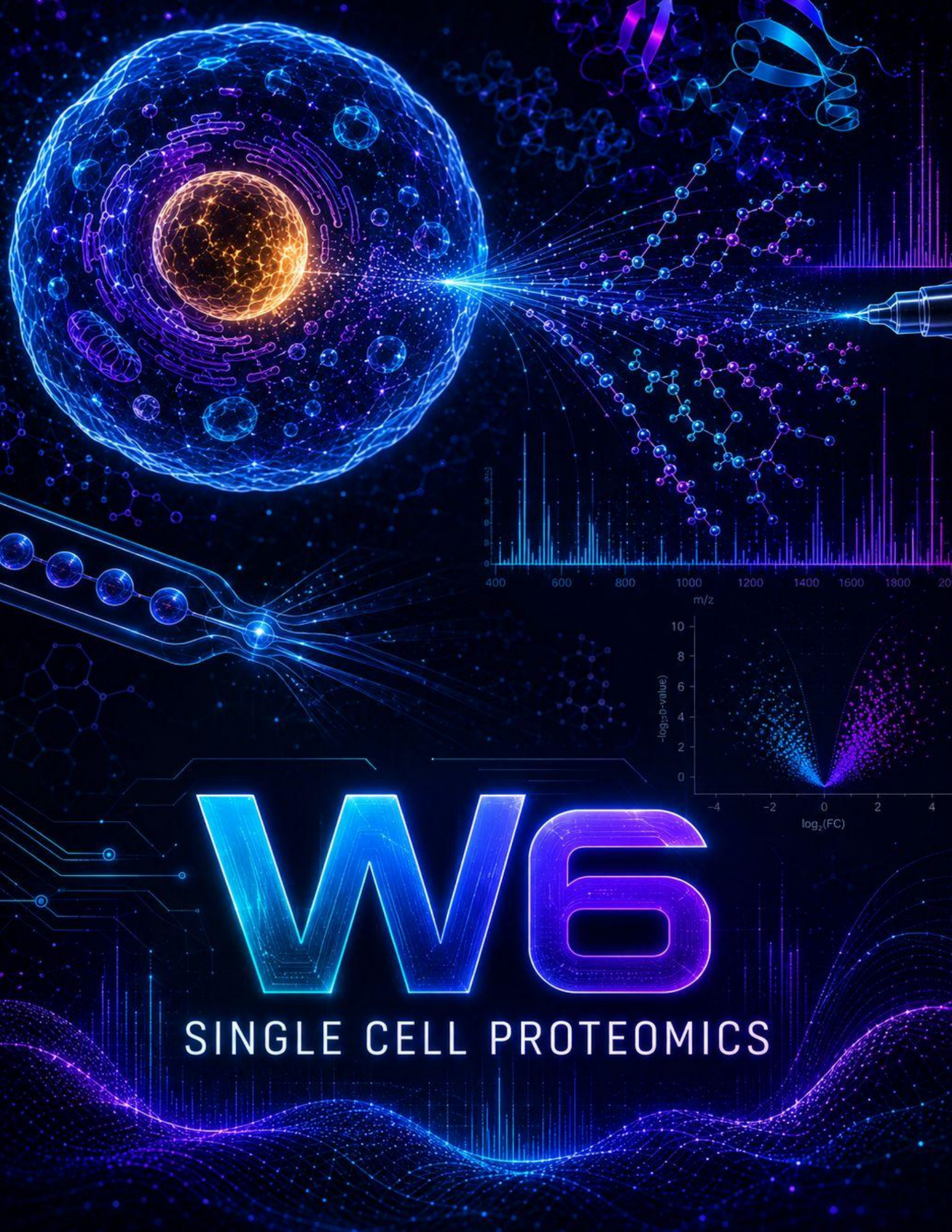
Current Challenges

Challenge	Impact	Current Mitigation
Large data volumes	Raw files of 5-50 GB require substantial storage and fast processing infrastructure	Compressed raw data formats; cloud computing; tiered storage strategies
Specialized software expertise	4D data analysis tools have steeper learning curves than conventional proteomics software	Growing community tutorials; university training programs; vendor-provided workshops
4D spectral library availability	Comprehensive 4D libraries exist for human proteome but are limited for other organisms	In-silico library prediction tools (DIA-NN, Prosit-IMS) now cover most sequenced proteomes
CCS standardization	CCS values are instrument- and buffer-gas-dependent; cross-platform comparisons require calibration harmonization	Community CCS reference standards; standardized calibration protocols under development
Cost and availability	TIMS-equipped instruments represent a significant capital investment	Expanding availability through core facilities; decreasing instrument costs over time

W 5.16: Future Directions

- Artificial intelligence integration: Deep learning models for CCS prediction, spectral library generation, and data analysis are rapidly improving. Future AI systems will generate near-perfect in-silico 4D libraries for any organism, eliminating the need for experimental library generation.
- Single-cell 4D proteomics: Continuing sensitivity improvements will push detection limits below 100 proteins per cell, enabling routine single-cell proteomics of primary clinical samples and rare cell populations.
- Spatial 4D proteomics: Combining tissue imaging mass spectrometry with ion mobility will enable spatial mapping of protein expression with CCS-filtered specificity — spatial 4D proteomics.
- Real-time clinical diagnostics: Fast 4D proteomics workflows (15-20 min gradient, >2,000 proteins) combined with automated data analysis pipelines will enable same-day clinical proteomics results for diagnostics and treatment monitoring.

- Native 4D proteomics: Applying TIMS to native, non-denatured protein complexes at scale will provide structural proteomics information on entire interactomes.
- Multi-omics integration: Combining 4D proteomics with metabolomics (also benefiting from IMS) and genomics in unified analysis frameworks will enable true molecular phenotyping.


m/z
400
600
800
1000
1200
1400
1600
1800
-log10(p-value)
log2(FC)
W6
SINGLE CELL PROTEOMICS





Single Cell & Deep Visual Proteomics

SCIENTIFIC PROGRAMME

Overview

Workshop 6 at APT-2026 focuses on the emerging and transformative field of Single Cell Proteomics, which enables analysis of proteins at the individual-cell level to uncover cellular diversity, heterogeneity, and functional complexity. This workshop is designed to introduce participants to cutting-edge technologies and analytical strategies that are reshaping biological and clinical research.

The workshop will cover key concepts and workflows in single-cell and spatial proteomics, highlighting how ultra-sensitive proteomics technologies can profile low-abundance proteins with exceptional sensitivity and resolution. Participants will gain insights into approaches for studying cellular microenvironments, tissue architecture, and disease-associated molecular variations.

A major emphasis of the workshop will be on data analysis and bioinformatics, including computational tools used for integrative analysis and interpretation of complex single-cell proteomics datasets. The sessions will also demonstrate applications of single-cell proteomics in precision medicine, disease biology, biomarker discovery, and therapeutic research.

Designed for students, researchers, and clinicians, this workshop provides exposure to next-generation proteomics approaches that are enabling unprecedented understanding of cellular function in health and disease.

KEY LEARNING AREAS

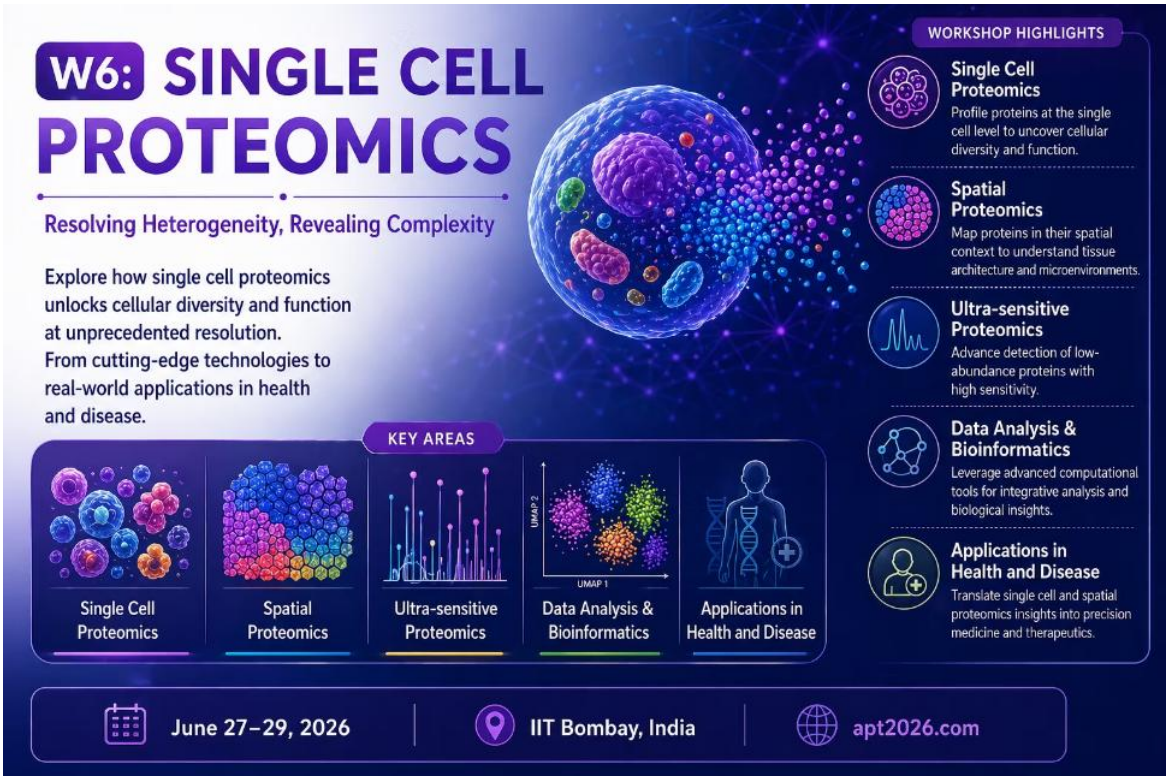
Key Learning Areas

- Single-cell proteomics workflows
- Spatial proteomics and tissue mapping
- Ultra-sensitive proteomics technologies
- Data analysis and bioinformatics
- Applications in health and disease research

WHAT PARTICIPANTS WILL GAIN

What Participants Will Gain

- Understanding of cellular heterogeneity and complexity
- Exposure to advanced single-cell proteomics technologies
- Knowledge of computational and bioinformatics tools
- Insights into translational and precision medicine applications
- Understanding of emerging trends in next-generation proteomics



DETAILED WORKSHOP CONTENT

Single Cell & Deep Visual Proteomics (Detailed)

Foundations of Single-Cell Proteomics

W 6.1: Introduction to Proteomics

Proteomics is the large-scale study of all proteins expressed by a cell, tissue, or organism at a particular time under specific conditions. Unlike the genome, which remains relatively stable, the proteome, or the complete set of proteins in a biological system, changes continuously in response to disease, environmental factors, cell cycle progression, differentiation, and stress. Proteins are the primary functional molecules of the cell. They catalyse biochemical reactions, transmit signals, provide structural support, and protect against pathogens. Understanding which proteins are present, how abundant they are, and where they are located within cells provides direct insight into biological function and disease processes, something that cannot be fully captured by studying the genome or transcriptome alone.

Note: mRNA levels (the transcriptome) predict protein abundance with only ~40-60% accuracy. Post-translational modifications, differences in protein stability, and translational regulation all influence protein levels, making direct protein measurement essential for understanding cell biology.

W 6.2: Limitations of Bulk Proteomics

Traditional proteomics analyses millions of cells together after they have been homogenised into a single sample. While this provides an overall protein profile, it masks the substantial biological variation that exists between individual cells within a tissue. Major limitations include:

- **Cellular heterogeneity:** A tumour contains cancer cells, immune cells, fibroblasts, and endothelial cells, each with its own distinct proteome. When analysed together, these differences are averaged out and individual cellular identities are lost.
- **Rare cell populations:** A drug-resistant cancer cell may represent only 0.1% of the cells in a tumour. Its unique protein signature is often undetectable in bulk proteomic measurements.

- **Cell state transitions:** Cells undergoing differentiation, division, or apoptosis exhibit distinct proteomic states that become diluted when mixed with large numbers of other cells.
- **Spatial context:** Proteins expressed in hepatocytes near the portal vein can differ substantially from those expressed near the central vein. Tissue homogenisation removes this spatial information entirely.

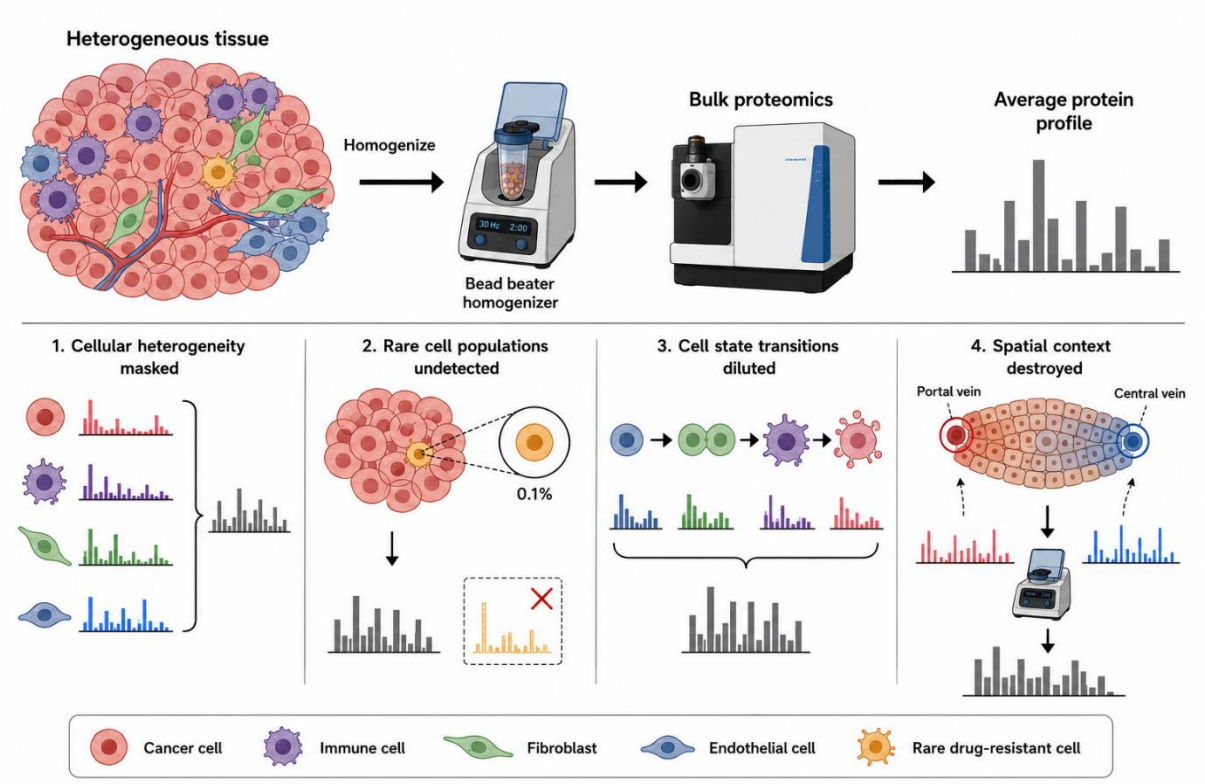


Figure 6.1. Key limitations of bulk proteomics in heterogeneous tissues.

Note: Many biological tissues are composed of diverse cell types that perform specialised functions and respond differently to their local environment. When all cells are combined into a single sample, the resulting protein profile represents an average signal that may not accurately reflect the behaviour of any individual cell population. As a result, biologically important differences can remain hidden in bulk measurements.

W 6.3: Emergence of Single-Cell Biology

The rapid advances in single-cell RNA sequencing (scRNA-seq) during the 2010s transformed our understanding of tissue organisation and cellular diversity. Projects such as the Human Cell Atlas have used transcriptomics to catalogue millions of cells across a wide range of tissues. However, mRNA does not always reflect protein abundance or activity. Cells with very similar transcriptomes can exhibit markedly different proteomes due to post-translational modifications (PTMs), differences in protein degradation rates, translational regulation by microRNAs and RNA-binding proteins, and the dynamics of protein complex assembly. These limitations highlighted the need for single-cell proteomics (SCP), which aims to measure thousands of proteins directly from individual cells.

W 6.4: Technical Challenges in Single-Cell Proteomics

A single mammalian cell contains approximately 10,000-30,000 different proteins, yet its total protein content is only about 50-250 picograms (pg), roughly 200,000 times less than the amount used in a conventional proteomics experiment. This creates several major technical challenges:

- **No Amplification:** Unlike DNA or RNA, proteins cannot be amplified by PCR. Every protein molecule must be detected directly from the extremely small amount of material present in a single-cell lysate.
- **Massive Dynamic Range:** Protein abundances span a concentration range of approximately 10^7-fold, ranging from a single copy of a transcription factor to around 10 million copies of abundant housekeeping enzymes within the same cell.

- **Sample Loss:** Proteins readily adsorb to tube walls, filter membranes, and pipette tips. Losing even 10% of the protein content from a single cell can significantly compromise the experiment.
- **Missing Data:** Mass spectrometers sample peptides in a stochastic manner. As a result, many proteins may be detected in some cells but not in others, leading to missing values in the final dataset.

W 6.5: Technologies Behind Single-Cell Proteomics

Cell Isolation Methods

Fluorescence-Activated Cell Sorting (FACS)

FACS remains the most widely used method for isolating individual cells. Cells are labelled with fluorescent antibodies and sorted at speeds up to 50,000 cells/second into 96- or 384-well plates. Surface antibodies conjugated to fluorescent dyes (FITC, PE, APC, BV421) are applied at titrated concentrations (~1-5 µg/mL). The FACS instrument uses hydrodynamic focusing to pass cells single-file through laser interrogation points. Viability dyes (DAPI, 7-AAD) exclude dead cells. Sort purity should exceed 95% for SCP work.

Laser Capture Microdissection (LCM/LMD)

LCM uses a focused UV laser to precisely excise cells or regions from tissue sections mounted on polyethylene naphthalate (PEN) membrane slides. This is critical for spatial proteomics since it preserves tissue context and allows isolation of specific cells based on morphology and location. The Leica LMD7 achieves ~200 nm spatial accuracy and can process 700 cell contours per hour in automated mode.

Microfluidic Platforms: nanoPOTS

The nanoPOTS (Nanodroplet Processing in One-pot for Trace Samples) chip confines cell lysis and digestion to 10-200 nL volumes. The core principle: by reducing sample volume, the surface-area-to-volume ratio decreases dramatically, and protein recovery improves proportionally. In a standard 1.5 mL tube with 100 µL buffer, most low-abundance proteins from a single cell adsorb to the tube wall. In a 10 nL nanoPOTS droplet, the same protein is 10,000x more concentrated — thermodynamic equilibrium favours proteins remaining in solution.

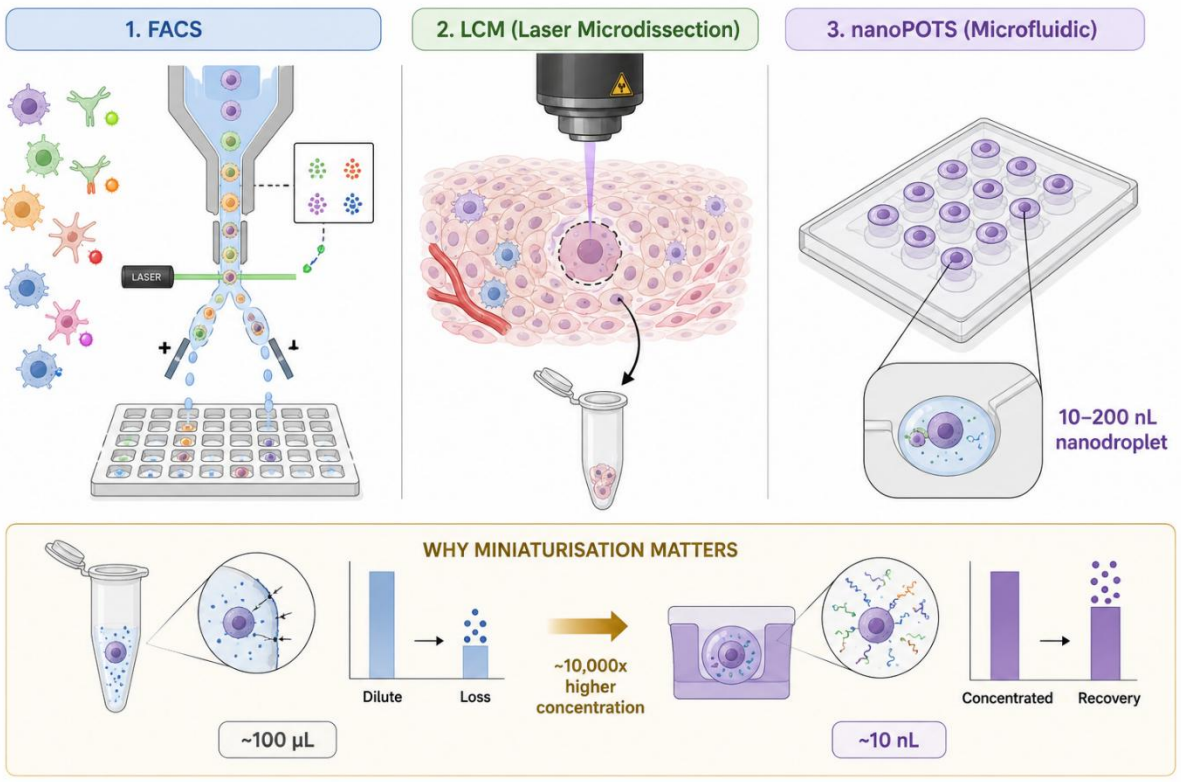


Figure 6.2. Key technologies enabling modern single-cell proteomics workflows.

Note: In a standard 1.5 mL tube, a protein from a single cell is dissolved in ~100 µL buffer. At such low concentrations, proteins stick to surfaces and are lost. In a 10 nL nanoPOTS droplet, the same protein is 10,000x more concentrated — dramatically improving peptide recovery and MS signal.

W 6.6: Sample Preparation Strategies

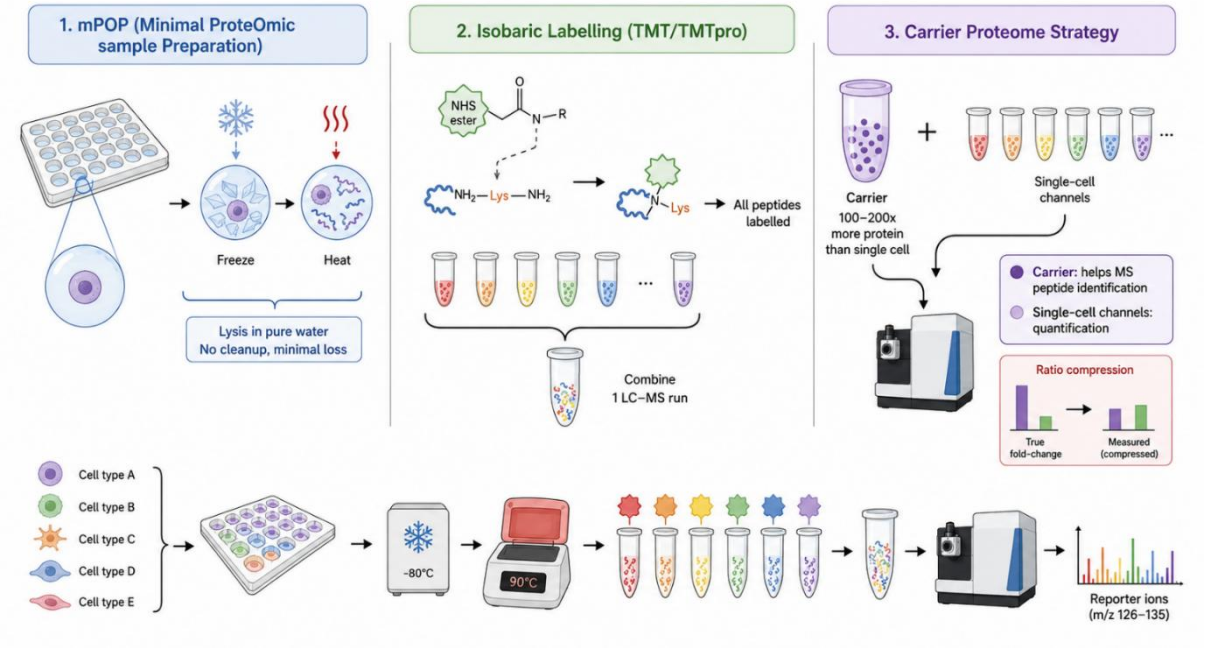


Figure 6.3. mPOP, isobaric labeling, and carrier-assisted quantification in single-cell proteomics.

mPOP: Minimal ProteOmic sample Preparation

Developed by the Slavov lab (Northeastern University), mPOP uses a simple freeze-heat cycle to lyse cells directly in water within multiwell plates. The freeze step forms ice crystals that physically disrupt the plasma membrane. The heat step (90°C, 10 min in a PCR thermocycler) denatures endogenous proteases and phosphatases. This clean lysis in pure water avoids detergents and buffers that would require removal before TMT labelling, eliminating all cleanup-associated sample losses.

Isobaric Labelling with TMT and TMTpro

TMT (Tandem Mass Tag) reagents are NHS ester-activated compounds that react with primary amines, the epsilon-amino group of lysine side chains and peptide N-termini. This ensures every peptide is labelled. Multiple TMT-labelled samples are combined and analysed together in one LC-MS run. Upon fragmentation, unique reporter ions (m/z 126-135) are released, each reflecting protein abundance in a specific sample. TMTpro allows up to 18-plex experiments. Labelling efficiency should exceed 95%.

W 6.7: Carrier-Assisted Quantification

In SCoPE-MS and SCoPE2, a 'carrier' channel containing 100-200x more protein than a single cell is added to each TMT batch. The carrier provides abundant peptide signal that guides the mass spectrometer to select the correct peptides for fragmentation, while quantification comes from the individual single-cell channels. However, the carrier can cause ratio compression — measured fold-changes between cells are compressed toward 1 because co-isolated peptides contribute more to the single-cell channels. Optimal carrier size is 100-200x (not 1000x).

W 6.8: Mass Spectrometry Instruments

Instrument	Key Features for Single-Cell Proteomics
Orbitrap Astral (Thermo Fisher, 2023)	~200 Hz scan speed; narrow-window DIA (4 m/z); 1,500-2,500 proteins per single HeLa cell label-free. Ideal for DVP workflows and spatial proteomics.
timsTOF Ultra 2 (Bruker, 2024-25)	Adds Trapped Ion Mobility Spectrometry (TIMS) for 4D separation. Athena Ion Processor (2025) enables 4,000-5,000 proteins per single HeLa cell. Dedicated timsTOF SCP model for single-cell work.

diaPASEF	Parallel Accumulation-Serial Fragmentation + DIA. Uses ion mobility to separate co-eluting peptides. Near 100% duty cycle. Standard acquisition on timsTOF for DVP and scDVP workflows.
Evosep ONE LC	Pre-loaded Evotip SPE tips enable 20-120 samples/day at 100-200 nL/min. Whisper 40-120 SPD gradients. Eliminates traditional gradient pump. Critical for tissue-scale DVP throughput.

W 6.9: Acquisition Strategies: DDA and DIA

Data-Dependent Acquisition (DDA) selects the top-N most abundant peptide ions for fragmentation — stochastic, creating run-to-run variation and high missing data rates in SCP. Data-Independent Acquisition (DIA) systematically fragments all ions within predefined m/z windows in every cycle, achieving high reproducibility and low missing data, at the cost of requiring spectral library-based analysis (DIA-NN, Spectronaut). DIA is now preferred for DVP and label-free SCP. DDA remains standard for SCoPE2 where the carrier channel dominates MS1 signal selection.

W 6.10: Deep Visual Proteomics and Spatial Proteome Mapping

Introduction to Deep Visual Proteomics (DVP)

Deep Visual Proteomics, introduced by Mund, Coscia, Mann et al. (Nature Biotechnology, 2022), is a landmark technology that integrates four powerful technologies into a single workflow to enable protein profiling at single-cell-type resolution while preserving spatial context in tissues. DVP inverts the conventional proteomics workflow: instead of dissociating tissue and hoping that mass spectrometry will reveal cell-type-specific proteins post-hoc, DVP first visually identifies every cell type in its native spatial context using AI-guided microscopy, then directly isolates the cells of interest using a laser, and finally measures their complete proteome by ultra-sensitive MS.

The Central Concept of DVP

DVP combines the strengths of imaging and mass spectrometry in a single experiment, providing both spatial context and deep proteome coverage. It performs 'biological fractionation' by collecting groups of morphologically similar cells from specific locations within a tissue, allowing sensitivity, throughput, and spatial information to be captured together in the same workflow.

W 6.11: Key Components of the DVP Workflow

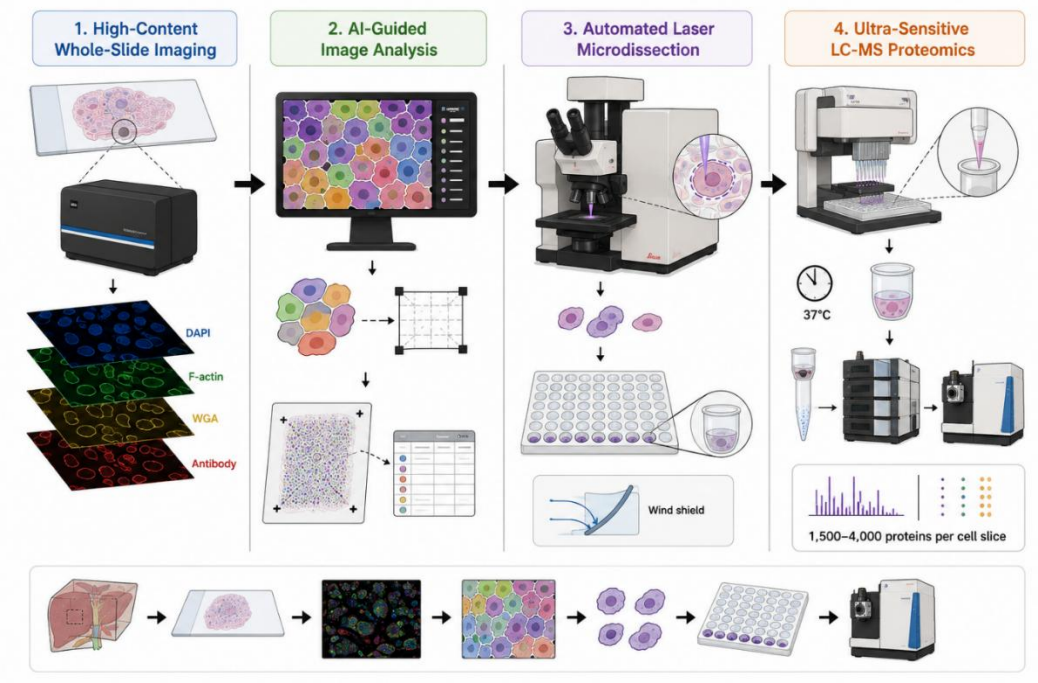


Figure 6.4. Overview of the Deep Visual Proteomics (DVP) workflow.

Component 1: High-Content Whole-Slide Imaging

Tissue sections (5-10 µm) on PEN membrane slides are stained with 3-6 fluorescent markers: DAPI (nuclear counterstain), phalloidin-Alexa Fluor (F-actin/cell body), WGA-Alexa Fluor (membranes), and cell-type-specific antibodies. A high-content scanner (Zeiss AxioScan, Leica THUNDER) images the entire slide at 20x-40x magnification, generating multi-channel whole-slide images (1-10 GB). At 20x with 0.3-0.5 µm/pixel resolution, cell nuclei (5-10 µm diameter) are resolved with ~20-30 pixels.

Component 2: AI-Guided Image Analysis (BIAS Software)

The BIAS (BioImage Analysis Software) platform, developed by Peter Horvath's group, serves as the central informatics hub. Deep learning models (CellPose 2.0, nucleAIzer/U-Net) segment individual cells from tissue images, assigning every pixel to a specific cell. Machine learning classifies cells into types based on morphological and intensity features. BIAS computes an affine transformation matrix (rotation, translation, scaling, shear) using 4-8 fiducial markers to map scanner coordinates to the LMD instrument's coordinate system with ~200 nm accuracy.

Component 3: Automated Laser Microdissection

Segmented cell contours are exported to the Leica LMD7, which uses a 355 nm pulsed UV laser to excise tissue with micrometre precision. Key operational parameters: Laser power 45, Aperture 1, Speed 40, Pulse frequency ~2,982 Hz, offset 190 µm (laser cuts outside cell contour to avoid UV protein damage). Excised pieces fall by gravity into 384-well plates (Eppendorf 0030129547) positioned below the stage. A wind-shield plate prevents air currents from deflecting falling tissue pieces. The LMD processes 700 contours/hour in fully automated mode.

Component 4: Ultra-Sensitive LC-MS Proteomics

Excised tissue is processed directly in the 384-well collection plate (no transfer to other vessels). The BRAVO robotic liquid handler adds 1 µL of extraction buffer containing 0.1-0.2% DDM detergent, 5 mM TCEP, 50-100 mM TEAB, and sequencing-grade trypsin (20-50 ng/µL). Simultaneous lysis, reduction, and digestion proceed at 37°C for 4-16 hours. Peptides are loaded onto Evotips and separated on the Evosep ONE, then analysed on timsTOF SCP (diaPASEF) or Orbitrap Astral (narrow-window DIA). DIA-NN with predicted spectral libraries and Match Between Runs provides 1,500-4,000 protein identifications per cell slice.

W 6.12: Applications of Deep Visual Proteomics

Liver Zonation (scDVP, Nature Methods, 2023)

Rosenberger, Thielert, Strauss et al. extended DVP to true single-cell resolution in tissue (scDVP). Applied to mouse liver, scDVP profiled individual hepatocytes at ~1,700 proteins/cell and discovered that ~50% of the hepatocyte proteome varies spatially along the porto-central axis. Machine learning models could infer a hepatocyte's spatial position from its protein profile alone. This was the first demonstration of liver metabolic zonation at protein level with true single-cell resolution.

Background: Liver Zonation

Hepatocytes near the portal vein specialise in amino acid metabolism; those near the central vein in lipid metabolism and detoxification. scDVP revealed these metabolic differences are encoded at the protein level with dramatic spatial gradients, impossible to detect by bulk proteomics, transcriptomics, or conventional immunohistochemistry.

Toxic Epidermal Necrolysis, First Clinical DVP Application (Nature, 2024)

Nordmann, Mann et al. applied DVP to skin biopsies from a patient with toxic epidermal necrolysis (TEN), a life-threatening blistering disease. DVP identified activated JAK-STAT signalling as the key molecular driver of keratinocyte death. Targeted JAK inhibitor therapy (baricitinib) was administered, the patient recovered within weeks. This represents the first case of single-cell spatial proteomics directly guiding clinical therapy in real time.

Alpha-1 Antitrypsin Deficiency: Application in Genetic Liver Disease (Nature, 2025)

DVP applied to FFPE liver biopsies from AATD patients resolved cell-type-specific proteotoxic stress responses, distinguishing hepatocytes loaded with misfolded Z-AAT protein from adjacent stress-compensating cells and immune infiltrates. This demonstrated DVP as a powerful tool for rare disease research and precision medicine using routinely archived clinical tissue.

Overview of Single-Cell Proteomics Approaches

Single-cell proteomics workflows fall into four paradigms. Understanding their trade-offs is essential for experimental design:

Parameter	SCoPE2	nanoPOTS LF	One-Pot 384w	DVP (pooled)	scDVP	plexDIA
Cell input	1 cell/channel	1 cell	1 cell	5-200 cells	1 cell slice	1 cell/channel
Sample volume	0.2-0.5 µL	10-200 nL	1 µL	1 µL	1 µL	0.2 µL
Proteins/cell	~1,000-3,000*	500-3,000	1,000-4,000	3,000-5,000+	1,500-2,500	~1,000-2,500
Cells/run	14 (TMTpro16)	1	1	1 cell type pool	1	3 (mTRAQ)
Throughput/day	~200 cells	~20-40 cells	~80-120 cells	~20-40 regions	~40-100 cells	~300-600 cells
Spatial context	No	No	No	Yes	Yes	No
MS acquisition	DDA + TMT	DIA label-free	DIA label-free	diaPASEF / DIA	diaPASEF / DIA	DIA + mTRAQ
Key limitation	Ratio compression	Low throughput	High missing data	Not truly s-c	LMD setup needed	Only 3-plex

** Across the full experiment; individual cells may have 500-1,500 proteins detected.*

nanoPOTS: Detailed Workflow

Understanding Surface Loss in Low-Input Proteomics

In a standard 1.5 mL tube with 100 µL buffer, proteins from a single cell (~200 pg total) are at ~10^-20 M concentration, far below the Kd for non-specific surface adsorption (~10^-10 to 10^-8 M). All low-abundance proteins adsorb to the tube wall and are lost. In a 10 nL nanoPOTS droplet, the same protein concentration is increased 10,000-fold. Thermodynamic equilibrium now strongly favours proteins remaining in solution, dramatically improving recovery.

nanoPOTS Step-by-Step Protocol

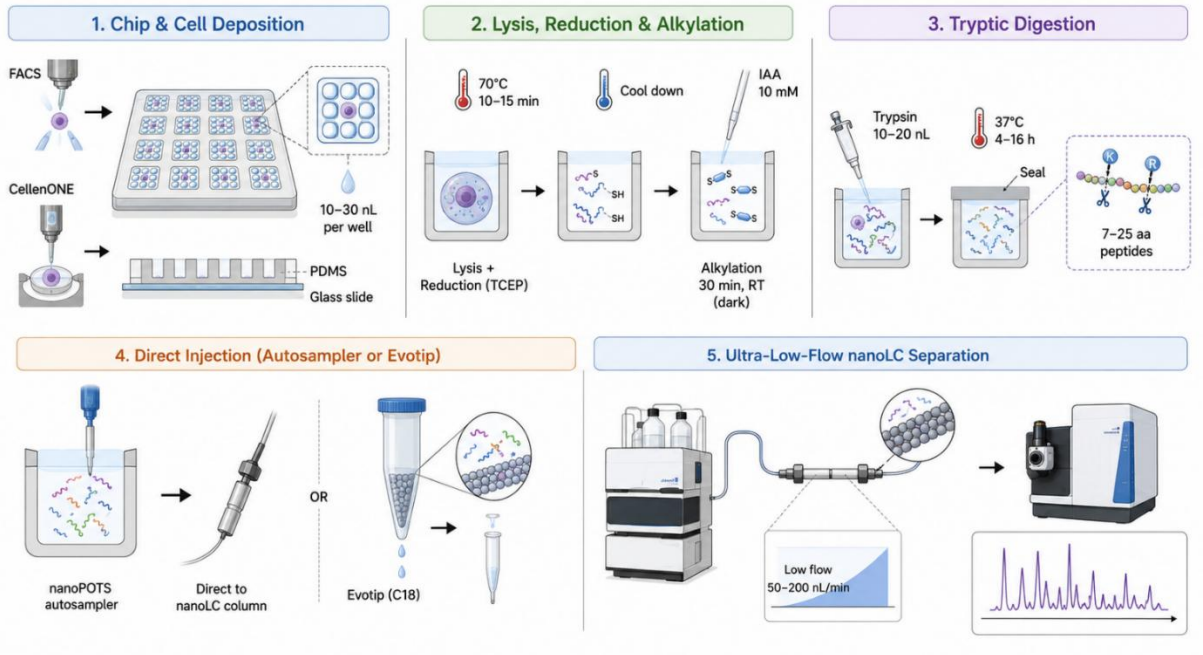


Figure 6.5. Overview of the nanoPOTS workflow for single-cell proteomics.

Step 1: Chip Design and Cell Deposition

nanoPOTS chips are fabricated from PDMS bonded to glass slides with BSA-passivated nanowell surfaces. The N2 (nested nanoPOTS) chip features 27 clusters of 9 nanowells (<30 nL each, 243 wells total). Individual cells are deposited by FACS or CellenONE into nanowells pre-wetted with 100 nL of 0.2% DDM (n-dodecyl beta-D-maltoside) in 100 mM TEAB buffer. Total volume after cell deposition is kept to 200-300 nL maximum to maintain high protein concentration.

Step 2: Cell Lysis, Reduction, and Alkylation

The chip is incubated at 70°C for 10-15 minutes. DDM detergent assists membrane protein extraction without precipitation or MS interference. TCEP (5 mM) in the lysis buffer reduces disulfide bonds at 70°C, unfolding proteins for complete digestion. After cooling, iodoacetamide (10 mM) is added for 30 min at room temperature in darkness, carbamidomethylating free thiols to prevent re-oxidation and ensure reproducible cysteine coverage.

Step 3: Tryptic Digestion

Sequencing-grade trypsin (Promega Gold or Platinum grade, free of chymotryptic contamination) is added at 10-20 nL per well (~0.5-1 ng trypsin for ~200 pg protein, approximately 1:200 mass ratio). Digestion proceeds at 37°C for 4-16 hours in a sealed, humidity-controlled incubator. The chip is sealed with optical adhesive film. Trypsin cleaves C-terminal to arginine and lysine residues (except when followed by proline), generating 7-25 amino acid peptides optimal for LC-MS/MS identification.

Step 4: Direct Injection via nanoPOTS Autosampler or Evotips

After digestion, peptides are extracted using a nanoPOTS autosampler, a custom capillary device aspirating the entire droplet (100-200 nL) and injecting directly onto the nanoLC column without intermediate storage. Alternatively, Evotips (single-use C18 SPE tips) trap peptides from the droplet while allowing salts and DDM to flow through. Sample transfer to any other vessel is avoided, even StageTip desalting causes 30-50% peptide loss from surface adsorption in these ultra-low-input samples.

Step 5: Ultra-Low-Flow nanoLC Separation

Peptides are separated on a reversed-phase nanoLC column (C18, 50-75 µm ID, 15-25 cm length, 1.7-2 µm particles) at 50-200 nL/min, lower than standard nanoLC (300-400 nL/min) to increase ionisation efficiency and extend elution windows. The Evosep ONE enables 20-120 samples/day using Whisper gradients (12-70 min active). Column temperature is thermostatted at 50-60°C for reproducible peak shapes.

SCoPE2: Detailed Workflow

Principle of SCoPE2

SCoPE2 uses isobaric TMT mass tags to chemically label peptides from multiple single cells, a 5-cell reference channel, and a 200-cell carrier channel, then combines them into a single LC-MS/MS run. In the mass spectrometer, all labelled peptides appear at the same nominal mass. Upon HCD fragmentation, each TMT tag releases a unique reporter ion (m/z 126-135) whose intensity directly reflects relative protein abundance in each cell vs. the reference. The carrier channel (200x concentrated) ensures the MS selects the correct peptides for fragmentation, bypassing the sensitivity threshold that would otherwise make single-cell signal invisible.

SCoPE2 Experimental Design: TMTpro16 Channel Layout

TMT Channel	Content	Cell Equivalent	Purpose
Channel 1 (126)	Carrier proteome (same cell type)	200 cells	Boosts peptide fragment ion signal for MS2 identification; reduces surface losses of single-cell peptides; guides instrument to select correct peptides.
Channel 2 (127N)	Reference channel (same cell type)	5 cells	Normalises across different SCoPE2 sets throughout the experiment; enables data integration from multiple LC-MS runs; removes run-to-run variation.

Channels 3-16 (127C-135N)	Individual single cells	1 cell each (x14)	The actual single-cell proteome measurements. Reporter ion intensities divided by reference channel give reference-normalised protein abundances comparable across all runs.

SCoPE2 Step-by-Step Protocol

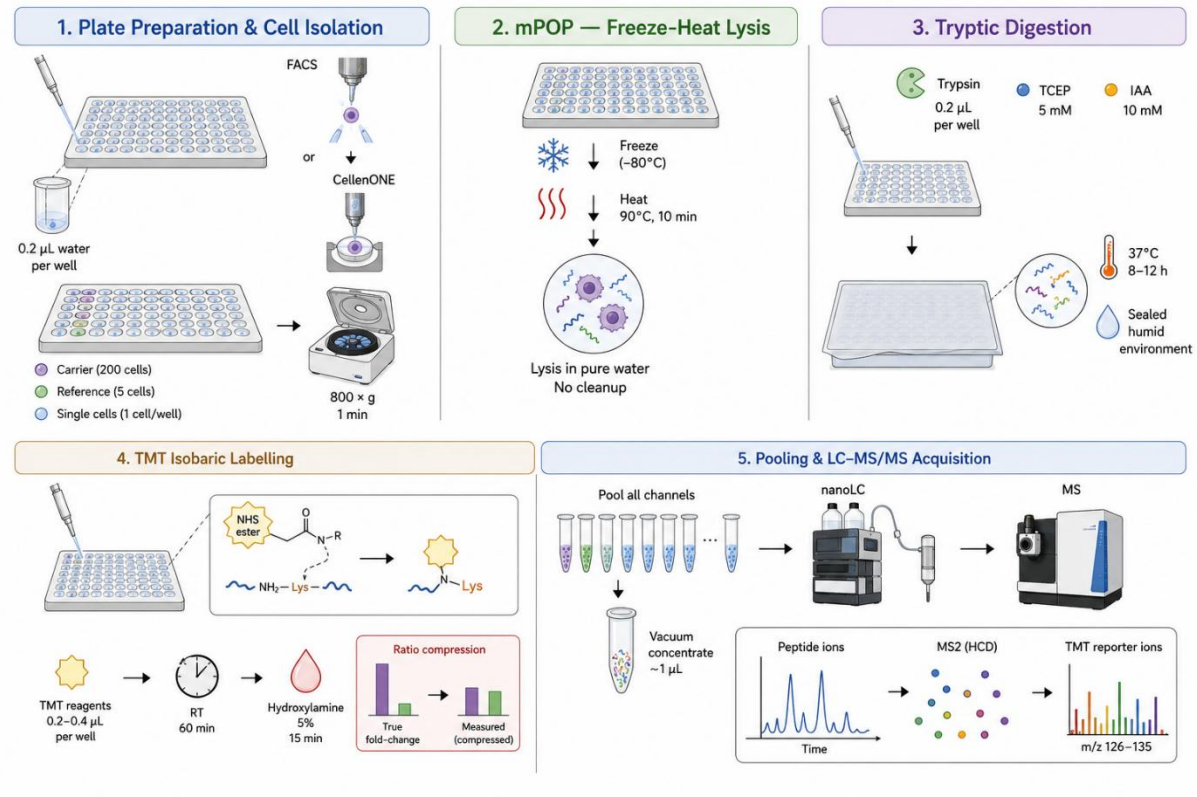


Figure W6.6. Overview of the SCoPE2 workflow for single-cell proteomics.

Step 1: Plate Preparation and Cell Isolation

384-well plates are prepared with 0.2 µL of ultrapure water per designated single-cell well. Carrier wells (200 cells) and reference wells (5 cells) are also prepared. Cells are sorted by FACS (depositing ~0.3 µL sheath fluid per cell) or CellenONE into designated wells. The plate is centrifuged at 800 x g for 1 min immediately after sorting to consolidate droplets. Empty wells (sort failures) and doublets (detected by FACS imaging) are flagged and excluded from downstream analysis. Sort purity must exceed 95%.

Step 2: mPOP, Minimal ProteOmic sample Preparation

mPOP achieves cell lysis by a two-step freeze-heat cycle performed directly in the sort plate with no additional reagents beyond water. The freeze step (already achieved during sort plate storage at -80°C) forms ice crystals that physically disrupt cell membranes. The heat step: the plate is transferred to a PCR thermocycler pre-set to 90°C and incubated for exactly 10 minutes. This rapid heating denatures endogenous proteases and phosphatases (preventing protein degradation and dephosphorylation), completes membrane disruption, and unfolds proteins for trypsin access. The total lysis volume is 0.2-0.5 µL, clean water lysate with no cleanup required.

Advantages of mPOP Over Sonication

The original SCoPE-MS used focused acoustic sonication (Covaris) to lyse cells in RIPA buffer, requiring StageTip cleanup that caused massive protein losses from single cells. mPOP's freeze-heat cycle achieves equivalent lysis in pure water, eliminating all cleanup steps. This single improvement increased protein recovery from single cells by an estimated 3-5-fold.

Step 3: Tryptic Digestion

After mPOP, the plate is cooled to room temperature. Trypsin in 100 mM TEAB (triethylammonium bicarbonate, used instead of ammonium bicarbonate because it is more volatile and leaves a cleaner MS background) is added: 0.2 µL containing ~0.5-1 ng sequencing-grade trypsin per well. TCEP (5 mM final) reduces disulfide bonds; iodoacetamide or acrylamide (10 mM) alkylates free cysteines. Digestion proceeds at 37°C for 8-12 hours overnight in a sealed plate with humidity control to prevent nanolitre-volume evaporation.

Step 4: TMT Isobaric Labelling

TMT reagents (dissolved in anhydrous acetonitrile immediately before use to prevent NHS-ester hydrolysis) are added to each well: 0.2-0.4 µL providing a large molar excess over the ~200 pg protein input. The NHS-ester reacts with primary amines (lysine epsilon-NH2 and peptide N-termini) at room temperature for 60 minutes. Reaction efficiency should exceed 95%, verifiable by the absence of unlabelled peptide peaks in the MS1 survey scan. The reaction is quenched by adding hydroxylamine (5% final, 15 min) to reverse any off-target serine/threonine/tyrosine ester bonds while preserving the stable amide-linked TMT on lysine and N-termini.

TMT Ratio Compression

When carrier (200 cells) and single cells are combined in one MS2 spectrum, the carrier's reporter ions dominate. Co-isolated peptides from other proteins contribute proportionally more to single-cell channels, compressing the measured fold-changes toward 1. This is the primary limitation of carrier-based SCP. Using 100-200x carrier (not 1000x) minimises compression while maintaining identification boost. Statistical correction methods (IsobaricQuant, DART) can partially mitigate this.

Step 5: Pooling and LC-MS/MS Acquisition

After individual labelling, all 16 wells of a SCoPE2 set are pooled by pipetting into a single tube (~6-10 µL total), vacuum-concentrated to ~1 µL, and injected onto the nanoLC column. LC-MS/MS parameters are optimised for SCoPE2 multiplexed data:

- MS1 survey scan: Orbitrap at 70,000 resolution, 3x10^6 AGC target, 50 ms maximum injection time.
- Peptide selection: Top 10 to Top 15 most abundant precursors selected per cycle. 30-second dynamic exclusion to prevent repeated selection.
- Isolation window: 0.7 m/z, much narrower than standard 2.0 m/z. Critical for reducing co-isolation interference in multiplexed data.
- Fragmentation: Higher-energy Collision Dissociation (HCD) at 33% normalised collision energy, generates both b/y sequence ions AND TMT reporter ions simultaneously.
- MS2 detection: Orbitrap at 45,000-70,000 resolution with 300-500 ms maximum injection time; long injection time accumulates enough single-cell channel signal for quantification.

W 6.14: SCoPE2 Data Analysis Pipeline

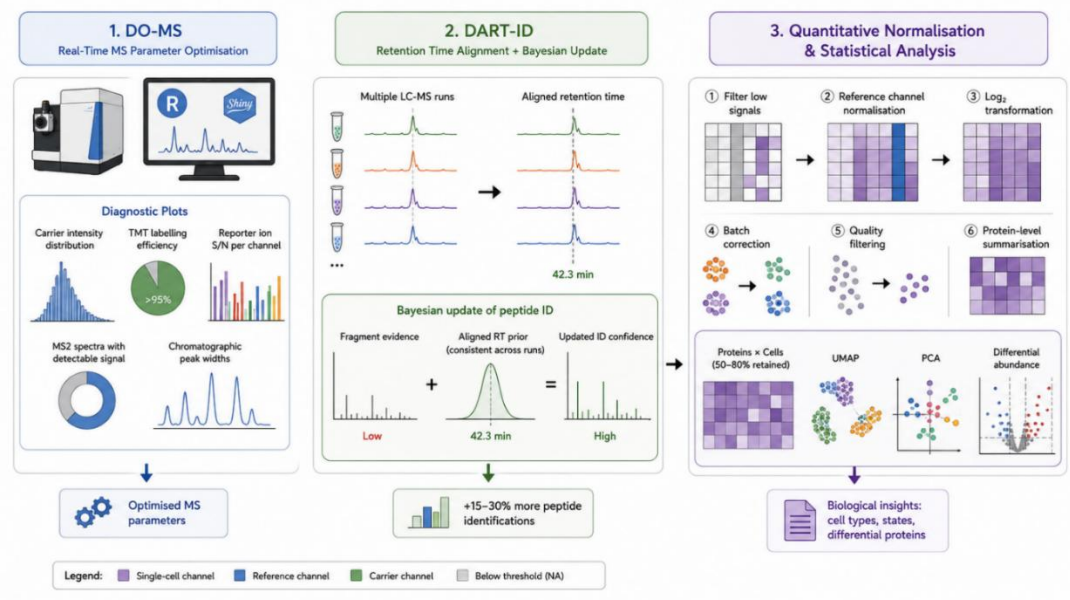


Figure 7. Overview of the SCoPE2 data analysis workflow.

DO-MS: Real-Time MS Parameter Optimisation

DO-MS (Data-driven Optimisation of Mass Spectrometry) is an R/Shiny interactive dashboard run on pilot LC-MS/MS data before the main experiment. It generates diagnostic plots: carrier channel intensity distributions (guides AGC target and injection time), TMT labelling efficiency (>95% required), reporter ion signal-to-noise ratio per channel, fraction of MS2 spectra with detectable single-cell reporter ions, and chromatographic peak widths. DO-MS prevents wasting days of instrument time on suboptimal settings.

DART-ID: Retention Time-Based Identification Enhancement

DART-ID (Data-driven Alignment of Retention Times for IDentification) addresses a key SCP challenge: spectra with enough TMT reporter signal for quantification but insufficient b/y fragment ions for confident sequence identification. DART-ID aligns retention times across hundreds of LC-MS runs using a generalised additive model, then applies a Bayesian update to peptide identification scores using the aligned retention time as a prior. A peptide consistently eluting at exactly 42.3 minutes across all runs gains additional identification confidence even if its fragment score alone is borderline. DART-ID consistently recovers 15-30% additional peptide identifications per SCoPE2 experiment.

Data Normalisation and Statistical Analysis

The SCoPE2 R pipeline and scp Bioconductor package perform: (1) filtering reporter ions below minimum threshold (~500 counts in single-cell channels, set to NA); (2) reference channel normalisation, each single-cell reporter ion divided by the corresponding reference channel ion in the same MS2 spectrum, removing run-to-run variation; (3) log2-transformation; (4) ComBat or scran-based batch correction if multiple experimental batches; (5) cell quality filtering (minimum 200-500 proteins quantified; suspicious total intensity outliers removed); (6) protein-level summarisation by median of reference-normalised peptide ratios. The final matrix (proteins x cells, 50-80% retained) feeds into UMAP/PCA, Seurat-based clustering, and differential abundance testing.

Deep Visual Proteomics Workflow

DVP Step 1: Tissue Preparation

Fresh-frozen tissue: Embedded in OCT compound, snap-frozen in liquid nitrogen, sectioned at 5-10 µm on a cryostat, mounted on PEN (polyethylene naphthalate) membrane slides. PEN membrane has UV-absorbing properties required for laser cutting. No coverslip is applied — the LMD laser must reach the tissue surface directly. FFPE tissue: Deparaffinised (2 x 5 min xylene, ethanol series), antigen retrieval (citrate buffer pH 6.0, 95-100°C, 20 min), then stained using the same immunofluorescence protocol as frozen sections. FFPE protocol enables use of clinically archived tissue biobanks.

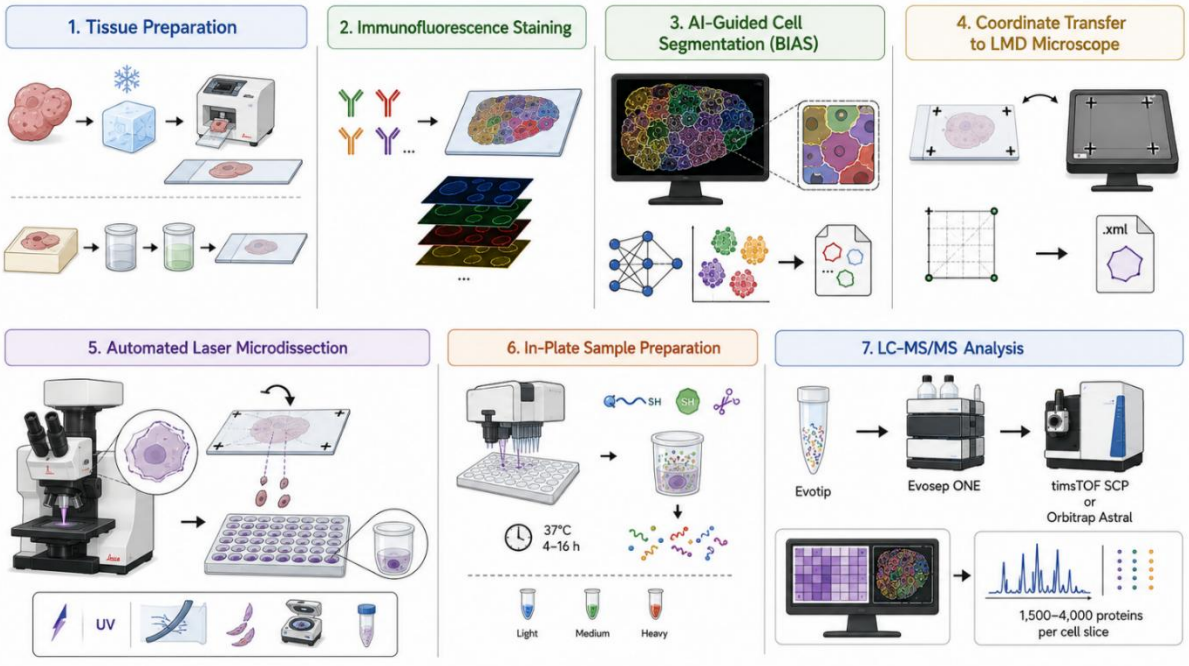


Figure 8. Overview of the Deep Visual Proteomics workflow from tissue imaging to protein analysis.

DVP Step 2: Immunofluorescence Staining

Blocking: 5% normal donkey serum in PBS + 0.1% Triton X-100 for 60 min at RT. Primary antibodies (3-6 targets per panel) at 1-5 µg/mL in blocking buffer, 4°C overnight in humidified chamber. For the liver zonation study: E-cadherin (portal vein marker), glutamine synthetase (central vein marker), phalloidin-Alexa Fluor (F-actin), wheat germ agglutinin (membranes/nuclei). For DVP melanoma: S100B (melanocytes), HMB45 (melanoma). Directly-conjugated primary antibodies (no secondary antibody required) reduce background and shorten protocol. Washing: 3 x 5 min gentle PBS washes to avoid section detachment.

DVP Step 3: AI-Guided Cell Segmentation in BIAS

The stitched multi-channel whole-slide image is imported into BIAS. Deep learning segmentation (CellPose 2.0 or nucleAIzer/U-Net architecture) processes the DAPI channel to generate nuclear instance masks, assigning every pixel to a specific nucleus with separation of touching nuclei. Whole-cell masks are generated by expanding nuclear masks using membrane channels. The 'Phenotype Finder' model in BIAS trains a classifier iteratively on user-labelled cells, then predicts cell types for the entire slide. Unsupervised clustering groups cells by morphological/intensity features without prior knowledge. BIAS generates a polygon coordinate set for each identified cell of interest, plus quality scores for each segmented object.

DVP Step 4: Coordinate Transfer to LMD Microscope

The scanner and LMD microscope have different pixel sizes, stage origins, orientations, and optical distortions. BIAS computes an affine transformation matrix using 4-8 fiducial markers (ink marks on slide edges or fluorescent beads) visible in both systems. The user clicks on the same fiducials in both coordinate systems; BIAS solves for rotation, translation, scaling, and shear parameters. After transformation, cell contours are exported as LMD7-readable files (.xml with stage coordinates and cutting paths). Practical spatial accuracy achieved: ~200 nm, sufficient for cell-level isolation.

DVP Step 5: Automated Laser Microdissection

The Leica LMD7 uses a 355 nm pulsed UV laser focused through the objective. Exact parameters used in published DVP protocols: Power 45 (0-100 scale), Aperture 1, Speed 40, Pulse frequency 2,982 Hz, Offset 190 µm. The cutting offset ensures the laser cuts just outside each cell contour, preventing UV photodamage to the proteins of interest. The PEN membrane beneath the tissue section absorbs the UV energy, cleanly cutting through both tissue and membrane. The slide is oriented tissue-side down; excised pieces fall by gravity into 384-well plates (Eppendorf 0030129547) positioned below the stage. A wind-shield plate on the sample stage prevents air currents from deflecting falling pieces into incorrect wells. After collection: plate sealed, centrifuged at 1,000 x g for 5 min, frozen at -20°C.

DVP Step 6: In-Plate Loss-Minimised Sample Preparation

Excised tissue is processed directly in the 384-well collection plate, no transfer. The BRAVO robotic liquid handler (Agilent) adds 1 µL per well of extraction/digestion master mix: 0.1-0.2% DDM (MS-compatible non-ionic detergent, assists membrane protein extraction), 50-100 mM TEAB (pH 8.0), 5 mM TCEP (disulfide reduction), 20-50 ng/µL sequencing-grade trypsin. Simultaneous lysis-reduction-digestion proceeds at 37°C for 4-16 hours. For multiplexed DVP comparing cell types or conditions, stable isotope dimethyl labelling (light: CH_2O; medium: CD_2O; heavy: $^{13}CD_2O$ + $NaBD_3CN$) provides 3-channel quantification compatible with DIA acquisition.

DVP Step 7: LC-MS/MS with timsTOF SCP or Orbitrap Astral

Peptides loaded onto Evotips directly from the 384-well plate, then separated on the Evosep ONE. For timsTOF SCP: diaPASEF acquisition with TIMS separation (30-60 ms TIMS accumulation time), 16-32 DIA windows synchronised with ion mobility elution, near-100% duty cycle. For Orbitrap Astral: narrow-window DIA (4 m/z windows), ~200 Hz scan speed, sample-tailored DIA method adjusting window widths based on precursor density. DIA-NN analysis uses predicted spectral libraries (DeepLC + ms2pip) with retention time alignment and MBR (transfer learning) across all DVP samples. Result: 1,500-4,000 protein groups per hepatocyte slice linked to spatial tissue coordinates.

Protein Yield from Microdissected Cells

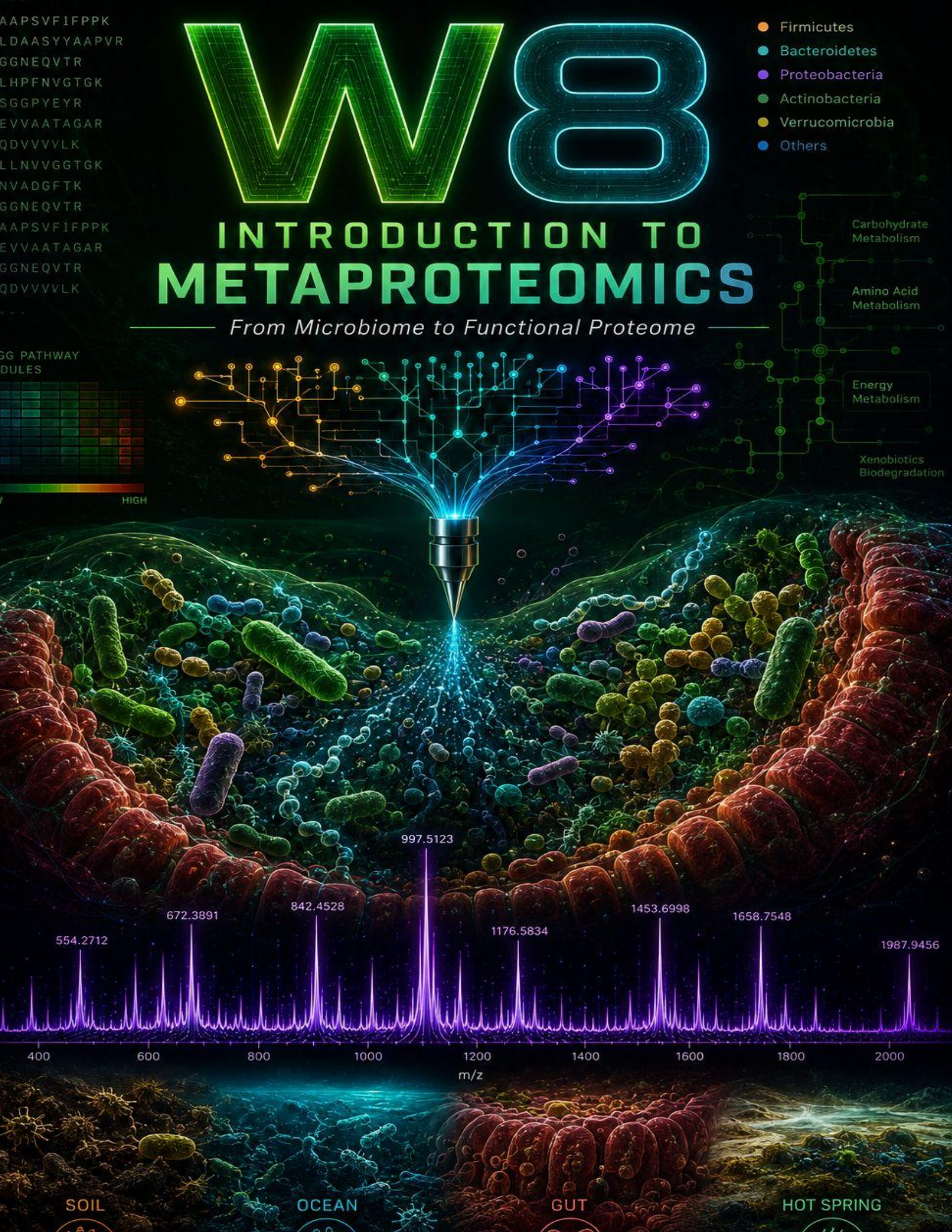
A single hepatocyte slice (20-30 µm cell diameter, 10 µm section thickness) contains approximately 250 pg of protein, equivalent to a single HeLa cell in suspension. This means single-cell tissue proteomics operates at the same sensitivity threshold as solution-based SCP. The key breakthrough was demonstrating that in-plate processing + Evotip loading + Evosep ONE chromatography recovers enough peptides from this input for 1,700-2,500 protein identifications.

W 6.15: Mass Spectrometry Concepts for Single-Cell Proteomics

TIMS: Principles of Trapped Ion Mobility Spectrometry

The timsTOF SCP and Ultra 2 instruments add a crucial separation dimension called Trapped Ion Mobility Spectrometry (TIMS). In the TIMS analyser, ions are trapped against a nitrogen gas flow by an electric field gradient. The trapping voltage is then ramped, and ions are released sequentially based on their collision cross section (CCS) — their effective three-dimensional shape in the gas phase. Two peptides with identical m/z but different 3D shapes are separated before mass measurement. In single-cell proteomics, where sample complexity is high and signal is low, this 4th dimension of separation dramatically reduces background noise and interference, improving signal-to-noise for each peptide.

PASEF (Parallel Accumulation-Serial Fragmentation) exploits TIMS by synchronising ion accumulation with fragmentation cycles: while one group of ions is being analysed in the TOF mass analyser, the next group is being accumulated in the TIMS. This achieves near-100% duty cycle, virtually no ions are wasted between acquisition cycles. diaPASEF applies this to multiple DIA isolation windows simultaneously, cycling through 16-32 defined m/z/mobility windows per second. The result is DIA-level proteome completeness combined with near-DDA sensitivity, the optimal combination for single cells and low-input spatial proteomics.


AAPSVFIFPPK
LDAASYYAAPVR
GGNEQVTR
LHPFNVGTGK
SGGPYEYR
EVVAATAGAR
QDVVVVLK
LLNVVGGTGK
NVADGFTK
GGNEQVTR
AAPSVFIFPPK
EVVAATAGAR
GGNEQVTR
QDVVVVLK
GG PATHWAY
DULES
HIGH
W8
INTRODUCTION TO
METAPROTEOMICS
From Microbiome to Functional Proteome
Firmicutes
Bacteroidetes
Proteobacteria
Actinobacteria
Verrucomicrobia
Others
Carbohydrate Metabolism
Amino Acid Metabolism
Energy Metabolism
Xenobiotics Biodegradation
997.5123
842.4528
672.3891
554.2712
1176.5834
1453.6998
1658.7548
1987.9456
400
600
800
1000
1200
1400
1600
1800
2000
m/z
SOIL
OCEAN
GUT
HOT SPRING

Introduction to Metaproteomics

SCIENTIFIC PROGRAMME

Overview

Workshop 8 at APT-2026 focuses on the emerging field of Metaproteomics, which enables large-scale analysis of proteins expressed by complex microbial communities. The workshop is designed to provide participants with a practical and conceptual understanding of metaproteomics workflows used in environmental, clinical, and microbiome research.

The workshop will cover key areas, including sample preparation, protein extraction, mass spectrometry-based data acquisition, protein identification and quantification, and bioinformatics analysis for microbiome studies. Participants will gain insights into how metaproteomics helps reveal microbial functions, biological pathways, and ecosystem interactions.

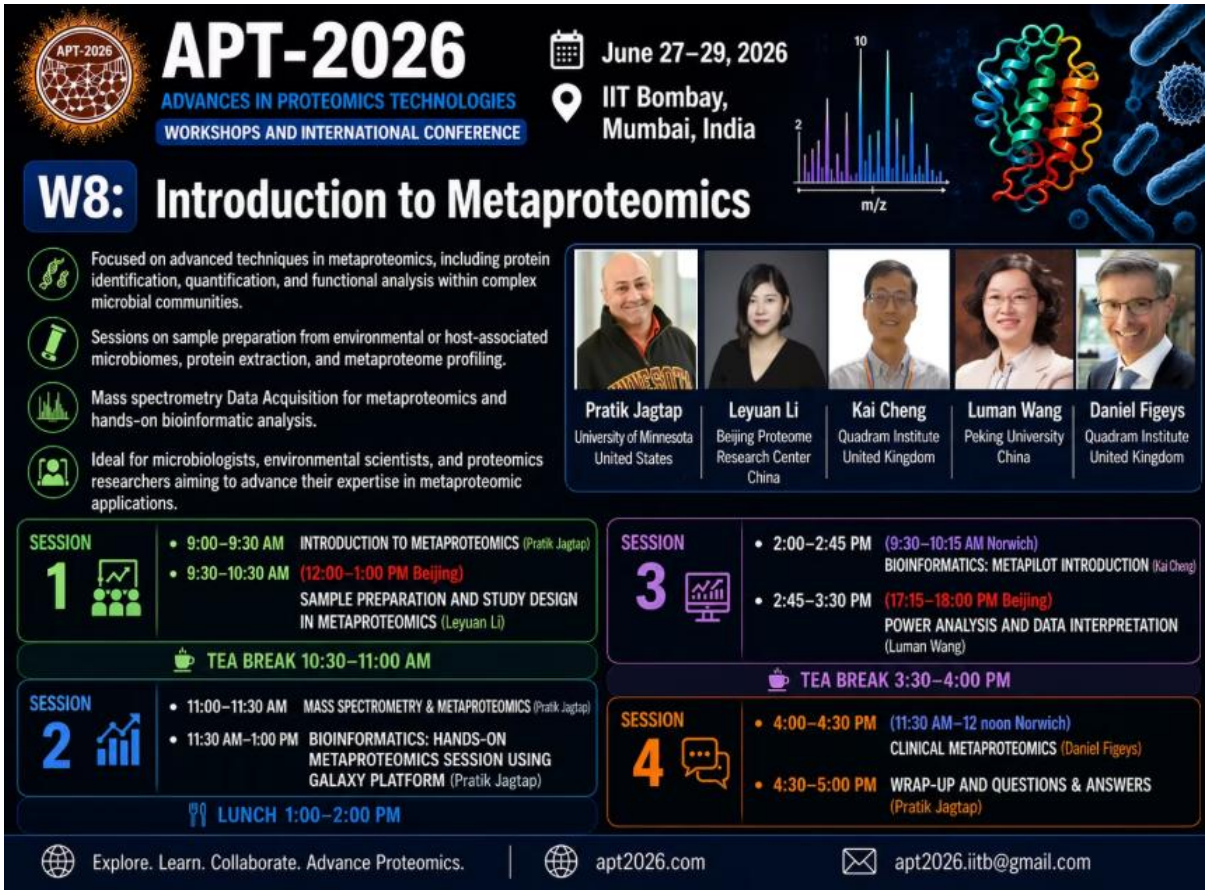
The sessions will be conducted by internationally recognized experts from the USA, China, and the United Kingdom. Dr. Pratik Jagtap (University of Minnesota, USA) will introduce concepts in metaproteomics, mass spectrometry workflows, and hands-on data analysis using the Galaxy platform. Dr. Leyuan Li (Beijing Proteome Research Center, China) will discuss sample preparation and study design for microbiome samples. Dr. Kai Cheng (Quadram Institute, UK) will introduce bioinformatics approaches and the MetaPilot platform, while Dr. Luman Wang (Peking University, China) will focus on data interpretation and power analysis. Dr. Daniel Figeys (Quadram Institute, UK) will present applications of clinical metaproteomics in translational research.

This workshop is ideal for microbiologists, environmental scientists, proteomics researchers, and students interested in advanced microbiome analysis and functional proteomics.

AT A GLANCE

Key Highlights

Introduction to metaproteomics workflows	Sample preparation and microbiome study design
Mass spectrometry-based metaproteomics analysis	Hands-on bioinformatics and data interpretation
Clinical and environmental microbiome applications	Interaction with international experts in metaproteomics



INTRODUCTION TO METAPROTEOMICS (D E T A I L E D)

Introduction to Metaproteomics

W 8.1: What Is Metaproteomics?

Metaproteomics was originally defined by Wilmes and Bond (2004) as the comprehensive, large-scale characterisation of all proteins expressed by a microbial community at a given point in time. The term was coined to describe an approach that, unlike traditional single-organism proteomics, does not require isolating or culturing individual community members. Instead, it directly extracts and identifies proteins from an entire environmental or host-associated sample, capturing a snapshot of the combined molecular activity of every organism present.

To understand where metaproteomics sits within the broader landscape of community-level molecular biology, it is useful to compare it with the other "meta-omics" disciplines. Each layer of the central dogma of molecular biology — DNA, RNA, protein, and metabolite — has a corresponding community-scale analytical approach, summarized in Table 1.

Omics Layer	Molecule Measured	Primary Question Answered
(Meta)genomics	DNA	Which organisms are present, and what is their genetic potential?
(Meta)transcriptomics	RNA (transcripts)	Which genes are being actively transcribed at this moment?

(Meta)proteomics	Proteins	Which gene products are actually expressed and functionally active?
(Meta)bolomics	Small molecules / metabolites	What chemical end-products result from this biological activity?

Table 1. The multi-omics landscape, illustrating where metaproteomics sits relative to genomic, transcriptomic, and metabolomic approaches.

Proteins are, in this sense, the molecules that most directly carry out cellular function. Because of this, metaproteomics is widely regarded as the meta-omics layer that comes closest to directly measuring phenotype — what a microbial community is actually doing — rather than what it is merely capable of doing.

W 8.2: Why Metaproteomics Matters

A microbial community's genome, recovered through metagenomic sequencing, describes its full catalogue of genetic potential: every gene that any member of the community could, in principle, express. However, only a subset of that potential is realized at any given moment, under any given set of environmental conditions. Metaproteomics closes this gap by directly measuring which proteins are present and in what relative abundance, providing a functional read-out that genomic sequencing alone cannot supply (Kleiner, 2019; VerBerkmoes et al., 2009).

> **Key Concept: Genomic Potential vs. Expressed Function**
> A metagenome tells you what a community could do. A metaproteome tells you what a community is doing right now. The two are complementary: metagenomic sequencing is typically used to build the protein sequence database against which metaproteomic spectra are searched, while the metaproteome itself reveals which of those genetically encoded functions are actually being expressed under the sampled conditions.

This functional perspective has made metaproteomics valuable across a wide range of research domains:

- Environmental ecology — characterizing the active metabolic roles of microbial communities in marine, soil, sediment, and freshwater ecosystems, and their contribution to biogeochemical cycling (VerBerkmoes et al., 2009).
- Engineered and industrial systems — monitoring and optimizing microbial consortia in wastewater treatment plants, anaerobic digesters, and biogas reactors, where functional shifts often precede measurable changes in process performance.
- Host-associated microbiomes — investigating the functional contribution of gut, oral, skin, and respiratory tract microbiota to host health, immunity, and disease.
- Clinical and diagnostic research — profiling host–microbe and microbe–microbe interactions directly from clinical specimens, including the identification of coinfecting organisms (Bihani et al., 2023, 2024).

W 8.3: A Brief History of the Field

Metaproteomics emerged from, and remains closely tied to, parallel advances in mass spectrometry instrumentation and metagenomic sequencing. Its development can be traced through a series of conceptual and technical milestones, summarized in Table 2.

Year	Milestone
2004	Wilmes and Bond coin the term "metaproteomics," using two-dimensional gel electrophoresis to characterize the protein complement of an activated sludge community.
2005	Ram et al. apply shotgun LC-MS/MS, rather than gel-based separation, to a natural acid mine drainage biofilm, establishing community proteogenomics as a scalable approach.

2009	VerBerkmoes et al. formalize the conceptual framework of microbial community proteogenomics, linking metagenomic sequencing directly to community-scale protein identification.
2012	Mesuere et al. release UniPept, enabling rapid, peptide-based taxonomic biodiversity analysis against the full UniProt knowledgebase.
2016	May et al. introduce an alignment-free "metapeptide" database strategy for marine metaproteomics — the same approach underlying the Bering Strait dataset used in the accompanying tutorial.
2017	Timmins-Schiffman et al. publish systematic guidance on metaproteomic database selection and false discovery rate control.
2019	Kleiner reframes metaproteomics as extending beyond gene-expression measurement to per-species biomass estimation and substrate-uptake tracking.
2021	The Metaproteomics Initiative launches as a community-wide hub for standardization and training (Van Den Bossche et al., 2021a), alongside the first large-scale, multi-laboratory benchmarking study, CAMPI (Van Den Bossche et al., 2021b).
2023–2024	Clinical metaproteomics workflows are applied to upper respiratory tract specimens to profile host–microbe coinfection dynamics during COVID-19 (Bihani et al., 2023, 2024).

Table 2. Selected milestones in the development of metaproteomics as an analytical field.

W 8.4: The Conceptual Workflow: From Sample to Insight

Although specific instrumentation and software choices vary across laboratories, nearly all metaproteomic experiments follow the same general conceptual sequence:

- Sample collection and preservation — the environmental or host-associated sample is collected and immediately stabilized (e.g., snap-frozen) to halt ongoing protein turnover and prevent degradation.
- Protein extraction — microbial cells are lysed and their proteins solubilized, typically through a combination of mechanical disruption and chemical denaturation.
- Proteolytic digestion — extracted proteins are enzymatically cleaved, most commonly with trypsin, into shorter peptides suitable for mass spectrometric analysis.
- LC-MS/MS acquisition — the resulting peptide mixture is separated by liquid chromatography and introduced into a tandem mass spectrometer, which records the mass and fragmentation pattern of each peptide ion.
- Database-dependent peptide identification — observed spectra are computationally matched against candidate peptide sequences drawn from a protein sequence database. Unlike single-organism proteomics, this database must represent an entire, often uncultured, community — typically derived from paired metagenomic sequencing of the same sample.
- Protein inference and confidence filtering — validated peptide-spectrum matches are aggregated into protein identifications and filtered to a defined confidence threshold.
- Downstream interpretation — the resulting high-confidence peptide and protein lists are mined for taxonomic origin and functional annotation, yielding an integrated picture of community composition and activity.

> **Tip: Mapping This Primer to the Hands-On Tutorial**
>
> These seven conceptual stages map directly onto the tools used in the accompanying hands-on tutorial. SearchGUI, running the X!Tandem search engine, performs Stage 5 (database-dependent peptide identification). PeptideShaker performs Stage 6 (validation and protein inference). UniPept's pept2lca and pept2prot functions perform Stage 7 (taxonomic and functional annotation). Keeping this mapping in mind will make the purpose of each tutorial exercise immediately clear.

W 8.5: Core Analytical Challenges

Metaproteomics inherits the technical challenges of conventional shotgun proteomics while introducing several additional layers of complexity unique to multi-organism samples:

Database completeness and construction. Unlike single-organism proteomics, there is rarely a single definitive reference proteome. Search databases must be constructed from metagenomic sequencing of the same or a closely matched sample, balancing comprehensiveness against the substantially increased search space and computation time that large databases impose (Timmins-Schiffman et al., 2017).

Protein inference ambiguity. Peptides that are identical across multiple related taxa cannot be unambiguously assigned to a single organism. Resolving this typically requires a lowest-common-ancestor strategy rather than forcing an arbitrary single assignment (Mesuere et al., 2012).

Quantification complexity. Translating peptide and spectral counts into meaningful estimates of relative protein abundance, and ultimately per-species biomass contribution, remains analytically demanding in highly diverse communities (Kleiner, 2019).

Computational scale. Searching large, metagenome-derived databases against high-resolution MS/MS data is computationally intensive, often requiring substantially more processing time and memory than single-organism workflows of comparable size.

Reproducibility and standardization. A 2021 multi-laboratory benchmarking study found that variability introduced during sample preparation generally exceeds variability introduced by choice of bioinformatic pipeline, and that peptide-level differences across workflows largely converge once results are aggregated to the protein level (Van Den Bossche et al., 2021b).

W 8.6: Taxonomic Profiling Concepts

Once a high-confidence peptide list has been generated, the next question is typically: which organisms produced these peptides? Because many peptides are shared across closely related taxa, simply discarding ambiguous matches would waste a substantial fraction of the available evidence. The lowest common ancestor (LCA) approach, implemented in UniPept, addresses this by assigning each peptide to the most specific taxonomic rank consistent with every organism in which that exact peptide sequence has been observed (Mesuere et al., 2012). A peptide found only in a single genus is assigned to that genus; a peptide shared across an entire phylum is assigned only to that phylum, preserving the maximum taxonomic precision the data can support without overstating confidence. This approach is exactly what the hands-on tutorial applies via UniPept's pept2lca function, and what underlies the interactive taxonomy tree visualization and genus-level summary participants will generate.

W 8.7: Functional Profiling Concepts

Alongside taxonomic origin, identified peptides can be mapped to the biological functions of the proteins from which they derive. Several controlled vocabularies are used across the field for this purpose. The Gene Ontology (GO), used throughout the accompanying tutorial, organizes gene product function along three independent aspects: molecular function (the biochemical activity of a gene product), biological process (the larger pathway or program a gene product contributes to), and cellular component (the cellular location at which a gene product is active). Other common functional vocabularies include the Kyoto Encyclopedia of Genes and Genomes (KEGG), which organizes proteins into metabolic and signaling pathways, Enzyme Commission (EC) numbers, which classify enzymatic activity, and clusters of orthologous groups (COG/eggNOG), which group proteins by inferred evolutionary and functional relationships. While this tutorial relies exclusively on GO, participants working with other metaproteomics platforms will frequently encounter these alternative schemes, often used in combination.

W 8.8: Common Tools and Platforms

A range of software tools and platforms have been developed specifically for, or widely adapted to, metaproteomic data analysis. Table 3 summarizes several of the most widely used, including those applied directly in the accompanying tutorial.

Tool / Platform	Primary Role

SearchGUI	Unified interface to multiple peptide-spectrum matching search engines, including X!Tandem
PeptideShaker	Validation of peptide-spectrum matches and protein inference from SearchGUI results
UniPept	Peptide-based taxonomic (pept2lca) and functional (pept2prot) annotation against the UniProt knowledgebase
Galaxy / Galaxy-P	Web-based platform for building, sharing, and reproducibly executing complete metaproteomics workflows
MetaProteomeAnalyzer (MPA)	Open-source platform for metaproteomic database searching, taxonomic binning, and functional annotation
MEGAN	Visualization and analysis of taxonomic and functional content from large-scale meta-omics datasets
MaxQuant	Quantitative proteomics software increasingly adapted for metaproteomic quantification workflows

Table 3. Selected software tools and platforms commonly used in metaproteomic data analysis.

W 8.9: Applications and Real-World Impact

Environmental and Marine Ecology

Metaproteomics has been used extensively to characterize the active metabolic roles of microbial communities in marine, soil, and sediment environments, directly informing our understanding of global biogeochemical cycling (VerBerkmoes et al., 2009). The Bering Strait chlorophyll maximum layer dataset used in the accompanying tutorial, originally generated by May et al. (2016), is itself an example of this application domain: it characterizes the taxonomic and functional composition of an active marine microbial community at a specific oceanographic depth and location.

Engineered and Industrial Systems

In engineered microbial systems such as wastewater treatment plants and anaerobic biogas digesters, metaproteomics provides a functional readout of process-relevant microbial activity, complementing taxonomic monitoring with direct evidence of which metabolic pathways are operating under given conditions. This functional resolution is particularly valuable for diagnosing process instability or optimizing operating parameters in real time.

Host-Associated and Clinical Microbiomes

Metaproteomics has become an increasingly important tool in human and animal microbiome research, where it provides functional insight into host–microbe interactions that taxonomic profiling alone cannot supply. Within the host institution of this conference, researchers at IIT Bombay have applied clinical metaproteomics workflows to profile microbial coinfections in nasopharyngeal swab samples from COVID-19 patients, identifying bacterial and fungal taxa co-occurring with SARS-CoV-2 in the upper respiratory tract (Bihani et al., 2023, 2024). This work illustrates the translational potential of the same analytical logic — peptide identification, taxonomic assignment, and functional annotation — that participants will apply to an environmental dataset in the accompanying tutorial.

W 8.10: Emerging Trends and Future Directions

Several trends are actively shaping the next phase of metaproteomics research. Community-wide standardization efforts, coordinated through resources such as the Metaproteomics Initiative, aim to harmonize sample preparation, instrumentation, and bioinformatic protocols across laboratories, building on benchmarking findings from large-scale comparisons such as CAMPI (Van Den Bossche et al., 2021a, 2021b). Methodologically, the field is moving beyond simple presence/absence or relative-abundance measurements toward quantitative estimation of per-species biomass contribution and in situ substrate uptake (Kleiner, 2019). There is also growing emphasis on multi-omics integration, combining metaproteomic data with paired metagenomic, metatranscriptomic, and metabolomic measurements of the same sample to build a more complete picture of microbiome structure and function. Finally, as in proteomics more broadly, machine learning approaches are increasingly being applied to peptide-spectrum matching, protein inference,

and functional annotation, with the potential to improve both the sensitivity and the speed of metaproteomic data analysis.

W 8.10: Glossary of Key Terms

Term	Definition
Metaproteomics	Large-scale characterization of the entire protein complement expressed by a microbial community at a given point in time.
Metagenomics	Sequencing-based characterization of the collective genetic material of a microbial community, without prior culturing of individual members.
Shotgun proteomics	A bottom-up proteomic strategy in which proteins are enzymatically digested into peptides prior to mass spectrometric analysis, rather than analyzed intact.
LC-MS/MS	Liquid chromatography coupled to tandem mass spectrometry; separates peptides before recording their mass and fragmentation pattern.
Peptide-spectrum match (PSM)	An assignment linking an observed MS/MS spectrum to a specific candidate peptide sequence from the search database.
Protein inference	The process of aggregating identified peptides into protein-level identifications and confidence assessments.
False discovery rate (FDR)	The estimated proportion of false-positive identifications within a set of reported peptide or protein matches, typically controlled using a decoy database strategy.
Decoy database	A reversed or randomized version of the search database used to estimate the rate of false-positive matches during FDR control.
Tryptic peptide	A peptide generated by digestion with trypsin, which cleaves proteins at the carboxyl side of lysine and arginine residues.
Metapeptide	A peptide sequence predicted directly from assembled metagenomic sequence data, used to construct sample-specific metaproteomic search databases.
Lowest common ancestor (LCA)	The most specific taxonomic rank consistent with all organisms known to share a given peptide sequence.
Gene Ontology (GO)	A structured, controlled vocabulary describing gene product function across molecular function, biological process, and cellular component aspects.
Taxonomic profiling	Estimation of the taxonomic composition of a sample based on the inferred origin of identified peptides or proteins.
Functional annotation	Assignment of identified peptides or proteins to known biological functions, pathways, or molecular activities.

W 8.11: Preparing for the Hands-On Tutorial

With these concepts in hand, participants are ready to proceed to the accompanying hands-on chapter. A few points are worth keeping in mind while working through it:

- The tutorial uses a real marine metaproteomic dataset (Bering Strait chlorophyll maximum layer; May et al., 2016), not simulated data — the taxonomic and functional results you generate reflect an actual sampled microbial community.
- Each Galaxy tool used in the tutorial corresponds to one of the seven conceptual stages introduced in Section 4 of this primer; if a step's purpose is ever unclear, refer back to that mapping.
- The confidence and database-selection considerations discussed in Section 5 directly motivate several of the specific parameter choices — such as the 95% PSM confidence threshold — used throughout the tutorial.
- The taxonomic and functional annotation steps in the tutorial apply the LCA and Gene Ontology concepts introduced in Sections 6 and 7 — understanding the underlying logic will make the resulting outputs easier to interpret, not just easier to produce.

Readers are encouraged to keep this primer alongside the tutorial chapter for reference as they work through each exercise.

TUTORIAL

W 8.12: Metaproteomics Tutorial

Questions

• How can I match metaproteomic mass spectrometry data to peptide sequences derived from shotgun metagenomic data?
• How can I perform taxonomy analysis and visualize metaproteomics data?
• How can I perform functional analysis on this metaproteomics data?

Objectives

• A taxonomy and functional analysis of metaproteomic mass spectrometry data.

In this metaproteomics tutorial we will identify expressed proteins from a complex bacterial community sample. For this MS/MS data will be matched to peptide sequences provided through a FASTA file.

Metaproteomics is the large-scale characterization of the entire protein complement of environmental microbiota at a given point in time. It has the potential to unravel the mechanistic details of microbial interactions with the host / environment by analyzing the functional dynamics of the microbiome.

In this tutorial, we will analyze a sample of sea water that was collected in August of 2013 from the Bering Strait chlorophyll maximum layer (7m depth, 65° 43.44” N, 168° 57.42” W). The data were originally published in May et al. 2016.

Agenda

In this tutorial, we will deal with:
• Pretreatments
• Data upload
• Analysis
• Match peptide sequences
• Taxonomy analysis
• Genus's taxonomy level summary
• Functional Analysis

Pretreatments

Data upload

There are three ways to upload your data.

- Upload/Import the files from your computer
- Using a direct link
- Import from the data library if your instance provides the files

In this tutorial, we will get the data from Zenodo.

> **Hands On: Data upload and organization**
> • Create a new history and name it something meaningful (e.g. Metaproteomics tutorial)
> • Import the three MGF MS/MS files and the FASTA sequence file from Zenodo:
> - https://zenodo.org/record/839701/files/2016_Jan_12_QE2_45.mgf
> - https://zenodo.org/record/839701/files/2016_Jan_12_QE2_46.mgf
> - https://zenodo.org/record/839701/files/2016_Jan_12_QE2_47.mgf
> - https://zenodo.org/record/839701/files/FASTA_Bering_Strait_Trimmed_metapeptides_cRAP.fasta
> - https://zenodo.org/record/839701/files/Gene_Ontology_Terms.tabular
> • As default, Galaxy takes the link as name.
> • Rename the datasets to a more descriptive name
> • Build a Dataset list for the three MGF files

We have a choice to run all these steps using a single workflow, then discuss each step and the results in more detail.

> **Hands On: Pretreatments**
> • Import the workflow into Galaxy
> • Run Workflow using the following parameters:
> - "Send results to a new history": No
> - "1: SixGill generated protein fasta file": FASTA_Bering_Strait_Trimmed_metapeptides_cRAP.fasta
> - "2: Dataset collection of Bering Strait MGF files": Dataset collection of bering MGF
> - "3: GeneOntology terms (selected)": Gene_Ontology_terms.tabular

Analysis

Match peptide sequences

The search database labelled FASTA_Bering_Strait_Trimmed_metapeptides_cRAP.FASTA is the input database that will be used to match MS/MS to peptide sequences via a sequence database search. It is a small excerpt of the original database, which was constructed based on a metagenomic screening of the sea water samples (see May et al. 2016). The full original database is available online. The contaminant database (cRAP) was merged with the original database.

For this, the sequence database-searching program called SearchGUI will be used. The created dataset collection of the three MGF files in the history is used as the MS/MS input.

SearchGUI

> **Hands On: SearchGUI**
> • Search GUI (Galaxy version 3.3.10.1) with the following parameters:
> • Protein Database: FASTA_Bering_Strait_Trimmed_metapeptides_cRAP.FASTA
> • Input Peak lists (mgf): MGF files dataset collection
> Section Search Engine Options:
> • Search Engines: X!Tandem
> Section Precursor Options:
> • Fragment Tolerance Units: Daltons
> • Fragment Tolerance: 0.2 — this is high resolution MS/MS data
> • Maximum Charge: 6

Section Protein Modification Options:
• Fixed Modifications: Carbamidomethylation of C
• Variable modifications: Oxidation of M
Section Advanced Options:
• X!Tandem Options: Advanced
• X!Tandem: Quick Acetyl: No
• X!Tandem: Quick Pyrolidone: No
• X!Tandem: Protein stP Bias: No
• X!Tandem: Maximum Valid Expectation Value: 100
• leave everything else as default
• Click Run Tool.

Once the database search is completed, the SearchGUI tool will output a file (called a SearchGUI archive file) that will serve as an input for the next section, PeptideShaker.

Comment

Note that sequence databases used for metaproteomics are usually much larger than the excerpt used in this tutorial. When using large databases, the peptide identification step can take much more time for computation. In metaproteomics, choosing the optimal database is a crucial step of your workflow, for further reading see Timmins-Schiffman et al (2017).
To learn more about database construction in general, like integrating contaminant databases or using a decoy strategy for FDR searching, please consult our tutorial on Database Handling.

PeptideShaker

PeptideShaker is a post-processing software tool that processes data from the SearchGUI software tool. It serves to organize the Peptide-Spectral Matches (PSMs) generated from SearchGUI processing and is contained in the SearchGUI archive. It provides an assessment of confidence of the data, inferring proteins identified from the matched peptide sequences and generates outputs that can be visualized by users to interpret results. PeptideShaker has been wrapped in Galaxy to work in combination with SearchGUI outputs.

Hands On: PeptideShaker

• Peptide Shaker (Galaxy version 1.16.36.3) with the following parameters:
• Compressed SearchGUI results: The SearchGUI archive file
• Specify Advanced PeptideShaker Processing Options: Default Processing Options
• Specify Advanced Filtering Options: Advanced Filtering Options
• Maximum Precursor Error Type: Daltons
• Specify Contact Information for mzIdendML: You can leave the default dummy options for now, but feel free to enter custom contact information.
• Include the protein sequences in mzIdentML: No
• Output options: Select the PSM Report (Peptide-Spectral Match) and the Certificate of Analysis
• Click Run Tool and inspect the resulting files after they turned green with the View data icon.

A number of new items will appear in your history, each corresponding to the outputs selected in the PeptideShaker parameters. Most relevant for this tutorial is the PSM report.

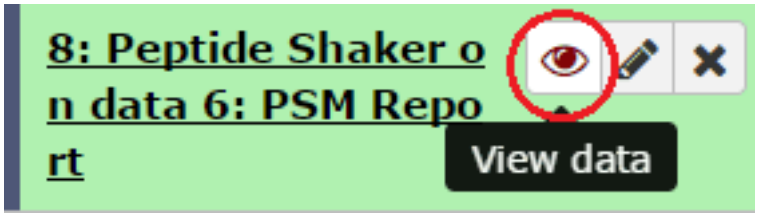


Figure W 8.1: The PSM report. Scrolling towards left will show the sequence for the PSM that matched to these metapeptide entries. Column 3 is the sequence matched for each PSM entry. Every identified PSM is a new row in the tabular output.

In the following steps of this tutorial, selected portions of this output will be extracted and used for analysis of the taxonomic make-up of the sample as well as the biochemical functions represented by the proteins identified.

Taxonomy analysis

In the previous section, the genome sequencing and mass spectrometry data from processing of biological samples was used to identify peptides present in those samples. Now those peptides are used as evidence to infer which organisms are represented in the sample, and what biological functions those peptides and associated proteins suggest are occurring.

The UniProt organization collects and annotates all known proteins for organisms. A UniProt entry includes the protein amino acid sequence, the NCBI taxonomy, and any annotations about structure and function of the protein. The UniPept web resource developed by Ghent University will be used to match the sample peptides to proteins. UniPept indexes all Uniprot proteins and provides a fast-matching algorithm for peptides.

> **Comment: Unipept**
> Users can access UniPept via a web page and paste peptide sequences into the search form to retrieve protein information. But we'll use the Galaxy Unipept tool to automate the process. The Unipept tool sends the peptide list to the UniPept REST API service, then transforms the results into datasets that can be further analyzed or operated on within Galaxy.

Receiving the list of peptides: Query Tabular

In order to use Unipept, a list containing the peptide sequences has to be generated. The tool Query Tabular can load tabular data (the PSM report in this case) into a SQLite data base. As a tabular file is being read, line filters may be applied and an SQL query can be performed.

> **Hands On: Query Tabular**
> • Query Tabular (Galaxy version 3.0.0) with the following parameters:
> • Database Table: Click on + Insert Database Table
> • Tabular Dataset for Table: The PSM report
> Section Filter Dataset Input:
> • Filter Tabular Input Lines: Click on + Insert Filter Tabular Input Lines
> • Filter By: Select by regex expression matching
> • regex pattern: ^\d
> • action for regex match: include line on pattern match
> Section Table Options:
> • Specify Name for Table: psm
> • Specify Column Names (comma-separated list): id,,sequence,,,,,,,,,,,,,,,,,,confidence,validation
> • Only load the columns you have named into database: Yes
> • Save the sqlite database in your history: Yes
> • SQL Query to generate tabular output:
> ```
> SELECT distinct sequence
> FROM psm
> WHERE confidence >= 95
> ORDER BY sequence
> ```

• include query result column headers: No
• Click Run Tool and inspect the query results file after it turned green.

While we can proceed with this list of peptides, let's practice using the created SQLite database for further queries. We might not only be interested in all the distinct peptides, but also on how many PSMs a single peptide had.

Hands On: SQLite to tabular

• SQLite to tabular (Galaxy version 2.0.0) with the following parameters:
• SQL Query:

```
SELECT sequence as "peptide", count(id) as "PSMs"
FROM psm
WHERE confidence >= 95
GROUP BY sequence
ORDER BY sequence
```

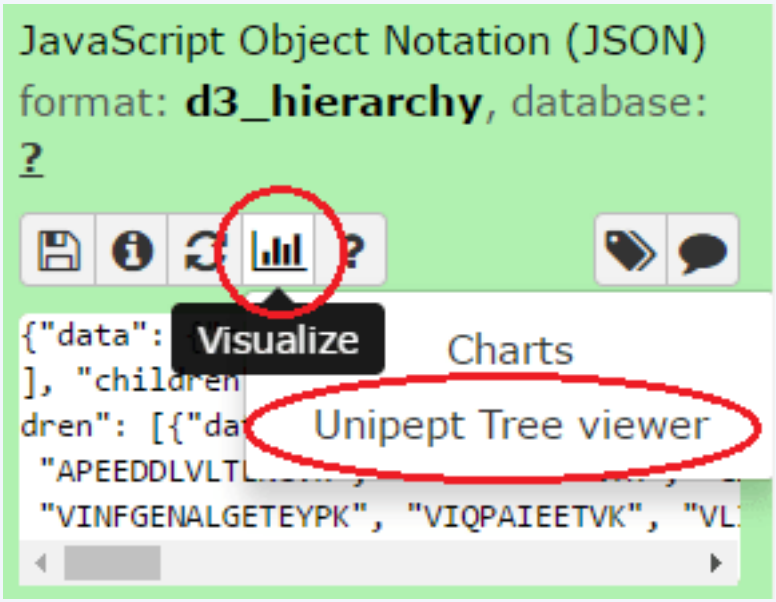
• Click Run Tool. The resulting file should have two columns, one with the distinct peptides, the other with the count number of PSMs.

Retrieve taxonomy for peptides: Unipept

The generated list of peptides can now be used to search via Unipept. We do a taxonomy analysis using the UniPept pept2lca function to return the taxonomic lowest common ancestor for each peptide:

Hands On: Unipept

• Unipept (Galaxy version 6.2.4+galaxy1) with the following parameters:
• Unipept application: pept2lca: lowest common ancestor
• Peptides input format: tabular
• Tabular Input Containing Peptide column: The query results file.
• Select column with peptides: Column 1
• Choose outputs: Select tabular and JSON taxonomy tree
• Click Run Tool. The history should grow by two files. View each to see the difference.
• Visualize the data: Click on the JSON output file from the Unipept tool to expand it. Click on the Visualize button and select Unipept Tree viewer.
• A new window should appear with a visualization of the taxonomy tree of your data.



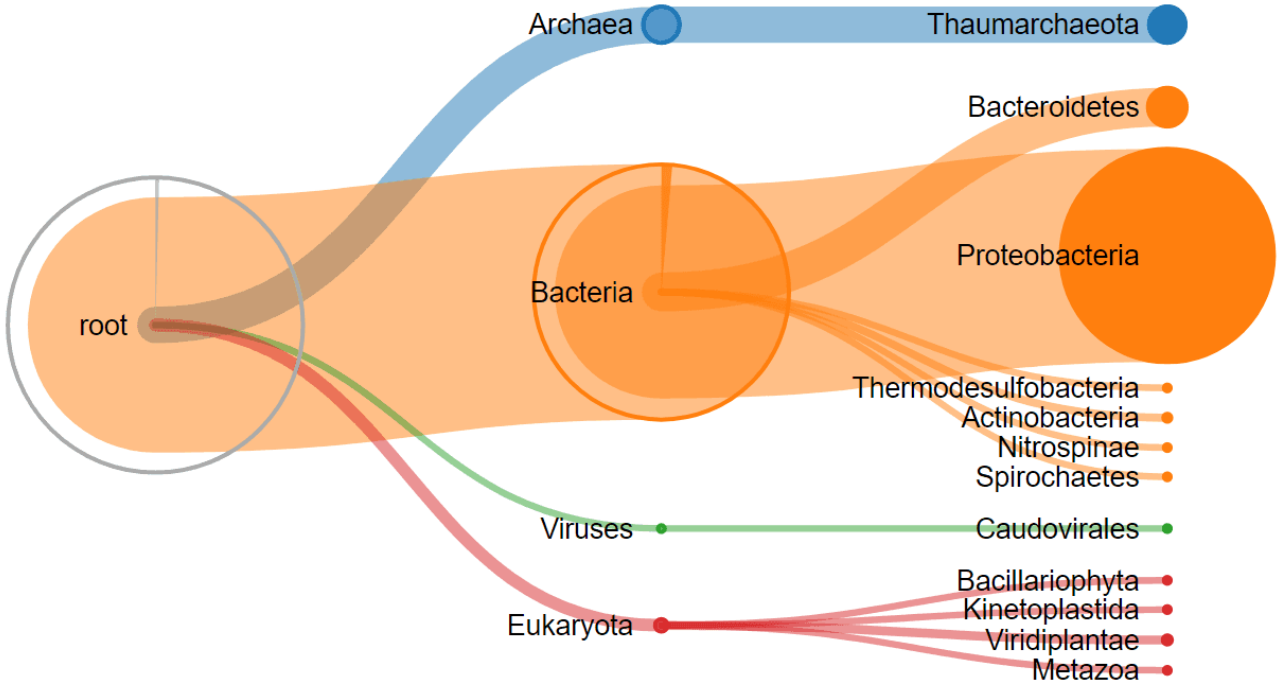


Figure 3: Interactive visualization from the Unipept Tree viewer plugin.

Genus taxonomy level summary

The tabular Unipept output lists the taxonomy assignments for each peptide. To create a meaningful summary, the Query Tabular tool is once again used, aggregating the number of peptides and PSMs for each genus level taxonomy assignment:

Hands On: Query Tabular

- Query Tabular (Galaxy version 3.0.0) with the following parameters:
- Database Table: Click on + Insert Database Table
- Tabular Dataset for Table: The PSM report

Section Table Options:

- Specify Name for Table: psm
- Specify Column Names: ,,sequence,,,,,,,,,,,,,,,,,,confidence,validation

- Repeat this step to have a second Database Table for the Unipept tabular/tsv output
- Specify Name for Table: lca
- Specify Column Names: peptide,,,,,,,,,,,,,,,,,,,genus
- Save the sqlite database in your history: Yes
- SQL Query to generate tabular output:

```
SELECT lca.genus, count(psm.sequence) as "PSMs", count(distinct psm.sequence) as "DISTINCT PEPTIDES"
FROM psm LEFT JOIN lca ON psm.sequence = lca.peptide
WHERE confidence >= 95
GROUP BY lca.genus
ORDER BY PSMs desc, 'DISTINCT PEPTIDES' desc
```

- Click Run Tool and inspect the query results file after it turned green.

1	2	3
#genus	PSMs	DISTINCT PEPTIDES
	596	92
Candidatus Pelagibacter	466	68
Planktomarina	127	15
Nitrosopumilus	121	26
Candidatus Thioglobus	83	1
Rhodobacter	57	9
Polaribacter	37	12
Octadecabacter	27	1
Pseudomonas	23	2
Elstera	21	2
Shewanella	20	1
Photobacterium	18	1
Haematobacter	17	2
Roseobacter	17	3
Candidatus Ruthia	10	1
Nitrospina	10	1
Sulfitobacter	10	3
Colwellia	9	1
Oceanimonas	9	1
Erythrobacter	8	1
Leisingera	8	1

Figure 4: Query Tabular output.

Functional Analysis

Recent advances in microbiome research indicate that functional characterization via metaproteomics analysis has the potential to accurately measure the microbial response to perturbations. In particular, metaproteomics enables the estimation of the function of the microbial community based on expressed microbial proteome.

In the following chapter, a functional analysis will be performed using the UniPept application pept2prot in order to match the list of peptides with the correlated Gene Ontology terms. This allows to get an insight of the biological process, the molecular function and the cellular component related to the sample data.

> **Comment: Gene Ontology (GO) Consortium**
>
> The Gene Ontology Consortium provides with its Ontology a framework for the model of biology. The GO defines concepts/classes used to describe gene function, and relationships between these concepts. It classifies functions along three aspects:
> • molecular function — molecular activities of gene products
> • cellular component — where gene products are active
> • biological process — pathways and larger processes made up of the activities of multiple gene products.

Data upload

For this tutorial, a tabular file containing the relevant GO terms has been created. It contains the GO aspect, the ID and the name. It is available at Zenodo.

> **Hands On: Data upload**
>
> • Import the file Gene_Ontology_Terms.tabular from Zenodo.
> • Rename the datasets to a more descriptive name, e.g. Gene Ontology Terms

Retrieve GO IDs for peptides: Unipept

The UniPept application pept2prot can be used to return the list of proteins containing each peptide. The option retrieve extra information option is set to yes so that we retrieve Gene Ontology assignments (go_references) for each protein.

> **Hands On: Unipept**
>
> • Unipept (Galaxy version 6.2.4+galaxy1) with the following parameters:
> • Unipept application: pept2prot: UniProt entries containing a given tryptic peptide
> • retrieve extra information: Yes
> • Peptides input format: tabular
> • Tabular Input Containing Peptide column: The first query results file.
> • Select column with peptides: Column 1
> • Choose outputs: Select tabular
> • Click Run Tool.
> • The output should be a tabular file containing a column labeled go_references.

Combine all information to quantify the GO results

As a final step we will use Query Tabular in a more sophisticated way to combine all information to quantify the GO analysis. The three used files and the extracted information are:

Gene Ontology Terms:

- go_id to match with Normalized UniPept output
- The GO aspect to group the results in three separate files
- The GO description to annotate the results

Normalized UniPept output:

- peptide to match with PSM Report and to count distinct peptides per GO term
- go_reference to match with Gene Ontology Terms

PSM Report:

- sequence to match with Normalized UniPept output
- id to count distinct PSM's per GO term

Hands On: Query Tabular

• Query Tabular (Galaxy version 3.0.0) with the following parameters:
• First Database Table: Gene Ontology Terms file
  - Specify Name for Table: go
  - Specify Column Names: aspect,go_id,description
• Second Database Table: Unipept tabular/tsv output
  - Specify Name for Table: bering_prot
  - Specify Column Names:
id,peptide,uniprot_id,taxon_id,taxon_name,ec_references,go_references,refseq_ids,refseq_protein_ids,insdc_ids,insdc_protein_ids
• Third Database Table: Same Unipept tabular/tsv output (normalized)
  - Specify Name for Table: bering_prot_go
  - Specify Column Names: id,go_reference
• Fourth Database Table: PSM Report
  - Specify Name for Table: bering_psms
  - Specify Column Names: id,sequence,confidence,validation
• SQL Query:

```
SELECT sequence as "peptide", count(id) as "PSMs"
FROM bering_psms
WHERE confidence >= 95
GROUP BY sequence
ORDER BY sequence
```

• Click Run Tool.

Hands On: SQLite to tabular

• SQLite to tabular (Galaxy version 2.0.0) with the following parameters:
• SQLite Database: The created SQLite database from the former step
• SQL Query:

```
SELECT go.description,
count(distinct bering_psms.sequence) as "bering_peptides", count(distinct bering_psms.id) as "bering_psms"
FROM go JOIN bering_prot_go ON go.go_id = bering_prot_go.go_reference JOIN bering_prot on bering_prot_go.id = bering_prot.id JOIN
bering_psms ON bering_prot.peptide = bering_psms.sequence
WHERE go.aspect = 'molecular_function'
GROUP BY go.description
ORDER BY bering_peptides desc, bering_psms desc
```

• Click Run Tool.
• Repeat these steps two times by replacing molecular_function with biological_process and cellular_component.

With these three output files the functional analysis of this tutorial is finished. Each record contains the name of a GO term, the amount of peptides related to it and the amount of PSMs for these peptides.

Key points

- Use dataset collections
- With SearchGUI and PeptideShaker you can gain access to multiple search engines
- Learning the basics of SQL queries can pay off

Frequently Asked Questions

Have questions about this tutorial? Have a look at the available FAQ pages and support channels:

- Tutorial FAQs: https://training.galaxyproject.org/training-material/topics/proteomics/tutorials/metaproteomics/faqs/
- Topic FAQs: https://training.galaxyproject.org/training-material/topics/proteomics/faqs/
- Galaxy FAQs: https://training.galaxyproject.org/training-material/faqs/galaxy/
- GTN Matrix Chat: https://gitter.im/Galaxy-Training-Network/Lobby
- Galaxy Help Forum: https://help.galaxyproject.org/

Useful literature

Further information, including links to documentation and original publications, regarding the tools, analysis techniques and the interpretation of results described in this tutorial can be found at: https://training.galaxyproject.org/training-material/topics/proteomics

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May, D. H., E. Timmins-Schiffman, M. P. Mikan, H. R. Harvey, E. Borenstein et al., 2016 An Alignment-Free "Metapeptide" Strategy for Metaproteomic Characterization of Microbiome Samples Using Shotgun Metagenomic Sequencing. Journal of Proteome Research 15: 2697–2705. 10.1021/acs.jproteome.6b00239

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Hiltemann, Saskia, Rasche, Helena et al., 2023 Galaxy Training: A Powerful Framework for Teaching! PLOS Computational Biology 10.1371/journal.pcbi.1010752

Batut et al., 2018 Community-Driven Data Analysis Training for Biology Cell Systems 10.1016/j.cels.2018.05.012

MORE TUTORIALS

- https://training.galaxyproject.org/training-material/topics/proteomics/#st-clinical-metaproteomics
- https://training.galaxyproject.org/training-material/topics/proteomics/tutorials/metaquantome-data-creation/tutorial.html
- https://training.galaxyproject.org/training-material/topics/proteomics/tutorials/metaquantome-taxonomy/tutorial.html
- https://training.galaxyproject.org/training-material/topics/proteomics/tutorials/metaquantome-function/tutorial.html

SECTION III



ABOUT IIT BOMBAY

Introduction

The Indian Institute of Technology Bombay (IIT Bombay) stands among the most distinguished institutions of higher education, research, innovation, and technological advancement in India. Since its establishment in 1958, IIT Bombay has played a transformative role in shaping the scientific, engineering, entrepreneurial, and technological landscape of the nation. Widely recognized for its academic excellence, world-class research infrastructure, interdisciplinary culture, and vibrant innovation ecosystem, the institute has emerged as a globally respected center for education and discovery.

Nestled in the scenic Powai region of Mumbai, IIT Bombay provides an intellectually stimulating environment where students, researchers, entrepreneurs, and industry leaders converge to address some of the most pressing challenges facing society. Over the decades, the institute has nurtured generations of scientists, engineers, innovators, policymakers, and business leaders who have made significant contributions across academia, healthcare, industry, government, and entrepreneurship.

Today, IIT Bombay is recognized not only as one of India's leading academic institutions but also as a catalyst for innovation-driven growth. Through cutting-edge research, technology development, startup incubation, and international collaborations, the institute continues to influence scientific progress and societal transformation on a national and global scale.

As the host institution of the Advances in Proteomics Technologies (APT-2026) Conference and Workshops, IIT Bombay provides an ideal platform for fostering interdisciplinary collaborations and advancing the frontiers of proteomics, multi-omics, artificial intelligence, precision medicine, and translational healthcare.

HISTORICAL FOUNDATIONS

Establishment and Early Vision

The Indian Institutes of Technology were conceived in the years following India's independence as institutions that would serve as engines of scientific and technological progress. IIT Bombay was established in 1958 as the second IIT in the country, reflecting the national vision of developing highly skilled scientists, engineers, and technologists capable of supporting India's industrial and economic development.

The institute was founded with technical and financial assistance from the United Nations Educational, Scientific and Cultural Organization (UNESCO) and the Government of the former Soviet Union. This collaboration represented one of the earliest large-scale international partnerships in higher technical education in India and laid the foundation for IIT Bombay's global outlook.

IIT BOMBAY MAIN GATE

Initially established with a limited number of departments and academic programs, the institute rapidly expanded its educational and research activities. Over the subsequent decades, IIT Bombay evolved from a traditional engineering institution into a comprehensive center for interdisciplinary education and research spanning engineering, science, healthcare, design, management, public policy, and entrepreneurship.



IIT BOMBAY MAIN GATE

Evolution into a Global Institution

The growth of IIT Bombay mirrors the evolution of modern India itself. As the nation transitioned into a knowledge-based economy, the institute continuously expanded its capabilities to address emerging scientific and technological challenges.

Today, IIT Bombay hosts a broad spectrum of academic departments, centers, schools, and interdisciplinary initiatives. The institute attracts some of the brightest students and researchers from India and around the world, creating a dynamic environment that fosters creativity, innovation, and scientific excellence.

Its alumni network spans more than seventy countries and includes globally recognized leaders in academia, technology, healthcare, business, public service, and entrepreneurship. Through their achievements, IIT Bombay's influence extends far beyond the boundaries of the campus.

CAMPUS & FACILITIES

A Unique Academic Environment

Located in Powai, Mumbai, IIT Bombay occupies a sprawling campus of approximately 550 acres. Surrounded by the natural beauty of Powai Lake, Vihar Lake, and the Sanjay Gandhi National Park ecosystem, the campus offers a unique combination of academic intensity and environmental tranquillity.

The campus is widely regarded as one of the most beautiful university campuses in India. Its lush greenery, diverse biodiversity, and thoughtfully designed infrastructure create an inspiring setting for learning and research.



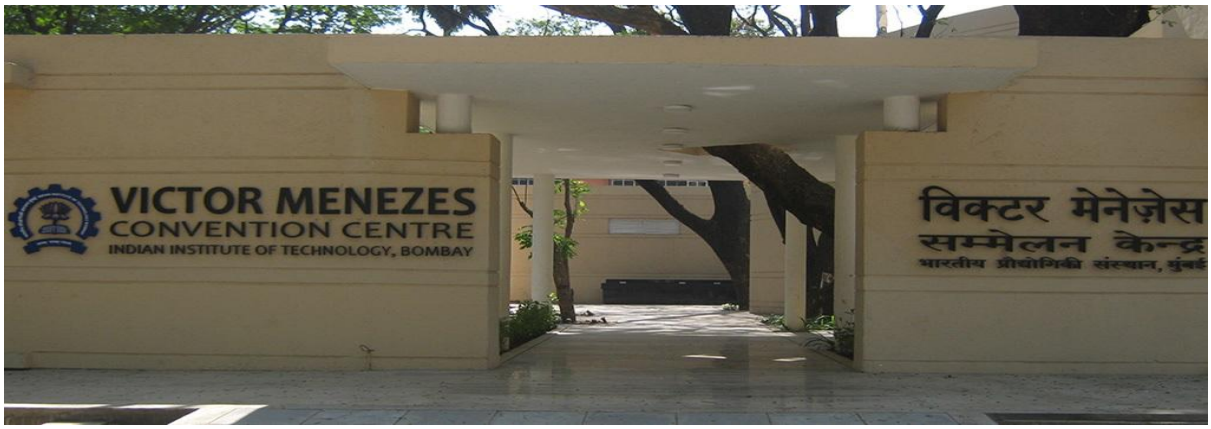
The IIT Bombay Campus

Powai Lake | Infinity Corridor, IITB | IIT Bombay Research Park

Infrastructure and Facilities

The institute hosts state-of-the-art facilities designed to support education, research, innovation, and community engagement. These include:

- Modern academic complexes
- Advanced research laboratories
- Central instrumentation facilities
- High-performance computing infrastructure
- Libraries and digital knowledge repositories
- Residential hostels
- Sports complexes
- Innovation and incubation centers
- Auditoriums and conference facilities



Among its premier venues, the Victor Menezes Convention Centre (VMCC) serves as a focal point for international conferences, workshops, symposia, and scientific gatherings. Such facilities enable IIT Bombay to host major global events, including APT-2026.

Sustainability and Environmental Stewardship

IIT Bombay has consistently demonstrated a commitment to environmental sustainability. The institute promotes green campus initiatives, energy-efficient infrastructure, waste management programs, water conservation measures, and biodiversity preservation.

The coexistence of modern scientific infrastructure with a rich natural environment reflects the institute's broader commitment to sustainable development and responsible innovation.



ACADEMIC EXCELLENCE

Undergraduate Education

IIT Bombay's undergraduate programs are internationally recognized for their rigor, innovation, and emphasis on problem-solving. Students are encouraged to develop strong analytical abilities while engaging in hands-on learning and interdisciplinary exploration.

The curriculum combines foundational knowledge with opportunities for research, entrepreneurship, design thinking, and societal engagement.

Postgraduate and Doctoral Programs

The institute offers a wide range of master's and doctoral programs across engineering, science, healthcare technologies, management, design, and interdisciplinary fields.

Graduate students play a central role in the institute's research ecosystem, contributing to scientific discovery, technology development, and innovation.

Doctoral scholars at IIT Bombay are engaged in cutting-edge research addressing global challenges in healthcare, sustainability, digital technologies, advanced materials, energy systems, and biological sciences.

Interdisciplinary Education

A defining characteristic of IIT Bombay is its emphasis on interdisciplinary learning. Complex real-world challenges often require expertise spanning multiple domains, and the institute actively promotes collaboration across traditional disciplinary boundaries.

This philosophy has contributed significantly to the growth of emerging areas such as systems biology, artificial intelligence, bioengineering, precision medicine, and multi-omics research.

RESEARCH & INNOVATION

Research and Innovation Ecosystem

Research represents one of the core pillars of IIT Bombay's mission. Faculty members, students, and researchers are actively engaged in advancing knowledge across a wide range of scientific and technological domains.

Strategic Research Areas

Major research themes include:

- Artificial Intelligence and Machine Learning
- Biotechnology and Healthcare
- Omics Sciences
- Precision Medicine
- Energy and Sustainability
- Climate Science
- Advanced Materials
- Quantum Technologies
- Robotics and Automation
- Data Science
- Space Technologies

The institute hosts numerous interdisciplinary centers and national facilities that facilitate collaborative research and innovation.

Research Funding and Partnerships

Research activities at IIT Bombay are supported by national agencies, international organizations, philanthropic foundations, healthcare institutions, and industry partners.

Collaborative projects frequently involve partnerships with hospitals, biotechnology companies, pharmaceutical organizations, government agencies, and global academic institutions.

These collaborations enable the translation of scientific discoveries into technologies and solutions with tangible societal impact.

ENTREPRENEURSHIP

Entrepreneurship and Technology Translation

One of the distinguishing features of IIT Bombay is its strong culture of innovation and entrepreneurship.



Society for Innovation and Entrepreneurship (SINE)

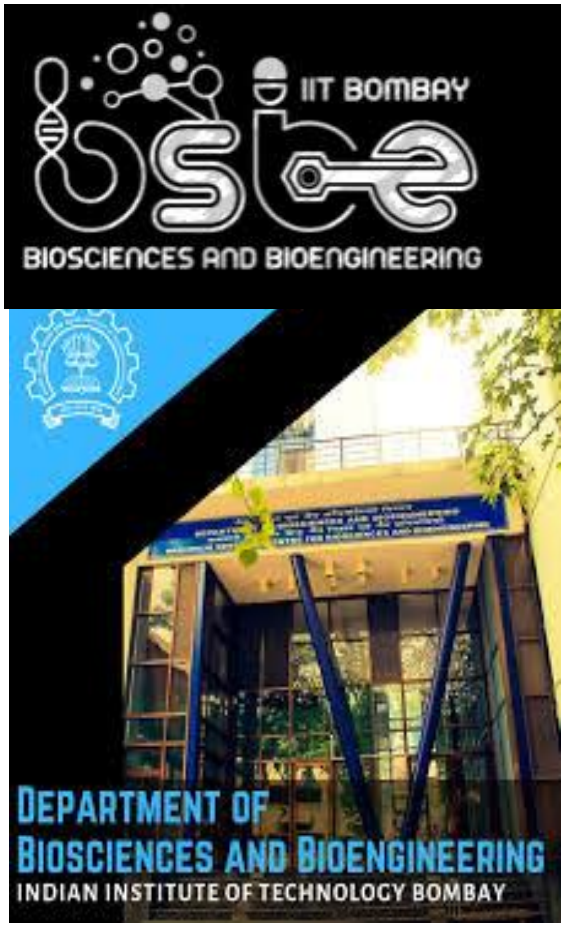
The Society for Innovation and Entrepreneurship (SINE) has become one of India's most successful academic incubators. Established to support technology-based startups, SINE provides mentoring, infrastructure, funding support, and industry connections to aspiring entrepreneurs.

Over the years, hundreds of startups have emerged from the IIT Bombay ecosystem, creating solutions in healthcare, biotechnology, artificial intelligence, clean energy, education, manufacturing, and digital technologies.

From Laboratory to Society

The institute actively promotes technology transfer and commercialization. Faculty members and researchers are encouraged to translate discoveries into products, services, and enterprises that address societal challenges.

The emergence of **Proteomica International Private Limited** as a biotechnology and omics-focused venture represents an example of this translational philosophy in action.



BIOSCIENCES & BIOENGINEERING

Biosciences and Bioengineering at IIT Bombay

The Department of Biosciences and Bioengineering (BSBE) represents IIT Bombay's commitment to integrating engineering principles with modern biological sciences.

Research within BSBE spans:

- Proteomics
- Genomics
- Bioinformatics
- Systems Biology
- Synthetic Biology
- Biomedical Engineering

- Cancer Biology
- Infectious Diseases
- Precision Medicine
- Translational Healthcare

The department has established strong collaborations with hospitals, research institutes, biotechnology companies, and international partners.

Through its educational and research programs, BSBE has contributed significantly to India's growing leadership in biological and biomedical sciences.

PROTEOMICS LEADERSHIP

Leadership in Proteomics and Multi-Omics Research

Over the past two decades, IIT Bombay has emerged as a leading center for proteomics and multi-omics research in India.

The institute has contributed to:

- Discovery Proteomics
- Targeted Proteomics
- Clinical Proteomics
- Biomarker Discovery
- Systems Biology
- Translational Medicine
- Precision Healthcare
- Multi-Omics Integration

In addition to scientific research, IIT Bombay has played an important role in capacity building through workshops, training programs, international symposia, and collaborative initiatives.

These efforts have helped create a vibrant proteomics community within India and strengthened international partnerships across the global proteomics ecosystem.

APT-2026

IIT Bombay as Host of APT-2026

The Advances in Proteomics Technologies (APT-2026) Conference and Workshops builds upon IIT Bombay's longstanding commitment to excellence in proteomics research, education, and innovation.

APT-2026 brings together scientists, clinicians, students, industry leaders, and technology developers from across the world to explore emerging advances in:

- Proteomics
- Multi-Omics
- Artificial Intelligence
- Biomarker Discovery
- Precision Medicine

- Clinical Diagnostics
- Translational Healthcare

The conference reflects the institute's broader vision of fostering interdisciplinary collaboration and accelerating scientific discoveries that improve human health and well-being.

Looking Ahead

As the boundaries between biology, engineering, medicine, and data science continue to dissolve, IIT Bombay is uniquely positioned to lead the next generation of scientific innovation.

By integrating advanced technologies with fundamental scientific inquiry, the institute is helping shape the future of precision medicine, digital biology, sustainable development, and knowledge-driven societal progress.

The hosting of APT-2026 represents not only a celebration of scientific achievement but also a reaffirmation of IIT Bombay's commitment to advancing research, education, innovation, and global collaboration for the benefit of humanity.

ABOUT THE DEPARTMENT

Department of Biosciences and Bioengineering (BSBE), IIT Bombay

INTRODUCTION

About the Department

The Department of Biosciences and Bioengineering (BSBE) at the Indian Institute of Technology Bombay represents one of India's most successful examples of interdisciplinary convergence between biology, engineering, medicine, and computational sciences. Established with the vision of addressing complex biological and healthcare challenges through engineering principles and quantitative approaches, BSBE has emerged as a nationally and internationally recognized center of excellence in education, research, innovation, and translational science.

Over the past two decades, BSBE has played a pivotal role in advancing modern biological sciences in India. The department has cultivated a unique ecosystem where engineers, biologists, clinicians, computational scientists, chemists, physicists, and data scientists collaborate to solve pressing challenges in human health, agriculture, environmental sustainability, and biotechnology.

Today, BSBE stands at the forefront of emerging scientific disciplines such as systems biology, proteomics, genomics, bioinformatics, synthetic biology, biomedical engineering, artificial intelligence in healthcare, and precision medicine. Its contributions have significantly strengthened India's scientific capabilities while fostering global collaborations and innovation-driven research.

As one of the principal academic units associated with the Advances in Proteomics Technologies (APT-2026) Conference, BSBE reflects the interdisciplinary spirit that underpins modern omics research and translational healthcare.

THE VISION BEHIND BSBE

Bridging Biology and Engineering

The rapid advances in biological sciences during the late twentieth and early twenty-first centuries created a growing need for professionals capable of integrating engineering methodologies with biological understanding. Traditional disciplinary boundaries were increasingly inadequate for addressing complex biological systems and healthcare challenges.

Recognizing this need, IIT Bombay established BSBE with a vision of creating a multidisciplinary academic environment where biological problems could be addressed using quantitative, computational, and engineering approaches.

The department was designed to serve as a bridge between:

- Biology and Engineering
- Medicine and Technology
- Computation and Experimentation
- Basic Science and Clinical Translation
- Academic Discovery and Industrial Innovation

This interdisciplinary philosophy remains central to the department's identity today.

ACADEMIC PROGRAMS

Undergraduate Education

BSBE offers undergraduate programs designed to provide students with a strong foundation in both biological sciences and engineering principles. Students are trained in Molecular Biology, Cell Biology, Genetics, Biochemistry, Bioinformatics, Computational Biology, Biomedical Engineering, and Systems Biology. The curriculum encourages students to develop analytical thinking, experimental skills, quantitative reasoning, and problem-solving capabilities. Through laboratory training, project-based learning, and research exposure, undergraduate students gain firsthand experience in addressing real-world scientific challenges.

Postgraduate Programs

The department offers advanced master's programs that enable students to specialize in diverse areas of biosciences and bioengineering. Graduate education emphasizes research-driven learning, advanced analytical techniques, computational approaches, and translational applications. Students benefit from interactions with faculty members working on cutting-edge research problems spanning healthcare, biotechnology, agriculture, and environmental sciences.

Doctoral Research

Doctoral training forms a cornerstone of BSBE's research mission. Ph.D. scholars contribute significantly to the department's scientific output through fundamental biological discoveries, technology development, clinical research collaborations, computational modeling, and omics-based investigations. The department has produced numerous doctoral graduates who have subsequently established successful careers in academia, industry, healthcare, and entrepreneurship worldwide.

RESEARCH EXCELLENCE AND INNOVATION

Major Research Areas

BSBE has developed a strong reputation for conducting high-impact research across multiple domains of biological and biomedical sciences. The department's research philosophy emphasizes both scientific excellence and societal relevance. Faculty members lead projects supported by national and international funding agencies, often working in collaboration with hospitals, government organizations, biotechnology companies, and academic institutions across the world.

Proteomics and Multi-Omics Research

Proteomics has become one of BSBE's most prominent research strengths. Faculty and researchers investigate protein expression dynamics, biomarker discovery, clinical proteomics, quantitative proteomics, targeted proteomics, and systems-level biological regulation. Recent advances have expanded research activities into broader multi-omics

approaches that integrate genomics, transcriptomics, proteomics, metabolomics, and lipidomics. BSBE has played an important role in establishing proteomics education and training initiatives that have benefited researchers throughout India and beyond.

Genomics and Systems Biology

Genomics research within BSBE focuses on understanding the genetic basis of biological processes and disease, including functional genomics, gene regulation, genome-wide analysis, personalized medicine, and disease susceptibility. Systems biology complements these efforts by examining how genes, proteins, metabolites, and cellular networks interact to generate biological function.

Bioinformatics and Computational Biology

BSBE has established strong expertise in bioinformatics, machine learning, artificial intelligence, data mining, network biology, and statistical genomics. Researchers develop algorithms and computational frameworks capable of extracting meaningful biological insights from large-scale datasets. These capabilities are increasingly important for precision medicine, digital health, and multi-omics integration.

Synthetic Biology and Biotechnology

Synthetic biology represents a rapidly expanding area within BSBE. Researchers work on genetic circuit design, metabolic engineering, microbial engineering, bioprocess optimization, and industrial biotechnology, combining engineering principles with biological systems to create innovative solutions for healthcare, agriculture, energy, and sustainability.

Biomedical Engineering

Research activities include biosensors, diagnostic technologies, medical devices, tissue engineering, drug delivery systems, and wearable health technologies. Many projects are conducted in collaboration with clinicians and healthcare institutions, facilitating the translation of research into practical healthcare solutions.

Translational Healthcare Research

One of the defining characteristics of BSBE is its commitment to translational science. Rather than limiting research to laboratory discoveries, the department actively seeks to convert scientific knowledge into solutions that improve human health. Collaborative projects address cancer, infectious diseases, maternal and child health, neurological disorders, metabolic diseases, and precision medicine.

RESEARCH INFRASTRUCTURE

BSBE benefits from access to some of the most advanced scientific infrastructure available within India, including high-resolution mass spectrometry platforms, genomics facilities, cell culture laboratories, imaging systems, computational infrastructure, biophysical characterization facilities, and advanced analytical instrumentation. The department also benefits from access to central facilities across IIT Bombay and collaborative infrastructure through national and international partnerships.

GLOBAL COLLABORATIONS

BSBE maintains active partnerships with universities, research institutes, hospitals, biotechnology companies, and government organizations that support joint research projects, student exchanges, faculty exchanges, technology development, international workshops, and collaborative publications.

CONTRIBUTIONS TO PROTEOMICS EDUCATION

BSBE has played a significant role in developing India's proteomics ecosystem. Faculty members have organized international workshops, hands-on training programs, symposia, scientific conferences, and educational outreach activities including PSI-related activities, TPWIS conferences, proteomics boot camps, advanced training courses, and the Advances in Proteomics Technologies (APT) conference series.

ENTREPRENEURSHIP AND INNOVATION

BSBE strongly encourages innovation and entrepreneurship. Research generated within the department has led to patents, technology transfers, startup ventures, and industrial collaborations. The emergence of omics-focused enterprises such as Proteomica International Private Limited illustrates the department's commitment to translating academic discoveries into practical solutions. Through IIT Bombay's innovation ecosystem and SINE incubator, BSBE researchers have access to mentorship, funding opportunities, and commercialization support.

BSBE AND THE FUTURE OF PRECISION MEDICINE

Healthcare is undergoing a profound transformation driven by advances in genomics, proteomics, artificial intelligence, and digital technologies. BSBE's expertise in multi-omics, systems biology, artificial intelligence, clinical research, and biomedical engineering provides a strong foundation for advancing precision medicine and personalized healthcare. Future directions are expected to include single-cell omics, spatial biology, digital health signatures, predictive diagnostics, AI-driven healthcare, and precision therapeutics.

BSBE AND APT-2026

The Advances in Proteomics Technologies (APT-2026) Conference reflects many of the scientific themes that define BSBE's research mission. Areas such as proteomics, multi-omics, artificial intelligence, biomarker discovery, precision medicine, and translational healthcare are central both to the conference and to the department's activities. By bringing together leading researchers, clinicians, students, and industry experts, APT-2026 provides an ideal platform for advancing interdisciplinary collaborations and accelerating scientific innovation.



PROTEOMICS LABORATORY

The Proteomics Laboratory, IIT Bombay

Advancing Proteomics, Precision Medicine, and Global Scientific Collaboration

INTRODUCTION

The Proteomics Laboratory at the Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, has emerged as one of India's leading centers for proteomics, mass spectrometry, systems biology, and multi-omics research. Since its establishment in 2009 under the leadership of Professor Sanjeeva Srivastava, the laboratory has evolved into a nationally and internationally recognized hub for scientific discovery, technology development, education, innovation, and translational healthcare research.

Over the past decade and a half, the laboratory has played a transformative role in shaping the proteomics landscape in India. Through pioneering research, establishment of advanced analytical facilities, development of educational resources, organization of international conferences and workshops, and active participation in global proteomics initiatives, the laboratory has significantly contributed to strengthening India's presence in the worldwide proteomics community.

Today, the Proteomics Laboratory serves as an interdisciplinary platform where biologists, engineers, clinicians, computational scientists, chemists, and data scientists collaborate to understand complex biological systems and develop innovative solutions for healthcare challenges. The laboratory's research spans proteomics, metabolomics, lipidomics, systems biology, biomarker discovery, artificial intelligence, precision medicine, infectious diseases, cancer biology, and translational healthcare.

As one of the driving forces behind Advances in Proteomics Technologies (APT-2026), the laboratory exemplifies IIT Bombay's vision of integrating research excellence, education, innovation, and societal impact.

ESTABLISHMENT

Establishment of the Proteomics Laboratory



Dr. Sanjeeva Srivastava

The Proteomics Laboratory was established following Professor Sanjeeva Srivastava's return to India after completing his doctoral studies at the University of Alberta, Canada, and postdoctoral training at Harvard Medical School, USA. Inspired by the vision of creating a globally competitive proteomics ecosystem in India, he joined IIT Bombay in 2009 as an Assistant Professor and initiated efforts to establish a world-class proteomics research and training facility.

At that time, proteomics research infrastructure in India was still developing. Advanced mass spectrometry technologies, specialized training programs, and dedicated proteomics facilities were limited. Recognizing this gap, the laboratory was envisioned not merely as a research group but as a national resource that would contribute to scientific discovery, education, infrastructure development, and community building.

Over the years, the laboratory has grown into a vibrant research ecosystem with extensive collaborations across academia, hospitals, government agencies, biotechnology companies, and international research institutions.

VISION AND MISSION

To advance biological discovery and improve human health through innovative proteomics and multi-omics research while fostering education, collaboration, entrepreneurship, and societal impact.

The laboratory's mission encompasses advancing proteomics and multi-omics technologies, understanding disease mechanisms, discovering clinically relevant biomarkers, developing precision medicine strategies, training future generations of scientists, promoting interdisciplinary collaborations, and translating scientific discoveries into healthcare solutions.

RESEARCH EXCELLENCE

Research Excellence and Scientific Contributions

Since its inception, the Proteomics Laboratory has established a strong international reputation for high-quality research in proteomics and systems biology. The group has published more than 200 peer-reviewed research articles, authored books and book chapters, and generated numerous intellectual property assets through patents and technology innovations.

Cancer Proteomics

Cancer has been one of the major focus areas of the laboratory. Research investigations have covered glioblastoma, meningioma, oral cancer, cervical cancer, triple-negative breast cancer, and pancreatic cancer. Using advanced proteomics, metabolomics, lipidomics, and systems biology approaches, the laboratory has identified molecular pathways associated with tumor progression, drug resistance, prognosis, and therapeutic response.

Infectious Diseases and Global Health

The laboratory has made significant contributions to understanding infectious diseases through proteomics and multi-omics approaches, including malaria, dengue, COVID-19, respiratory infections, and host-pathogen interactions. The laboratory has contributed extensively to malaria proteomics and biomarker discovery efforts, including studies on Plasmodium vivax and severe malaria. During the COVID-19 pandemic, the group rapidly mobilized its expertise to investigate disease mechanisms, severity markers, immune responses, and multi-omics signatures.

Neurological Disorders and Brain Proteomics

The laboratory has established internationally recognized expertise in brain tumor proteomics and neurological research, including investigations into gliomas, meningiomas, medulloblastomas, and human brain proteome studies.

Multi-Omics and Systems Biology

Recognizing that biological systems cannot be understood through a single molecular layer, the laboratory actively integrates genomics, transcriptomics, proteomics, metabolomics, and lipidomics for a systems-level understanding of biological regulation and disease mechanisms.



Thermo Scientific Vanquish UHPLC System



SPR Instrument SMCxPRO



Q Exactive Orbitrap

TSQ Altis LC-MS/MS



Orbitrap Fusion Tribrid MS

RESEARCH INFRASTRUCTURE

One of the most significant contributions of the laboratory has been the creation of advanced research infrastructure at IIT Bombay. Professor Srivastava established and led the development of the MASSFIITB National Proteomics Facility, providing researchers access to state-of-the-art mass spectrometry technologies including high-resolution LC-MS/MS platforms, MALDI-TOF/TOF systems, Surface Plasmon Resonance (SPR) facilities, advanced computational resources, and bioinformatics pipelines.

EDUCATION AND CAPACITY BUILDING

One of the defining characteristics of the Proteomics Laboratory is its strong commitment to education. Professor Srivastava has consistently viewed teaching and mentorship as integral components of scientific leadership. Over the years, he has taught undergraduate and postgraduate courses to thousands of students at IIT Bombay and other institutions. The laboratory has trained undergraduate students, M.Sc. students, M.Tech. students, Ph.D. scholars, postdoctoral researchers, clinicians, and industry professionals. To date, the laboratory has successfully mentored numerous doctoral graduates and more than seventy-five postgraduate theses.

INNOVATIONS IN DIGITAL LEARNING

Beyond traditional classroom teaching, the laboratory has been a pioneer in educational innovation through NPTEL MOOCs, Virtual Labs, OSCAR educational resources, flipped classrooms, simulation-based learning, interactive assessments, and gamification approaches. The laboratory's online courses have reached tens of thousands of learners globally and have contributed significantly to capacity building in biotechnology, bioengineering, and proteomics.

INTERNATIONAL COLLABORATIONS

The Proteomics Laboratory has established strong partnerships with leading institutions worldwide, including Harvard Medical School, University of California San Francisco, Arizona State University, Institute for Systems Biology, Nottingham Trent University, Central South University, and multiple HUPO-affiliated research groups. These collaborations have facilitated joint research projects, student exchanges, faculty exchanges, technology development, international workshops, and collaborative publications.

LEADERSHIP IN GLOBAL PROTEOMICS

The laboratory has actively contributed to international efforts aimed at advancing proteomics and systems biology, including the Human Proteome Organization (HUPO), Biology and Disease-driven Human Proteome Project (B/D-HPP), Cancer-HPP, Human Infectious Diseases-HPP, Proteomics Society India (PSI), and π-HuB: Proteomic Navigator of the Human Body.

BUILDING THE PROTEOMICS COMMUNITY IN INDIA

A defining contribution of the laboratory has been its role in community building. Over the years, the laboratory has organized numerous national and international events that have trained researchers and fostered scientific interactions.

PSI-2014: Proteomics from Discovery to Function

One of the largest proteomics meetings organized in India, attracting approximately 800 participants and bringing together leading researchers from around the world.

TPWIS-2015: Targeted Proteomics Workshop and International Symposium

A landmark event that introduced advanced targeted proteomics technologies and training programs to a broader Indian audience.

TPWIS-2018

An expanded international platform integrating proteomics, mass spectrometry, bioinformatics, and translational research.

APT Series

The evolution of these efforts eventually led to the launch of the Advances in Proteomics Technologies (APT) conference series, which has become one of the premier platforms for proteomics and multi-omics research in India.

4D Omics Symposium

The inauguration of advanced omics infrastructure and the introduction of next-generation technologies further strengthened India's proteomics ecosystem.

FROM RESEARCH TO ENTREPRENEURSHIP

A major milestone was the establishment of Proteomica International Private Limited, an IIT Bombay-incubated startup focused on proteomics, metabolomics, lipidomics, diagnostics, and precision healthcare. Proteomica represents the laboratory's commitment to bridging academia and industry while contributing to India's vision of self-reliance in advanced healthcare technologies.

TOWARDS PRECISION MEDICINE

The future of healthcare increasingly depends upon understanding the molecular complexity of human biology. The Proteomics Laboratory is actively contributing to this transformation through research in biomarker discovery, precision medicine, multi-omics integration, artificial intelligence, digital health, and predictive diagnostics. These efforts seek to move healthcare from reactive treatment toward predictive, preventive, personalized, and participatory models of medicine.

PROFESSOR SANJEEVA SRIVASTAVA

Founder and Visionary Leader

The growth and success of the Proteomics Laboratory at IIT Bombay are closely intertwined with the scientific vision, leadership, and dedication of Professor Sanjeeva Srivastava. After completing his doctoral training at the University of Alberta, Canada, and postdoctoral research at Harvard Medical School, USA, Professor Srivastava returned to India with a mission to establish a world-class proteomics ecosystem that could contribute not only to scientific discovery but also to healthcare innovation, education, and national capacity building.

Since joining IIT Bombay in 2009, Professor Srivastava has pursued a multidisciplinary vision that integrates proteomics, systems biology, bioinformatics, engineering, clinical sciences, and translational medicine. His leadership roles in HUPO, B/D-HPP, Cancer-HPP, Human Infectious Diseases-HPP, Proteomics Society India, and the π-HuB initiative reflect his active involvement in shaping the future direction of proteomics worldwide.

LABORATORY MILESTONES

A Journey of Growth and Innovation

2009	Professor Sanjeeva Srivastava joined IIT Bombay and established the Proteomics Laboratory.

2010–2013	Development of foundational research infrastructure and initiation of proteomics-focused research programs.
2014	Organization of the 6th Annual Meeting of Proteomics Society, India (PSI-2014), one of the largest proteomics meetings held in India.
2015	Organization of the Targeted Proteomics Workshop and International Symposium (TPWIS-2015), introducing advanced targeted proteomics technologies to the Indian scientific community.
2018	Expansion of TPWIS into a broader international scientific platform involving mass spectrometry, bioinformatics, and translational research.
2020	Recognition of excellence in education through the prestigious Prof. S. P. Sukhatme Excellence in Teaching Award.
2022	Organization of the Rinti Banerjee Memorial Conference and expansion of multi-omics initiatives.
2024	Launch of Proteomica International Private Limited and establishment of advanced next-generation omics infrastructure.
2025	Introduction of Advances in Proteomics Technologies (APT) and MOOD-OMICS.
2026	APT-2026 represents the culmination of nearly two decades of scientific leadership, education, innovation, and community building.

PUBLICATIONS, PATENTS, AND SCIENTIFIC IMPACT

The laboratory has generated a substantial body of scientific work spanning fundamental biology, clinical proteomics, biomarker discovery, infectious diseases, cancer research, and systems biology. Key indicators of impact include more than 200 peer-reviewed publications, multiple books and book chapters, dozens of patent applications and granted patents, extensive citation records, contributions to international scientific initiatives, and development of novel methodologies and analytical workflows.

TRAINING FUTURE SCIENTIFIC LEADERS

One of the most enduring contributions of the Proteomics Laboratory lies in its commitment to mentorship and human resource development. The laboratory has trained Ph.D. scholars, M.Tech. students, M.Sc. students, undergraduate researchers, postdoctoral fellows, clinicians, and industry scientists. Many former trainees now occupy positions at prestigious institutions worldwide. The laboratory views student success as one of its most important achievements.

VISION 2030

The next phase of growth will focus on emerging technologies and healthcare paradigms including single-cell proteomics, spatial biology, artificial intelligence, digital twins, precision medicine, preventive healthcare, multi-omics integration, and translational diagnostics. The laboratory aims to contribute to the development of next-generation healthcare systems that are predictive, preventive, personalized, and participatory.

INDUSTRY PARTNER

Proteomica International Private Limited

Translating Omics Discoveries into Healthcare Solutions

INTRODUCTION

The rapid advancement of proteomics, metabolomics, lipidomics, genomics, and systems biology has transformed our understanding of human health and disease. Despite remarkable scientific discoveries, translating these findings into practical healthcare solutions remains one of the greatest challenges in biomedical research. Recognizing this critical gap, Proteomica International Private Limited was established with the vision of accelerating the journey from scientific discovery to clinical application.

Founded by Professor Sanjeeva Srivastava and his former doctoral student Dr. Arghya Banerjee, Proteomica emerged from years of pioneering research and innovation conducted at the Indian Institute of Technology Bombay. The company was conceived as a translational platform that would bridge academic research, healthcare institutions, industry, and technology development to create impactful solutions for precision medicine and personalized healthcare.

Since its inception, Proteomica has positioned itself at the forefront of India's rapidly evolving omics ecosystem, combining advanced analytical technologies, clinical collaborations, artificial intelligence, and translational research to address some of the most pressing healthcare challenges of our time.

ORIGINS

From Academic Research to Entrepreneurship

The foundation of Proteomica lies in nearly two decades of proteomics and systems biology research conducted at IIT Bombay. While discoveries in cancer biology, infectious diseases, neurological disorders, biomarker discovery, precision medicine, and multi-omics research provided important biological insights, a recurring challenge remained: how could promising biomarkers and molecular signatures be translated into clinically useful products and technologies?

Proteomica was established to address this challenge. The company represents a natural evolution of the laboratory's translational philosophy, creating a dedicated platform capable of moving scientific discoveries beyond academic publications and into healthcare applications. By integrating expertise from biology, engineering, medicine, bioinformatics, and entrepreneurship, Proteomica aims to accelerate the translation of omics research into diagnostics, prognostics, therapeutics, and digital health solutions.

VISION AND MISSION

Vision

To transform healthcare through omics-driven innovation, enabling predictive, preventive, personalized, and precision medicine for populations worldwide.

Mission

Proteomica seeks to advance proteomics and multi-omics technologies, accelerate biomarker translation, develop clinically actionable solutions, enable personalized healthcare, support healthcare innovation through partnerships, and foster collaboration between academia, hospitals, and industry.

BRINGING 4D OMICS TO INDIA

A defining milestone in Proteomica's journey has been the establishment of next-generation 4D omics capabilities. The company introduced advanced timsTOF mass spectrometry technology from Bruker, enabling researchers and clinicians to explore biological systems with unprecedented sensitivity, depth, and throughput. The incorporation of trapped ion mobility spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) technologies has significantly expanded the analytical capabilities available within India. These platforms support deep proteome profiling, quantitative proteomics, clinical proteomics, metabolomics, lipidomics, biomarker discovery, and multi-omics integration.

OMICS SERVICES AND ANALYTICAL EXCELLENCE

Services and Capabilities

Proteomics Excellence

Proteomics remains one of the company's core strengths. Capabilities include discovery proteomics, quantitative proteomics, DIA-PASEF workflows, targeted proteomics, PRM-based validation, and biomarker discovery. These approaches enable comprehensive characterization of protein expression and biological pathways associated with health and disease.

Advanced Metabolomics

Metabolomics investigations provide critical insights into cellular metabolism and physiological regulation. Applications include disease progression studies, drug response analysis, pathway characterization, and clinical biomarker identification.

Comprehensive Lipidomics

Lipidomics is increasingly recognized as an essential component of systems biology and precision medicine. Proteomica offers high-throughput lipid profiling to investigate metabolic disorders, cardiovascular diseases, neurological disorders, inflammatory diseases, and cancer biology.

Key Research Areas

Maternal and Child Health

Maternal and child health remains a major public health priority. Proteomica utilizes proteomics and metabolomics approaches to identify molecular signatures associated with maternal nutrition, pregnancy outcomes, neonatal health, and child development, with the goal of facilitating early intervention and improving health outcomes.

Empowering Cancer Care

Cancer represents one of the most significant healthcare challenges worldwide. Proteomica applies multi-omics technologies to discover biomarkers, improve disease classification, predict therapeutic response, and support precision oncology. Through collaborations with clinicians and hospitals, the company seeks to advance personalized cancer care and improve patient outcomes.

Personalized Healthcare

Proteomica aims to develop 'digital health signatures' by integrating proteomic profiles, metabolic profiles, clinical information, and genetic information. These signatures have the potential to guide personalized healthcare decisions and enable earlier disease detection.

Aging and Wellness

The company is investigating molecular markers associated with biological aging, age-related diseases, wellness trajectories, and preventive healthcare. The objective is to move healthcare from reactive treatment toward proactive health management.

COLLABORATIONS

A key differentiator of Proteomica is its close engagement with clinicians and healthcare institutions. The company actively collaborates with medical colleges, hospitals, clinical researchers, and public health organizations to facilitate access to clinically relevant samples, biomarker validation studies, translational research projects, and development of diagnostic solutions.



Use of AI in Health Care

ARTIFICIAL INTELLIGENCE AND DIGITAL HEALTH

The future of healthcare will increasingly depend on the integration of omics data with artificial intelligence. Proteomica is developing capabilities in machine learning, predictive analytics, data integration, digital health signatures, and clinical decision support systems. These technologies will play a crucial role in transforming large-scale biological data into actionable healthcare insights.

SUPPORTING INDIA'S OMICS ECOSYSTEM

Beyond research and commercial activities, Proteomica contributes actively to the broader scientific community, supporting workshops, training programs, scientific conferences, student engagement, technology demonstrations, and industry-academia partnerships. Its involvement in APT, MOOD-OMICS, and related initiatives reflects a commitment to strengthening India's scientific and innovation ecosystem.

LOOKING AHEAD

Proteomica International Private Limited

Where Innovation Meets Excellence

Proteomica International Private Limited represents a unique convergence of academic excellence, scientific innovation, clinical collaboration, and entrepreneurial vision. What began as a vision shared by Professor Sanjeeva Srivastava and Dr. Arghya Banerjee has evolved into a platform dedicated to transforming omics discoveries into real-world healthcare solutions. As technologies such as single-cell proteomics, spatial biology, artificial intelligence, and precision medicine continue to advance, Proteomica is well positioned to play a leading role in shaping the future of healthcare in India and beyond.

PROFESSIONAL SOCIETY

Proteomics Society, India (PSI)

PSI

Proteomics Society, India

Advancing Proteomics Research, Education, and Collaboration in India

INTRODUCTION

The Proteomics Society, India (PSI) serves as the premier professional organization dedicated to promoting proteomics research, education, technology development, and scientific collaboration in India. Since its inception, PSI has played a transformative role in nurturing the growth of proteomics and mass spectrometry-based research across the country, bringing together scientists, clinicians, students, industry professionals, and policymakers under a common platform.

As proteomics emerged globally as a powerful tool for understanding biological systems, disease mechanisms, and therapeutic interventions, India recognized the need for a dedicated scientific society that could coordinate national

efforts, facilitate collaboration, and accelerate capacity building. PSI was established to fulfill this vision and has since become the focal point of India's proteomics community.

Today, PSI represents a vibrant network of researchers working across academia, healthcare institutions, biotechnology industries, pharmaceutical organizations, research laboratories, and government agencies. Through conferences, workshops, training programs, collaborative initiatives, and international partnerships, the society continues to strengthen India's position within the global proteomics landscape.

THE EMERGENCE OF PROTEOMICS IN INDIA

The completion of the Human Genome Project marked a new era in biological sciences. While genomic information provided a blueprint of life, scientists increasingly realized that proteins are the primary functional molecules responsible for cellular processes, signaling pathways, physiological regulation, and disease progression.

The emergence of proteomics created new opportunities to understand disease mechanisms, discover biomarkers, develop targeted therapeutics, advance precision medicine, and investigate complex biological systems. As research groups across India began adopting proteomics technologies, the need for a coordinated national platform became evident. The formation of PSI represented an important milestone in addressing these needs and fostering a cohesive proteomics ecosystem within India.

VISION AND MISSION

Vision

To promote excellence in proteomics research, education, innovation, and clinical translation while strengthening India's contributions to global proteomics initiatives.

Mission

The Proteomics Society, India seeks to advance proteomics research and technology development, facilitate scientific collaboration, promote education and training, support young investigators and students, foster industry-academia partnerships, enhance international engagement, and accelerate translational applications of proteomics.

BUILDING A NATIONAL PROTEOMICS COMMUNITY

One of PSI's most significant achievements has been the creation of a national network connecting researchers across diverse disciplines. Members of PSI represent expertise in proteomics, mass spectrometry, bioinformatics, systems biology, clinical research, biotechnology, pharmaceutical sciences, agricultural sciences, and environmental sciences. The society provides opportunities for interdisciplinary interactions that often lead to new collaborations and innovative research directions.

ANNUAL CONFERENCES

The annual meetings of PSI have become important platforms for disseminating scientific advances and fostering collaborations. These meetings bring together national and international experts, early-career researchers, students, industry representatives, and technology developers to present research findings, learn emerging technologies, establish collaborations, interact with global leaders, and explore career opportunities.

PSI-2014: A LANDMARK EVENT AT IIT BOMBAY

One of the most significant milestones in the history of PSI was the organization of the 6th Annual Meeting of Proteomics Society, India and International Conference on Proteomics from Discovery to Function at IIT Bombay. Organized under the leadership of Professor Sanjeeva Srivastava and his team, PSI-2014 emerged as one of the largest proteomics gatherings ever held in India, bringing together leading international proteomics researchers, national scientific leaders, industry

partners, students, and trainees. The event showcased advances in clinical proteomics, quantitative proteomics, biomarker discovery, cancer proteomics, infectious disease research, and systems biology.

EDUCATION AND CAPACITY BUILDING

A major objective of PSI has been to strengthen education and workforce development in proteomics. The society actively promotes workshops, hands-on training programs, educational courses, summer schools, and student engagement activities. These initiatives help bridge the gap between theoretical knowledge and practical expertise in biology, chemistry, instrumentation, data analysis, bioinformatics, and statistics.

SUPPORTING YOUNG INVESTIGATORS

Recognizing that the future of any scientific discipline depends upon its next generation of researchers, PSI has consistently prioritized student participation, travel fellowships, young investigator awards, poster competitions, and mentorship opportunities. Many young researchers who first presented their work at PSI meetings have subsequently established successful careers in academia, industry, and healthcare.

INDUSTRY ENGAGEMENT

Proteomics is inherently technology-driven, making interactions with industry essential for scientific progress. PSI actively encourages partnerships between academic institutions, biotechnology companies, pharmaceutical organizations, instrument manufacturers, and clinical laboratories. Industry participation in PSI meetings facilitates technology dissemination, product demonstrations, collaborative research, and workforce development.

INTERNATIONAL PARTNERSHIPS

From its early years, PSI recognized the importance of global engagement. The society has developed strong relationships with the Human Proteome Organization (HUPO), Asia Oceania Human Proteome Organization (AOHUPO), US HUPO, and the American Society for Mass Spectrometry (ASMS), enabling international speaker exchanges, collaborative projects, joint educational initiatives, and participation in global scientific programs.

CONTRIBUTIONS TO HUMAN HEALTH AND PRECISION MEDICINE

Research conducted by PSI members has contributed significantly to cancer research (identification of biomarkers, therapeutic targets, and molecular pathways), infectious diseases (proteomics investigations related to malaria, dengue, tuberculosis, COVID-19), neurological disorders (molecular mechanisms underlying brain diseases), precision medicine (integration of omics technologies for personalized healthcare strategies), and translational research (conversion of scientific discoveries into clinically relevant diagnostic applications).

PSI AND APT-2026

The scientific themes of APT-2026 closely align with the mission and vision of PSI. Topics such as proteomics, multi-omics, artificial intelligence, biomarker discovery, precision medicine, clinical diagnostics, and translational healthcare represent areas where PSI members have made substantial contributions. APT-2026 builds upon the strong foundation established through PSI activities over the past two decades and provides an important platform for advancing the next generation of proteomics research and innovation.

LOOKING AHEAD

As biology enters an era defined by artificial intelligence, single-cell technologies, spatial biology, and precision medicine, PSI is uniquely positioned to guide this transformation. Future priorities include expanding national proteomics infrastructure, strengthening multi-omics research, enhancing international collaborations, supporting translational healthcare initiatives, developing educational programs, and empowering young investigators.

INTERNATIONAL PARTNERSHIPS

International Partnerships

From its early years, PSI recognized the importance of global engagement.

The society has developed strong relationships with international organizations such as:

- Human Proteome Organization (HUPO)
- Asia Oceania Human Proteome Organization (AOHUPO)
- US HUPO
- American Society for Mass Spectrometry (ASMS)

These partnerships have enabled:

- International speaker exchanges
- Collaborative projects
- Joint educational initiatives
- Participation in global scientific programs

Such interactions ensure that Indian researchers remain connected to the latest developments in proteomics and systems biology.

CONTRIBUTIONS TO HUMAN HEALTH

Contributions to Human Health and Precision Medicine

The impact of PSI extends beyond scientific meetings and educational programs.

Research conducted by PSI members has contributed significantly to:

Cancer Research

Identification of biomarkers, therapeutic targets, and molecular pathways associated with diverse cancers.

Infectious Diseases

Proteomics investigations related to malaria, dengue, tuberculosis, COVID-19, and emerging infectious diseases.

Neurological Disorders

Studies exploring molecular mechanisms underlying brain diseases and neurological conditions.

Precision Medicine

Integration of omics technologies to develop personalized healthcare strategies.

Translational Research

Conversion of scientific discoveries into clinically relevant applications and diagnostic solutions.

Through these contributions, PSI has helped advance India's capabilities in biomedical research and healthcare innovation.

EVOLUTION OF PROTEOMICS IN INDIA

PSI and the Evolution of Proteomics in India

The growth of proteomics in India is closely intertwined with the growth of PSI.

Over the years, the society has witnessed the evolution of:

- Proteomics technologies
- Mass spectrometry platforms
- Computational approaches
- Multi-omics integration
- Artificial intelligence applications
- Clinical translation

PSI has consistently adapted to these developments while serving as a catalyst for scientific progress.

The society has helped transform proteomics from a niche discipline into a major component of contemporary biological and biomedical research

PSI & APT-2026

PSI and APT-2026

The scientific themes of APT-2026 closely align with the mission and vision of PSI.

Topics such as:

- Proteomics
- Multi-omics
- Artificial intelligence
- Biomarker discovery
- Precision medicine
- Clinical diagnostics
- Translational healthcare

represent areas where PSI members have made substantial contributions.

APT-2026 builds upon the strong foundation established through PSI activities over the past two decades and provides an important platform for advancing the next generation of proteomics research and innovation.

The conference also reflects the continued commitment of PSI members to fostering scientific excellence, collaboration, and education.

LOOKING AHEAD

Looking Ahead

As biology enters an era defined by artificial intelligence, single-cell technologies, spatial biology, and precision medicine, the role of proteomics will become increasingly important.

The Proteomics Society, India is uniquely positioned to guide this transformation.

Future priorities include:

- Expanding national proteomics infrastructure

- Strengthening multi-omics research
- Enhancing international collaborations
- Supporting translational healthcare initiatives
- Developing educational programs
- Empowering young investigators

The society's continued growth will play a critical role in shaping the future of biological and biomedical research in India.

By fostering collaboration, innovation, education, and scientific excellence, PSI will continue to serve as a cornerstone of India's proteomics ecosystem and a vital contributor to global efforts aimed at improving human health and understanding biological complexity.

GLOBAL PROTEOMICS ORGANIZATION

Human Proteome Organization (HUPO)

Advancing the Global Understanding of Human Biology Through Proteomics



INTRODUCTION

The Human Proteome Organization (HUPO) is the world's leading international scientific organization dedicated to promoting proteomics research, technology development, education, standardization, and global collaboration. Since its establishment in 2001, HUPO has served as the central platform connecting scientists, clinicians, technology developers, bioinformaticians, industry leaders, and policymakers working to understand the complexity of the human proteome.

Just as the Human Genome Project transformed our understanding of the genetic blueprint of life, HUPO was founded with the vision of comprehensively characterizing the proteins that execute biological functions within cells, tissues, organs, and entire organisms. While genes provide instructions, proteins are the dynamic molecular machines that regulate virtually every biological process.

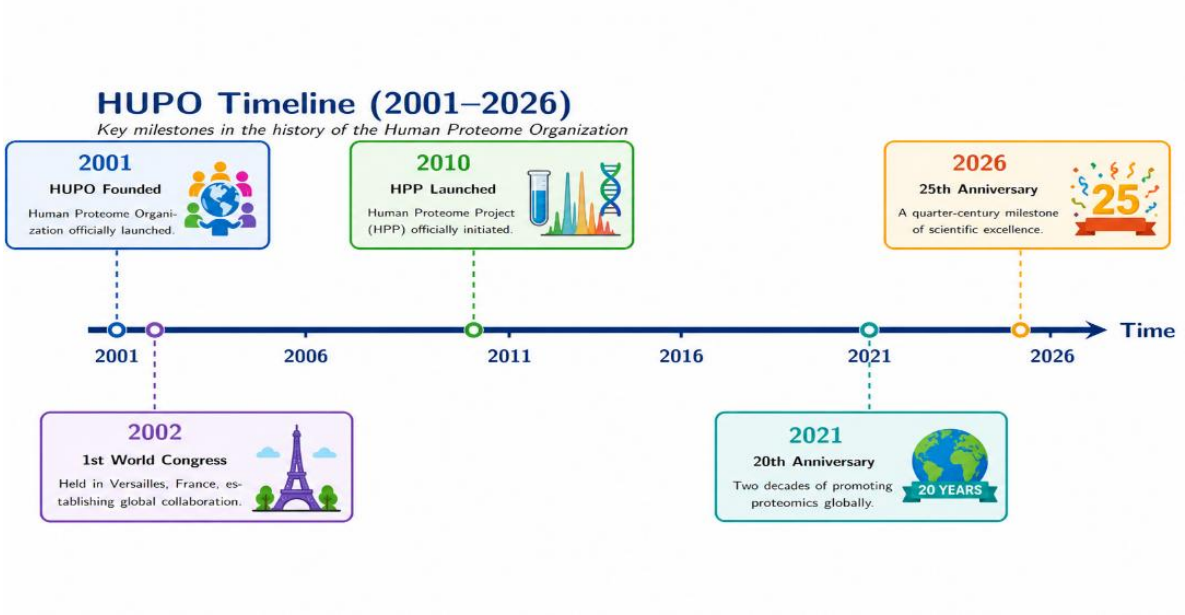
Over the past two decades, HUPO has evolved into a truly global scientific movement involving researchers from more than 70 countries. Through its scientific initiatives, international congresses, educational programs, and collaborative projects, HUPO has played a transformative role in shaping modern proteomics and systems biology. Today, HUPO stands at the forefront of efforts to integrate proteomics, genomics, metabolomics, artificial intelligence, and precision medicine to create a comprehensive molecular understanding of human biology.

THE BIRTH OF HUPO

A Vision Beyond the Genome

The completion of the Human Genome Project in the early 2000s marked a historic milestone in biological sciences. However, researchers quickly recognized that understanding the genome alone would not fully explain the complexity of living systems. Critical questions remained about which genes are actively expressed, which proteins are present in specific tissues, how proteins interact, how protein modifications regulate biological functions, and how protein networks change in disease. These questions gave rise to the field of proteomics.

Recognizing the need for an international organization to coordinate proteomics research efforts, scientific leaders established the Human Proteome Organization (HUPO) in 2001 with an ambitious mission: to advance the comprehensive characterization of the human proteome and promote international collaboration in proteomics research.

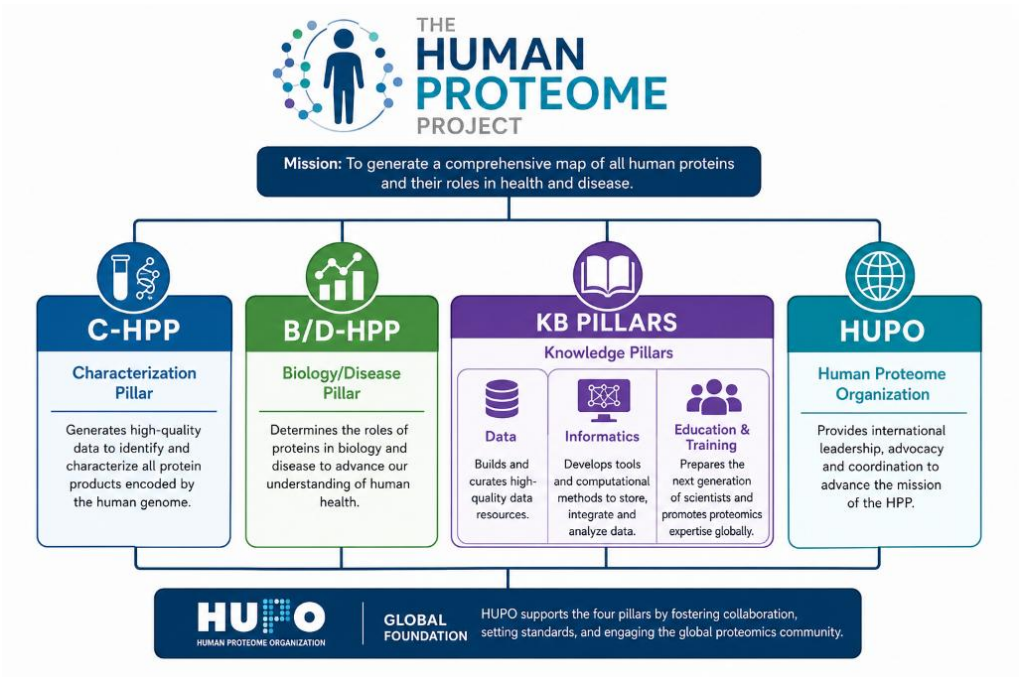


Timeline of HUPO (2001-2026)

WHY PROTEINS MATTER

Proteins are often described as the 'workhorses of the cell.' They perform virtually every biological function, including enzymatic catalysis, signal transduction, cell communication, immune responses, structural support, transport processes, and gene regulation. Unlike the relatively static genome, the proteome is highly dynamic and continuously changes in response to development, environmental stimuli, nutrition, infection, drug treatment, and disease progression. Because proteins directly reflect biological activity, proteomics provides a powerful window into human health and disease.

MISSION AND VISION



Structure of the Human Proteome Project

Vision

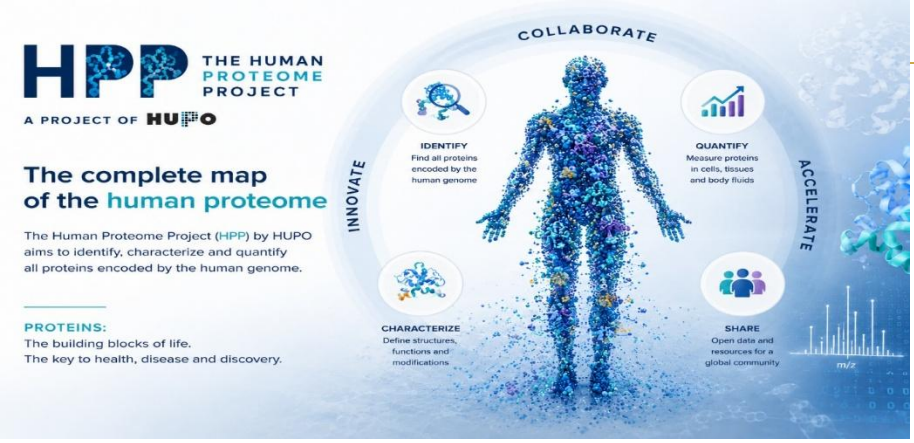
To advance the understanding of human biology and improve global health through proteomics research and international collaboration.

Mission

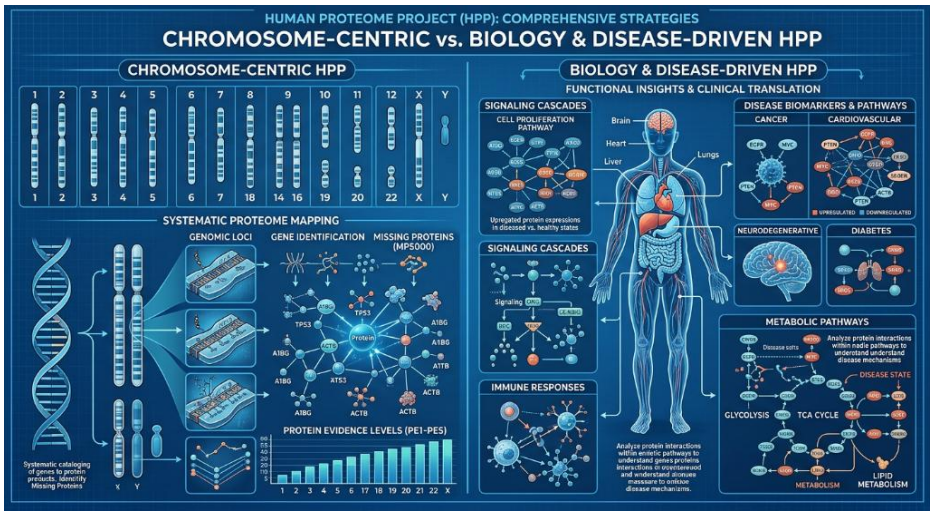
HUPO seeks to promote proteomics research worldwide, facilitate international collaborations, develop scientific standards, support education and training, advance technology development, accelerate clinical translation, and foster the next generation of proteomics scientists.

THE HUMAN PROTEOME PROJECT

A Global Scientific G



Among HUPO's most ambitious initiatives is the Human Proteome Project (HPP), launched in 2010. The HPP is often regarded as the proteomics counterpart to the Human Genome Project. Its overarching goal is to identify, characterize, and understand the complete set of proteins encoded by the human genome. The project seeks to answer fundamental questions about which proteins exist in the human body, where they are expressed, what functions they perform, and how they contribute to health and disease.



The Chromosome-Centric Human Proteome Project (C-HPP)

In this initiative, individual chromosomes were assigned to different countries and research groups. Teams worked collaboratively to identify proteins encoded by specific chromosomes and missing proteins became major targets for investigation. The project accelerated global collaboration and significantly improved our understanding of the human proteome. Today, thousands of previously uncharacterized proteins have been identified through these efforts, HUPO aims to improve scientific understanding and contribute to better healthcare outcomes worldwide.

Biology and Disease-driven Human Proteome Project (B/D-HPP)

As proteomics matured, HUPO expanded its focus from cataloguing proteins to understanding biological function and disease mechanisms. The B/D-HPP investigates cancer, cardiovascular diseases, infectious diseases, neurological disorders, liver diseases, kidney diseases, and metabolic disorders. Professor Sanjeeva Srivastava has been actively involved in several HUPO initiatives, including leadership roles within the B/D-HPP and related disease-focused programs, contributing to global efforts aimed at advancing proteomics-driven healthcare.

DISEASE-FOCUSED INITIATIVES

Cancer Human Proteome Project (Cancer-HPP)

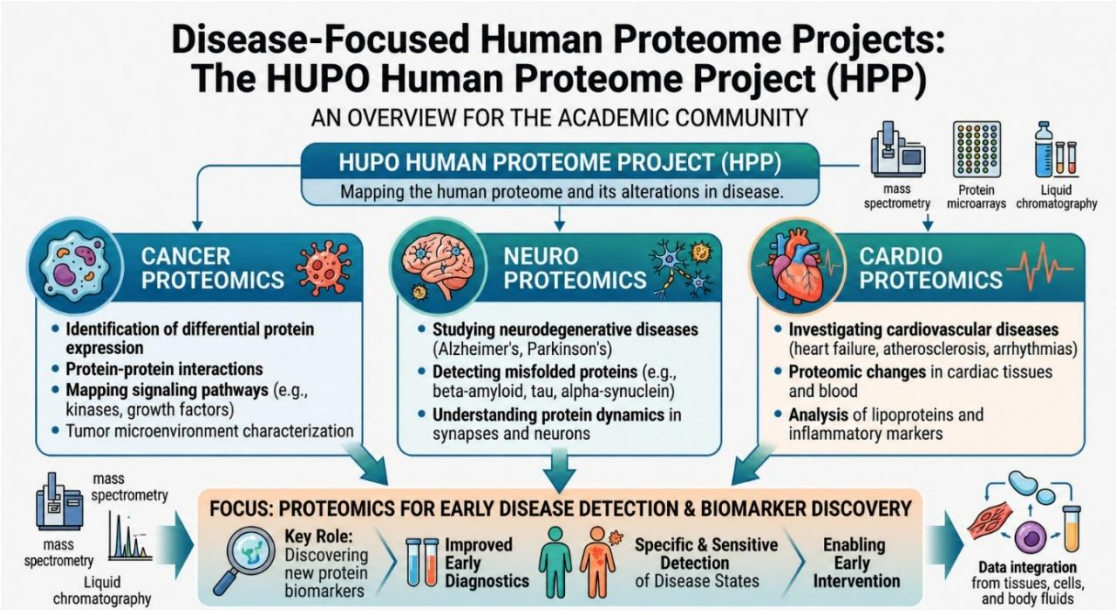
The Cancer-HPP seeks to understand tumor biology, cancer heterogeneity, biomarker discovery, therapeutic targets, and precision oncology. Proteomics has become increasingly important in understanding cancer beyond genomic information alone.

Human Infectious Diseases Human Proteome Project (HID-HPP)

The HID-HPP focuses on host-pathogen interactions, emerging infectious diseases, immune responses, and biomarker development. These efforts became particularly important during global outbreaks such as COVID-19.

Other Disease Programs

Additional projects address cardiovascular diseases, neurological disorders, rare diseases, and metabolic conditions. Collectively, these initiatives contribute to a deeper understanding of human disease biology.



Disease-Focused Human Proteome Projects

HUPO WORLD CONGRESS

The annual HUPO World Congress is among the most important scientific meetings in proteomics. Each year, the congress brings together scientists, clinicians, industry leaders, technology developers, students, and policymakers to discuss advances in proteomics technologies, mass spectrometry, bioinformatics, multi-omics, clinical translation, and artificial intelligence. The congress serves as a platform for exchanging ideas, establishing collaborations, and shaping future scientific directions.



HUPO World Congress

TECHNOLOGY AND INNOVATION

HUPO has played a major role in promoting technological advances that have transformed proteomics research, including advances in high-resolution mass spectrometry, ion mobility spectrometry, data-independent acquisition, and targeted proteomics. The organization has also supported the development of data repositories, analytical pipelines, computational standards, and artificial intelligence tools. Increasingly, proteomics is integrated with genomics, transcriptomics, metabolomics, and lipidomics to provide comprehensive biological insights.

EDUCATION AND CAPACITY BUILDING

Education has always been central to HUPO's mission. The organization supports training workshops, summer schools, educational courses, mentorship programs, and young investigator initiatives. These activities help ensure that researchers worldwide have access to modern proteomics knowledge and technologies. HUPO's educational efforts have contributed significantly to the growth of proteomics communities in developing nations, including India.

HUPO AND INDIA

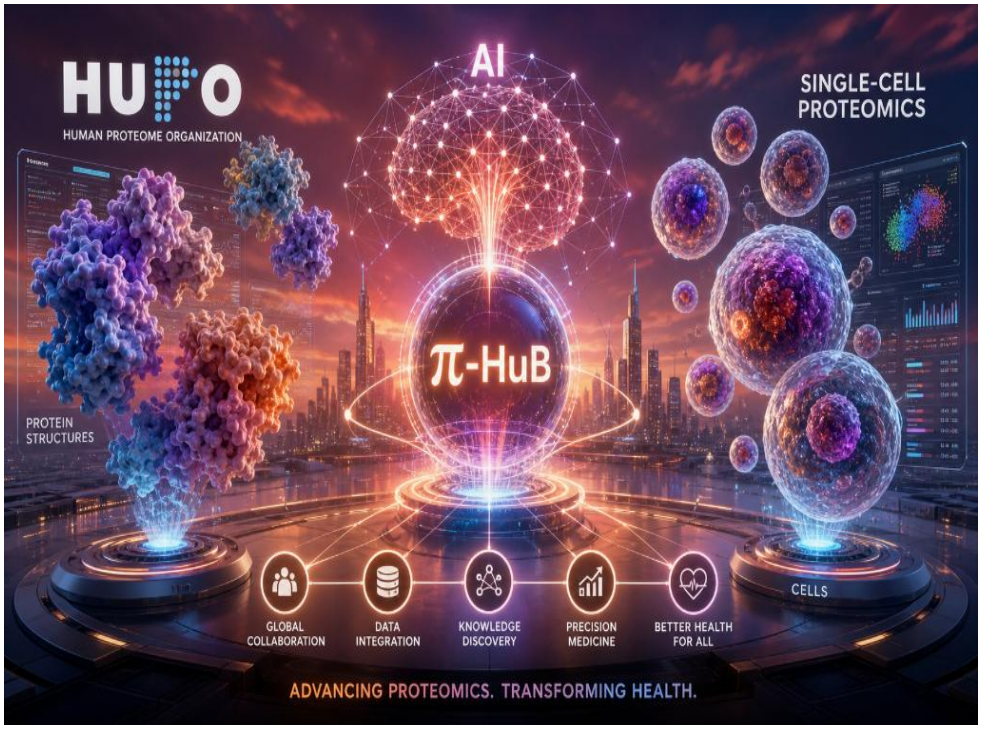
India has become an increasingly important contributor to global proteomics research. Indian scientists have actively participated in HUPO congresses, Human Proteome Project initiatives, disease-focused programs, educational activities, and international collaborations. Organizations such as the Proteomics Society, India (PSI) have strengthened the connection between Indian researchers and the global HUPO community. The leadership contributions of Indian scientists, including Professor Sanjeeva Srivastava and several PSI members, have further enhanced India's visibility within international proteomics initiatives.

HUPO AND PRECISION MEDICINE

HUPO's research initiatives directly contribute to biomarker discovery, precision diagnostics, personalized therapies, drug development, and predictive healthcare. Proteomics provides critical information that complements genomic and clinical data, enabling more accurate healthcare decisions. These efforts are helping move medicine toward a future that is predictive, preventive, personalized, and participatory.

HUPO AND THE FUTURE OF HUMAN BIOLOGY

The next frontier of proteomics extends beyond protein identification. Emerging priorities include single-cell proteomics for understanding cellular heterogeneity at unprecedented resolution, spatial biology for mapping proteins within tissues and organs, artificial intelligence for applying machine learning to large-scale biological datasets, and digital human models for creating computational representations of human biology. The π-HuB (Proteomic Navigator of the Human Body) initiative aims to understand health and disease at a systems level, redefining how scientists study biology and how clinicians practice medicine.



Future Vision: HUPO, AI, Single-Cell Proteomics, and π-hub

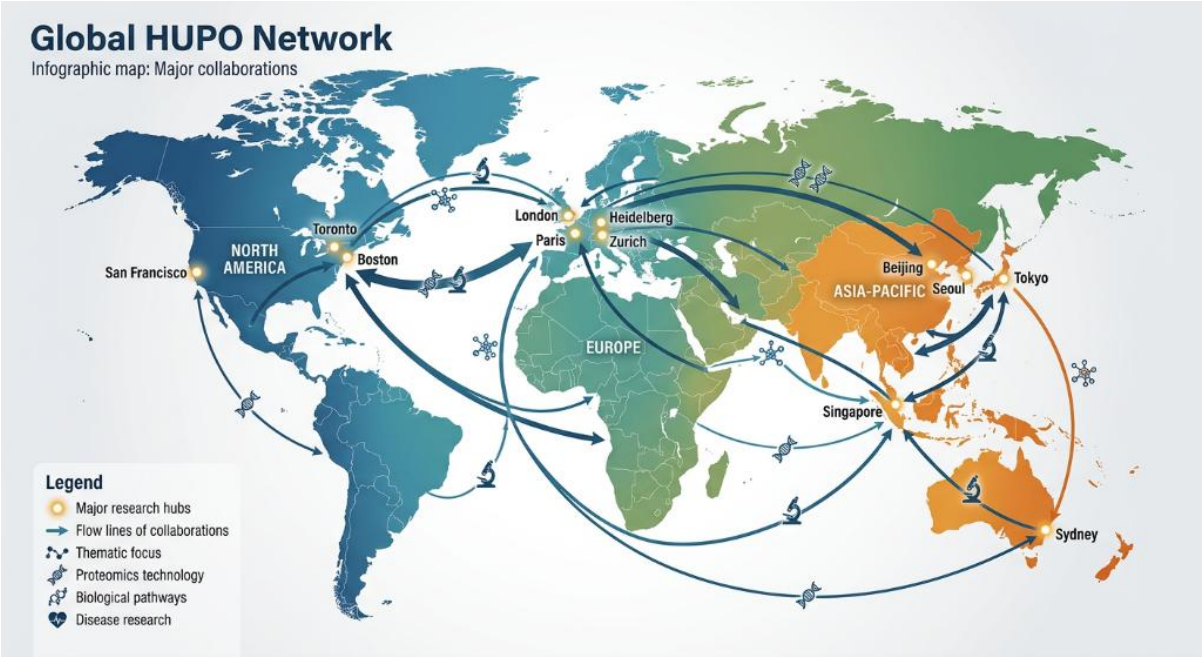
HUPO AND APT-2026

The scientific themes of APT-2026 closely mirror many of HUPO's strategic priorities. Areas such as proteomics, multi-omics, artificial intelligence, precision medicine, biomarker discovery, clinical translation, and systems biology are central to both HUPO and APT. The conference provides an important platform for disseminating emerging technologies, fostering collaborations, and training future leaders in proteomics. By connecting national initiatives with global scientific efforts, APT-2026 contributes to the broader vision advanced by HUPO.

LOOKING AHEAD

Over the past two decades, the Human Proteome Organization has transformed proteomics from an emerging discipline into a cornerstone of modern biological and biomedical research. Its achievements have advanced our understanding of human biology, accelerated technological innovation, fostered international collaboration, and laid the foundation for precision medicine. As science enters an era defined by artificial intelligence, single-cell biology, spatial omics, and digital

health, HUPO's role will become even more important. By bringing together scientists from across disciplines and continents, HUPO continues to drive one of humanity's most ambitious scientific endeavors: understanding the complexity of life through the language of proteins.



Global HUPO Network

SCIENTIFIC OVERVIEW

American Society for Mass Spectrometry (ASMS)

The American Society for Mass Spectrometry (ASMS) is the world's largest and most influential professional organization dedicated to the advancement of mass spectrometry and its applications across science, medicine, engineering, industry, and technology. Since its establishment in 1969, ASMS has played a pivotal role in shaping the development of modern analytical sciences and has become the premier global platform for scientific exchange in mass spectrometry.

Mass spectrometry lies at the heart of modern proteomics, metabolomics, lipidomics, clinical diagnostics, pharmaceutical research, environmental monitoring, and systems biology. Virtually every major technological breakthrough that has transformed contemporary omics research has been influenced by innovations presented, discussed, and disseminated through the ASMS community.

Today, ASMS serves as a global network of researchers, instrument developers, clinicians, bioinformaticians, industry leaders, and students who share a common mission: advancing science through mass spectrometry.

For the proteomics community, ASMS represents far more than a professional society; it serves as a primary engine of technological innovation that continually expands our ability to explore the molecular complexity of life.

Origins of ASMS

The Emergence of Modern Mass Spectrometry

Mass spectrometry has a rich scientific history dating back to the early twentieth century. Initially developed as a tool for studying atomic and molecular masses, the technology gradually evolved into one of the most powerful analytical platforms in modern science.

As applications expanded across chemistry, biology, medicine, and industry, the need for a dedicated scientific organization became increasingly apparent.

In 1969, a group of pioneering scientists established the American Society for Mass Spectrometry to:

- Promote scientific exchange
- Foster technological innovation
- Support education and training
- Advance analytical methodologies
- Build a collaborative scientific community

Over the subsequent decades, ASMS became the leading international forum for mass spectrometry research and development.

The Foundation of Modern Omics Sciences

The extraordinary growth of proteomics and multi-omics research would not have been possible without advances in mass spectrometry.

Mass spectrometry enables scientists to:

- Identify proteins
- Quantify biomolecules

- Characterize metabolites
- Analyze lipids
- Study post-translational modifications
- Investigate molecular interactions

The evolution of these capabilities has fundamentally transformed biological and biomedical research.

Many of the technologies routinely used today in proteomics laboratories around the world were first introduced and refined through scientific interactions within the ASMS community.

Mission and Vision

Vision

To advance scientific discovery and innovation through the development and application of mass spectrometry.

Mission

ASMS seeks to:

- Promote excellence in mass spectrometry research
- Foster education and training
- Encourage interdisciplinary collaboration
- Support technological innovation
- Advance scientific communication
- Mentor future generations of scientists

Through these efforts, ASMS continues to influence virtually every field that relies on molecular analysis.

The ASMS Annual Conference

The World's Premier Mass Spectrometry Meeting

The ASMS Annual Conference on Mass Spectrometry and Allied Topics is widely regarded as the most important gathering of mass spectrometry scientists in the world.

Each year, thousands of participants attend the conference, including:

- Academic researchers
- Clinicians
- Industry scientists
- Instrument developers
- Bioinformaticians
- Graduate students
- Technology innovators



ASMS Annual ConferenceASMS Annual Conference

The conference serves as a platform for unveiling groundbreaking discoveries, emerging technologies, and next-generation analytical approaches.

For many researchers, attending ASMS provides a first glimpse into technologies that will shape scientific research over the coming decade.

ASMS and Proteomics

Proteomics has been among the fields most profoundly influenced by ASMS.

Major advances presented through the ASMS community include:

High-Resolution Mass Spectrometry

Development of instruments capable of analyzing complex biological samples with exceptional sensitivity and accuracy.

Quantitative Proteomics

Methods enabling reliable measurement of protein abundance across biological conditions.

Targeted Proteomics

Technologies such as:

- Selected Reaction Monitoring (SRM)
- Parallel Reaction Monitoring (PRM)

that support biomarker verification and clinical translation.

Data Independent Acquisition (DIA)

Transforming large-scale protein quantification and reproducibility.

Ion Mobility Spectrometry

Adding an additional dimension of molecular separation and enhancing analytical performance.

Collectively, these innovations have revolutionized biological research and precision medicine.

The Rise of 4D Proteomics

One of the most exciting developments in recent years has been the emergence of 4D proteomics.

Technologies incorporating:

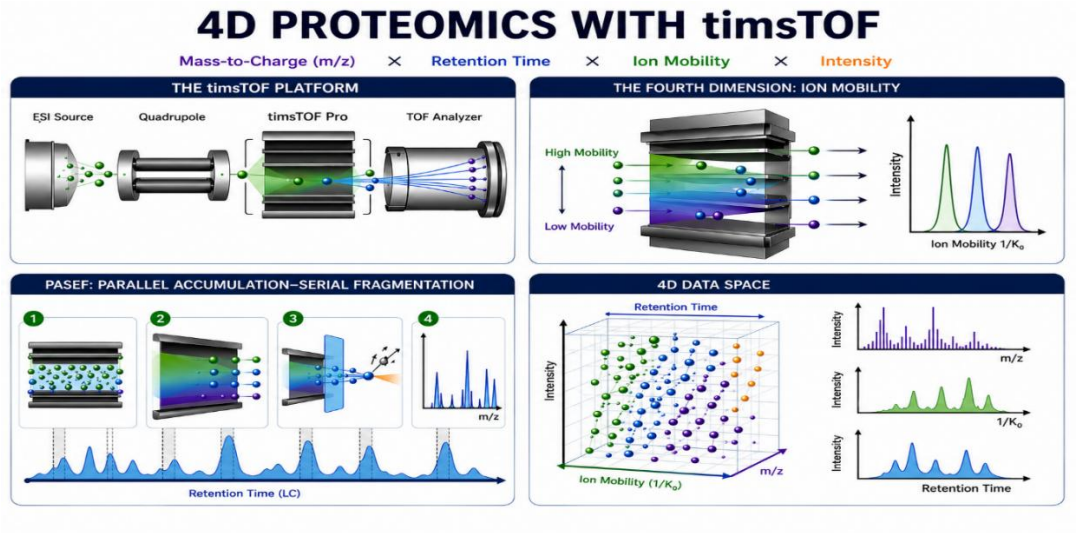
- Retention time
- Mass-to-charge ratio

- Signal intensity
- Ion mobility

have dramatically expanded analytical capabilities.

The introduction of trapped ion mobility spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) has enabled unprecedented depth, speed, and sensitivity.

These innovations form the technological foundation of modern platforms such as the timsTOF systems being utilized within advanced proteomics ecosystems, including those supporting APT-2026.



ASMS and Clinical Translation

Mass spectrometry is increasingly moving beyond research laboratories into clinical practice.

Applications now include:

Clinical Proteomics

Identification of biomarkers for:

- Cancer
- Neurological disorders
- Infectious diseases
- Cardiovascular diseases

Precision Medicine

Supporting patient stratification and individualized treatment strategies.

Therapeutic Monitoring

Enabling accurate measurement of drug responses and treatment outcomes.

Translational Diagnostics

Facilitating development of clinically actionable assays.

These developments are transforming healthcare and creating new opportunities for precision medicine.

Instrumentation Innovation

ASMS has served as a major platform for introducing revolutionary instrumentation.

Technological advances frequently highlighted at ASMS include:

- Orbitrap technologies
- Time-of-flight instruments
- Hybrid mass spectrometers
- Ion mobility platforms
- Imaging mass spectrometry
- Single-cell proteomics technologies

Instrument manufacturers often unveil their newest innovations at ASMS, making the conference a major driver of scientific progress.

Education and Training

ASMS places strong emphasis on scientific education and workforce development.

Educational activities include:

Short Courses

Providing intensive training in specialized topics.

Workshops

Covering emerging technologies and methodologies.

Student Programs

Supporting graduate students and early-career researchers.

Mentoring Initiatives

Facilitating interactions between established leaders and future scientists.

These activities help ensure that researchers remain current with rapidly evolving technologies.

Supporting the Next Generation

The future of science depends upon nurturing young investigators.

ASMS actively supports:

- Student travel awards
- Young investigator awards
- Poster competitions
- Career development activities
- Networking opportunities

Many leading scientists in proteomics and mass spectrometry first gained visibility through ASMS presentations and interactions.

ASMS and Artificial Intelligence

The future of mass spectrometry increasingly involves artificial intelligence and advanced computational approaches.

Emerging areas include:

- Machine learning
- Deep learning
- Predictive analytics
- Automated data interpretation
- Digital biology

These technologies are helping scientists extract meaningful insights from increasingly complex datasets.

The integration of AI with mass spectrometry is expected to transform biological discovery and clinical diagnostics over the coming decade.

ASMS and the Future of Omics Sciences

The next generation of scientific discovery will be driven by the convergence of:

- Mass spectrometry
- Artificial intelligence
- Multi-omics integration
- Single-cell analysis
- Spatial biology
- Digital health

ASMS continues to serve as one of the primary global platforms where these advances are developed, discussed, and disseminated.

Many of the innovations shaping the future of precision medicine will likely emerge from scientific interactions within the ASMS community.

ASMS and APT-2026

The scientific themes highlighted at APT-2026 closely mirror many of the advances regularly featured at ASMS.

These include:

- Proteomics
- Metabolomics
- Lipidomics
- Multi-omics integration
- Biomarker discovery
- Clinical translation
- Artificial intelligence
- Precision medicine

Researchers participating in APT-2026 are part of a broader international community that benefits from technological and methodological advances disseminated through ASMS.

The conference therefore serves as an important bridge connecting global innovations in mass spectrometry with emerging scientific opportunities in India and beyond.

Looking Ahead

For more than five decades, the American Society for Mass Spectrometry has served as a driving force behind scientific and technological innovation.

Its contributions extend far beyond instrumentation, influencing how scientists study biology, understand disease, develop therapeutics, and practice medicine.

As emerging technologies continue to push the boundaries of analytical science, ASMS will remain at the forefront of discovery, enabling researchers to explore biological systems with increasing depth, precision, and resolution.

The future of proteomics, metabolomics, lipidomics, systems biology, and precision medicine will continue to be shaped by the innovations, collaborations, and scientific excellence fostered by the global ASMS community.

GLOBAL INITIATIVE

π-HuB: Proteomic Navigator of the Human Body

The twenty-first century has witnessed remarkable advances in genomics, proteomics, artificial intelligence, systems biology, and digital technologies. Together, these developments have revolutionized our understanding of life and disease. Yet despite these achievements, a fundamental challenge remains: how can we integrate vast amounts of biological information to create a comprehensive and actionable understanding of the human body?

To address this challenge, an international consortium of scientists introduced the concept of π-HuB (Proteomic Navigator of the Human Body)—an ambitious global initiative designed to create a dynamic proteomic framework capable of mapping human biology across tissues, organs, cell types, physiological states, and disease conditions.

Published in Nature in 2024, π-HuB represents one of the most visionary scientific roadmaps ever proposed in proteomics. The initiative brings together leading scientists from around the world with expertise spanning proteomics, genomics, artificial intelligence, medicine, systems biology, computational sciences, and clinical research.

Rather than simply cataloging proteins, π-HuB seeks to understand how proteins function collectively to govern health, disease, aging, development, and therapeutic responses. Its ultimate goal is to transform biological knowledge into actionable healthcare intelligence.

Why Do We Need π-HuB?

Beyond the Genome

The Human Genome Project provided an invaluable blueprint of human life. However, genes alone do not determine biological function.

Proteins serve as the primary functional molecules responsible for:

- Cellular communication
- Signal transduction
- Immune responses
- Metabolism
- Tissue homeostasis
- Disease progression

Unlike the relatively stable genome, proteins are highly dynamic and continuously respond to:

- Environmental changes
- Nutrition
- Lifestyle
- Disease states
- Drug interventions
- Aging

Consequently, understanding the human proteome is essential for understanding human biology itself.

While significant progress has been achieved through the Human Proteome Project, the scientific community increasingly recognizes the need for a more comprehensive framework capable of integrating biological information across multiple dimensions.

π-HuB was conceived to fulfill this need.

A New Paradigm for Human Biology

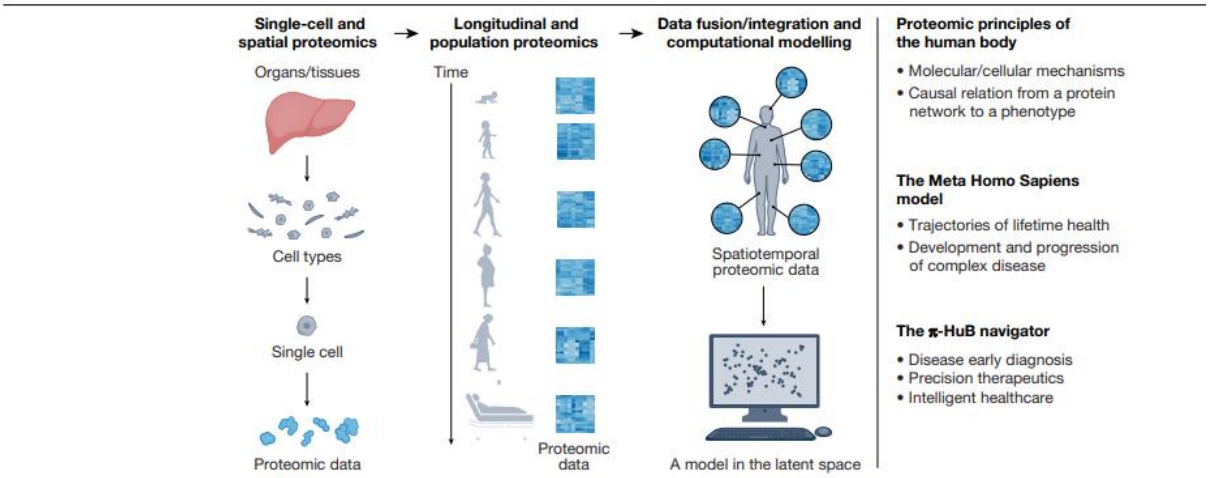
π-HuB represents a transition from static biological catalogs toward dynamic biological navigation.

The initiative envisions a future in which scientists and clinicians can:

- Monitor molecular changes in real time
- Predict disease development
- Identify personalized therapeutic strategies
- Understand biological aging
- Detect disease before symptoms appear

This shift has the potential to transform medicine from a reactive discipline into a proactive and predictive science.

The Three Grand Goals of π-HuB



Goal 1: Discover the Principles Governing the Human Body

One of the primary objectives of π-HuB is to uncover the fundamental biological principles that govern human life.

Researchers seek to understand:

- Protein networks
- Cellular communication
- Tissue organization
- Organ-level regulation
- System-wide interactions

By identifying these governing principles, scientists can develop a deeper understanding of both health and disease.

Goal 2: Develop the Meta Homo Sapiens Model

A central concept of π-HuB is the creation of a digital representation of human biology known as the Meta Homo Sapiens Model.

This model aims to integrate information from:

- Genomics
- Transcriptomics
- Proteomics
- Metabolomics
- Lipidomics
- Clinical data
- Environmental information

The resulting framework would provide a comprehensive representation of human biological systems across multiple scales.

Such a model could eventually enable simulation of disease progression, prediction of treatment outcomes, and optimization of healthcare interventions.

Goal 3: Build the Proteomic Navigator

The third goal involves developing a navigational system capable of guiding researchers and clinicians through the complexity of human biology.

Much like GPS systems guide travelers through geographic landscapes, the Proteomic Navigator aims to guide scientists through molecular landscapes.

Potential applications include:

- Disease prediction
- Biomarker discovery
- Drug target identification
- Precision medicine
- Personalized healthcare

This capability could fundamentally transform how healthcare is practiced.

From Precision Medicine to Phronesis Medicine

One of the most innovative concepts introduced by π-HuB is the idea of Phronesis Medicine.

Derived from the Greek concept of phronesis, meaning practical wisdom, this framework extends beyond traditional precision medicine.

While precision medicine focuses on tailoring treatments to individuals, phronesis medicine seeks to provide intelligent guidance throughout the entire healthcare journey.

The approach emphasizes:

- Prevention
- Prediction
- Personalization
- Participation
- Practical decision-making

The goal is not simply to treat disease but to maintain health and optimize human well-being.

Scientific Pillars of π-HuB

The success of π-HuB depends upon multiple interconnected scientific pillars.

Human Biospecimens

Large-scale collection and characterization of tissues, cells, and biological samples.

Advanced Technologies

Development of next-generation analytical platforms, including:

- High-resolution mass spectrometry
- Single-cell proteomics
- Spatial proteomics
- Imaging technologies

Computational Sciences

Application of:

- Artificial intelligence
- Machine learning
- Data science
- Network biology

to extract knowledge from massive biological datasets.

Open Data Resources

Creation of accessible databases and computational resources to support global scientific collaboration.

International Partnerships

Building a worldwide network of researchers working toward common scientific goals.

Artificial Intelligence and Digital Biology

Artificial intelligence plays a central role in the π-HuB vision.

Modern proteomics generates enormous volumes of data that exceed the capacity of traditional analytical methods.

AI technologies enable:

- Pattern recognition
- Predictive modeling
- Disease classification
- Biomarker discovery
- Knowledge generation

The integration of AI with proteomics is expected to accelerate scientific discovery and enhance clinical decision-making.

Global Collaboration at an Unprecedented Scale

The π-HuB initiative brings together researchers from leading institutions across North America, Europe, Asia, and Australia.

Participants include experts in:

- Proteomics
- Systems biology
- Medicine
- Artificial intelligence
- Computational sciences
- Biotechnology

The consortium reflects the growing recognition that solving complex biological problems requires international cooperation and interdisciplinary expertise.

The participation of scientists from India, including contributors associated with IIT Bombay and the Proteomics Society, India, highlights the country's growing role in global proteomics initiatives.

Relevance to Human Health

The long-term impact of π-HuB extends across multiple healthcare domains.

Cancer

Understanding tumor evolution and therapeutic responses.

Infectious Diseases

Characterizing host-pathogen interactions and immune responses.

Neurological Disorders

Investigating molecular mechanisms underlying neurodegeneration and brain diseases.

Aging

Defining molecular signatures associated with healthy and pathological aging.

Precision Medicine

Developing personalized approaches to disease prevention, diagnosis, and treatment.

Collectively, these efforts have the potential to transform healthcare worldwide.

π-HuB and APT-2026

Many of the scientific themes highlighted at APT-2026 align directly with the vision of π-HuB.

These include:

- Proteomics
- Multi-omics integration
- Artificial intelligence
- Biomarker discovery
- Precision medicine
- Clinical translation
- Digital health
- Systems biology

APT-2026 therefore serves as an important platform for discussing technologies and strategies that contribute to the realization of the π-HuB vision.

The conference brings together many of the scientific communities whose expertise will be essential for building the future envisioned by π-HuB.

Looking Ahead

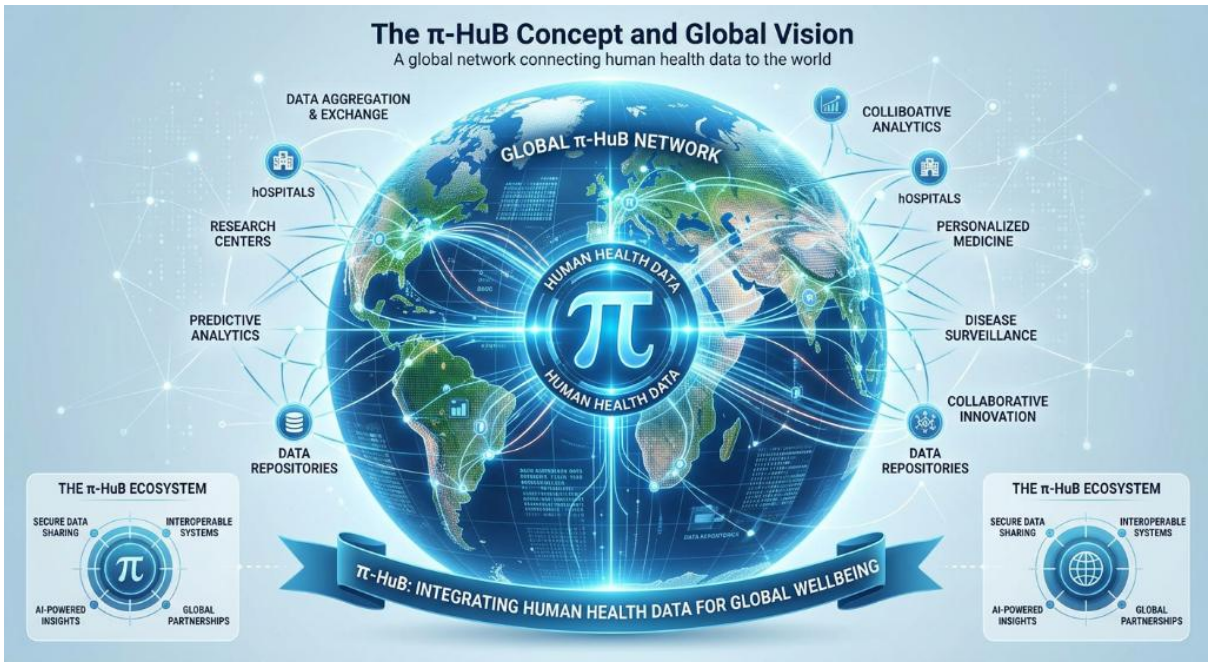
The Proteomic Navigator of the Human Body represents one of the most ambitious scientific initiatives of the modern era.

By integrating proteomics, multi-omics, artificial intelligence, computational modeling, and international collaboration, π-HuB seeks to create an unprecedented understanding of human biology.

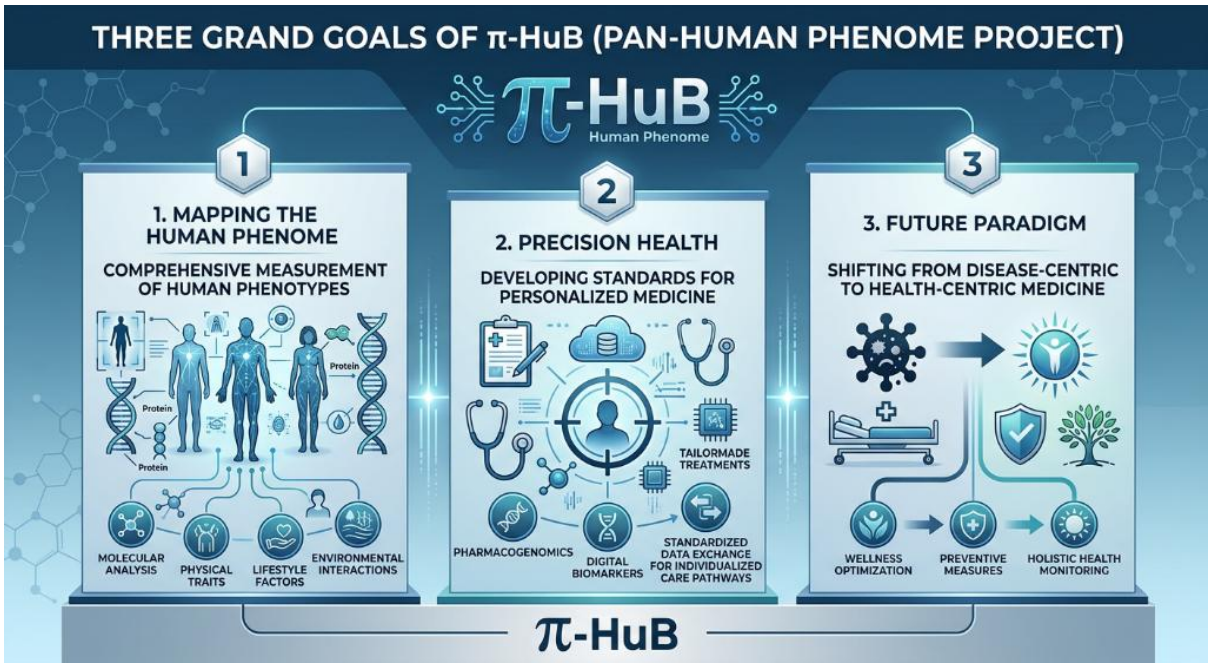
Its vision extends beyond scientific discovery toward a future in which healthcare becomes predictive, preventive, personalized, and intelligent.

As proteomics continues to evolve and technologies become increasingly powerful, initiatives such as π-HuB will help shape the future of biology, medicine, and global health.

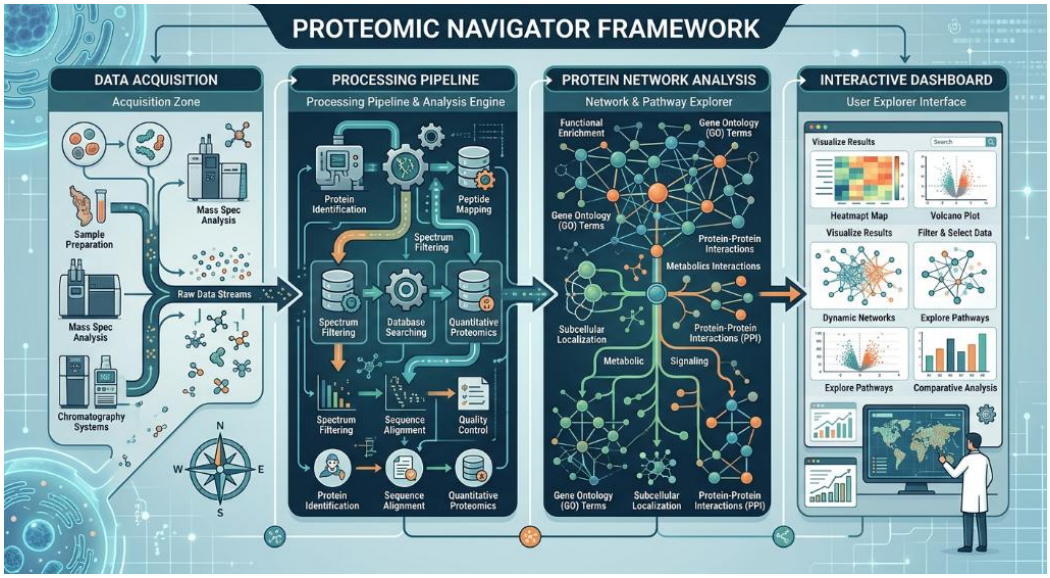
For researchers, clinicians, and innovators participating in APT-2026, π-HuB offers not only a scientific roadmap but also an inspiring vision of what can be achieved when the global scientific community works together to understand the complexity of life.



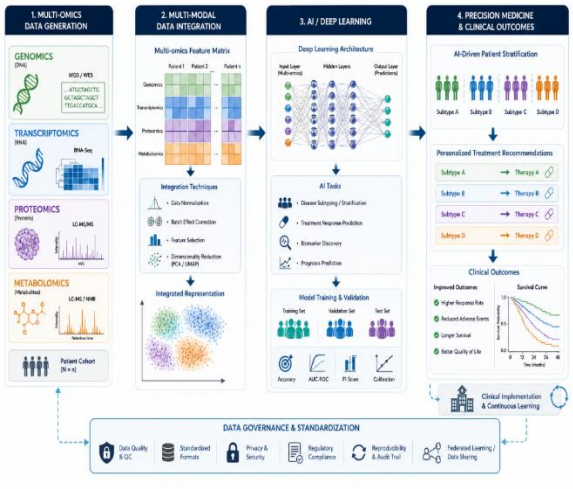
The π-HuB Concept and Global Vision



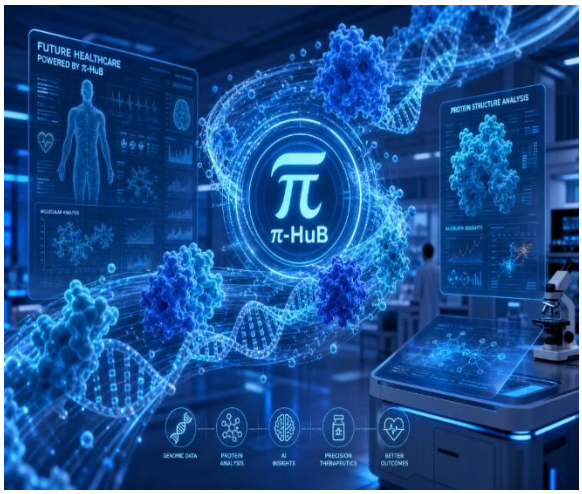
Three Grand Goals of π-HuB



Proteomic Navigator Framework



Integration of Multi-Omics and AI



Future Healthcare Powered by π-HuB

The π-HuB Council: A Global Leadership Network

A distinguishing feature of the π-HuB initiative is its commitment to fostering international scientific leadership through the establishment of the π-HuB Council, a global body comprising leading scientists, clinicians, technologists, and innovators from diverse disciplines and geographic regions.

The Council serves as a strategic advisory and leadership platform that helps guide the scientific vision, priorities, collaborative frameworks, and long-term roadmap of the π-HuB initiative. By bringing together experts from multiple countries and scientific domains, the Council ensures that π-HuB remains a truly global effort aimed at addressing challenges relevant to humanity as a whole.

Members of the π-HuB Council represent internationally recognized expertise in proteomics, systems biology, artificial intelligence, clinical medicine, computational sciences, biotechnology, and precision healthcare. The Council promotes cross-disciplinary interactions and facilitates collaboration among academic institutions, healthcare organizations, industry partners, and governmental agencies worldwide.

India's growing leadership in global proteomics initiatives is reflected through the participation of Professor Sanjeeva Srivastava, Indian Institute of Technology Bombay, as a member of the π-HuB Council. As one of the leading proteomics researchers from India, Professor Srivastava contributes to the international vision of π-HuB while helping strengthen connections between Indian scientific initiatives and the broader global proteomics community.

His involvement further reflects India's expanding role in international efforts aimed at advancing proteomics, multi-omics integration, artificial intelligence-driven biology, and precision medicine. Through such participation, Indian researchers continue to contribute to shaping the future directions of global biomedical research and healthcare innovation.

The establishment of the π-HuB Council underscores a central philosophy of the initiative: that understanding the complexity of human biology and transforming healthcare requires not only technological innovation but also sustained international cooperation, shared scientific leadership, and collective global vision.

MOOCs, NPTEL, SWAYAM & Digital Science Education

The twenty-first century has witnessed a profound transformation in education driven by digital technologies, online learning platforms, and global connectivity. Traditional classroom-based teaching is increasingly complemented by technology-enabled learning environments that provide students with access to high-quality educational resources regardless of geographic location, institutional affiliation, or socioeconomic background.

Among the most important developments in this transformation has been the emergence of Massive Open Online Courses (MOOCs), which have democratized access to education on an unprecedented scale. MOOCs enable learners to access lectures, assignments, reading materials, assessments, and certifications from leading institutions and experts across diverse disciplines.

The MOOC revolution has significantly expanded opportunities for lifelong learning, workforce development, interdisciplinary education, and professional skill enhancement. In scientific disciplines such as biotechnology, bioengineering, proteomics, systems biology, artificial intelligence, and precision medicine, MOOCs have become powerful tools for training the next generation of researchers, clinicians, innovators, and entrepreneurs.

SWAYAM: India's National Digital Learning Platform

To promote equitable access to quality education, the Government of India launched SWAYAM (Study Webs of Active-Learning for Young Aspiring Minds), one of the world's largest national MOOC initiatives. SWAYAM was established to achieve the three fundamental principles of educational policy: access, equity, and quality. The platform seeks to bridge the digital divide and make high-quality learning resources available to learners across the country.

SWAYAM provides free online courses spanning school education, undergraduate studies, postgraduate programs, engineering, science, humanities, management, teacher training, and professional development. The platform allows learners to access educational content at their own pace, anytime and anywhere.

The SWAYAM framework incorporates four major learning components:

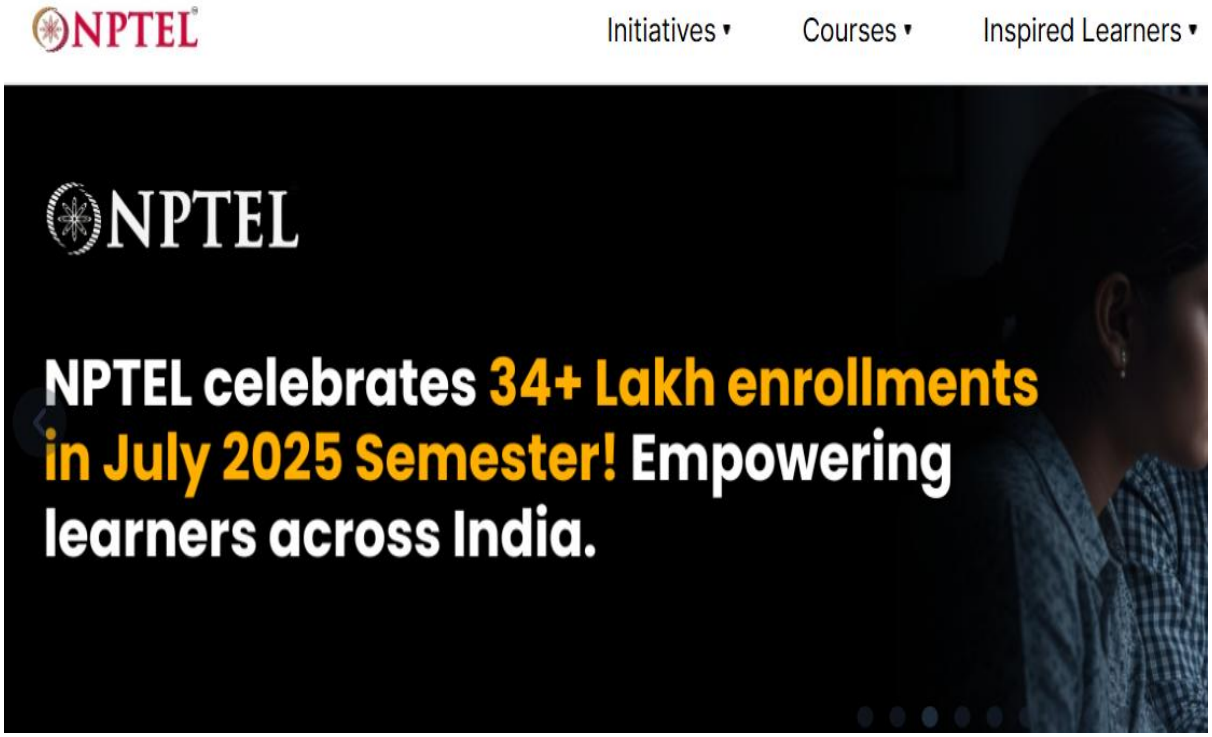
- Video lectures
- Downloadable study materials
- Self-assessment exercises and quizzes
- Interactive discussion forums

This integrated learning model promotes active engagement and enhances learning outcomes through modern pedagogical approaches.

To ensure academic quality and national reach, multiple national coordinators have been appointed, including NPTEL, UGC, AICTE, CEC, IGNOU, NCERT, IIM Bangalore, NIOS, and other premier educational organizations.

Today, SWAYAM represents a major pillar of India's digital education ecosystem and has become a globally recognized model for large-scale online learning.

NPTEL: Transforming Technical and Scientific Education in India NPTEL has played a transformative role in:



- The National Programme on Technology Enhanced Learning (NPTEL) is one of India's most successful educational initiatives and serves as the primary national coordinator for engineering, science, technology, and interdisciplinary higher education courses on SWAYAM.NPTEL was established as a collaborative initiative of the Indian Institutes of Technology (IITs) and the Indian Institute of Science (IISc), with support from the Ministry of Education, Government of India. Its mission is to enhance the quality of higher education through technology-enabled learning and to make world-class educational content accessible to all learners.Since launching its online certification model, NPTEL has evolved into one of the largest educational repositories in the world, offering thousands of courses across engineering, sciences, humanities, management, and emerging interdisciplinary fields. Millions of learners have benefited from NPTEL courses, making it one of the most influential digital education initiatives in India.The National Programme on Technology Enhanced Learning (NPTEL) is one of India's most successful educational initiatives and serves as the primary national coordinator for engineering, science, technology, and interdisciplinary higher education courses on SWAYAM.NPTEL was established as a collaborative initiative of the Indian Institutes of Technology (IITs) and the Indian Institute of Science (IISc), with support from the Ministry of Education, Government of India. Its mission is to enhance the quality of higher education through technology-enabled learning and to make world-class educational content accessible to all learners.Since launching its online certification model, NPTEL has evolved into one of the largest educational repositories in the world, offering thousands of courses across engineering, sciences, humanities, management, and emerging interdisciplinary fields. Millions of learners have benefited from NPTEL courses, making it one of the most influential digital education initiatives in India.Expanding access to

quality education

- Supporting faculty

Development

- Enhancing employability

Skills

- Promoting

interdisciplinary learning

- Strengthening industry-

academia interactions

- Supporting lifelong

learning

Importantly, NPTEL has enabled students from institutions across India to learn directly from faculty members of premier institutions including IITs and IISc. This democratization of educational access has significantly contributed to capacity building in science, technology, engineering, and healthcare disciplines.

Educational Vision of Professor Sanjeeva Srivastava

Alongside his research contributions in proteomics, systems biology, biomarker discovery, and precision medicine, Professor Sanjeeva Srivastava has consistently viewed education as a central component of scientific leadership.

Over the years, he has taught and mentored thousands of undergraduate, postgraduate, doctoral, and professional learners through classroom teaching, workshops, virtual laboratories, educational outreach programs, and online learning platforms.

His educational philosophy emphasizes:

- Concept-based learning
- Interdisciplinary thinking
- Research-integrated education
- Technology-enabled learning
- Student-centered pedagogy
- Scientific curiosity and innovation

This philosophy has guided the development of multiple MOOCs that introduce learners to modern biological sciences, biotechnology, proteomics, systems biology, and emerging omics technologies.

MOOCs Developed and Delivered by Professor Sanjeeva Srivastava

Professor Sanjeeva Srivastava has developed and delivered multiple MOOCs through NPTEL and SWAYAM that have helped train students, researchers, faculty members, clinicians, and industry professionals across India and internationally.

These courses serve as important educational resources for learners interested in proteomics, bioinformatics, systems biology, biotechnology, precision medicine, and multi-omics sciences.

Introduction to Proteomics

This course introduces learners to the fundamental principles of proteomics and its applications in biological and biomedical research. Topics include protein structure and function, protein separation technologies, protein identification methods, biomarker discovery, quantitative proteomics, and systems-level investigations of cellular processes.

The course provides a strong foundation for students seeking to understand how proteins regulate biological functions and contribute to human health and disease.

Gel-Based Proteomics

Gel-based proteomics remains a foundational methodology for protein separation and characterization. This course covers one-dimensional and two-dimensional gel electrophoresis, protein staining approaches, image analysis, comparative proteomics, and downstream protein identification workflows.

Learners gain practical understanding of classical proteomics methodologies that continue to play important roles in biological research.



Mass Spectrometry-Based Proteomics

Mass spectrometry has transformed modern biological research. This course provides comprehensive training in the principles of mass spectrometry, instrumentation, ionization techniques, peptide fragmentation, protein identification, database searching, quantitative proteomics, and clinical applications.

The course also introduces learners to advanced proteomics workflows and emerging technologies that drive contemporary omics research.

Quantitative Proteomics and Biomarker Discovery

This course focuses on quantitative measurement of proteins and the discovery of clinically relevant biomarkers. Topics include label-free quantification, isotope labeling strategies, targeted proteomics, statistical analysis, experimental design, biomarker validation, and translational applications.

The course bridges fundamental proteomics research with real-world clinical implementation.

Proteogenomics: Integrating Genomics and Proteomics

Proteogenomics represents one of the most exciting frontiers in precision medicine. This course explores the integration of genomic, transcriptomic, and proteomic information to understand disease mechanisms, identify novel proteins, and develop personalized healthcare strategies.

Applications discussed include cancer biology, biomarker discovery, therapeutic development, and multi-omics integration.

Interactomics: Understanding Molecular Interaction Networks

Cells function through highly coordinated networks of molecular interactions. This course introduces methodologies used to study protein-protein interactions, signaling pathways, molecular complexes, interaction databases, network biology, and systems-level analyses.

Learners gain insight into how biological networks regulate cellular behavior and disease processes.



Systems Biology

This course introduces systems-level approaches for understanding biological complexity. Topics include biological networks, mathematical modeling, pathway analysis, computational simulations, systems medicine, and integrative omics.

The course emphasizes the importance of studying biological systems as interconnected networks rather than isolated components.

Bioinformatics for Modern Biology

Modern biological research increasingly depends upon computational analysis. This course provides training in biological databases, sequence analysis, functional annotation, structural biology, omics data analysis, and computational tools used in contemporary life sciences research.

The course supports interdisciplinary training at the interface of biology and computational sciences.

Biotechnology and Human Welfare

This course explores the role of biotechnology in addressing societal challenges related to healthcare, agriculture, environmental sustainability, and industrial innovation. Learners are introduced to recombinant DNA technology, diagnostics, therapeutics, vaccines, and emerging biotechnological applications.

The course highlights how scientific innovation can contribute to improving human well-being.

Emerging Omics Technologies and Precision Medicine

This advanced course introduces learners to next-generation technologies including proteomics, metabolomics, lipidomics, single-cell biology, spatial biology, artificial intelligence, digital health, and precision medicine.

The course provides a forward-looking perspective on how converging technologies are transforming biomedical research and healthcare.

Educational Impact and Capacity Building

Collectively, these MOOCs have contributed significantly to capacity building in biotechnology, bioengineering, proteomics, systems biology, and healthcare research. Through NPTEL and SWAYAM, learners from universities, colleges, hospitals, research institutions, and industries have gained access to high-quality educational resources developed at IIT Bombay.

These efforts reflect a broader vision of democratizing scientific education and empowering future generations of scientists, engineers, clinicians, innovators, and entrepreneurs.

As advances in proteomics, artificial intelligence, systems biology, and precision medicine continue to reshape healthcare and biomedical research, educational initiatives such as these MOOCs will remain essential for developing the skilled workforce required to drive future scientific and technological progress.

About Mumbai: Financial Capital & Innovation Hub

Mumbai, often referred to as the "City of Dreams," is India's financial capital, commercial powerhouse, and one of the world's most dynamic metropolitan cities. Situated along the Arabian Sea on the western coast of India, Mumbai serves as the economic engine of the nation and is widely recognized as a center for finance, industry, healthcare, education, entertainment, technology, and entrepreneurship.

Home to more than twenty million people representing diverse cultures, languages, religions, and traditions, Mumbai embodies the spirit of modern India. The city is a unique blend of history and innovation, where colonial-era architecture coexists with modern skyscrapers, global financial institutions, cutting-edge research centers, world-class hospitals, and thriving startup ecosystems.

As the host city of the Advances in Proteomics Technologies (APT-2026) Conference, Mumbai offers an ideal environment for scientific exchange, international collaboration, technological innovation, and cultural exploration.

A Brief Historical Perspective

Mumbai's history spans several centuries and reflects its evolution from a group of fishing islands into one of the world's most influential urban centers.

Originally consisting of seven islands inhabited primarily by fishing communities, the region came under Portuguese control during the sixteenth century before being transferred to the British Crown in 1661.

Recognizing its strategic location and natural harbor, the British developed Bombay into a major trading and commercial center. During the nineteenth and twentieth centuries, the city became a focal point for:

- Maritime trade
- Textile industries
- Banking and finance
- Manufacturing
- Education

Following India's independence in 1947, Bombay continued its remarkable growth and emerged as the nation's financial and commercial capital. In 1995, the city officially adopted the name Mumbai, derived from the local deity Mumbadevi.

Today, Mumbai stands as one of the most influential cities in Asia and a major contributor to India's economic development.

India's Financial Capital

Mumbai serves as the headquarters of many of India's most important financial institutions.

The city hosts:

- Reserve Bank of India (RBI)
- Bombay Stock Exchange (BSE)
- National Stock Exchange (NSE)
- Securities and Exchange Board of India (SEBI)
- Major national and international banks
- Insurance companies
- Investment firms

A substantial portion of India's financial transactions and capital market activities originate from Mumbai.

The city's financial ecosystem has played a critical role in supporting industrial growth, technological innovation, entrepreneurship, and infrastructure development across the country.

A Center for Science, Technology, and Innovation

Beyond finance, Mumbai has emerged as one of India's leading centers for scientific research and technological innovation.

The city is home to several prestigious institutions, including:

Indian Institute of Technology Bombay (IIT Bombay)

A globally recognized center of excellence in engineering, science, healthcare technologies, entrepreneurship, and innovation.

Tata Institute of Fundamental Research (TIFR)

One of India's premier institutions for fundamental scientific research.

Bhabha Atomic Research Centre (BARC)

A leading center for nuclear science and technology.

Institute of Chemical Technology (ICT)

Internationally recognized for chemical engineering, pharmaceutical sciences, and biotechnology.

National Centre for Biological Sciences Collaborations

Numerous research networks involving biological and biomedical sciences.

Together, these institutions contribute significantly to India's scientific output and technological advancement.

Mumbai as a Healthcare and Biomedical Hub

Mumbai is also one of India's leading healthcare destinations.

The city hosts several internationally recognized hospitals and healthcare institutions, including:

- Tata Memorial Centre
- KEM Hospital
- Lilavati Hospital
- Hinduja Hospital
- Kokilaben Dhirubhai Ambani Hospital
- Breach Candy Hospital
- Jaslok Hospital

These hospitals serve millions of patients annually and actively participate in clinical research, translational medicine, and healthcare innovation.

The concentration of hospitals, clinicians, researchers, and biotechnology companies makes Mumbai an ideal location for advancing precision medicine, biomarker discovery, and omics-driven healthcare.

This healthcare ecosystem provides important opportunities for collaborations associated with APT-2026 and Proteomica.

Biotechnology and Life Sciences Ecosystem

Mumbai has become a major center for biotechnology, pharmaceuticals, diagnostics, and healthcare innovation.

The region hosts:

- Biotechnology startups
- Pharmaceutical companies

- Clinical research organizations
- Diagnostics companies
- Medical technology firms

The city's strong industrial base and access to scientific expertise have created a thriving life sciences ecosystem.

Recent growth in:

- Genomics
- Proteomics
- Artificial intelligence
- Digital health
- Precision medicine

has further strengthened Mumbai's position as a healthcare innovation hub.

Entrepreneurship and Startup Culture

Mumbai has witnessed remarkable growth in entrepreneurship and startup development.

The city provides access to:

- Venture capital
- Angel investors
- Incubators
- Accelerators
- Corporate partnerships

Institutions such as IIT Bombay and SINE have played important roles in fostering innovation-driven entrepreneurship.

Companies emerging from scientific research, including ventures focused on biotechnology, healthcare, and omics sciences, continue to contribute to Mumbai's innovation ecosystem.

This entrepreneurial environment aligns closely with the translational objectives of APT-2026.

The Cultural Capital of India

Mumbai is widely regarded as India's cultural capital.

The city is home to:

- Bollywood
- Theatre communities
- Art galleries
- Music festivals
- Literary events
- Cultural institutions

Its rich cultural landscape reflects the diversity and creativity of its residents.

Visitors can experience:

- Classical music
- Contemporary art
- Regional cuisines
- International cuisine
- Traditional festivals
- Modern entertainment

This cultural vibrancy contributes to Mumbai's unique identity and global appeal.

Iconic Landmarks

Mumbai offers numerous landmarks that reflect its history and character.

Gateway of India

One of India's most recognizable monuments and a symbol of Mumbai's maritime heritage.

Marine Drive

Often called the "Queen's Necklace," Marine Drive is among the city's most famous waterfront promenades.

Chhatrapati Shivaji Maharaj Terminus

A UNESCO World Heritage Site showcasing remarkable Victorian Gothic architecture.

Elephanta Caves

Ancient rock-cut cave temples located on Elephanta Island.

Haji Ali Dargah

A renowned spiritual and architectural landmark situated in the Arabian Sea.

Siddhivinayak Temple

One of Mumbai's most visited places of worship.

These attractions offer delegates an opportunity to experience Mumbai's rich historical and cultural heritage.



Marine Drive



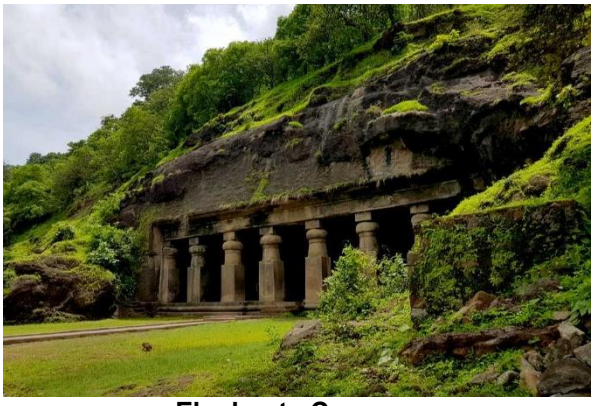
Gateway of India



Marine Drive



Chhatrapati Shivaji Maharaj Terminus



Elephanta Caves



Haji Ali Dargah



Siddhivinayak Temple

Mumbai and International Connectivity

Mumbai serves as one of India's primary gateways to the world.

The Chhatrapati Shivaji Maharaj International Airport connects the city to:

- North America
- Europe
- Asia
- Australia
- Africa
- Middle East

The city's extensive transportation infrastructure facilitates international travel and scientific collaboration.

Its global connectivity has been instrumental in attracting international conferences, business events, and research partnerships.

Why Mumbai is an Ideal Host for APT-2026

The selection of Mumbai as the host city for APT-2026 reflects several strategic advantages.

Mumbai offers:

Scientific Excellence

Home to leading research institutions and universities.

Healthcare Infrastructure

Access to major hospitals and clinical research networks.

Biotechnology Ecosystem

Strong interactions among academia, industry, and healthcare.

International Accessibility

Excellent global connectivity.

Entrepreneurial Culture

A thriving innovation and startup ecosystem.

Cultural Diversity

A welcoming environment for participants from around the world.

These strengths create a unique setting for scientific dialogue, collaboration, and innovation.



Looking Ahead

Mumbai continues to evolve as one of the world's most influential cities.

Its growing leadership in:

- Biotechnology
- Healthcare

- Artificial intelligence
- Entrepreneurship
- Precision medicine
- Digital innovation

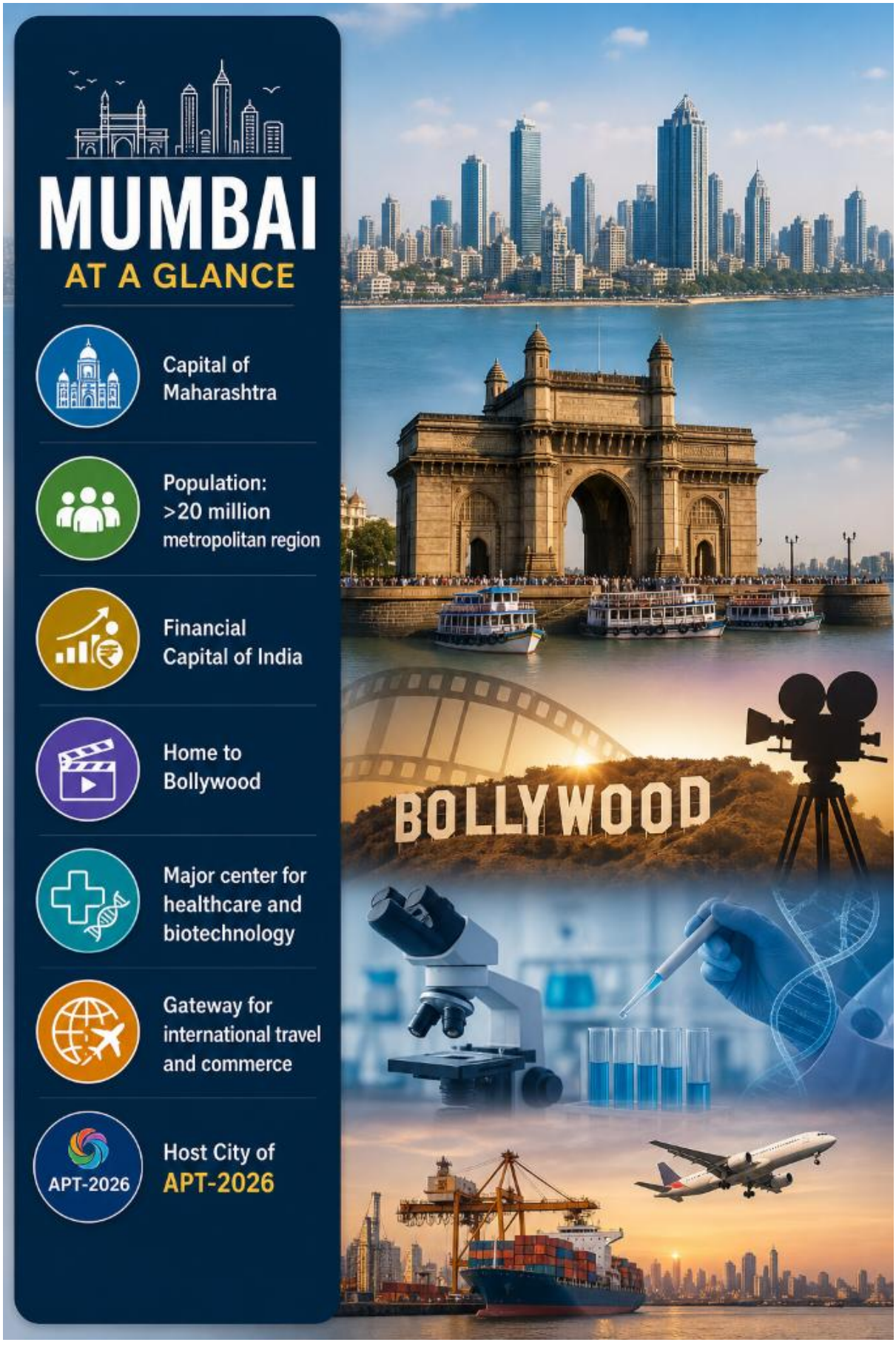
positions it as an important contributor to the future of science and technology.

As researchers, clinicians, entrepreneurs, and innovators gather for APT-2026, Mumbai provides more than a venue—it offers an ecosystem where ideas, discoveries, partnerships, and innovations can flourish.

The city's enduring spirit of resilience, ambition, diversity, and innovation makes it an ideal setting for advancing the future of proteomics, multi-omics, and precision healthcare.



Mumbai's Biotechnology and Healthcare Ecosystem


MUMBAI
AT A GLANCE
Capital of Maharashtra
Population: >20 million metropolitan region
Financial Capital of India
Home to Bollywood
Major center for healthcare and biotechnology
Gateway for international travel and commerce
APT-2026
Host City of APT-2026
BOLLYWOOD

About India: Knowledge, Innovation & Scientific Leadership

India is one of the world's oldest civilizations and one of its youngest nations in terms of demographic vitality, innovation potential, and economic growth. Home to more than 1.4 billion people, India represents an extraordinary blend of ancient wisdom, cultural diversity, scientific achievement, technological innovation, and entrepreneurial energy.

Over thousands of years, India has contributed significantly to mathematics, astronomy, medicine, metallurgy, philosophy, literature, and education. In the modern era, the nation has emerged as a global leader in information technology, space exploration, biotechnology, pharmaceuticals, healthcare innovation, and digital transformation.

Today, India stands among the world's fastest-growing major economies and is increasingly recognized as a key contributor to global scientific research and technological advancement. With a strong educational foundation, a rapidly expanding innovation ecosystem, and ambitious national initiatives in healthcare, artificial intelligence, biotechnology, and precision medicine, India is uniquely positioned to shape the future of science and human health.

As the host nation of the Advances in Proteomics Technologies (APT-2026) Conference, India offers a compelling example of how scientific excellence, technological innovation, and societal aspirations can converge to address global challenges and create opportunities for future generations.

A Civilization of Knowledge

India's intellectual heritage spans more than five millennia and has profoundly influenced human civilization.

Ancient centers of learning such as:

- Nalanda
- Takshashila
- Vikramashila

attracted scholars from across Asia and beyond.

India made foundational contributions to:

Mathematics

- Concept of zero
- Decimal number system
- Algebraic methods
- Trigonometry

Astronomy

- Planetary calculations
- Solar and lunar observations
- Celestial mechanics

Medicine

- Ayurveda
- Surgery
- Public health practices
- Herbal therapeutics

Philosophy and Ethics

- Logic
- Consciousness studies
- Human well-being
- Knowledge systems

These traditions laid the groundwork for a culture that values inquiry, learning, and innovation.

The World's Largest Democracy

India is the world's largest democracy, characterized by remarkable cultural, linguistic, ethnic, and religious diversity.

The nation consists of:

- 28 States
- 8 Union Territories
- Hundreds of languages and dialects
- Numerous cultural traditions

Despite this diversity, India remains united through shared constitutional values and democratic institutions.

The country's democratic framework has enabled sustained social, economic, and scientific development while fostering inclusivity and participation.

Economic Growth and Global Influence

Over the past three decades, India has undergone a remarkable economic transformation.

Today, India is among the world's largest economies and a major contributor to global growth.

Key sectors driving this transformation include:

- Information Technology
- Manufacturing
- Biotechnology
- Pharmaceuticals
- Healthcare
- Telecommunications
- Renewable Energy
- Financial Services

India's growing economic influence has strengthened its role in international trade, diplomacy, technology development, and scientific collaboration.

The nation increasingly serves as a bridge between developed and developing economies, contributing solutions to challenges affecting global health, sustainability, and development.

Science and Technology: Building a knowledge economy

India's commitment to science and technology has been a cornerstone of national development since independence.

Visionary leaders recognized that scientific capability would be essential for economic progress and societal advancement.

This vision led to the establishment of institutions such as:

- Indian Institutes of Technology (IITs)
- Indian Institutes of Science Education and Research (IISERs)
- Indian Institute of Science (IISc)
- Council of Scientific and Industrial Research (CSIR)
- Indian Council of Medical Research (ICMR)

- Department of Biotechnology (DBT)
- Department of Science and Technology (DST)

These institutions have played a pivotal role in advancing research, education, innovation, and technology development.

Today, India produces a large pool of scientists, engineers, healthcare professionals, and entrepreneurs who contribute to both national and international scientific ecosystems.

India's Leadership in Space Science

India's achievements in space exploration have attracted worldwide attention.

The Indian Space Research Organisation (ISRO) has demonstrated exceptional capabilities through missions involving:

- Satellite development
- Planetary exploration
- Lunar missions
- Mars exploration
- Human spaceflight preparation

Recent milestones such as Chandrayaan and Aditya missions have showcased India's growing leadership in advanced scientific and engineering endeavors.

These achievements reflect the nation's ability to pursue ambitious scientific goals while maintaining cost-effective innovation.

Biotechnology and Life Sciences Revolution

India has emerged as one of the world's leading biotechnology and pharmaceutical hubs.

The country's biotechnology ecosystem encompasses:

- Academic institutions
- Research laboratories
- Startups
- Pharmaceutical companies
- Clinical research organizations
- Healthcare providers

Major areas of growth include:

Genomics

Large-scale genome sequencing initiatives and population genomics studies.

Proteomics

Advanced proteomics research focused on biomarker discovery, disease mechanisms, and precision medicine.

Multi-Omics

Integration of genomics, proteomics, metabolomics, and lipidomics.

Synthetic Biology

Engineering biological systems for healthcare, agriculture, and industrial applications.

Biomanufacturing

Development of vaccines, biologics, and advanced therapeutics.

These advances are positioning India as a major contributor to the future of life sciences and healthcare innovation.

India's Global Role in Healthcare

India plays a crucial role in global healthcare through its contributions to pharmaceuticals, vaccines, diagnostics, and medical services.

The country is often referred to as:

"The Pharmacy of the World"

due to its extensive production of affordable medicines and vaccines.

India has contributed significantly to:

- Vaccine manufacturing
- Generic pharmaceuticals
- Medical research
- Public health initiatives
- Digital health solutions

The COVID-19 pandemic further highlighted India's importance in supporting global healthcare systems through vaccine production and international cooperation.

Digital India and Technological Transformation

India has become a global leader in digital innovation.

Programs such as:

- Digital India
- Aadhaar
- Unified Payments Interface (UPI)
- National Digital Health Mission

have transformed service delivery and digital infrastructure.

The rapid adoption of digital technologies has created new opportunities in:

- Artificial Intelligence
- Data Science
- Healthcare Informatics
- Precision Medicine
- Digital Health

These developments are enabling India to leapfrog traditional development pathways and create innovative solutions at scale.

Artificial Intelligence and Future Technologies

India is investing heavily in emerging technologies that are expected to define the future economy.

Priority areas include:

- Artificial Intelligence
- Quantum Computing
- Robotics
- Advanced Manufacturing
- Semiconductor Technologies
- Bioengineering
- Precision Healthcare

The integration of AI with biological sciences is creating exciting opportunities for:

- Biomarker discovery
- Clinical decision support
- Drug development
- Personalized medicine

These areas align closely with the scientific themes of APT-2026.

India's Emerging Leadership in Omics Sciences

India's contributions to omics research have expanded dramatically over the past two decades.

Research groups across the country are actively engaged in:

- Proteomics
- Genomics
- Metabolomics
- Lipidomics
- Systems Biology
- Precision Medicine

Organizations such as:

- Proteomics Society, India (PSI)
- HUPO-affiliated programs
- Academic institutions including IIT Bombay

have played important roles in building national capabilities.

The emergence of advanced infrastructure, including next-generation mass spectrometry platforms and multi-omics facilities, is accelerating India's contribution to global scientific initiatives.

India is increasingly participating in international efforts such as:

- Human Proteome Project
- Cancer-HPP
- Human Infectious Diseases-HPP
- π-HuB

demonstrating its growing leadership in global biomedical research.

Entrepreneurship and Innovation Ecosystem

India has become one of the world's most dynamic startup ecosystems.

The country hosts thousands of startups working across:

- Biotechnology
- Healthcare
- Artificial Intelligence
- Medical Devices
- Diagnostics
- Digital Health

Government initiatives such as:

- Startup India
- Atal Innovation Mission

- Biotechnology Industry Research Assistance Council (BIRAC)

have strengthened innovation and entrepreneurship.

Institutions such as IIT Bombay and incubators such as SINE continue to nurture technology-driven enterprises capable of generating global impact.

India's Demographic Advantage

India possesses one of the world's youngest populations.

This demographic strength provides:

- A large talent pool
- Scientific workforce growth
- Entrepreneurial energy
- Innovation potential

The country's universities, research institutions, and professional training programs continue to produce skilled graduates who contribute to global science and technology.

Investments in education and skill development are expected to further strengthen India's position in the knowledge economy.


INDIA
AT A GLANCE
Population: ~1.4 billion
World's Largest Democracy
One of the World's Fastest Growing Major Economies
Global Leader in Pharmaceuticals and Vaccines
Major Contributor to Information Technology and Digital Innovation
Emerging Leader in Biotechnology, Omics Sciences, and Precision Medicine
Host Nation of APT-2026
INFORMATION TECHNOLOGY & DIGITAL INNOVATION
VACCINE
PHARMA
PHARMACEUTICALS & VACCINES
BIOTECHNOLOGY, OMICS SCIENCES & PRECISION MEDICINE
APT-2026
ASIA PACIFIC THERAPEUTICS
HOSTED BY INDIA

Why India Matters for the Future of Precision Medicine

Several factors make India uniquely important for the future of precision healthcare:

Population Diversity

India's genetic, ethnic, environmental, and cultural diversity provides valuable opportunities for biomedical research.

Disease Burden

The coexistence of infectious diseases and non-communicable diseases creates important research challenges and opportunities.

Clinical Networks

Large healthcare systems facilitate translational and clinical studies.

Technological Expertise

Strong capabilities in engineering, computing, and biotechnology support innovation.

Global Partnerships

Growing participation in international scientific initiatives strengthens collaborative opportunities.

These factors position India as an important contributor to the future of precision medicine and multi-omics research.

India and APT-2026

The Advances in Proteomics Technologies (APT-2026) Conference reflects India's growing leadership in omics sciences and healthcare innovation.

APT-2026 brings together researchers, clinicians, industry leaders, students, and policymakers from around the world to discuss advances in:

- Proteomics
- Multi-omics
- Artificial Intelligence
- Precision Medicine
- Clinical Translation
- Digital Health

The conference highlights India's commitment to scientific excellence, innovation, and international collaboration.

It also showcases the country's expanding role in shaping the future of biomedical research and healthcare technologies.

Looking Ahead

India stands at a pivotal moment in its scientific and technological journey.

With a strong foundation in education, research, innovation, entrepreneurship, and healthcare, the nation is poised to play an increasingly influential role in addressing global challenges and advancing human well-being.

The convergence of biotechnology, artificial intelligence, precision medicine, digital health, and multi-omics sciences offers unprecedented opportunities for scientific discovery and societal impact.

As India continues its journey toward becoming a global knowledge and innovation leader, initiatives such as APT-2026 symbolize the nation's commitment to advancing science, fostering collaboration, and creating a healthier and more sustainable future for humanity.

From ancient centers of learning to cutting-edge research laboratories, India's story is one of continuous discovery, adaptation, and aspiration. It is a story that continues to inspire scientists, innovators, and dreamers around the world.





Map of India



India's Scientific and Technological Ecosystem

BrainProt: Integrative Omics Knowledgebase for Human Brain Diseases

The human brain remains one of the most complex biological systems known to science. Despite remarkable advances in neuroscience, understanding the molecular mechanisms underlying brain tumors and neurodegenerative disorders continues to be a major challenge. Modern omics technologies have generated vast amounts of genomic, transcriptomic, proteomic, and clinical data; however, much of this information remains scattered across repositories, publications, and specialized databases, limiting its accessibility and utility for researchers. To address this challenge, Professor Sanjeeva Srivastava and his team developed BrainProt, an integrative omics-driven knowledgebase designed to facilitate comprehensive exploration of the human brain and its associated diseases.

BrainProt was conceived as a community resource to support the global neuroscience and Human Proteome Project communities by bringing together multidimensional biological information into a single, intuitive platform. The latest version, BrainProt v3.0, represents a major advancement in neuroinformatics and translational neuroscience by integrating transcriptomics, proteomics, disease markers, therapeutic targets, and clinical trial information across a broad spectrum of brain diseases. The platform is freely accessible through BrainProt.org and serves as a bridge between fundamental neuroscience research and clinical translation.

A Comprehensive Atlas of Human Brain Diseases

At the heart of BrainProt is the Human Brain Disease Atlas (HBDA), which serves as a central navigation framework connecting multiple domains of brain disease information. The atlas encompasses information on 56 distinct human brain disorders and integrates disease-specific knowledge from thousands of scientific publications and established biomedical resources. By providing standardized disease identifiers and links to major biomedical repositories, HBDA enables researchers to rapidly access curated information on diverse neurological and neurodegenerative conditions.

The atlas was developed to simplify the exploration of complex brain disease information and to create a common framework for integrating molecular, clinical, and therapeutic data. This effort addresses a major bottleneck in neuroscience research, where relevant information is often dispersed across multiple databases and literature sources.

Brain Disease Transcriptome and Proteome Maps



A Comprehensive Atlas of Human Brain Diseases

One of the most innovative aspects of BrainProt is the integration of the Brain Disease Transcriptome Map (BDTM) and Brain Disease Proteome Map (BDPM). These modules provide researchers with the ability to examine gene and protein expression patterns across multiple brain diseases using harmonized analysis pipelines. The platform currently integrates data from 52 omics datasets representing 1,868 human samples and includes more than 6,200 differentially expressed genes and nearly 4,000 differentially expressed proteins.

These resources enable comparative analysis across major neurodegenerative disorders and brain tumors, including Alzheimer's disease, Parkinson's disease, Huntington's disease, Amyotrophic Lateral Sclerosis (ALS), Frontotemporal Lobar Degeneration, Multiple Sclerosis, Glioma, Glioblastoma, Meningioma, Medulloblastoma, and Pituitary Adenoma. Researchers can visualize disease-specific molecular signatures, compare expression trends across diseases, and identify candidate biomarkers and therapeutic targets.

By integrating transcriptomics and proteomics data within a common analytical framework, BrainProt provides a systems-level understanding of disease biology that is difficult to achieve through individual studies alone.

Brain Disease Marker Curator

Biomarker discovery remains a critical objective in neuroscience research. To support this goal, BrainProt includes the Brain Disease Marker Curator (BDMC), a specialized module that integrates disease-gene associations from multiple public resources and develops ranking strategies for identifying high-confidence disease markers. Through the integration of seven major knowledgebases, BrainProt compiles information on more than 20,000 disease-associated genes and systematically prioritizes them based on evidence and association strength.

This capability allows researchers to identify key molecular markers involved in disease progression and pathology. The platform further provides visualization tools that facilitate comparative analyses among diseases and enable exploration of common and unique molecular signatures across different neurological disorders.

Brain Disease Drug Finder

Translating molecular discoveries into therapeutic opportunities is one of the most important challenges in biomedical research. To support translational neuroscience, BrainProt incorporates the Brain Disease Drug Finder (BDDF), a dedicated resource linking disease-associated markers with therapeutic compounds, drug targets, and clinical trial information.

The BDDF integrates information from multiple drug databases and clinical repositories, including more than 136,000 chemical-target interactions and over 2,100 clinical trial records. Researchers can explore therapeutic candidates associated with specific disease markers, investigate mechanisms of action, and identify ongoing or completed clinical studies. This functionality transforms BrainProt from a purely descriptive database into a powerful translational research platform that supports hypothesis generation, drug repurposing, and precision medicine initiatives.

Understanding Cross-Talk Between Brain Tumors and Neurodegenerative Diseases

A particularly important contribution of BrainProt is its ability to explore molecular relationships between seemingly distinct neurological conditions. Using integrated omics analyses, the platform enables systematic comparisons between brain tumors and neurodegenerative disorders, revealing shared pathways, disease-associated markers, and potential mechanistic connections.

Such analyses have highlighted common molecular signatures among Glioma, Glioblastoma, Meningioma, Alzheimer's disease, Parkinson's disease, and other disorders. These findings provide valuable insights into disease pathobiology and offer new opportunities for understanding how diverse neurological conditions may share underlying biological mechanisms.

Supporting the Human Brain Proteome Project

BrainProt has been developed as an important resource supporting the goals of the Human Brain Proteome Project (HBPP) and the broader international proteomics community. The platform facilitates the integration of proteomics data with transcriptomics and clinical information, thereby helping researchers better understand brain function and disease at a systems level.

The resource exemplifies the vision of modern proteomics: moving beyond data generation toward data integration, interpretation, and knowledge discovery. By providing intuitive visualization tools and curated datasets, BrainProt lowers barriers for researchers entering the field and enables more effective utilization of publicly available omics resources.

Scientific and Societal Impact

BrainProt represents a significant contribution to open science and scientific outreach. Unlike many specialized databases that focus on a single disease or data type, BrainProt provides an integrated framework encompassing molecular biology, clinical information, biomarkers, therapeutic targets, and translational applications. The platform empowers scientists, clinicians, students, and educators to explore complex neurological disorders through a unified interface.

More broadly, BrainProt reflects Professor Sanjeeva Srivastava's vision of democratizing access to scientific knowledge. By transforming large-scale omics datasets into accessible and interpretable resources, BrainProt contributes to global efforts aimed at accelerating discoveries in neuroscience, improving disease diagnosis, identifying therapeutic opportunities, and ultimately enhancing patient care.

As omics technologies continue to generate increasingly large and complex datasets, platforms such as BrainProt will play a vital role in translating data into biological understanding and clinical impact. The development of BrainProt demonstrates how integrative bioinformatics, proteomics, and systems biology can converge to create resources that serve both the scientific community and society at large.

Student-Led Innovation and Collaborative Development

One of the most remarkable aspects of BrainProt is that it exemplifies the power of student-driven innovation and collaborative scientific research. The project was conceived and developed under the mentorship of Professor Sanjeeva Srivastava at the Proteomics Laboratory, Department of Biosciences and Bioengineering, IIT Bombay, with substantial contributions from a large multidisciplinary team of students, research scholars, and interns.

The scientific development of BrainProt was spearheaded by Dr. Deeptarup Biswas, who served as the lead author and principal contributor to the BrainProt project. During his doctoral research at IIT Bombay, Dr. Biswas demonstrated exceptional scientific leadership and technical expertise in proteomics, bioinformatics, data integration, and systems biology. His vision for creating an integrative and user-friendly brain disease knowledgebase played a pivotal role in transforming BrainProt from an initial concept into a globally accessible scientific resource.

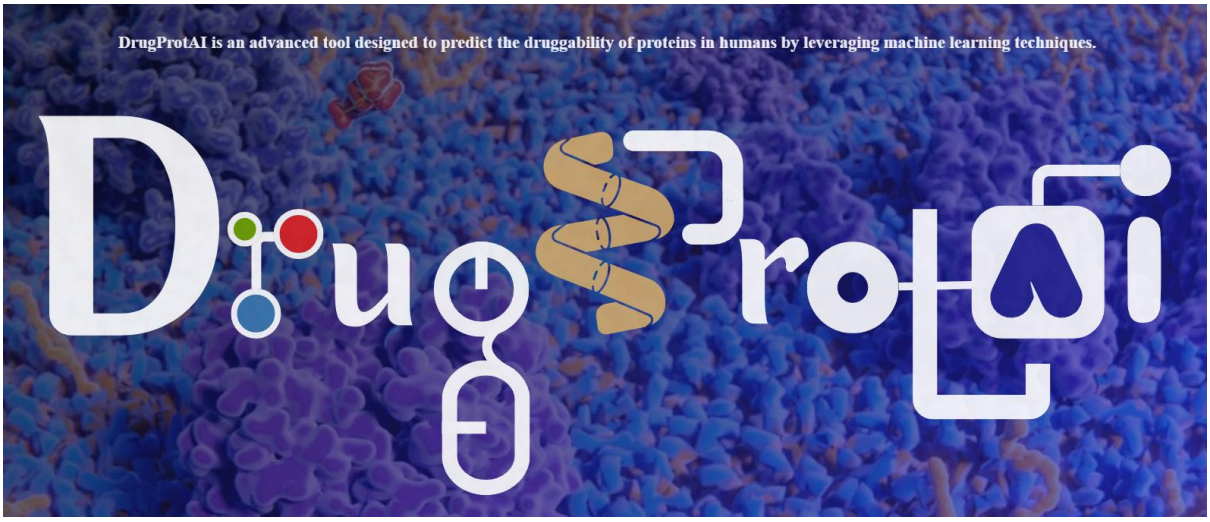
Dr. Biswas led the design, curation, analysis, and integration of large-scale transcriptomics, proteomics, biomarker, therapeutic, and clinical trial datasets. He worked extensively on developing computational workflows, disease-marker ranking strategies, and biological interpretation frameworks that form the foundation of BrainProt. His efforts culminated in the publication of BrainProt v3.0 in the Journal of Proteome Research, establishing the platform as an important contribution to neuroscience and proteomics research.

The success of BrainProt was also made possible through the collective efforts of numerous undergraduate students, postgraduate students, doctoral scholars, project staff, and interns associated with the Proteomics Laboratory. These contributors participated in diverse aspects of the project, including data mining, literature curation, bioinformatics analysis, software development, visualization design, quality control, validation, and database testing. Importantly, the project also provided a unique training platform for students from IIT Bombay and several academic institutions across India, enabling them to gain hands-on experience in big-data biology, computational proteomics, systems neuroscience, and translational research.

The collaborative nature of BrainProt reflects the educational philosophy of the Proteomics Laboratory, where research, innovation, mentorship, and capacity building go hand in hand. Through projects such as BrainProt, students are encouraged to tackle complex biological questions, develop interdisciplinary expertise, and contribute to resources that serve the broader scientific community.

The BrainProt initiative stands as a testament to how mentorship, teamwork, and scientific curiosity can collectively create resources of international significance. Beyond its scientific impact, the project has helped train the next generation of

researchers in proteomics, bioinformatics, neuroscience, and data science, thereby contributing to the growth of India's scientific ecosystem and strengthening global efforts toward understanding human brain diseases.



AI IN DRUG DISCOVERY

DrugProtAI: AI Platform for Protein Druggability Prediction

The identification of effective therapeutic targets remains one of the greatest challenges in modern drug discovery. Despite enormous investments in pharmaceutical research, nearly 90% of drug development programs fail before reaching clinical application, often due to the selection of unsuitable or poorly characterized targets. Recognizing this critical bottleneck, researchers in the Proteomics Laboratory at the Department of Biosciences and Bioengineering, IIT Bombay developed DrugProtAI, an advanced artificial intelligence–driven platform designed to predict the druggability of proteins and facilitate rational target prioritization for drug discovery.

DrugProtAI represents the convergence of proteomics, bioinformatics, machine learning, systems biology, and translational medicine. The platform was conceived under the leadership of Professor Sanjeeva Srivastava and developed through the dedicated efforts of a multidisciplinary team of students and researchers from IIT Bombay. By integrating large-scale protein information with state-of-the-art machine learning approaches, DrugProtAI enables researchers to evaluate the therapeutic potential of proteins across the human proteome and identify promising targets for future drug development.

Unlike conventional target-selection strategies that often depend on limited biological information or structural characteristics, DrugProtAI employs a comprehensive feature-driven framework capable of analyzing hundreds of molecular and biological properties simultaneously. The platform serves as an intelligent decision-support system that helps researchers prioritize proteins with the highest likelihood of successful therapeutic intervention.

Scientific Vision Behind DrugProtAI

The rapid expansion of omics technologies has generated an unprecedented volume of biological information. Large-scale genomics, transcriptomics, proteomics, metabolomics, and systems biology studies routinely identify thousands of molecules associated with diseases. However, converting these discoveries into actionable therapeutic targets remains extremely challenging.

DrugProtAI was developed to bridge this gap.

The central vision behind DrugProtAI is to transform vast biological datasets into actionable knowledge by answering a fundamental question:

"Can a particular protein serve as an effective therapeutic target?"

To address this challenge, the platform integrates diverse biological features, including:

- Protein sequence characteristics
- Physicochemical properties
- Protein-protein interaction networks
- Post-translational modifications
- Structural properties
- Subcellular localization information
- Functional annotations
- Drug-target associations
- Systems biology parameters

Through machine learning–based analysis of these multidimensional datasets, DrugProtAI generates a quantitative measure known as the Druggability Index, which estimates the likelihood that a protein can be successfully targeted by therapeutic interventions.

Technological Innovation

DrugProtAI introduces several methodological innovations that distinguish it from existing druggability prediction tools.

A major challenge in druggability prediction arises from highly imbalanced biological datasets. While only a relatively small fraction of human proteins are known drug targets, the vast majority remain unexplored. Traditional machine learning models often perform poorly under such circumstances.

To overcome this limitation, the IIT Bombay team developed novel machine-learning frameworks known as:

- Partition Ensemble Classifier (PEC)
- Partition Leave-One-Out Ensemble Classifier (PLOEC)

These approaches employ partition-based ensemble learning strategies that significantly improve prediction accuracy while minimizing bias. By combining multiple machine-learning models, including Random Forest and XGBoost algorithms, DrugProtAI achieves robust and reliable predictions across thousands of proteins.

The platform analyzes over 180 biological features and incorporates explainable artificial intelligence methodologies, enabling users not only to obtain predictions but also to understand which biological characteristics contribute most strongly to druggability.

This combination of predictive accuracy and interpretability represents a major advance in computational drug discovery.

Scientific Impact

DrugProtAI extends beyond simple prediction and contributes significantly to our understanding of protein biology.

Analysis performed through the platform identified several key determinants of protein druggability, including:

- Kinase activity
- Protein stability
- Secondary structural characteristics
- Glycosylation patterns
- Post-translational modifications
- Network connectivity
- Physicochemical properties

These findings provide important biological insights into why certain proteins become successful drug targets while others remain therapeutically inaccessible.

The platform therefore functions not only as a predictive tool but also as a discovery engine capable of uncovering fundamental principles governing therapeutic target selection.

Student Leadership and Collaborative Development

One of the most inspiring aspects of DrugProtAI is its emergence as a student-driven innovation originating from the Proteomics Laboratory at IIT Bombay.

The scientific development of DrugProtAI was spearheaded by Mr. Ankit Halder, who served as the lead author and principal contributor to the project. Through exceptional dedication and interdisciplinary expertise spanning proteomics, bioinformatics, machine learning, systems biology, and drug discovery, Ankit played a central role in transforming the initial concept into a fully functional and scientifically validated platform.

Working under the mentorship of Professor Sanjeeva Srivastava, Ankit led multiple aspects of the project, including:

- Data acquisition and curation
- Feature engineering
- Machine learning model development
- Biological interpretation
- Tool validation
- Manuscript preparation
- Platform deployment

The project also benefited from substantial contributions from Sabyasachi Samantaray, Sahil Barbade, and Aditya Gupta, who participated in computational development, algorithm implementation, data analysis, and web platform construction.

Importantly, DrugProtAI reflects the collaborative culture of the Proteomics Laboratory, where students from multiple disciplines—including biosciences, computer science, mechanical engineering, and computational biology—work together to address complex biomedical challenges.

The project further highlights the laboratory's commitment to training future leaders in artificial intelligence, computational biology, proteomics, and translational medicine.

Educational and Training Impact

Beyond its scientific contributions, DrugProtAI has served as an exceptional educational platform.

The development of the resource provided students and interns with hands-on exposure to:

- Machine learning
- Artificial intelligence
- Drug discovery
- Systems biology
- Big-data analytics
- Computational proteomics
- Biomedical informatics
- Translational research

The project demonstrates how interdisciplinary training can empower young scientists to develop solutions with real-world biomedical impact.

It further exemplifies Professor Sanjeeva Srivastava's long-standing philosophy of integrating research excellence with student mentorship and capacity building.

Global Relevance and Future Directions

DrugProtAI represents an important step toward AI-enabled drug discovery and precision medicine.

Future versions are expected to expand toward:

- Multi-species druggability prediction
- Precision medicine applications
- Antibody target prioritization
- Drug repurposing studies
- Cancer target discovery
- Infectious disease target identification
- Integration with proteogenomics data
- Generative AI–assisted therapeutic design

As global pharmaceutical research increasingly adopts artificial intelligence–based strategies, platforms such as DrugProtAI are expected to play a critical role in accelerating target identification and reducing the cost and time associated with drug development.

Legacy and Significance

DrugProtAI stands as a powerful example of how advances in proteomics, bioinformatics, artificial intelligence, and translational medicine can converge to address one of the most challenging problems in biomedical research.

The platform highlights the growing international impact of the Proteomics Laboratory at IIT Bombay and showcases how student-led innovation can generate globally relevant scientific resources.

Through the visionary leadership of Professor Sanjeeva Srivastava, the outstanding contributions of Ankit Halder, and the collective efforts of students, collaborators, and researchers, DrugProtAI has emerged as a valuable contribution to the worldwide drug discovery community and a model for interdisciplinary scientific innovation.

STRUCTURAL BIOLOGY & AI

AlphaCross-XL: Crosslinking Proteomics & AI for Structural Biology

Proteins are not static molecules. Their biological functions are governed by dynamic structural rearrangements, conformational transitions, folding states, and molecular interactions that occur continuously within living systems. Understanding these conformational changes is fundamental to deciphering disease mechanisms, drug responses, cellular signaling pathways, and protein function.To address this challenge, a collaborative team led by Professor Sanjeeva Srivastava (IIT Bombay) and Dr. Arun Wiita (University of California, San Francisco) developed AlphaCross-XL, an innovative computational platform that integrates crosslinking mass spectrometry data with AlphaFold-predicted protein structures for large-scale structural analysis. The software provides an automated solution for mapping experimentally identified crosslinked peptides onto three-dimensional protein structures and identifying structural alterations across entire proteomes.

AlphaCross-XL represents a unique convergence of proteomics, structural biology, artificial intelligence, and computational science, creating a powerful resource for researchers investigating protein conformations in health and disease.

The Scientific Challenge

Crosslinking Mass Spectrometry (XL-MS) has emerged as one of the most promising approaches for studying protein structures in their native biological environment. By chemically linking amino acid residues that are spatially close within proteins, XL-MS provides valuable information about protein architecture and molecular interactions.

However, modern XL-MS experiments routinely generate thousands of crosslinks across hundreds or even thousands of proteins. Interpreting these large datasets has historically been a major bottleneck.

Before AlphaCross-XL, researchers often had to manually:

- Retrieve protein structures
- Map crosslinked residues
- Measure residue distances
- Validate structural compatibility
- Visualize protein conformations

Such manual workflows were labor-intensive and impractical for proteome-scale analyses.

Recognizing this challenge, the IIT Bombay–UCSF collaboration set out to create a seamless, automated platform capable of performing these analyses at unprecedented scale.

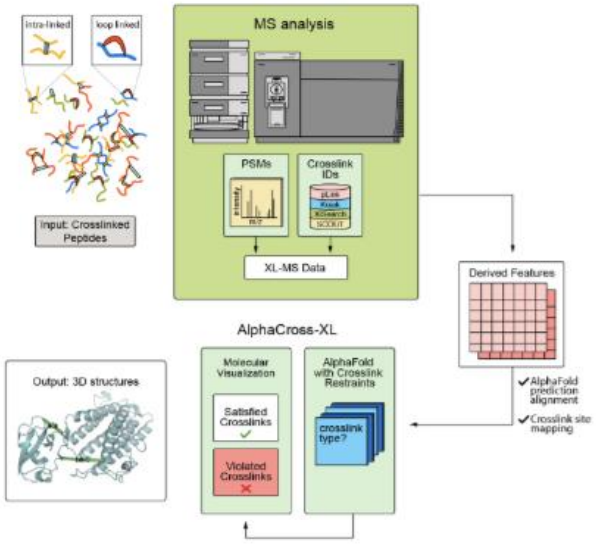
MCP RESEARCH

AlphaCross-XL: A Seamless Tool for Automated and Proteome-Scale Mapping of Cross-Linked Peptides Onto 3D Protein Structures

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Graphical Abstract



In Brief
Crosslinking mass spectrometry (XL-MS) has emerged as a powerful tool for proteome-scale structural analysis of proteins. However, a major bottleneck is interpretation and analysis of the thousands of experimentally identified crosslinks. Here, we present AlphaCross-XL, an open-source software enabling proteome-wide automated mapping of crosslinked peptides on to either AlphaFold-predicted or Protein Data Bank–determined structures. This tool allows rapid analysis and visualization to enable triaging proteome-scale XL-MS data, for mining structurally or conformationally altered state of proteins for further downstream biological investigation.

Vision Behind AlphaCross-XL

The core vision of AlphaCross-XL was simple yet transformative:

"Can we automatically integrate experimental crosslinking data with AI-predicted protein structures to understand protein conformations at proteome scale?"

The release of AlphaFold fundamentally changed structural biology by making high-quality protein structure predictions available for millions of proteins. AlphaCross-XL leverages this revolutionary resource by directly retrieving protein structures from the AlphaFold Protein Structure Database and combining them with experimentally derived XL-MS data.

The result is a highly scalable framework that allows researchers to:

- Map crosslinks automatically
- Measure residue distances
- Detect structural violations
- Identify conformational changes
- Visualize protein structures
- Prioritize biologically relevant targets

all within a single streamlined workflow.

Technological Innovation

AlphaCross-XL is among the first platforms specifically designed for automated proteome-wide structural mapping of crosslinked peptides onto protein structures.

The software performs several critical tasks automatically:

Structure Retrieval

The platform directly accesses the AlphaFold Protein Structure Database and retrieves protein structures using UniProt identifiers.

Crosslink Mapping

Experimentally identified crosslinked peptides are automatically mapped onto corresponding protein structures.

Distance Calculations

The software calculates Euclidean distances between crosslinked residues and determines whether they satisfy or violate user-defined distance constraints.

Structural Validation

AlphaCross-XL distinguishes between:

- Satisfied crosslinks
- Violated crosslinks

allowing researchers to identify potential conformational rearrangements.

Confidence Scoring

The software incorporates AlphaFold's pLDDT confidence scores, enabling users to evaluate the reliability of structural regions and prioritize high-confidence observations.

Visualization

A major strength of the platform is its generation of color-coded PyMOL visualizations:

- Green crosslinks represent structurally satisfied interactions.
- Red crosslinks indicate potential structural violations and conformational changes.

This visual framework allows rapid identification of proteins warranting further biological investigation.

A Powerful Community Resource

One of the distinguishing features of AlphaCross-XL is its commitment to accessibility.

The software was designed as:

- Open-source
- User-friendly
- GUI-enabled
- Cloud accessible through Google Colab
- Compatible with multiple XL-MS search engines

Researchers can use the platform without requiring extensive computational expertise, significantly lowering barriers to adoption across the structural biology and proteomics communities.

This democratization of advanced structural analysis reflects the broader philosophy of the IIT Bombay Proteomics Laboratory—developing technologies that benefit the global scientific community.

Student Leadership and Innovation

A particularly noteworthy aspect of AlphaCross-XL is the leadership demonstrated by Mr. Sanjyot Vinayak Shenoy, a student from IIT Bombay, who served as the lead author and primary driving force behind the software development.

Sanjyot played a central role in:

- Software architecture
- Algorithm development
- Workflow automation
- Integration with AlphaFold
- Visualization framework creation
- User-interface design
- Validation studies
- Manuscript preparation

The project exemplifies the laboratory's tradition of empowering students to lead ambitious interdisciplinary research initiatives that combine biology, engineering, artificial intelligence, and computational science.

The work also benefited from contributions from several researchers across IIT Bombay, UCSF, Thermo Fisher Scientific, the Chan Zuckerberg Biohub, and collaborating institutions, demonstrating the truly international nature of the effort.

International Collaboration Between IIT Bombay and UCSF

AlphaCross-XL represents a successful example of international scientific collaboration between:

- Professor Sanjeeva Srivastava's laboratory at IIT Bombay
- Dr. Arun Wiita’s team at UCSF

Together, the teams combined expertise in:

- Proteomics
- Structural biology
- Crosslinking mass spectrometry
- Artificial intelligence
- Computational modeling
- Biomedical research

This collaboration highlights how partnerships between leading institutions can accelerate innovation and create globally impactful scientific resources.

SCIENCE COMMUNICATION

Science Communication Through Film & Public Outreach

Science communication plays a critical role in bridging the gap between scientific discovery and society. While research publications, conferences, and academic lectures remain important avenues for disseminating knowledge, visual storytelling through films and documentaries offers a powerful medium for engaging broader audiences. Recognizing the importance of making science accessible and inspiring, Professor Sanjeeva Srivastava has actively explored filmmaking as an innovative approach to communicate scientific concepts, showcase the human side of research, and motivate future generations of scientists and innovators.

Over the years, several documentaries and short films have been conceptualized and developed to highlight themes such as scientific perseverance, innovation, healthcare challenges, proteomics research, cancer biology, entrepreneurship, and the societal impact of scientific discoveries. These productions have been screened at national and international film festivals and have received recognition through awards, official selections, and educational outreach programs.

RINTI: A Story of Courage, Science, and Inspiration

"RINTI" is a short film based on the true story of the late Professor Rinti Banerjee, a distinguished scientist, educator, and colleague whose life continues to inspire students and researchers. The film portrays the personal and professional journey of a scientist dedicated to advancing knowledge despite immense challenges. Through a compelling narrative, the film highlight's themes of resilience, commitment to education, scientific passion, and the transformative impact of mentorship.

Beyond being a biographical tribute, RINTI celebrates the human spirit that drives scientific discovery and innovation. The film received significant recognition at multiple film festivals and was honored with the Dadasaheb Phalke Film Puraskar (2024–25), reflecting its emotional depth and educational significance. It also received selections and awards at several national and international film festivals, bringing wider visibility to the inspirational story of a scientist whose legacy continues to influence future generations.

The Open Mind: Innovation for Society

The Open Mind is a documentary that explores the journey of scientific innovation and its potential to create meaningful societal impact. The film presents a broader perspective on how curiosity-driven research can evolve into technologies that improve healthcare, address societal challenges, and contribute to national development.

The documentary highlights the importance of interdisciplinary thinking, perseverance, and an openness to new ideas. Through real-life examples and personal experiences, the film demonstrates how scientific innovation can influence public health, biomedical research, and technology development. The documentary was recognized at multiple film festivals and received awards for educational filmmaking, underscoring its value as a tool for science communication and public engagement.

India Beckons: Returning Home to Build Scientific Excellence

India Beckons tells the inspiring story of a researcher trained at Harvard Medical School who chooses to return to India with a vision of contributing to the nation's scientific and technological advancement. The documentary highlights the opportunities and challenges associated with building research programs in a developing nation and emphasizes the importance of creating world-class scientific ecosystems within India.

The film explores themes of national service, scientific leadership, education, mentorship, and innovation. By documenting the journey of establishing advanced research programs and nurturing future scientists, the documentary presents a powerful message about the role of science in nation-building. The film received international recognition through

screenings and selections at multiple film festivals across different countries, reflecting its universal message of aspiration, commitment, and impact.

Proteomics: Translating the Code of Life

One of the earliest science communication initiatives focused directly on the field of proteomics. The documentary Proteomics: Translating the Code of Life was developed to introduce audiences to the emerging world of proteins, biological systems, and molecular medicine.

The film explains how proteomics enables scientists to understand complex biological processes, identify disease-associated biomarkers, and develop strategies for personalized healthcare. Featuring experts and state-of-the-art research facilities, the documentary serves as an educational resource for students, researchers, and members of the public interested in understanding the role of proteins in health and disease.

The documentary was featured at Human Proteome Organization (HUPO) activities and contributed to raising awareness about the growing importance of proteomics in biomedical research and healthcare innovation.

Cancer: Divide and Rule

Cancer remains one of the most complex and challenging diseases affecting humanity. Cancer: Divide and Rule was created to communicate the biological complexity of cancer and the ongoing efforts of researchers to understand and combat the disease.

The documentary explores how cancer cells evolve, adapt, and evade normal biological controls. Through visual storytelling and scientific explanations, the film introduces viewers to modern cancer research, biomarker discovery, precision medicine, and emerging therapeutic strategies.

The film received recognition at several international film festivals and educational forums. Beyond its scientific content, the documentary aims to foster awareness and appreciation of the research efforts dedicated to improving cancer diagnosis, treatment, and patient outcomes.

Triumph: Celebrating Scientific Perseverance

Triumph is a short one-shot film that captures the spirit of perseverance, determination, and innovation that characterizes scientific research. The film portrays the often-unseen journey behind scientific achievements, highlighting the dedication required to overcome challenges and pursue ambitious goals.

Through a concise yet impactful narrative, Triumph emphasizes that scientific success is rarely instantaneous; rather, it is the result of sustained effort, resilience, collaboration, and belief in a larger vision. The film was officially selected at multiple international film festivals and serves as an inspirational piece for students, researchers, and aspiring innovators.

Film as a Medium for Scientific Outreach

Collectively, these documentaries and short films represent an innovative approach to science communication and public engagement. They demonstrate how storytelling can be used to explain complex scientific concepts, highlight the human dimensions of research, inspire future generations, and build stronger connections between science and society.

By combining scientific rigor with creative expression, these initiatives have expanded the reach of proteomics, healthcare innovation, and biomedical research beyond traditional academic audiences. They also illustrate the importance of communicating not only scientific results but also the stories, values, and people behind scientific discovery.

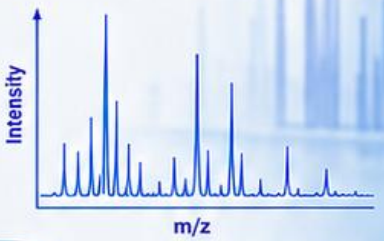
As science becomes increasingly interdisciplinary and globally connected, effective communication will remain essential for fostering public trust, inspiring young learners, and translating research into meaningful societal impact. These film-based outreach initiatives provide a compelling example of how scientific storytelling can contribute to education, awareness and innovation.

APT-2026

PROCEEDIINGS

ADVANCING PROTEOMICS, TRANSFORMING HEALTHCARE

This proceeding captures the knowledge, ideas and innovations shared at APT-2026. Together, we move closer to a future where proteomics drives precision medicine and improves lives worldwide.



Thank you

to all our speakers, delegates, partners and contributors for being part of this impactful journey.

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"From discovery to impact – together, we shape the future of proteomics."