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Neil KelleherNorthwestern University



Ljiljana Paša-Tolić EMSL, PNNL

THURSDAY, JANUARY 24

6:00 – 7:00 pm **Registration**, Outside of the Long/Bird/Indian Ballroom

6:30 – 8:00 pm Opening Session

Top Down Mass Spectrometry: Past, Present and Future

Session Chairs, Neil Kelleher, Northwestern University & Ljiljana Paša-Tolić, EMSL, PNNL

Long/Bird/Indian Ballroom

6:30 - 7:15 pm **Joseph Loo**, *UCLA*

Top-Down Mass Spectrometry – Where are we going? Are we there

yet?

7:15 - 8:00 pm **Fred McLafferty,** *Cornell University*

Charge Site Mass Spectra: Basic Mechanisms for Electron Capture Dissociation of Both Covalent and Noncovalent Bonds in Ionized

Proteins

8:00 - 10:00 pm Reception setup all posters

Banyan Breezeway

FRIDAY, JANUARY 25

	FRIDAT, JANUART 25
	8:30 – 9:30 am
Ins	trumentation for Top Down Mass Spectrometry
	on Chair: David Goodlett, University of Washington
	Long/Bird/Indian Ballroom
8:30 – 9:00 am	Alan Marshall, NHMFL/Florida State University
3.00 J.00 Mil	Determination of Site-Specific Protein Disulfide Bond Reduction
	Potentials by Top-Down FT-ICR MS/MS
9:00 – 9:30 am	Mike Senko, Thermo Fisher Scientific
7.00 7.50 um	Orbitrap Instrumentation for Top-Down Analysis
9:30 - 9:50 am	Coffee Break, Banyan Breezeway
	9:50 - 11:20 am
	Targeted strategies I
(Characteriza	tion of recombinants, immunoglobulins, phosphoproteins,
`	membrane proteins, histones, etc.)
Se	ssion Chair: Lloyd Smith, <i>University of Wisconsin</i>
	Long/Bird/Indian Ballroom
9:50 – 10:20 am	Julian Whitelegge, UCLA
7.50 10.20 am	Data-Directed Top-Down Mass Spectrometry for Precise
	Characterization of Integral Membrane Proteins
10:20 – 10:50 am	Yury Tsybin, Ecole Polytechnique Federale
10.20 10.50 um	Top-Down and Middle-Down Mass Spectrometry of Immunoglobulins
	and Beyond
10:50 – 11:20 am	John Yates, Scripps Research Institute
10.30 – 11.20 am	The CFTR Interactome: the Case for Protein Complex Variations
11:20 – 11:40 am	Coffee Break, Banyan Breezeway
	11:40 am - 12:40 pm
	Targeted strategies II
(Characteriza	ation of recombinants, immunoglobulins, phosphoproteins,
(membrane proteins, histones, etc.)
Session (Chair: Julia Chamot-Rooke, CNRS - Ecole Polytechnique
Session	Long/Bird/Indian Ballroom
11:40 am - 12:10 pm	Ying Ge, University of Wisconsin
11.70 am - 12.10 pm	Top-Down Targeted Proteomics for Deep Sequencing of
	Phosphoproteins
12:10 - 12:40 pm	Maarten Altelaar, Utrecht University
12.10 - 12.40 pm	Extending the Capabilities of the Orbitrap in Mass Range and
	Fragmentation Efficiency for Top-Down Proteomics
12.40 2.00	Croun Lunch Garden Courtward
12:40 - 2:00 pm	Group Lunch, Garden Courtyard

FRIDAY, JANUARY 25

2:00 - 3:30 pm	
Protein Conformation, Charging and Complexation	
	Session Chair: Joseph Loo, UCLA
Long/Bird/Indian Ballroom	
2:00 - 2:30 pm	Scott McLuckey, Purdue University
-	New Gas-Phase Ion Chemistries for Top-Down Tandem Mass
	Spectrometry
2:30 - 3:00 pm	Kathrin Breuker, University of Innsbruck
-	ECD and Protein Structure in the Gas Phase
3:00 - 3:30 pm	Evan Williams, UC Berkeley
•	Supercharging Approaches for Top-Down Native Mass Spectrometry

3:30 - 5:30 pm Consortium for Top Down Proteomics Long/Bird/Indian Ballroom

7:00 - 8:00 pm		
Promoted Talks I		
Sess	sion Chair: Catherine Costello, Boston University	
Long/Bird/Indian Ballroom		
7:00 - 7:15 pm	Xibei Dang, Florida State University	
	Poster 11 - Top-Down Analysis of Histone Post-Translational	
	Modifications by Electron Capture Dissociation Fourier Transform Ion	
	Cyclotron Resonance Mass Spectrometry	
7:15 - 7:30 pm	Frederik Lermyte, University of Antwerp	
	Poster 19 - Ion Mobility - Mass Spectrometry and top-down Electron	
	Transfer Dissociation of Intact Proteins on a Quadrupole/TOF Instrument	
7:30 - 7:45 pm	Jared Shaw, University of Texas	
	Poster 27 - 193 nm Ultraviolet Photodissociation in an Orbitrap Elite	
	Mass Spectrometer for Top-Down Proteomics	
7:45 - 8:00 pm	David Horn, Thermo Fisher Scientific	
	Poster 13 - Top-Down Identification of Case in Isoforms using a High	
	Performance Benchtop Quadrupole Orbitrap Mass Spectrometer	

8:00 - 10:00 pm **Poster Session I** odd-numbered posters present Banyan Breezeway

SATURDAY, JANUARY 26

8:30 - 10:30 am Intact Protein Separations and Top Down Mass Spectrometry on a Chromatographic Time Scale Session Chair: Yury Tsybin, Ecole Polytechnique Federale Long/Bird/Indian Ballroom	
8:30 - 9:00 am	Alan Doucette, Dalhousie University
	How to Analyze Twice as much Sample, in Half the Time
9:00 - 9:30 am	Ljiljana Paša-Tolić, EMSL, PNNL
	Defining Bacterial Proteomes from the Top-Down
9:30 - 10:00 am	Lloyd Smith, University of Wisconsin
10:00 - 10:30 am	Proteoform Analysis: New Technologies for Detection and Quantitation of Intact Proteins Neil Kelleher, Northwestern University
	Top Down Proteomics and the Human Proteome Project
10:30 - 10:50 am	Coffee Break, Banyan Breezeway

10.50 am 12.50 nm	
10:50 am - 12:50 pm	
Top Down Mass Spectrometry and Human Health	
S	ession Chair: Ying Ge, University of Wisconsin
	Long/Bird/Indian Ballroom
10:50 - 11:20 am	Julia Chamot-Rooke, CNRS - Ecole Polytechnique
	Top-Down Analysis of Bacterial Proteins Involved in Virulence
11:20 - 11:50 am	Jeffrey Agar, Brandeis University
	Proteoforms Put in Perspective: Toxic, Therapeutic, and Protective
11:50 am - 12:20 pm	Nathan Yates, University of Pittsburgh
_	Pharmaceutical Applications of Top-Down Differential Mass
	Spectrometry
12:20 - 12:50 pm	Catherine Costello, Boston University
-	Top-Down Analysis of Variant and/or Post-Translationally Modified
	Proteins
1:00 - 7:00 pm	Afternoon Free
1	or optional trip to the Dali Museum, shuttle will leave at 1 pm and return at
	3:45 pm and 5:00 pm, ask Brent at the registration desk if \$10 shuttle tickets are still available.

4:00 - 6:00 pm Consortium for Top Down Proteomics Long/Bird/Indian Ballroom

SATURDAY, JANUARY 26

	7:00 - 8:00 pm
	Promoted Talks II
	Session Chair: Evan Williams, UC Berkeley
	Long/Bird/Indian Ballroom
7:00 - 7:15 pm	Gary Van Berkel, Oak Ridge National Laboratory
	Poster 30 - Spatially Resolved Extraction of Proteins from Tissues and
	Blood Spots for Top Down Analysis using a Continuous Flow Liquid
	Microjunction Surface Sampling Probe (LMJ-SSP)
7:15 - 7:30 pm	Christophe Masselon, CEA, Institut de Biologie Structurale Jean-Pierre
-	Ebel
	Poster 20 - Top-down MS analysis reveals binding site between S.
	pneumoniae pilin domains
7:30 - 7:45 pm	Simone Nicolardi, Leiden University Medical Center (LUMC)
-	Poster 22 - Top-Down MS Identification of New O-Glycosylated
	Apolipoprotein-CIII Isoforms in Ultrahigh Resolution Human Serum
	Profiles
7:45 - 8:00 pm	Zhixin (Michael) Tian, Dalian Institute of Chemical Physics, CAS
•	Poster 28 - Interpreting Biological Mass Spectra as It Is Using Isotopic
	Mass-to-charge Ratio and Envelope Fingerprinting

8:00 - 10:00 pm Poster Session II even-numbered posters present Banyan Breezeway

SUNDAY, JANUARY 27

	8:30 - 10:30 am
	Bioinformatics
Se	ession Chair: Scott McLuckey, Purdue University
	Long/Bird/Indian Ballroom
8:30 - 9:00 am	Richard LeDuc, Indiana University
	Statistical Consideration for Identification and Quantification in Top-
	Down Proteomics
9:00 - 9:30 am	Pavel Pevzner, UCSD
	MS-Align: Identification of Top-Down Spectra with Unexpected
	Modifications
9:30 - 10:00 am	David Goodlett, University of Washington
	Exploring data-independent top-down proteomics
10:00 - 10:30 am	Nathan Edwards, Georgetown University
	Phyloproteomic Classification of Unsequenced Organisms by Top-Down
	Proteomics
10:30 - 11:00 am	Coffee Break, Banyan Breezeway

11:00 am- 12:00 pm	
	lass Spectrometry Imaging of Intact Proteins
Sess	ion Chairs, Neil Kelleher, Northwestern University
	& Ljiljana Paša-Tolić, <i>EMSL, PNNL</i>
	Long/Bird/Indian Ballroom
11:00 - 11:30 am	Sarah Trimpin, Wayne State University
	LSI Imaging and Characterization of Endogenous Peptides and Proteins
	Directly from Tissue on High Resolution Mass Spectrometers
11:30 am - 12:00 pm	Jeffrey Spraggins, Vanderbilt University
	Integrating the Spatial Domain and Top-Down Proteomics using Mass
	Accuracy: Enhancing Protein Mapping for Biological Applications
12:00 - 12:30 pm	Closing Remarks

Poster List

All posters are located in the Banyan Breezeway odd-numbered posters will be presented on Friday from 8:00 - 10:00 pm even-numbered posters will be presented on Saturday from 8:00 - 10:00 pm All posters should be set up by 7:00 pm on Thursday Remove all posters by 11:00 am on Sunday

- N-terminal Top-Down Protein Sequencing by ETD-UHR-TOF Mass Spectrometry; Christian Albers, Ralf Hartmer, Wolfgang Jabs; Bruker Daltonik GmbH, Bremen, Germany
- 2 LC-MS Analysis of Intact Enzymes using the Synapt G2 Mass Spectrometer; <u>Ioana M. Barbu</u>, Michiel Akeroyd, Rob A.M. van der Hoeven, Maurien M.A. Olsthoorn, Marcel W.E.M. van Tilborg; *DSM Biotechnology Center, Analysis Department, Delft, The Netherlands*
- 3 Identification of MALDI Imaging MS peaks by Top-Down Proteomics; Marshall Bern, Christopher Becker, Yong J. Kil, Peggi Angel, Kristie Rose, David Anderson, Dhananjay Sakrikar, Kevin Schey and Richard Caprioli; Protein Metrics Inc., San Carlos, CA; Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN
- 4 **Top-Down Proteomics using High Resolution Mass Spectrometry and Online Core-Shell HPLC Protein Separation;** Christopher Bolcato¹; Xianglin Yuan¹; Matthew Maust¹, Amy Flynn¹; Matthew Powell¹; ¹Protea Biosciences Group, Inc., Morgantown, WV

5

MS based Characterization of Soluble and Membrane-Bound Forms of Synaptic Proteins;

Ann Brinkmalm¹, Gunnar Brinkmalm¹, William G. Honer², Henrik Zetterberg¹, Joel Jakobsson¹,

Kaj Blennow¹, and Annika Öhrfelt¹; ¹Institute of Neuroscience and Physiology, The Sahlgrenska

Academy at University of Gothenburg, Sahlgrenska University Hospital, Mölndal, Sweden

²Centre for Complex Disorders, Department of Psychiatry, University of British Columbia,

Vancouver General Hospital Research Pavilion, Vancouver, BC, Canada

- Comprehensive Characterization of Amyloid β Peptides from Endogenous Peptides in Cerebrospinal Fluid to Synthetic Dimers; Gunnar Brinkmalm¹, Ann Brinkmalm¹, Tiernan O'Malley², Erik Portelius¹, Maria Olsson¹, Jessica M. Mc Donald², Dominic M. Walsh², Henrik Zetterberg¹, and Kaj Blennow¹; Institute of Neuroscience and Physiology, The Sahlgrenska Academy at University of Gothenburg, Sahlgrenska University Hospital, Mölndal, Sweden ²Brigham and Women's Hospital, Harvard Medical School, Boston, MA
- Characterising the Mouse Protamine PTMome* using Bottom-Up and Top-Down Proteomics * PTMome (pē tē em-ōm) = the Entire Set of Post-Translational Modifications (PTMs) on Proteins Expressed by a Genome, Cell, Tissue or Organism; Andrea M Brunner¹, Paolo Nanni², Isabelle M Mansuy¹; * Brain Research Institute, UZH/ETHZ, * Functional Genomics Center Zurich, UZH/ETHZ, Switzerland
- 9 Comparison of 193 nm UVPD, ETD, HCD and CID for Characterization of Multiple Engineered Green Fluorescent Protein Isoforms with Varying Isoelectric Points; Joe Cannon, Christian Kluewe, Andrew Ellington and Jennifer Brodbelt; *University of Texas, Austin, TX*
- 10 Comparative Study of Fractionation Methods for Top-down Analysis of Complex Protein Mixtures; Avantika Dhabaria¹; Yan Wang¹; Catherine Fenselau¹; Nathan Edwards²; ¹University of Maryland, College Park, MD ²Georgetown University Medical Center, Washington, D. C.

- Top-Down Analysis of Histone Post-Translational Modifications by Electron Capture
 Dissociation Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Xibei Dang¹,
 Jenna Scotcher², Yeqing Tao¹, Alan G. Marshall^{1,2}, and Nicolas L. Young²; ¹Department of
 Chemistry and Biochemistry, Florida State University, 95 Chieftain Way, Tallahassee, FL; ²Ion
 Cyclotron Resonance Program, National High Magnetic Field Laboratory, 1800 East Paul Dirac
 Drive, Tallahassee, FL
- Type IV pili of Pathogenic Neisseria meningitidis Sickly Sweet Appendages; Joseph Gault¹, Christian Malosse¹, Guillaume Duménil², Catherine Costello³, Julia Chamot-Rooke¹; Institut Pasteur, CNRS UMR3528, Unité de Spectrométrie de Masse Structurale et Protéomique, Paris 75015, France; INSERM U970, Paris Cardiovascular Research Center, Paris 75015, France; Center for Biomedical Mass Spectrometry, Department of Biochemistry, Boston University School of Medicine, Boston, MA
- Top-Down Identification of Casein Isoforms using a High Performance Benchtop Quadrupole Orbitrap Mass Spectrometer; <u>David M. Horn</u>, Terry Zhang, Yi Zhang, and Guifeng Jiang; *Thermo Fisher Scientific*
- Verification of Glycosylation of the Recombinant Human Granulocyte Colony Stimulating Factor (G-CSF) produced in HEK293 cells by Top-down Mass Spectrometry; Sergei Ilchenko¹; Alexander V. Gasparian²; Janna Kiselar¹; Natalia D. Tararova², Mark R. Chance¹; Anton A. Komar^{2,3}; 1-Case Western Reserve University, 2-DAPCEL Inc, 3-Cleveland State University, Cleveland, OH
- Mass Spectrometric Immunoassay Workflow for the Determination of Human IGF1; <u>Urban A. Kiernan¹</u>, David A. Phillips¹, Kemmons A. Tubbs¹, Dobrin Nedelkov¹, Bryan Krastins², Mary F. Lopez², and Eric E. Niederkofler¹; *ThermoFisher Scientific*, 2155 E. Conference Dr., Suite 104, Tempe, AZ; ² ThermoFisher Scientific BRIMS, 790 Memorial Dr., Cambridge, MA
- Top-Down Mass Spectrometry Approach for Structural Analysis of Proteins using Covalent Labeling; Sergei Ilchenko1; Janna Kiselar1; Alexandra Klinger2, Paul Axelsen2 and Mark R. Chance1; Case Western Reserve University, Cleveland, OH; University of Pennsylvania, PA
- 17 **Intact Protein (PTM) Characterization: Top-Down Proteomics Approach;** Ravi K Krovidi, *Agilent Technologies Pvt. Ltd, Bangalore, 560 048, India*
- Identification of Proteins with Multiple Post-Translational Modifications using Top-Down Tandem Mass Spectra; Xiaowen Liu^{1,3}, Shawna Hengel², Si Wu², Nikola Tolić², Ljiljana Pasa-Tolić², and Pavel A. Pevzner³; ^I School of Informatics, Indiana University-Purdue University Indianapolis; ² Biological Science Division, Pacific Northwest National Laboratory; ³ Department of Computer Science and Engineering, University of California, San Diego, CA
- 19 **Ion Mobility Mass Spectrometry and top-down Electron Transfer Dissociation of Intact Proteins on a Quadrupole/TOF Instrument;** Lermyte, F. a,b,c, Valkenborg, D. a,c, Sobott, F. a,b; a

 CFP-CeProMa, University of Antwerp, Belgium; b Department of Chemistry, University of

 Antwerp, Antwerp, Belgium; MANT, VITO, Mol, Belgium
- Top-Down MS Analysis Reveals Binding Site between S. pneumoniae Pilin Domains; Anne-Marie di Guilmi¹, Unige Laskay², Yuri Tsybin², Christophe Masselon³; CEA, Institut de Biologie Structurale Jean-Pierre Ebel, F-38027 Grenoble, France; Biomolecular Mass Spectrometry Laboratory, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland; CEA, IRTSV, Biologie à Grande Echelle, F-38054 Grenoble, France

- 21 Structure Determination, Specificity and Affinity of Fibril- Inhibiting β-Amyloid Epitopes Recognized by Serum Anti-Aβ-Autoantibodies; Claudia Cozma¹, Adrian Moise¹, Marius Iurascu¹, Gabriela Paraschiv¹, Madalina Maftei¹, Alina Petre^{1,3}, Gabor Mezo⁴, Ferenc Hudecz⁴ Marilena Manea^{1,2}, Michael Gross³ and Michael Przybylski¹*; ¹Department of Chemistry, Laboratory of Analytical Chemistry and Biopolymer Structure Analysis, and ²Zukunftskolleg, University of Konstanz, Konstanz, Germany; ³Department of Chemistry, Washington University St. Louis, St. Louis, MO; ⁴Department of Peptide Chemistry, Hungarian Academy of Sciences, Budapest, Hungary
- Top-Down MS Identification of New *O*-Glycosylated Apolipoprotein-CIII Isoforms in Ultrahigh Resolution Human Serum Profiles; Simone Nicolardi *, Yuri E.M. van der Burgt, Manfred Wuhrer, Paul J. Hensbergen, and André M. Deelder; Leiden University Medical Center (LUMC), Technology Focus Area Proteomics & Metabolomics, Albinusdreef 2, 2300 RC, Leiden, The Netherlands
- Examining the Charge State Protein Conformation Relationship by H/D Exchange Electrospray Ionization and Electron Capture Dissociation Mass Spectrometry; Teerapat Rojsajjakul, Fred L. King*; C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV
- 24 **Protein Unfolding & Refolding in the Gas Phase;** Moritz Schennach, <u>Kathrin Breuker</u>; *Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI)*; *University of Innsbruck, Innrain 80/82, 6020 Innsbruck, Austria*
- Suggestions for a Protein Species Terminology; <u>Hartmut Schlüter (1)</u>, Peter Jungblut (2), Hermann-Georg Holzhütter (3), Rolf Apweiler (4); (1) University Medical Center Hamburg-Eppendorf, Germany. (2) Max Planck Insitute of Infection Biology, Berlin, Germany. (3) Charité University Medicine, Berlin, Germany. (4) EMBL Outstation European Bioinformatics Institute, Hinxton, Cambridge, Great Britain.
- 26 **193 nm Ultraviolet Photodissociation in an Orbitrap Elite Mass Spectrometer for Top- Down Proteomics**; Jared B. Shaw and Jennifer S. Brodbelt; *The University of Texas, Austin, TX*
- The Ugly Duckling of Top-Down Mass Spectrometry; Shannon Cornett, Detlev Suckau, Rainer Paape and Anja Resemann; Bruker Daltonik GmbH, Bremen, Germany
- Using Isotopic Mass-to-charge Ratio and Envelope Fingerprinting to Decode Biological Mass Spectra; Li Li, ZhixinTian; Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Liaoning 116023, China
- 29 **Top-Down Analysis of Histone H4**; <u>Jeremy J. Wolff</u> and Christopher J. Thompson; *Bruker Daltonics*, *Billerica*, *MA*
- 30 Spatially Resolved Extraction of Proteins from Tissues and Blood Spots for Top Down Analysis using a Continuous Flow Liquid Microjunction Surface Sampling Probe (LMJ-SSP); Gary J. Van Berkel, Vilmos Kertesz, Joshua J. Nicklay, Kristie L. Rose, Kevin L. Schey, Richard M. Caprioli and Jeremy L. Norris; Oak Ridge National Laboratory, Oak Ridge, TN; Mass Spectrometry Research Center, Vanderbilt University School of Medicine, Nashville, TN

- Elucidating the Sites of Metal Binding Important in Fibrillation of α-Synuclein by Top-Down Mass Spectrometry; Piriya Wongkongkathep, Sheng Yin, and Joseph A. Loo; Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA
- Top-down Study for Heterocyclic Amine Hemoglobin Adducts; Min Yang 1, Neelam Zahoor 2, Maria Ospina 2, Hubert Vesper 2; 1 Battelle Memorial Institute, Atlanta, GA 30345, 2 Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA
- 33 **Systematic Evaluation of Ultrahigh Resolution MS Instrument Parameter to Optimize Topdown Analysis**; Martin Zeller, Mathias Mueller, Eugen Damoc, Eduard Denisov, Dirk
 Nolting and Thomas Moehring *Thermo Fisher Scientific, Bremen, Germany*
- Optimization of the High Performance Liquid Chromatography (HPLC) Separation for Characterization and Quantitation of Histone Proteoforms; Zhaorui Zhang¹, Si Wu¹, Rui Zhao¹, Nikola Tolić¹, David L. Stenoien², Rosalie K. Chu¹ and Ljiljana Paša-Tolić¹; Environmental Molecular Science Laboratory, Pacific Northwest National Laboratory; Fundamental & Computational Sciences Division, Pacific Northwest National Laboratory