WOF am 08:00
‘Eye-Tracking’ of Proteins from Human Intraocular Fluids – Qualitative and Quantitative Approaches Toward Understanding the Progression of Eye Disease; Keiryn L. Bennett1; Marion Funk2; Andreas Polleisz3; Marion Tschernutter1; Melanie Planyavsky1; Katja Parapatric1; Florian P. Breitwieser1; Cecereena Ubaida Mohien1; Andre Mueller1; Zlatko Trajanoski1; Jacques Colinge1; Giulio Superti-Furga1,2,3; Ursula Schmidt-Erfurth1
CeMM - Center for Molecular Medicine, Vienna, Austria; 1Medical University of Vienna, Vienna, Austria; 3Technical University of Graz, Graz, Austria

WOF am 09:00
Proteome Analysis of Cerebrospinal Fluid: Monitoring Changes in Protein Abundance over the Course of Antiretroviral Therapy in HIV Infected Individuals; Thomas Angel1; Jon Jacobs1; Richard Price2; Serena Spudich2; Marina Gritsenko1; Dietmar Fuchs3; Lars Rosengren4; 1German Sport University, Cologne, Germany; 2University of Turin, Turin, Italy; 3Technical University of Graz, Graz, Austria; 4Sahlgrenska Cancer Institute, Gothenburg, Sweden

WOF am 09:30
Quantitation by High Resolution Full Scan Accurate Mass – The Future of Discovery DMPK? Jonathan L. Josephs; Yanou Yang; Chiwuwa Emily Luk; Petia Shipkova; William Humphreys; Bristol-Myers Squibb, Pennington, NJ

WOF am 09:50
Evaluating the Intestinal Health of Premature Infants by NanoLC-MS Analysis of Excreted Oligosaccharides; Maria Lorna A. de Leoz1,2; Shuai Wu1; Mark Underwood3; Peggy Cheng1; John S. Strumi1; Rudolf Grimm1; Bruce German1; David Mills1; Carlito B. Lebrilla1; 1University of California, Davis, CA; 2Biocentre, Innsbruck Medical University, Innsbruck, Austria; 3Sahlgrenska Academy at University of Gothenburg, Gothenburg, Sweden

WOF am 10:10
Mass Spectrometric Characterization of Arylpropionamide-Derived Selective Androgen Receptor Modulators and their in-vitro and in-vivo Generated Metabolites; Mario Thevis1; Enrico Gerace2; Hans Geyer2; Wilhem Schänzer1; 1German Sport University, Cologne, Germany; 2University of Technology, Vienna, Austria

10:30 AM – 2:30 PM, WEDNESDAY POSTER SESSION
Exhibit Hall ABCDE

WOA pm 2:30
Gas-Phase Substitution and Elimination Reactions of Vinlyc and Aryl Halides; Allison Eanes; Diogo de Oliveira; Michele Khurana; Renan Joviliano; Scott Gronert; Virginia Commonwealth Uni, Richmond, VA

WOA pm 2:50
Original Formation and Reactivity on Double Bonds of Dichlorocarbene at Atmospheric Pressure Studied by Photoionization Mass Spectrometry; David Touboul1; Julie Allegrande1; Alexandre Giuliani1; Olivier Laprévote1; CNRS-ICSN, Gif-Sur-Yvette, France; 2Synchrotron Soleil, Gif-Sur-Yvette, France

WOA pm 3:10
Does the 2,6-Didehydroxyproridium Ion Exist? Bartlomiej J. Jankiewicz1,2; Nelson R. Viruzela1; Lindsey M. Kipkpatrick1; John J. Nash1; Hilkka I. Kenttämaa1; 1Department of Chemistry, Purdue University, West Lafayette, Indiana; 2Military University of Technology, Warsaw, Poland

WOA pm 3:30
Gas Phase Reactions of Carbanions with H Atoms; Zhibo Yang1; Oscar Martinez Jr.1; Brian Eichelberger2; Marshall Carpenter1; Theodore P. Snow1; Veronica M. Bierbaum1; 1Oak Ridge National Lab, Knoxville, TN; 2UTK-Oak Ridge National Lab, Knoxville, TN

WOA pm 3:50
Investigating the Role of Cation Recombination Energy as a Key Factor in ETD/ECD; Marija Mentinova1; David Crizer2; Takashi Baba2; Gary L. Glish3; Scott A. Eichelberger4; John J. Nash1; Hilkka I. Kenttämaa1; 1UTK-Oak Ridge National Lab, Knoxville, TN; 2Media University of California, Davis, CA; 3Univ. of California, San Diego, San Diego, CA; 4Institute for Systems Biology, Seattle, WA

8:30 – 10:30 AM, WEDNESDAY MORNING CHARACTERIZING PTMs
Andy Tao, presiding
Room: Hall 4

WOG am 08:30
Quantitative Mass Spectrometry Reveals Complexity and Function of Protein Ubiquitination; Junmin Peng; Emory University, Atlanta, GA

WOG am 08:50
Improved Methodologies for the Identification of Ubiquitin and Ubiquitin-Like Protein (Ubl) Conjugation Sites Identifies Novel Ubl Chain Linkages; Tharan Srikumar1,2; Stanley Jeram1,2; Xiang-Dong Zhang1; H. Anne Eisenhauer1; Richard Rogers1; Patrick G.A. Pedrioli1; Michael Matunis3; Henry Lam1; Brian Raught1,2; 1Ontario Cancer Institute, Toronto, Canada; 2Medical Biophysics, University of Toronto, Toronto, Canada; 3Dept. Biological Sciences, Wayne State University, Detroit, MI; 4Institute for Systems Biology, Seattle, WA; 5Institute of Biochemistry ETH, Zurich, Switzerland; 6Biochem. and Mol. Biol. The Johns Hopkins Univ., Baltimore, MD; 7Dept Chem Biomol Engineer. Hong Kong Univ Sci Tech, Clear Water Bay, Hong Kong

58th ASMS Conference on Mass Spectrometry

2:30 – 4:30 PM, WEDNESDAY AFTERNOON FUNDAMENTALS: ION/MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS
Hilkka Kenttämaa, presiding
Room: Ballroom IJ

University, Detroit, MI; 1Institute for Systems Biology, Seattle, WA; 2Institute of Biochemistry ETH, Zurich, Switzerland; 3Biochem. and Mol. Biol. The Johns Hopkins Univ., Baltimore, MD; 7Dept Chem Biomol Engineer. Hong Kong Univ Sci Tech, Clear Water Bay, Hong Kong

10:00 AM – 12:00 PM, WEDNESDAY AFTERNOON FUNDAMENTALS: ION/MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS
Hilkka Kenttämaa, presiding
Room: Ballroom IJ

10:00 AM – 12:00 PM, WEDNESDAY AFTERNOON FUNDAMENTALS: ION/MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS
Hilkka Kenttämaa, presiding
Room: Ballroom IJ
### FTMS: INSTRUMENTATION AND APPLICATIONS

#### 2:30 – 4:30 PM, WEDNESDAY AFTERNOON

**Room:** Ballroom ACE

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<th>Session</th>
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<tr>
<td>WOB pm 2:30</td>
<td><strong>Overview:</strong> Recent Advances in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry</td>
<td>Alan G. Marshall; Ion Cyclotron Resonance Prog, Tallahassee, FL</td>
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<tr>
<td>WOB pm 2:50</td>
<td><strong>Harmonization of Electric Field in FT ICR Cell, The New Approaches</strong></td>
<td>Ivan Boldin; Eugene Nikolaev; The Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation</td>
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<tr>
<td>WOB pm 3:10</td>
<td><strong>Examining Time-Dependent Space-Charge Effects in FT ICR Mass Spectrometry With Multiparticle Simulations of Ion Motion</strong></td>
<td>Jon Amster1; Franklin E. Leach III1; Andriy Kharchenko; Ron M.A. Heeren2; Eugene Nikolaev3; Konstantin Aizikov; Peter B. O’connor; 1University of Georgia, Athens, GA; 2FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands; 3BUSM, Boston, MA; 4The Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; 5FOM Inst. Atomic/Molecular Phy, Amsterdam, Netherlands; 6University of Warwick, Coventry, UK</td>
</tr>
<tr>
<td>WOB pm 3:30</td>
<td><strong>A Gas-Phase Reactivity Study of a σ,σ,σ- Tetra-radical Ion – the 2,4,6-Tridehydroxypridine Radical Cation</strong></td>
<td>Vanessa Gallardo1; Bartlomiej Jankiewicz2; Nelson Vinueza3; John Nash4; Hilka Kettamaa5; 1Purdue University, West Lafayette, IN; 2Military University of Technology, Warsaw, Poland</td>
</tr>
<tr>
<td>WOB pm 3:50</td>
<td><strong>Tailored Ion Spatial Distribution in FT-ICR MS for Improved Analysis of Complex Mixtures</strong></td>
<td>Nathan K. Kaiser1; Joshua J. Savory2; Amy M. McKenna3; Christopher L. Hendrickson4; Alan G. Marshall5; National High Magnetic Field Laboratory, Tallahassee, FL; 1Ion Cyclotron Resonance Prog, Tallahassee, FL</td>
</tr>
<tr>
<td>WOB pm 4:10</td>
<td><strong>Top-Down Proteomic Identification of Heavy Isootope Depleted Yeast Proteins Using LC-FTICR MS With Funnel-Skimmer Dissociation Fragmentation</strong></td>
<td>Jennifer S. Cobbs1,2; Aimée M. Morris3; Michael L. Easterling4; Jeffrey N. Agar5; 1Brandeis University, Waltham, MA; 2Braker Daltonics, Inc., Billerica, MA</td>
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### MS IN ENVIRONMENTAL TOXICOLOGY

#### 2:30 – 4:30 PM, WEDNESDAY AFTERNOON

**Room:** Ballroom BDF

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<tr>
<td>WOC pm 2:30</td>
<td><strong>Linking Mass Spectrometry with Toxicology for Emerging Water Contaminants</strong></td>
<td>Susan Richardson; US EPA, NERL, Athens, GA</td>
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<tr>
<td>WOC pm 2:50</td>
<td><strong>Arsenic Interaction with Proteins and Detecting Arsenic-Binding Proteins in Human Cells Using Mass Spectrometry and Affinity Chromatography</strong></td>
<td>Huiming Yan1; Michael Weinfield2; William Cullen3; Xiufen Lu4; Baowei Chen5; Meiling Lu6; Zhongwen Wang7; Anthony McKnight-Whitford8; X. Chris Le9; 1University of Alberta, Edmonton, Canada; 2University of British Columbia, Vancouver, Canada</td>
</tr>
<tr>
<td>WOC pm 3:10</td>
<td><strong>Quantitative Analysis of 6-Thioguanine-Induced Changes in the Proteome of Jurkat-T Cells</strong></td>
<td>Fan Zhang; Yinheng Wang; University of California, Riverside, CA</td>
</tr>
<tr>
<td>WOC pm 3:30</td>
<td><strong>Quantification of the HSP 70 and HSP 90 Response to Environmental Stress in Pacific Oysters Using Orthologue-Based Multiple Reaction Monitoring</strong></td>
<td>David Cassis; Shujun Lin; Cordula Klockenbusch; Juergen Kast; University of British Columbia, Vancouver, Canada</td>
</tr>
<tr>
<td>WOC pm 3:50</td>
<td><strong>Inhibition of 4-Aminobiphenyl-Induced DNA Damage by Sulforaphane and 5,6-Dihydrocyclopenta[c]-Dithiole-3(4H)-Thione in Bladder Cells and Tissues</strong></td>
<td>Kristen L. Randall1; Dayana Argoti2; Yi Ding3; Joseph D. Paonessa4; Rex Munday5; Yuesheng Zhang6; Paul Vouros7; 1Northeastern University, Boston, MA; 2Protein Forest, Lexington, MA; 3Roswell Park Cancer Institute, Buffalo, NY; 4Ruakura Research Center, Hamilton, New Zealand</td>
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<td>WOC pm 4:10</td>
<td><strong>Determination of Chlorpyrifos and Chlorpyrifos-Oxon in Rat Blood Using Isotope Dilution Technique by GC Quadrupole and Magnetic Sector MS</strong></td>
<td>Yvacheslav N. Fishman1; Alaine Sledz2; Kathy A. Brzak3; Michael J. Bartels4; 1The Dow Chemical Company, Midland, MI; 2Kelly Services Inc., Midland, MI</td>
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#### MS OF GLYCOPROTEINS

**Room:** Room 155

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<th>Session</th>
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<tr>
<td>WOD pm 2:30</td>
<td><strong>Influence of Peptide Length on the Gas-Phase Fragmentation of Pronase-Derived Glycopeptides</strong></td>
<td>Wen Zhou; Kristina Hakansson; University of Michigan, Ann Arbor, MI</td>
</tr>
<tr>
<td>WOD pm 2:50</td>
<td><strong>Development of a Hyphenated Ion Mobility - Mass Spectrometry Technique for the Characterization of Glycosylated Peptides</strong></td>
<td>Craig Dorschel1,2; Jim Langridge1,2; Scott Geromano3,4; 1Waters Corporation, Milford, MA; 2Kelly Services Inc., Midland, MI</td>
</tr>
<tr>
<td>WOD pm 3:10</td>
<td><strong>Monitoring Quantitative Changes in Protein Specific Glycosylation during Lactation Using MALDI-FTICR MS and Its Effect on Interactions with Pathogenic Bacteria</strong></td>
<td>Mariana Barboza1; John W. Froehlich; Janneth Pinzon2; Isabelle Moeller; J. Bruce Germ; Bart Weimer; Carlito Lebrilla; University of California Davis, Davis, CA</td>
</tr>
<tr>
<td>WOD pm 3:30</td>
<td><strong>A Novel Tandem Mass Spectrometry Approach for the Detection and Identification of O-GlcNAc-Modified Peptides</strong></td>
<td>Hannes Hahne; Simone Lemeer; Bernhard Kuster; Technical University Munich, Freising, Germany</td>
</tr>
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</table>
| WOD pm 3:50 | **Complementary N-Linked Glycoproteomics of Myocardial Ischemia / Reperfusion Injury Reveals Complex Changes in Extracellular Environments** | Benjamin Parker1; Giuseppe Palmisano2; Alistair Edwards3; Melanie White4,5; Kasper Engholm-Keller3; Brett Hamby1; Albert Lee1; Daniel Kolarich2; Nicki Packer1; Martin Larsen1; Stuart Cordwell1,2; 1The University of Sydney, NSW, Australia; 2The University of
2:30 – 4:30 PM, WEDNESDAY AFTERNOON
LC-MS OF REACTIVE XENOBIOTIC METABOLITES
JinPing Gan, presiding
Room: Hall 2

WOE pm 2:30 Overview of LC-MS Techniques to Characterize Reactive Xenobiotic Metabolites; Raju Subramanian; Pharmacokinetics and Drug Metabolism, Thousand Oaks, CA

WOE pm 2:50 High-Throughput Screening of Drug Reactive Metabolites Using Accurate Mass Based Background Subtraction and Noise Reduction Algorithm; Shuguang Ma; Yuan Yuan; Xiaowen Lu; Anima Ghosal; Keun-Joong Lee; Peijuan Zhu; Wei Tong; Kevin Alton; Swapan Chowdhury; Merck Research Laboratory, Kenilworth, NJ

WOE pm 3:10 Characterization of Stereo Conformation of the Reactive Metabolites of the Chlorogenic Acid by UPLC/ Ion Mobility/TOF MS; Cen Xie1; Kate Yu2; Xiaoyan Chen3; Tao Yuan4; Daofang Zhong5; Hayley Crowe6; John P. Shockcor2; Alan L Millar2; 1Chemical & Systems Biology, Stanford University, Stanford, CA; 2AB SCIEX, Concord, ON

WOE pm 3:30 Screening of Glutathione and Cyanide Adducts Using Precursor Ion and Neutral Loss Scans-Dependent Acquisition of Enhanced MS and MS/MS Spectra; Hua-Fen Liu1; Weiping Zhao2; Wenyong Jian3; Elliott Jones4; Mingshe Zhu5; 1AB SCIEX, Foster City, CA; 2Bristol-Myers Squibb, Princeton, NJ; 3Johnson & Johnson PRD, Raritan, NJ

WOE pm 3:50 Human Serum Albumin Cys34 Adducts as a Biomarker for Exposure to Unknown Reactive Chemicals; Jian Cai; Frederick W. Benz; Donald E. Nerland; Harrell E. Hurst; William M. Pierce, Jr.; University of Louisville, Louisville, KY

WOE pm 4:10 Reactive Intermediates in the Oxidative Pathway of Haloperidol to its Neurotoxic Pyridinium Metabolite Identified by On-Line Electrochemistry/ Mass Spectrometry; Tove Johansson Malin1,2; Lars Weidolf1; Neal Castagnoli, Jr.3; Ulrik Jurva4; 1AstraZeneca R&D Mölnal, Mölnal, Sweden; 2University of Gothenburg, Gothenburg, Sweden; 3Virginia Tech and The Edward Via Virginia College, Blacksburg, VA

2:30 – 4:30 PM, WEDNESDAY AFTERNOON
MS OF PHARMACEUTICALS AND PERSONAL CARE PRODUCTS IN WATER
Dil Ramanathan, presiding
Room: Hall 3

WOF pm 2:30 Pharmaceuticals and their Metabolites in Drinking-Water: Breaking the Part-Per-Trillion Concentration Barrier with

WOF pm 2:50 Quantification of Protein Copy Number and Robustness in the Store-Operated Calcium Signaling Network Using Selective Reaction Monitoring (SRM) Mass Spectrometry; Ellen Abell1; Paola Picotti2; Tobias Meyer1; Ruedi Aebersold1; 1Chemical & Systems Biology, Stanford University, Stanford, CA; 2Institute for Molecular Systems Biology, ETH Zurich, Zurich, Switzerland

WOF pm 3:30 A Global Protein Kinase and Phosphatase Interaction Network in Yeast; Ashton Breitkreuz1; Hyungwon Choi2; Jeff Sharom1; Lorrie Boucher1; Victor Nedeva1; Brett Larsen1; Zhen-Yuan Lin3; Bobby-Joe Breitkreuz4; Chris Stark1; Guomoin Liu1; Gloria Kreitinger1; Mark Tervo5; Ron Stewart2; James A Thomson1, 2; 1AstraZeneca R&D, Macclesfield, UK; 2University of Michigan, Ann Arbor, MI

WOF pm 3:50 Rapid Quantitation of mRNA, Proteins, and PTMs Applied to a Systems-Level Analysis of Human ES, iPS, and Fibroblast Cells; Doug Phanstiel1; Justin Brumbaugh1; Craig Wenger1; Danielle L Swaney1; Gloria Kreitinger1; Mark Tervo5; Ron Stewart2; James A Thomson1, 2; 1AstraZeneca R&D, Macclesfield, UK; 2University of Michigan, Ann Arbor, MI