### TUESDAY MORNING ORAL SESSIONS, MAY 30

- **8:00 – 8:45 am:** PLENARY LECTURE
  - Recipient of the Award for a Distinguished Contribution in Mass Spectrometry

- **8:45 – 10:15 am:** POSTER SESSION AND EXHIBITS

- **10:15 am – 12:15 pm:** PARALLEL SESSIONS

### METABOLITE IDENTIFICATION USING HYPHENATED MS TECHNIQUES

**James A. Yergey,** presiding

**TOA am 10:15**
- Data Independent Acquisition for Metabolite Identification Using Alternating High and Low Energy Scans with a QToF Instrument; **Russell Mortishire-Smith**; **Mark Wrana**; **Desmond O’Connor**; **Kevin P. Bateman**; **Merck Sharp and Dohme, Harlow, United Kingdom**

**TOA am 10:35**
- Towards Comprehensive Detection of Metabolites Using Polarity Switching Data Collection and Post-Acquisition Data Mining Strategies; **Carmat Seto**; **Gary Impye**; **Applied Biosystems/MDS Sciex, Concord, Canada**

**TOA am 10:55**
- Characterization of *in vivo* and *in vitro* Metabolites of a PDE4 Inhibitor By LC-MS/MS and 1H NMR; **Chandra Prakash**; **Miao Zhang**; **Pfizer Global Research & Development, Groton, CT**

**TOA am 11:15**
- Cross Correlation Algorithms Combined with MS/MS Spectral Libraries of Structural Analogues for the Automated Regional Assignment of Metabolic Modification; **Jonathan Josephs**; **Stephen Johnson**; **Brian Claus**; **Robert Langish**; **Bristol-Myers Squibb, Hopewell, New Jersey**

**TOA am 11:35**
- Metabolite Prediction and a Two-Step Metabolite Identification Approach in Early Drug Discovery; **Peter L Jacobs**; **Harrie AM Peters**; **Lars Ridder**; **Markus Wagener**; **NV Organon, Oss, The Netherlands**

**TOA am 11:55**
- What and How Much Information Can We Really Extract in an Automated Manner from LC/MS Data? **Robyn A. Rourke**; **John P. Walsh**; **Bayliss"
**DETECTION AND DECONTAMINATION OF INDOOR ENVIRONMENTS**

Scott A Gerber; Steven P Gygé; Harvard Medical School, Boston, MA; Dartmouth Medical School, Hanover, NH

**TOC am 11:35**

Novel Strategy for Rapid Screening and Quantification of Biomarkers in Serum; Bruno Domon; Jianru Zeng-Stahl; Ruedi Aebersold; IMSB - ETH Zurich, Zurich, Switzerland; Applied Biosystems, Darmstadt, Germany

**TOC am 11:55**

XMudPIT – A Novel Approach for Multidimensional Separation of Peptides with Liquid Chromatography/Mass Spectrometry; Johannes A. Hewel; John R. Yates III; The Scripps Research Institute, La Jolla, CA

**GLYCOMICS**

Heather Desaire, presiding

**TOD am 10:15**

Specificity of Glycosaminoglycan Binding to CCR2 Chemokines: Significance of Sulfation Binding sites; Julie A. Leary; Matthew D. Sweeney; University of California, Davis, CA

**TOD am 10:35**

Comparative Glycoproteomics of the Trypanosoma Cruzi Lifecycle; Ron Orlando; James Atwood; Art Nuccio; Fernanda Ludolf; Brent Weatherly; Rick Tarleton; CCRG/UGA, Athens, GA; Department of Cellular Biology, UGA, Athens, GA

**TOD am 10:55**

Comparative Glycomic Profiling through Solid-phase Deuteromethylation and Permethylation; Yehia Mechref; Pilsoo Kang; Milos V Novotny; METACyt Biochemical Analysis Center, Bloomington, IN 47405; Department of Chemistry, Indiana University, Bloomington, IN 47405

**TOD am 11:15**

Novel Tags for the Stable Isotopic Labeling of Carbohydrates and Quantitative Analysis by Mass Spectrometry; Michael J. Bowman; Joseph Zaia; Boston University School of Medicine, Boston, MA

**TOD am 11:35**

Using Ion-Pairing for Acidic Glycopeptide Analysis; Ying Zhang; Hui Jiang; Edward P. Go; Janet Irunгу; Dilusha S. Dalpathado; George R. Bousfield; Heather Desaire; Department of Chemistry, University of Kansas, Lawrence, KS; Department of Biology, Wichita State University, Wichita, KS

**TOD am 11:55**

Quantification, Isobar Resolution and High Throughput Analysis of Carbohydrate Glycans; Vernon N. Reinhold; David J. Ashline; Anthony J. Lapadula; Hailong Zhang; Justin M. Prien; Center for Structural Biology, UNH, Durham, NH

**INTACT PROTEIN SEPARATIONS AND MS**

Martha M. Vestling, presiding

**TOD am 10:15**

Analysis of Human Esophagus Tissue Proteins through Automated Integration of Monolithic-LC with On-Plate Digestion for MALDI-MS and Intact MW Analysis; David M. Lubman; Chul Yoo; Suping Zheng; Jia Zhao; Manoj Pal; Katie Hersberger; Christian G. Huber; David G. Beer; University of Michigan, Ann Arbor, MI; Saarland University, Saarbrucken, Germany

**TOD am 10:35**

When Mass Spectrometry “Gels”; Rachel R. Ogorzalek Loo; Yanan Yang; Ivory Peng; Jason Dunsmore; Jentiae Shiea; Joseph A. Loo; University of California, Los Angeles, CA; National Sun Yat-Sen University, Kaohsiung, Taiwan

**TOD am 10:55**

High-throughput Identification of Intact Proteins and Comparative Analysis of Saccharomyces Cerevisiae using 15N/15N Metabolic Labeling and Top-Down Proteomics; Bryan A. Parks; Jon T. Ferguson; Yi Du; Patricia Burke; Kurt Kwast; Allen Marshall; Chris Hendrickson; Tanner Schaub; Neil Kelleher; Univ. of Illinois, Champaign, Illinois; National High Magnetic Field Laboratory, Tallahassee, Florida

**TOD am 11:15**

Reversed-Phase LC/UV/MS for Characterizing Heterogeneity of Intact Monoclonal Antibodies; Thomas M. Dillon; Douglas S. Rehder; Gary D. Pipes; Margaret Ricci; Himanshu S. Gadgil; Dirk Chelius; Da Ren; Pavel V. Bondarenko; Angen, Department of Pharmaceutical, Thousand Oaks, California

**TOD am 11:35**

MALDI Proteomics Chip; Harrison K. Musyimi; Hamed Shadpour; Steven A. Soper; Kermit K. Murray; Louisiana State University, Baton Rouge, LA; Center for BioModular Multi-Scale Systems (CBM2), Baton Rouge, LA

**TOD am 11:55**

Rapid, Comprehensive and High-Resolution Intact Protein Separation for Proteomics; Andrew R Pitt; Karl E V Burgess; Ken Cook; Remco Swart; University of Glasgow, Glasgow, UK; Dionex UK, Camberley, UK; Dionex, Amsterdam, Netherlands

**DETECTION AND DECONTAMINATION OF INDOOR ENVIRONMENTS**

Gary Groenewold, presiding

**TOE am 10:15**

Addressing Physio-chemical Controls on Indoor Detection and Decontamination of Chemical Warfare Agents; Adam H Love; Carolyn J Koester; William J Smith; Bradley R Hart; M. Lee Davison; Sharon J Shields; Armando Alcaraz; John G Reynolds; Lawrence Livermore National Laboratory, Livermore, CA

**TOE am 10:35**

Analysis and Detection of Chemical Warfare Agent Surrogates on Polyurethane Foams and Fabrics by Thermal Desorption with Mass Spectrometry Detection; Theodore T. Borek; Deborah Hunka; Sandra National Laboratories, Albuquerque, NM

**TOE am 10:55**

Modification of Metal Contaminants on Oxide Surfaces by Laser Irradiation; Anita K. Gianotto; Recep Avci; Muhammed Deliorman; Eric Williams; Marnie M. Cortez; Robert V. Fox; Gary S. Groenewold; Idaho National Laboratory, Idaho Falls, ID; Montana State University, Bozeman, MT

**TOE am 11:15**

Rapid Separation and Identification of CBW Agents in Food and Consumer Matrices using FAIMS-MS Technology; Beata M. Kolakowski; Margaret A. McCooye; Zoltan Mester; Paul A. D’Agostino; NRC Institute for National Measurement Standards, Ottawa, Canada; Defence Research and Development Canada, Suffield, Canada

**TOE am 11:35**

Detection of Ricin in Food Matrices by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry; Fredrick J. Cox; Lindy Dejarme; Edward R. Richter; Battelle Eastern Science & Tech Center, Aberdeen, MD; Battelle, Columbus, OH; Richter International, Columbus, OH

**TOE am 11:55**

Rapid Identification and Area Delineation of Dispersed Chemicals using a Surface-Sampling TOFMS, Ion Correlation Program, and Inexpensive Autosampler; Andrew H. Grange; Robert J. Cody, Jr.; Wayne Sovcuck; U.S. EPA, ORD, NERL, ESD, Las Vegas, NV; JEOL USA, Inc., Peabody, MA
**ORGANIC REACTION MECHANISMS**
Douglas P. Ridge, presiding

**TOG am 10:15**  Organic Reaction Mechanisms in Mass Spectrometry; Hilkka I. Kenttamaa1; 1Purdue University, West Lafayette, IN

**TOG am 10:35**  Gas Phase Studies of Nucleophilic Substitution and Elimination Reactions Utilizing Deuterium Kinetic Isotope Effects; Veronica M. Bierbaum1; Stephanie M. Villano1; Nicole Eyet1; Shuji Kato1; 1University of Colorado, Boulder, CO

**TOG am 10:55**  Gas Phase Reactivity of Adenine and Derivatives: How Damaged Bases Differ from Natural Nucleobases and Unusual C-H Acidities; Seema Sharma1; Xiaofeng Shi1; Meng Xu1; Jeehiun K. Lee1; 1Rutgers University, Piscataway, NJ

**TOG am 11:15**  H/D Exchange of Deprotonated Amino Acids; Zhixin Tian1; Dana Reed1; Steven R Kass1; 1University of Minnesota, Minneapolis, MN

**TOG am 11:35**  Reactions of Distonic Radical Anions with Molecular Oxygen: Trapping Peroxyl Radicals in the Gas Phase; David G. Harman1; Stephen J. Blanksby1; 1University of Wollongong, Wollongong, Australia

**TOG am 11:55**  Investigation of Aromatic s,s-Biradicals’ Reactions with Nucleosides and Oligonucleotides in an FT-ICR Mass Spectrometer; Linan Yang1; Ryan C. Shea1; Hilkka I. Kenttamaa1; 1Purdue University, West Lafayette, IN

**TUESDAY AFTERNOON, MAY 30**

12:30 – 1:30 pm: INTEREST GROUP MEETINGS

1:30 – 3:00 pm: FOSTER SESSION AND EXHIBITS

3:00 – 5:00 pm: PARALLEL SESSIONS

5:30 – 7:00 pm: WORKSHOPS

**METABOLITE PROFILING**
Oliver Fiehn, presiding

**TOA pm 03:00**  Metabolomics by Chip Based Nanospray Infusion and its Application in Drug Development; Olaf Boerensen1; Stephan Gatzek1; 1Novartis Pharma AG, Basel, Switzerland

**TOA pm 03:20**  Investigation of Analytical Variation in Metabonomic Analysis Using LC-MS; Tim Sangster1; Toby Athersuch2; Ian Wilson2; Lyle Burton3; Julie Wingate4; 1Huntingdon Life Sciences, East Millstone, NJ; 2Imperial College London, London, UK; 3AstraZeneca, Macclesfield, UK; 4Applied Biosystems / MDS Sciex, Toronto, Canada

**TOA pm 03:40**  The Use of Isotope Ratio Measurements to Reduce the Number of Candidate Elemental Compositions from Accurate Mass Determination; Kirsten Hobby1; Robert Bateman1; 1Water Corporation, Micromass MS Technologies, Manchester, UK

**TOA pm 04:00**  Ionizable Isotopic Labeling Reagents for Relative Quantification and Structural Elucidation of Metabolites; Michael R. Shortreed1; Shane M. Lamos1; Brian L. Frey2; Margaret F. Philips1; Peter J. Belshaw1; Lloyd M. Smith1; 1University of Wisconsin, Madison, WI

**TOA pm 04:20**  Metabolomic Profiling of Brain Tissue Extracts from Alcohol Preferring and Non-Preferring Rats; Toward Identification of Alcoholism Biomarkers; Yehia Mechref1; Jason Starkey1; Tatiana Rojkovicova1; Ali Kettani2; Catherine Stacey3; William J. McBride4; Milos V. Novotny1; 1Department of Chemistry, Indiana University, Bloomington, IN; 2METAcyt Biochemical Analysis Center, Bloomington, IN; 3Bruker Daltonics, Billerica, MA; 4Department of Psychiatry, Indiana University, Indianapolis, IN

**54th ASMS Conference on Mass Spectrometry**

**MS CONTRIBUTION TO THE IMMUNOLOGY OF DISEASE**
Anthony W. Purcell, presiding

**TOB pm 03:00**  Characterization of Immune Responses to Pathogen Challenge by MS Based Epitope Excision; Kenneth B. Tomet1; Christine Hager-Braun1; Roxana Jacob1; Jason Williams1; Jeffery F. Kuhn1; 1NIH/NCI, Bethesda, MD; 2Texas Tech University, Carlsbad, CA

**TOB pm 03:20**  Proteomics in Islet Diabetes Research Using Surface Enhanced Laser Desorption/Ionization Time-of-Flight Mass Spectrometry; Peter Bergsten1; Jian-Man Lin1; Henrik Ortsäter1; Tea Sundsten1; 1Uppsala University, Uppsala, Sweden

**TOB pm 03:40**  Direct Discovery of Class I HLA Antigens that Distinguish Virus-Infected and Cancerous Cells; William H. Hildebrand1; Angela Wahl1; Wilfried Bardet1; Melva Gonzalez1; Ken W. Jackson1; Jon Weidanz1; Fredda Schauer1; 1University of Oklahoma HSC, Oklahoma City, OK; 2Texas Tech University, Amarillo, TX

**TOB pm 04:00**  Mass Spectrometry Contributions to Immunology of Disease; Nina Hillen1; 1Institute for Cell Biology, Tuebingen, Germany

**TOB pm 04:20**  Assessing the Diversity of the Immunopeptidome; Frank R Rooney1; Nicholas A Williamson1; 1Applied Biosystems, Melbourne, Australia; 2Bio21, University of Melbourne, Victoria, Australasia

**TOB pm 04:40**  Identification of Modified MHC Class II Self Peptides from Spleen of Listeria Infected Mice; James J Walters1; Anish Suri1; Jamie Ireland1; Shirley Petzold1; Emil R Unnaue1; Michael L Gross1; 1Washington University in St. Louis, St. Louis, MO

**CLINICAL MASS SPECTROMETRY ASSAYS**
Donald H. Chace, presiding

**TOC pm 03:00**  The Growing Acceptance of Mass Spectrometry in Routine Clinical Analysis; Michael Morris1; 1Waters Corporation, Manchester, UK

**TOC pm 03:20**  Analysis of Variance-Principal Component Analysis: A Soft Tool for Proteomic Discovery of MALDI-MS Biomarkers from Amniotic Fluids; Alfred L. Yergey1; Peter de B Harrington1; Nancy E Vieira1; Roberto Romero1; 1NICHD, NIH, Bethesda, MD; 2Chemistry & Biochemistry, Ohio University, Athens, OH

**TOC pm 03:40**  MS-Based High Throughput Identification and Strain Typing of Clinically Relevant Bacteria: Acelinobacter baumanii and Other Drug Resistant Pathogens; Steven A. Hofstadler1; Peter de B Harrington1; Nancy E Vieira1; Roberto Romero1; 1NICHD, NIH, Bethesda, MD; 2Chemistry & Biochemistry, Ohio University, Athens, OH
54th ASMS Conference on Mass Spectrometry

TOC pm 03:00 Clinical Mass Spectrometry Based Immunoassays; Urban A. Kiernan; Kemmons A. Tubbs; Eric E. Niederkofer; Dobrin Nedelkov; Allan L. Bieber; Randall W. Nelson; Intrinsic Bioprobes, Inc, Tempe, AZ

TOC pm 03:20 Profiling Oligosaccharides Shed By Cells for Disease Marker Discovery; Crystal Kirmiz; Bensheng Li; Caroline Chu; Brian Clowers; Hyunjoo An; Suzanne Miyamoto; Ralph DeVere White; Carlito Lebrilla; University of California, Davis, Davis, CA

TOC pm 04:00 Selective Profiling of Proteins in Cancer Cells from Fine Needle Aspirates by MALDI-TOF Mass Spectrometry; Pierre Chaurand; Joseph M Amann; Adriana Gonzalez; James A. Mobley; Pierre P. Massion; David P. Carbone; Richard M. Caprioli; Vanderbilt University Medical Center, Nashville, TN

COSTY pm 03:00 IRMPD of Potential Glycan Markers for Diseases; Carlito B. Lebrilla; University of California, Davis, Davis, CA

TOC pm 03:20 Online Normal-phase Capillary Liquid Chromatography – MALDI-TOF/TOF Tandem Mass Spectrometry for the Detailed Structure Elucidation of Oligosaccharides; Elaing Stephens; Sarah L Maslen; Alex Adam; Chemistry Department, Cambridge University, Cambridge, UK; Dionex UK Ltd, Camberley, UK

TOC pm 03:40 Structural Glycomics of the Human Parasite Schistosoma mansoni; Manfred Wurher; Cornelis H. Hokke; André M. Deelder; Leiden University Medical Center, Leiden, the Netherlands

TOC pm 04:00 Structural Characterization of Lipoooligosaccharides from Gram Negative Bacteria Using Multiple-Stage MS on a qMALDI Linear Ion Trap Mass Spectrometer; Simon Allen; Deborah M. Post; Bradford W. Gibson; Buck Institute for Age Research, Novato, CA

TOC pm 04:20 Structure Studies of Sulfated Carbohydrates Using ECD and EDD; Jeremy J. Wolff; Jonathan Amster; University of Georgia, Athens, GA

TOC pm 04:40 Comparison of Methods for the Simultaneous Detection of O-GlcNAc Modified and Phosphopeptides; Lauren E Ball; Maria G Buse; Medical University of South Carolina, Charleston, SC

NEW AND EMERGING CONTAMINANTS
Enrico Davoli, presiding

TOE pm 03:00 Emerging Environmental Contaminants and Current Issues; Susan D. Richardson; U.S. EPA, National Exposure Research Laboratory, Athens, GA

TOE pm 03:40 Illicit Drugs as Emerging Contaminants: Residues in Surface Waters Allow Monitoring of Community Drug Abuse; Roberto Fanelli; Sara Castiglioni; Chiara Chiarando; Renzo Bagnati; Ettore Zuccato; Istituto Mario Negri, Milano, Italy; University of Insulbia, Varese, Italy

TOE pm 04:00 Mass Spectrometric Study of Environmental Contamination Related to Military Training; Denise K. MacMillan; Randy D. Laubscher; Sally L. Yost; Judy C. Pennington; Engineer Research and Development Center, Omaha, NE; SpecPro Incorporated, Huntsville, AL; Engineer Research and Development Center, Vicksburg, MS

TOE pm 04:20 Real-Time Measurement of Woodsmoke and Hydrocarbon Tracer Species in Urban Airshed Transects by Mobile Membrane Introduction Tandem Mass Spectrometry (MIMS-MS/MS); Alexander J. Thompson; Charles W. LeBlanc; Chris D. Simpson; Erik T. Krogh; Chris G. Gill; Applied Environmental Research Labs, Malaspinia, Nanaimo, BC, Canada; Environmental Division, Cantest Ltd., Burnaby, BC, Canada; University of Washington, Seattle, WA

TOE pm 04:40 Proteomics Methods for the Detection and Quantification of Toxins and Allergens in Foods; John H. Callahan; Kevin J. Shefcheck; Steven M. Musser; FDA/CFSAN, College Park, MD

HYDROCARBONS TO PETROLEUM
William J. Simonnick, presiding

TOF pm 03:00 Soft Photon Ionization TOFMS Coupled to Gas Chromatography: Novel GCxMS Approach for Comprehensive Characterization of Complex Hydrocarbon Samples; Ralf Zimmermann; Werner Welthagen; Marc Gonin; Katrin Fuhrer; Fabian Mühler; GSF Research Centre and University Augsburg, Oberrechleisheim, Germany; TOFWERK, Thun, Switzerland

TOF pm 03:20 Molecular Profiling of Petroleum and Petrochemicals by GC-FIMS; Chang Hsu; Charles Yarbrough; Ricky Pujol; Haven Aldrich; ExxonMobil Process Research Laboratories, Baton Rouge, LA; ExxonMobil Chemical Co., Baton Rouge, LA

TOF pm 03:40 Detailed Characterization of GPC Fractionated Athabasca Asphaltenes by FT-ICR Mass Spectrometry; Brandi M. Craven; Tanner M. Schaub; Ryan P. Rodgers; Heather D. Dettman; Sara L. Salmon; Alan G. Marshall; National High Magnetic Field Laboratory, FSU, Tallahassee, Florida; Department of Chemistry and Biochemistry, FSU, Tallahassee, Florida; National Centre for Upgrading Technology, Devon, Alberta

TOF pm 04:00 Self-Association of Polar Organics in Petroleum Derived Materials Determined by Mass Spectrometry; Ryan P. Rodgers; Tanner M. Schaub; Donald F. Smith; Parviz Rahimi; Alan G. Marshall; National High Magnetic Field Laboratory, FSU, Tallahassee, Florida; Department of Chemistry and Biochemistry, FSU, Tallahassee, Florida; National Centre for Upgrading Technology, Devon, Alberta

TOF pm 04:20 Positive and Negative Mode ESI Analysis on Heavy Crude Oils; Katianna A. Phihak; Anding Fan; Robert T. McIver; IonSpec corporation, Lake Forest, CA

TOF pm 04:40 Molecular Characterization and Reactivity of Marine Humic Acids by High Resolution Electrospray Fourier Transform-Ion Cyclotron Mass Spectrometry; Sarah A. L. Cacamis; Rachel L. Sleightor; Susan A. Hatcher; Old Dominion University, Norfolk, VA; Ohio State University, Columbus, OH