## 21st International Mass Spectrometry Conference

# August 20–26, 2016 Metro Toronto Convention Centre 255 Front Street, West Toronto, ON, Canada

# **Conference Program**

Hosted by The Canadian Society for Mass Spectrometry



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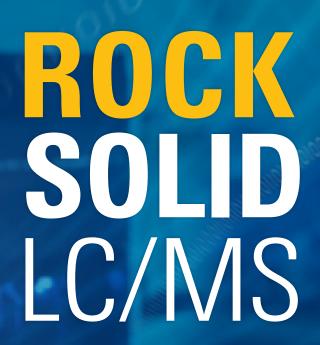
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# Welcome from the IMSC Executive Committee

On behalf of the Canadian Society for Mass Spectrometry, we welcome you to the 21<sup>st</sup> International Mass Spectrometry Conference in Toronto, Canada.

Canada has a proud and outstanding tradition in mass spectrometry research. The home of pioneers such as Fred Lossing, Alex Harrison, John Holmes, Paul Kebarle, Ken Standing, Mel Comisarow, Bob Boyd, Ray March, Henry Thode and Ted Litherland, Canadians have contributed to every facet of mass spectrometry development. It is the home of SCIEX, one of the world's premier mass spectrometer companies. Mass spectrometry is represented in every university and analytical government laboratory in Canada, and as is evident from the scientific organizing committee, Canada is host to some of the very finest mass spectrometrists in the world, in every mass spectrometry-related discipline.

Toronto is one of the most culturally-diverse cities in the world, where everyone can safely stroll and enjoy public transportation at all hours of the day. Conference participants can enjoy dining in one of the over 9000 restaurants featuring cuisine from across the globe. Whether you take in the Canadian National Exhibition, Ripley's Aquarium, the Hockey Hall of Fame, a relaxing break on Centre Island Park, or a short get-away to visit one of the natural wonders of the world, Niagara Falls, Toronto has venues that will excite everyone.

We are proud to have assembled an outstanding cast of scientific speakers in 40 oral and poster sessions for the conference, covering a wide variety of mass spectrometry disciplines in five major themes: Integrated Omics, Physical and Biophysical Mass Spectrometry, Environmental Mass Spectrometry, Mass Spectrometry in Drug Discovery and Novel Instrumentation. We know you will find the meeting stimulating and return home full of new ideas. Enjoy the meeting!

Your IMSC 2016 executive committee



Paul M Mayer, Chair



Lekha Sleno



Michael Siu



Terry Cyr



Kerry M Peru

# Welcome from the IMSF President

Dear Participants at the 21st IMSC,

I'm delighted to welcome all of you to the vibrant city of Toronto and especially to this first IMSC meeting in the Americas! The Executive Board and the representatives of our associated societies from around the world join our hosts, the Canadian Society for Mass Spectrometry, in wishing that you will have a productive and enjoyable stay in Toronto.

I especially want to thank the Executive Committee, Paul Mayer, Terry Cyr, Kerry Peru, and K.W. Michael Siu, who have organized an excellent meeting and the Scientific Committee, whose 23 members have worked so long and hard to produce the dynamic and exciting program.

This is only the second IMSC to be held outside of Europe. The first, held in Kyoto, Japan, in 2012, brought a new dimension to the IMSC conferences and I am sure that this week's events will also prove memorable. Toronto has one of the world's most diverse populations and there will be many opportunities for attendees to share their expertise and experiences with colleagues from around the world and local citizens. We are especially happy for the participation of a large number of students and early-career scientists. Please also watch for information about the 22<sup>nd</sup> IMSC, to be held in the beautiful city of Florence in 2018.

The International Mass Spectrometry Foundation continues to expand its range of activities to support the growth of our field. Do visit our newly revised website. The Executive Committee is pleased with the success of our first two International Mass Spectrometry Schools, held in Italy (2013) and Brazil (2015), and looks forward to the vote of our Affiliates to select the next locales. We also sponsor visiting speakers and will now add smaller, focused Workshops. We welcome suggestions for other activities.

We hope you enjoy the 21st IMSC and this wonderful city and return home full of enthusiasm for mass spectrometry, stimulating collaborations, and new friends!



Catherine E Costello





#### PRIME MINISTER . PREMIER MINISTRE

August 20-26, 2016

#### Dear Friends:

I am pleased to extend my warmest greetings to everyone attending the 21st International Mass Spectrometry Conference (IMSC), hosted by the Canadian Society for Mass Spectrometry.



This year's conference provides an ideal framework to showcase the latest developments in practice and instrumentation, to discuss issues of concern to the scientific community and to offer a variety of professional development activities. The commercial exhibition also gives delegates a chance to view emerging tools and scientific and industrial applications in mass spectrometry.

I would like to thank the organizers for putting together an informative and stimulating program. I also wish to commend everyone taking part in this weeklong gathering for their efforts to advance our understanding of our world by seeking out the technological discoveries of tomorrow.

Please accept my best wishes for a memorable and productive event in Toronto.

Sincerely,

The Rt. Hon. Justin P.J. Trudeau, P.C., M.P.

Prime Minister of Canada





August 20 – 26, 2016

#### A Personal Message from the Premier

On behalf of the Government of Ontario, I am pleased to extend warm greetings to everyone attending the 21<sup>st</sup> International Mass Spectrometry Conference (IMSC 2016), hosted by the Canadian Society for Mass Spectrometry and the Canadian scientific community.

Since its inception, the International Mass Spectrometry Foundation (IMSF) has worked diligently to advance the science and application of mass spectrometry worldwide by the promotion and dissemination of knowledge.

This conference provides a forum for students, delegates and leaders in industrial mass spectrometry to come together to enhance and exchange their knowledge and skills. I extend my appreciation to the organizers for efforts to draw enlightening speakers, prepare useful workshops and create innovative sessions.

Please accept my best wishes for a successful and productive conference.

Kathleen Wynne

Kathlin luyme

**Premier** 







#### Message from the Mayor

It is my pleasure to extend greetings and a warm welcome to everyone attending the 21<sup>st</sup> International Mass Spectrometry Conference.

This year's conference will be an opportunity for attendees to discuss matters of mutual interest in a setting designed for professional development.

I wish to welcome everyone to our city and encourage you to enjoy Toronto at this time of year as well as learn about our vibrant neighbourhoods.

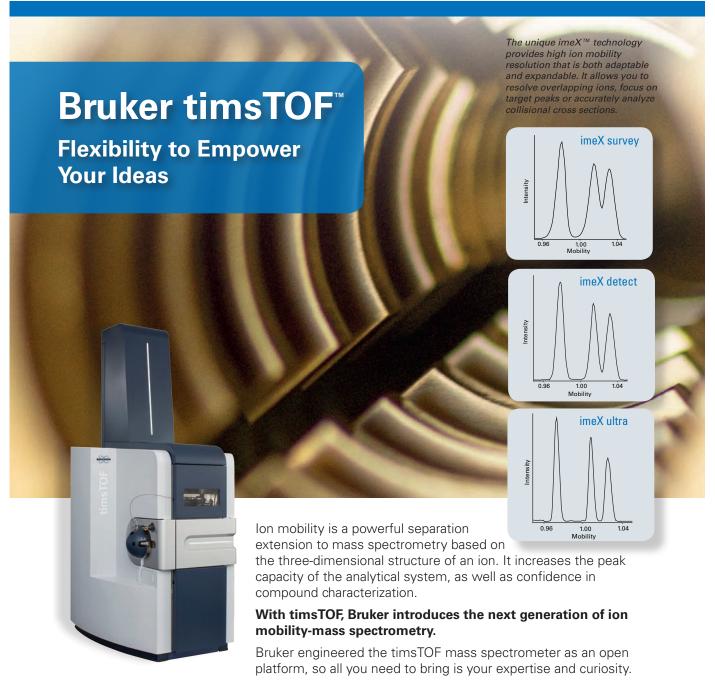
On behalf of Toronto City Council, please accept my best wishes for an informative and enjoyable conference.

Yours truly,

Mayor John Tory
City of Toronto







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# International Mass Spectrometry Conferences

1 <sup>st</sup> IMSC – London, UK	1958
2 <sup>nd</sup> IMSC - Oxford, UK	1961
3 <sup>rd</sup> IMSC - Paris, FR	1964
4 <sup>th</sup> IMSC - Berlin, GE	1967
5 <sup>th</sup> IMSC - Brussels, BE	1970
6 <sup>th</sup> IMSC – Edinburgh, UK	1973
7 <sup>th</sup> IMSC – Florence, IT	1976
8 <sup>th</sup> IMSC - Oslo, NO	1979

9 <sup>th</sup> IMSC – Vienna, AT	1982
10 <sup>th</sup> IMSC – Swansea, UK	1985
11 <sup>th</sup> IMSC – Bordeaux, FR	1988
12 <sup>th</sup> IMSC – Amsterdam, NL	1991
13 <sup>th</sup> IMSC – Budapest, HU	1994
14 <sup>th</sup> IMSC – Tampere, FI	1997
15 <sup>th</sup> IMSC – Barcelona, SP	2000
16 <sup>th</sup> IMSC – Edinburgh, UK	2003

17 <sup>th</sup> IMSC - Prague, CZ	2006
18 <sup>th</sup> IMSC - Bremen, GE	2009
19 <sup>th</sup> IMSC – Kyoto, JP	2012
20 <sup>th</sup> IMSC – Geneva, CH	2014
21 <sup>st</sup> IMSC – Toronto, CA	2016
22 <sup>nd</sup> IMSC –Florence, IT	2018

# IMSF Executive Committee, IMSF National Affiliates, and Scientific Committee

#### International Mass Spectrometry Foundation (IMSF)

#### **Executive Committee**

- Prof. Catherine E. Costello (US) President
- Prof. Marcos N. Eberlin (BR) Past President
- Dr. G. John Langley (US) Vice President (Society)
- Prof. Paul Mayer (Ca) Vice President (Conference)
- Prof. Marcos N. Eberlin (BR) Vice President (Education)
- Prof. Ron Heeren (NL) Treasurer
- Prof. Stephan Blanksby (AU) Secretary
- Prof. Gianluca Giorgi (IT) Region A Representative
- Prof. Jen-taie Shiea (TW) Region B Representative
- Prof. Dr. Scott A. McLuckey (US) Region C Representative
- Prof. Marcos N. Eberlin (BR) Region D Representative

#### **National Affiliates**

- Argentina Rosa Erra Balsells
- Australia/New Zealand Andrew McAnoy
- Austria Günter Allmaier
- Belgium Jeff Rozenski
- Brazil Fabio Gozzo

- Canada Paul Mayer
- Croatia Mario Cindric
- Czech Republic Jan Preisler
- Denmark Steen Pontoppidan
- Egypt Ezzat Selim





Biology is complex and elucidating the roles that proteins play can be challenging. In addition to profiling which proteins are present, understanding specific isoform structures and their function in complexes and networks can provide essential insights. Top-down protein analysis, chemical cross-linking mass spectrometry, and hydrogen-deuterium exchange have become increasingly powerful methods to probe the structure of protein complexes and interactions. High resolution accurate mass Orbitrap technology, in combination with enhanced fragmentation modes such as HCD, ETD, EThcD - and MS<sup>n</sup> modalities of hybrid Orbitrap technologies - is the ideal platform for general and structural proteomics studies.

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- Finland Tiina Kauppila
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- Germany Michael Linscheid
- Greece Despina Tsipi
- Hong Kong April S.Y. Wong
- Hungary Laszlo Lelik
- India Suresh Aggarwal
- Ireland Peter Kenny
- Israel Michal Sharon
- Italy Gianluca Giorgi
- Japan Yosinao Wada
- Korea Hyun Sik Kim
- Norway Einar Uggerud
- Peoples Republic of China Jin-Ying Li
- Poland Piotr Stefanowicz
- Portugal Maria Helena Florencio

- Romania Zaharie Moldovan
- Russia Albert Lebedev
- Serbia & Montenegro Mila Lausevic
- Singapore Manfred Raida
- Slovakia Vladimir Patoprsty
- Slovenia Helena Prosen
- South Africa Egmont Rohwer
- Spain Encarnación Moyano
- Sweden Jonas Bergquist
- Switzerland Bertran Gerrits
- Taiwan Pao-Chi Liao
- The Netherlands Rob Vreeken
- Ukraine Marina Kosevich
- United Kingdom Christine Eckers
- United States of America Jennifer Brodbelt

#### IMSC 2016 Executive Committee

- Paul Mayer, University of Ottawa (Chair, CSMS President)
- Lehka Sleno, Université du Québec à Montréal (CSMS Vice-President)
- Terry Cyr, Health Canada (CSMS Treasurer)
- Kerry Peru, Environment and Climate Change Canada (CSMS Secretary)
- K.W. Michael Siu, University of Windsor (CSMS Past-President)

#### IMSC 2016 Scientific Committee

- Christoph Borchers (University of Victoria, Genome BC Proteomics Centre)
- Pierre Chaurand (Départment de chimie, Université de Montréal)
- Travis Fridgen (Chemistry Department, Memorial University)
- Karl Jobst (Ministry of the Environment, Ontario)
- Rebecca Jockusch (Chemistry Department, University of Toronto)
- Juergan Kast (Chemistry Department, University of British Columbia)
- Liam Kieser (Department of Physics, University of Ottawa)
- John Klassen (Chemistry Department, University of Alberta)
- Lars Konermann (Chemistry Department, University of Western Ontario)
- Oleg Krokhin (Manitoba Centre for Proteomics and Systems Biology, University of Manitoba)
- Liang Li (Chemistry Department, University of

- Alberta)
- Paul Mayer (Chemistry Department, University of Ottawa)
- Terry McMahon (Chemistry Department, University of Waterloo)
- Randy Purves (National Research Council Saskatoon)
- Eric Reiner (Ministry of the Environment, Ontario)
- David Schriemer (Southern Alberta Cancer Research Institute, University of Calgary)
- Lekha Sleno (Départment de chimie, Université de Quebec a Montréal)
- Vince Taguchi (Ministry of the Environment, Province of Ontario)
- Pierre Thibault (Départment de chimie et Institut de Recherche en Immunologie et Cancérologie, Université de Montréal)
- Derek Wilson (Chemistry Department, York University)Thomson Medal Award



# Thomson Medal Award

The Thomson Medal Award is named after Sir J. J. Thomson, who was responsible for the first mass spectrograph and its resulting data more than 100 years ago. He also predicted many features of modern mass spectrometry. He discovered the electron using mass spectrometry and won the Nobel Prize in 1906 for his research.

The Thomson Medal Award is sponsored by the International Mass Spectrometry Foundation (IMSF), and the first awards were made in 1985.

#### 2016 Thomson Medal Winners are

Scott McLuckey, Purdue University, USA

Marcos Eberlin, UNICAMP, Brazil

The Thomson Medal Award presentations will take place during the Awards Morning on Wednesday, August 24 in Hall A.

The previous winners are:

2014	C. V. Robinson and R. Zenobi
2012	R. Aebersold, A. Makarov and F. Tureček
2009	C. E. Costello, C. C. Fenselau and P. Roepstorff
2006	J. H. Bowie, M. L. Gross and M. Karas
2003	R. M. Caprioli, F. Hillenkamp and V. L. Talrose
2000	J. B. Fenn, D. F. Hunt and A. G. Marshall
1997	M. T. Bowers, D. E. Games and J. F. J. Todd
1994	C. Brunnée, C. Djerassi and H. Schwarz
1991	K. Biemann, H. Matsuda and N. M. M. Nibbering
1985	J. H. Beynon, R. G. Cooks, K. R. Jennings, F. W. McLafferty and A. O. C. Nier



## Curt Brunnée Award

The Curt Brunnée Award will be presented on the occasion of the 21<sup>st</sup> IMSC in Toronto, August 20-26, 2016. The prize, of \$5,000 (USD), is generously sponsored by Thermo Fisher Scientific and will be made to an individual for "outstanding contributions to the development of instrumentation for mass spectrometry by a person under the age of 45 at the time of the award".



The 2016 recipient is **Dr. Yury Tsybin** (SpectroSwiss).

The Brunnée Award will be presented during the Awards Morning on Wednesday, August 24 in Hall A.

#### Previous winners of the award:

2014	Dr. Dimitris Papanastasiou, Fasmatech
2012	Prof. Zheng Ouyang, Purdue University
2009	Dr. Alexander Makarov, Thermo Scientific
2006	Prof. Roman Zubarev, Uppsala University
2003	Dr. Michisato Toyoda, Osaka University
2000	Prof. Scott McLuckey, Purdue University
1997	Prof. Michael Guilhaus, University of New South Wales
1994	Dr. Gareth Brenton, Swansea

# **CSMS** Awards

The Fred P. Lossing Award is awarded by the Canadian Society for Mass Spectrometry to an individual who has made distinguished contributions to mass spectrometry in Canada. Sponsored by **Agilent Technologies Canada**Inc., the 2016 Lossing Awardee is **Mel Comisarow**, UBC, for his role in the development of FT-ICR.

The Lossing Award will be presented during the Awards Morning on Wednesday, August 24 in Hall A.



# 2016 Journal for Mass Spectrometry Student Award Winners

Presentations will be made during the JMS symposium on Wednesday afternoon, Room 206E-F

Mario Francesco Mirabelli and Renato Zenobi. ETH Zurich, Switzerland

Observing proton transfer reactions inside the MALDI plume: experimental and theoretical insight into MALDI gas-phase processes

**German Augusto Gómez-Ríos**, Nathaly Reyes-Garcés, Ezel Boyacı, Emanuela Gionfriddo, Justen Poole, Barbara Bojko and J Pawliszyn. University of Waterloo, Canada

Fast quantitation of target analytes in complex matrices by solid phase microextraction-mass spectrometry (SPME-MS): recent developments and applications

**Gerard Bryan Gonzales**, Guy Smagghe, Sofie Coelus, Dieter Adriaenssens, Karel De Winter, Tom Desmet, Katleen Raes and John Van Camp. Ghent University, Belgium

Collision cross section prediction of deprotonated phenolics in a travelling-wave ion mobility spectrometer using molecular descriptors and chemometrics

Toru Takarada. Kobe Pharmaceutical University, Japan

New strategy for analysis of the splicing regulatory factors using high-resolution mass spectrometry

Pedro H. Vendramini, Rosana M. Alberici, Marcos N. Eberlin. University of Campinas, Brazil

EASI-MSI can be used in clinical analysis without loss chemical information?





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# Local Support Organizations

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## Conference Coordination provided by:



## Website & APP developed by:





# Sponsors of the 21st IMSC

#### Gold Level





Silver Level





# Exhibitors of the 21st IMSC

Organization Name	Booth	Hospitality
ACD Labs (Advanced Chemistry Development, Inc.)	1329	
Advion	1119	
Agilent Technologies: AFO Regional Columns & Supplies	1133/1230	716
Analytical Scientist / Texere	1316	
Bioinformtics Solutions Inc.	1333	
Biotage	1312	
Bruker Corporation	1217/1219	714
Hamamatsu	1239	
IM Publications	1123	
Ionbench	1418	
IonSense, Inc.	1218	
ISOSCIENCES	1214	
Jeol USA Inc	1319	
Leco	1223	
Markes International	1315	
MassTech Inc.	1129	
mSPEC group (MSPEC & MS PARTS)	1233/1332	
National Institute of Standards & Technology	1428	
Parker Hannifin Corporation - Filtration and Separation Division	1327	
Peak Scientific	1226	
PerkinElmer	1414	
Pfeiffer Vacuum GmbH	1113	
Photonis	1422	
Phytronix	1412	
Prosolia Inc.	1212	
Rapid Novor Inc.	1416	
Royal Society of Chemistry	1314	
Science Alert	1313	
Scientific Instrument Services	1216	
Sciex	1323/1325	713
Shimadzu Scientific Instruments Inc.	1229	
SpectraWorks Ltd	1318	
Springer	1215	
Themo Fisher Scientific	1322/1324/1326/1328	
VRS	1213	
Waters Coporation	1222/1224	715
Wiley	1115	
Zef Scientific	1317	

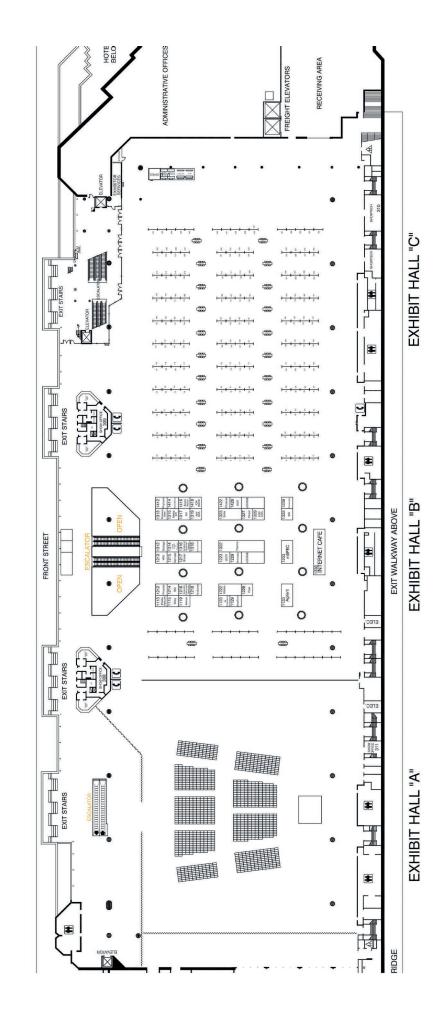




# Int'l Mass Spectometry Conference 2016

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NORTH EXHIBIT LEVEL 300

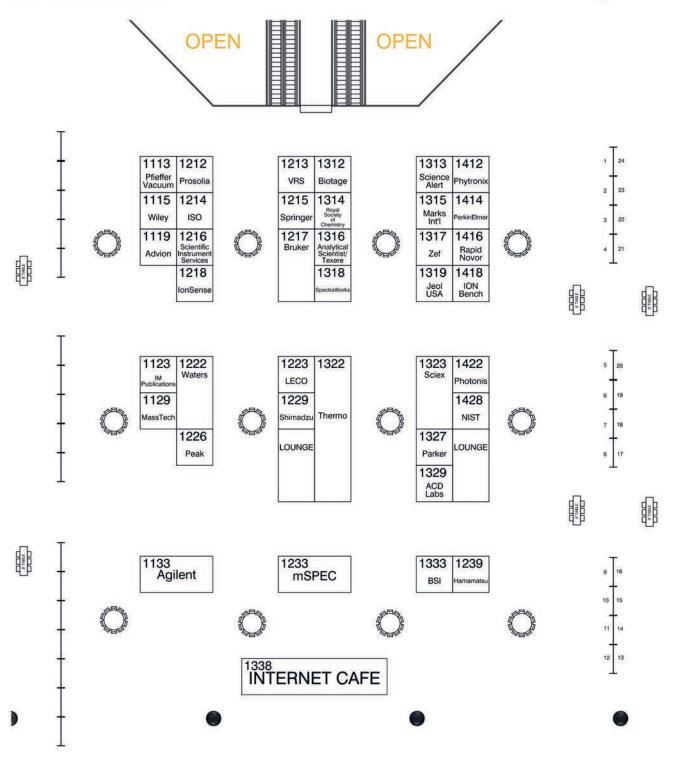




# Int'l Mass Spectometry Conference 2016 metro toronto convention centre

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NORTH EXHIBIT LEVEL 300





## **Exhibitors Information**



#### Advanced Chemistry Development, Inc. (ACD/Labs)

**Booth 1329** 

Advanced Chemistry Development, Inc. (ACD/Labs) is an informatics company that develops and commercializes solutions in support of R&D. We provide integrated knowledge management and a unified platform for chemical structure confirmation, verification, and elucidation using a variety of spectroscopic and spectrometric techniques; and chromatographic method development/optimization. Our solutions also enable scientists to extract and apply knowledge from predicted ADME-Tox and physicochemical property data. Advanced Chemistry Development, Inc. (ACD/Labs) is an informatics company that develops and commercializes solutions in support of R&D. We provide integrated knowledge management and a unified platform for chemical structure confirmation, verification, and elucidation using a variety of spectroscopic and spectrometric techniques; and chromatographic method development/optimization. Our solutions also enable scientists to extract and apply knowledge from predicted ADME-Tox and physicochemical property data.



#### Advion, Inc.

**Booth 1119** 

Advion, Inc. was founded in 1993 based on the novel techniques developed within the Cornell University laboratory of Dr. Jack Henion, a leading researcher in the field of Liquid Chromatography/Mass Spectrometry (LC/MS). Pioneers within the industry, Advion offers a variety of fit-for-purpose systems and consumables for life science research. With sales and support offices in North America and Europe and a large network of distributors, Advion is a global company with customers in all of the top pharmaceutical companies, government life science research agencies and universities. Advion continues to expand its diverse portfolio of innovative microfluidic sand mass spec-based products for the life science industry.



**Biotage** 

Booth 1312

Biotage is a leading provider of Instruments and Consumables for use in Medicinal Chemistry, Organic Chemistry, Peptide Synthesis and Analytical Testing. Check out the Extrahera<sup>TM</sup>, Simple automation, the Isolera<sup>TM</sup> Dalton, Mass Detection for Flash Systems, and the Isolera<sup>TM</sup> Spektra with ACITM Accelerated Chromatographic Isolation and Assist which purifies 250 mg in 5 minutes.



#### **Bioinformatics Solutions Inc. (BSI)**

**Booth 1333** 

Bioinformatics Solutions Inc (BSI) is well-known by their complete proteomic analysis software package, PEAKS. PEAKS provides a simple workflow for the identification and quantification of proteins in very complex biological samples with LC-MS. PEAKS includes key features such as de novo sequencing; PEAKS DB; PEAKS PTM; the homology search tool, SPIDER; and PEAKS Q. Through collaborative work, BSI has also been able to further their software by developing new technologies such as the PEAKS AB service, to allow quick and cost effective characterization of mAbs. PEAKS is used by users worldwide, and in numerous labs. Come stop by our booth to find out more.





#### **Hamamatsu Corporation**

Booth 1239

Hamamatsu Corporation is the North American subsidiary of Hamamatsu Photonics K.K. (Japan), a leading manufacturer of devices for the generation and measurement of infrared, visible, and ultraviolet light. These devices include photomultiplier tubes, photodiodes, image sensors, mini-spectrometers, and light sources. Hamamatsu Photonics is dedicated to the advancement of photonics through extensive research. This corporate philosophy results in state-of-the-art products which are used throughout the world in scientific, industrial, and commercial applications.



IONBENCH Booth 1418

IONBENCH - Manufacturer of laboratory furniture for mass spectrometry (LC/GC/MS) & Elevating UHPLC benches. Mass Spec IonBench products integrate MS peripherals, a built-in vacuum pump noise reduction enclosure and protect turbomolecular pumps by reducing vibration by 99%. There is up to 30% savings in laboratory space allocation. Solidly built lockable casters simplify moving the system. Our integrated vacuum pump enclosure reduces noise emissions by 80% down in perception. LC Elevating IonBench, on caster wheels, can be easily lifted up or down by commuting a switch, for a convenient & safe access to the top of your UHPLC



lonSense, Inc. Booth 1218

lonSense, Inc. provides open-air ionization products for use with mass spectrometry products from all major vendors. The company offers it automated Total Product Mass Spectrometry technology to the enhance quality control and production efforts in fields of food safety, forensics, drug development, and chemical analysis. IonSense manufactures (DART®) technology and distributes the atmospheric solids analysis probe (ASAPTM) licensed from M&M Mass Spec Consulting. The company endeavors to work with potential DART and ASAP users to provide customized interfaces for use with their existing LC/MS instruments. We invite you to inquire about the potential for using DART or ASAP to investigate your applications.



IsoSciences, LLC Booth 1214

IsoSciences, LLC is a leader in the custom synthesis of stable isotope labeled chemicals including vitamins, steroids, drug substances and metabolites. IsoSciences is ISO9001 certified and has an extensive catalog of stable isotope labeled standards available for immediate delivery both as solids and as CertiMass<sup>™</sup> exact concentrations solutions. IsoSciences has added over 200 new products over the past year including an extensive range of  $^{13}C_3$  labeled steroids, Vitamin D metabolites,  $^{13}C_7$ -Vitamin B12,  $^{13}C_6$ -Vitamin K2 MK4,MK7 and MK9. Visit us at www. isosciences.com for more information.





JEOL Booth 1319

JEOL introduced its first mass spectrometer in 1963 and is a world leader in mass spectrometry, NMR, ESR, and electron microscopy. JEOL MS products include quadrupole, time-of-flight and magnetic sector mass analyzers. JEOL TOF mass spectrometers include the AccuTOF GCx, a versatile high-resolution TOF system offering a variety of ionization methods (EI, CI+/-, FI/FD) that are compatible with GCxGC. The SpiralTOF high-performance MALDI-TOF/TOF system utilizes unique multi-turn ion optics to compress a 17-meter flight path into a compact space. The AccuTOF-DART 4G system is the third generation of the world's first commercial ambient ionization system introduced in 2005.



LECO Booth 1223

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#### **Markes International**

Booth 1315

Markes International, an industry leader in technology for trace organic analysis, manufactures instrumentation and software that enhances the analytical capability and productivity of gas chromatography. As well as having a long-established reputation for thermal desorption equipment, Markes manufactures BenchTOF™ mass spectrometers (and associated TOF-DS™ software) for single-run GC and GC×GC analysis of target compounds and screening of unknowns. Markes' technological innovation for mass spectrometry also includes ground-breaking Tandem Ionisation® technology, which uses a Select-eV® ion source to generate reference-quality 70 eV EI mass spectra at the same time as repeatable 'soft-ionisation' spectra with an enhanced molecular ion.



MassTech Inc. Booth 1129

MassTech Inc., located in, Columbia, Maryland USA, is a privately owned analytical instrumentation and technology company incorporated in 2001 for developing AP MALDI, field deployable ion trap mass spectrometer, and conducting on-going research and development. MassTech is the only licensed manufacturer of AP-MALDI ion sources. MassTech's AP MALDI ion source product has been adapted to commercial mass spectrometers from major equipment manufacturers: Agilent, Bruker Daltonics, JEOL, Sciex, Thermo Fisher Scientific, and Waters. MassTech's MT Explorer 50 ion trap mass spectrometer offers desktop performance in a transportable package, has customizable software, and has potential for a variety of applications.





#### mSPEC Group

#### Booth 1233/1332

At mSPEC Group we believe that products and relationships should be built to last, that knowledge should be shared and innovation should benefit everyone. Under the umbrella of mSPEC group of companies we have been supporting the mass spectrometry industry since 1996, offering a wide range of ISO certified comprehensive maintenance, application and production support programs designed to meet your needs, however unique they may be. Specialized in: Method development, validation & application support; Full service coverage, preventative maintenance & repairs; Staff proficiency training and production support; Turn-key LCMS laboratory instruments, accessories and consumables.



#### NIST Mass Spectrometry Data Center (MSDC)

Booth 1428

The NIST Mass Spectrometry Data Center (MSDC) is a part of Biomolecular Measurement Division of the National Institute of Standards and Technology located near Washington, DC. The MSDC is responsible for the development of evaluated reference mass spectral databases for the identification and analysis of chemical compounds by mass spectrometry: It includes the NIST/EPA/NIH Mass Spectral Library (for GC-MS), the NIST Tandem Mass Spectral Library (for LC-MS), the NIST Peptide Mass Spectral Libraries, and the NIST GC Retention Index library. More information can be found at http://chemdata.nist.gov/



#### Parker Balston

Booth 1327

Parker Balston Gas Generators for analytical instruments eliminate the expense and danger associated with high pressure compressed gas cylinders. The inconvenience of changing cylinders and supply interruptions will no longer be a concern. A Parker Balston Gas Generator offers price stability and eliminates long-term commitments, contract negotiations and tank rental fees. A continuous supply of consistent purity is available 24/7 without the need for operator attention. Parker Balston offers Gas Generators for a variety of analytical applications including LCMS, GC, FTIR, and NMR. Parker offers global distribution and support.



#### Peak Scientific

Booth 1226

With nearly two decades in pioneering reliable gas generator technology, Peak Scientific develops market-leading nitrogen, hydrogen and zero air systems mainly for the fields of LC-MS and GC. An on-site gas generator from Peak Scientific is the practical and cost-effective alternative to pressurized cylinders. Our forte is in providing our customers with unrivalled peace of mind and hassle free gas generation solutions for their specific laboratory demands, backed up by our world-class technical support and ongoing service care throughout the generator's lifespan. With a rapid response and offices on every continent we deliver a local service on a global scale.



PerkinElmer

Booth 1414





#### Pfeiffer Vacuum Booth 1113

Pfeiffer Vacuum is one of the world's leading providers of vacuum solutions. Our portfolio comprises a full range of hybrid and magnetically levitated turbopumps, backing pumps, measurement and analysis devices, components and vacuum chambers. Pfeiffer Vacuum enjoys a reputation for offering innovative, efficient and reliable vacuum solutions. Our products are constantly being optimized through close collaboration with customers from a wide variety of industries and through ongoing development work.



#### PHOTONIS Booth 1422

PHOTONIS is the market leader for mass spectrometer detectors and ion transport solutions. We offer an extensive array of Channeltrons® with Extended Dynamic Range, Custom Microchannel Plates with electro-optic housings, and a wide range of Time of Flight Detectors which reduce time jitter. We also provide patented Resistive Glass technology in capillary tubes, inlet tubes, ion guides, drift tubes, collision cells and monolithic reflectron lenses. Let PHOTONIS design your next instrument detector or ion transport product for reliable results and extended lifetime because better detectors produce better results.



#### Phytronix Booth 1412

The leader in quantitative ultra-fast high-throughput analysis solution for mass spectrometry presents the LDTD-96 and LDTD-384 ion sources. These platforms represent a unique shotgun approach that introduces the sample into the mass spectrometer using an ultra-fast Laser Diode Thermal Desorption (LDTD®). The LDTD Ion Source technology is the unique solution to increase your sample analysis throughput for your application needs.



#### Prosolia, Inc. Booth 1212

Prosolia, Inc. is a privately-held company engaged in the development, manufacturing and marketing of innovative life science tools that expand the use of mass spectrometers for translational research and molecular analysis. The company's technologies enable a wide variety of basic research, translational science and chemical analysis applications and deliver lower operating costs and faster results by eliminating the need for timeconsuming, costly and error-prone sample preparation steps. The DESI 2D™ and flowprobe™ directly profile hundreds of molecules simultaneously from cells and tissue sections, among other surfaces, while the Velox 360™ PaperSpray® System enables quantitative results on molecules in microliters of biological fluids using a single-use, disposable cartridge.



#### Rapid Novor Inc. Booth 1416

Rapid Novor Inc is dedicated to developing unparalleled analytical technologies to drastically change the processes in early stage drug research and development in the bio-pharmaceutical sector. Specializing in the field of mass spectrometry-based proteomics, the Novor team is up for the challenges to solve tough problems such as characterizing antibody proteins. We build bioinformatics software and services that deliver accurate, comprehensive and efficient results and enable the integration for pharmaceutical companies to bring the capabilities in-house.





http://www.scialert.net

Science Alert Booth 1313

Science Alert (www.scialert.net) is a leading ePublishing platform in Asia, committed to provide the services to independent scholarly publishers, societies, associations, and university presses to facilitate the digital dissemination of more than 175 journals. Science Alert also offers a complete manuscript submission, tracking, peer review, and publishing system for journal editors (www.scialert.com).



Shimadzu Booth 1229

Shimadzu is a leading manufacturer of a wide variety of mass spectrometers, including LCMS, GCMS and MALDI-TOF MS. Ideal for applications in a variety of industries, including foods, pharmaceuticals, toxicology, clinical and environmental, our platforms offer an incomparable fusion of speed and sensitivity to achieve new levels of data quality and throughput. We offer complete analysis platforms, with integrated, enabling software and reliable reagents/consumables. Visit us at IMSC 2016 (or online at Shimadzu.com) to discover why more and more labs are choosing Shimadzu as their most trusted partner for all of their analytical needs.

#### **SpectralWorks**

#### **SpectralWorks Limited**

**Booth 1318** 

SpectralWorks Limited is a leading UK based software development company. We provide innovative solutions targeted for markets within the life sciences industry including metabolomics. Coupled with our collaborations in academia and industry, this provides the perfect balance between scientific and software development expertise to provide the best solutions for the end user. As well as providing software consultancy and development services our off the shelf products, such as AnalyzerPro® and RemoteAnalyzer®, provide workflow oriented solutions for mass spectrometry data acquisition and processing. Coupled with our PCA tools we can provide an integrated workflow for your metabolomics projects.



VRS Booth 1213

VRS are the leading Recruitment Consultancy specialising in jobs within Analytical Chemistry, predominantly Mass Spectrometry & Chromatography (HPLC, GC, LC-MS, GC-MS, ICP-MS). With office locations in the US and Europe we provide unparalleled expertise to jobseekers and employers globally. To jobseekers VRS provide an exciting and diverse range of job opportunities within Analytical Chemistry, both laboratory-based and customer facing (Sales, Engineering, Marketing) roles. We can also provide you with in depth industry knowledge and advice. To employers we identify high calibre professionals at all levels of seniority across a wide spectrum of disciplines, meeting both temporary and permanent staffing needs.



ZefSci Booth 1317

ZefSci provides maintenance, service contracts, repair and compliance on state of the art Mass Spectrometers, Liquid Chromatographs, Gas Chromatographs (HPLC/UPLC, GC, LC-MS-MS, GC-MS), and other hyphenated analytical techniques used in the Pharmaceutical, Biotechnology, Chemical, Environmental and Food Industries – or anywhere analytical instruments are used. ZefSci started with the vision that a complex LC-MS-MS environment requires a highly technical team with multi-disciplinary knowledge and a strong dedication to customers and their applications. This vision and our strong business ethic have led us to be recognized as a premier independent Engineering and Scientific firm specializing in state of the art chromatography and mass spectrometry.



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# Short Courses and Workshops

#### **Short Courses**

Fundamentals of Mass Spectrometry
O. David Sparkman, Jürgen H. Gross
Saturday and Sunday, 9am to 5pm, Room 201

A two-day course on the interpretation of mass spectra of organic compounds.

Starting at the introductory level, the course is intended to provide the fundamentals for an understanding of the basic principles and applications of mass spectrometry of organic molecules.

Key topics of the short course are ionization processes, the formation and interpretation of isotopic patterns, uses of high-resolution and accurate mass for molecular formula determination, and an introduction to the fragmentation pathways of odd-electron and even-electron ions.

Information regarding available mass spectral databases will be provided along with how to use them with all types of organic mass spectrometry including MS/MS data. With an emphasis on the analysis of small molecules, you will learn to systematically employ all of the above mass spectral data for compound identification and structure elucidation.

To complete the course, compact lectures on instrumentation and its common modes of operation, as well as on the basics of widespread soft ionization methods such as chemical ionization (CI), field desorption (FD) including LIFIDI, electrospray ionization (ESI), and matrix-assisted laser desorption/ionization (MALDI) and ambient MS (DESI, DART) will be included.

Methodology Lectures (about 80% of the time) plus short simple exercises to assist understanding Language and Presentation English PowerPoint.

#### Advanced Interpretation of CID Mass Spectra from LC/MS/MS Robert D. Voyksner Saturday and Sunday, 9am to 5pm, Room 202

This advanced 2 day course will cover generation and interpretation of Collision Induced Dissociation (CID) mass spectra generated from positive and negative ions formed from the API techniques of electrospray, APCI or APPI.

The course will cover formation of ions, variables in CID mass spectra under tandem MS (triple quadrupole, q-TOF, ion trap) and API transport CID and interpretation of both the molecular ion and common molecular adduct ions and the product ion formed from these species after CID. The interpretation of the product ion mass spectra will be broken down into distinctive fragmentation mechanisms to aid the student to develop a systematic approach towards spectral interpretation. The fragmentation processes covered include single bond cleavage, multiple bond cleavage with charge retention and with charge migration, cyclization, ring opening fragmentation, hydrogen rearrangements, and charge remote fragmentation. The fragmentation



mechanisms will be applied to both positive and negative ions. Additionally, CID product ion formation from adducts such as  $[M+Na]^+$   $[M+NH_4]^+$  and  $[M+F, CI \text{ or } Br]^-$  will be covered. Each of the lectures have imbedded practical problems, which will allow a review of the various fragmentation mechanisms on a variety of compound types. The course will finish with a series of real world LC/MS/MS interpretation problems applicable to pharmaceuticals, clinical, industrial, and forensic and biochemical industry that the students will work on in groups and discuss at the end of the class.

The course is designed for the students who have completed a LC/MS Short Course or who have some working knowledge of LC/MS and want to improve their qualitative interpretation skills for problem solving in LC/MS.

# The NSERC CREATE Training program in Mass Spectrometry-enabled Science and Engineering (York University)

Courses are offered at a discount as they are linked to the CREATE program. Discounts are available to all participants.

# Career Paths for Mass Spectrometry in Academia Saturday, 9am to 5pm, Room 203

In this course, international academic leaders in mass spectrometry will share with you the story of the evolution of their careers in academia: How they got into to the buisness, how their research programs evolved over time and their involvement in major conceptual or technical advances in their fields. The course will provide ample time for formal and informal discussion with each speaker, culminating in a panel discussion on "Maximizing success in Academic Careers in Mass Spectrometry"

#### Career Paths for Mass Spectrometry in Industry Saturday, 9am to 5pm, Room 203

In this course, leaders in industrial mass spectrometry from a broad range of multinational companies including Sanofi-Pasteur, Sciex, Waters, Maxxam, Fluidigm, Ionics and many others will share stories on: Career paths in industry, historical perspectives on the development of their company / sector, entrepreneurial stories or 'case study' industrial research projects in mass spectrometry. The course will offer ample time for formal an informal discussion with each speaker, culminating in a panel discussion on "Maximizing Success in Industrial Careers in Mass Spectrometry" and "Industry / Academic Collaborations in Industrial Mass Spectrometry"



#### Workshops

All workshops are included with the price of registration, no extra fees are required. Light refreshments will be served.

You've got an idea; Now what? Torys LLP Monday, 5:45 pm to 7:00 pm, Room 201

#### Topics of discussion will include:

- Anatomy of a start-up
  - Making the most of limited resources; finding and attracting talent; getting to proof-of-concept and prototype
- Incorporating a company
  - Incorporation vs. unincorporation structure; shareholders' agreements; accounting needs
- Partnering with others
  - Confidentiality; cross-licensing; joint ownership of IP
- Finding financing
  - Bootstrapping; friends and family; angel investments; government grants
- How to be friendly (attractive) to further investment
  - Series A through IPO; tax structures

#### You've got a start-up; Now what's your IP play Torys LLP Tuesday, 5:45 pm to 7:00 pm, Room 201

#### Topics of discussion will include:

- Contributing IP to a start-up (or keeping the IP personally)
  - Control of IP; founder(s') assignments and grant-back licenses; employee and contractor assignments
- Why patent your innovation (and when to stop patenting)
  - Exclusionary rights granted by patents; term of patents; application deadlines and cost of obtaining patents
- What makes an innovation patentable?
  - Novelty, non-obviousness, utility, subject matter
- If you don't patent, will you still have protection? (hint: copyright and trade secrets)
  - Copyright, trade secrets, industrial designs
- To patent or not to patent: the case studies of Twitter vs. Alibaba
  - First movers' advantage; patent valuation in an IPO

#### About Torys LLP:

Torys LLP is an international business law firm that works with entrepreneurs and innovators who need strategic, nimble and cost-effective advice to launch their products and maximize their market share. Our corporate lawyers advise on founder and shareholder agreements, tax issues, financing and partnership agreements. Torys' dedication to excellence across practice areas and industries has resulted in an enviable record of experience in Canada and globally. Our patent lawyers and agents advise on strategy and are experienced in all stages of protecting your innovation, from securing patents to freedom to operate. Torys' legal team keeps pace with your industry—from our North American base in Toronto, New York, Calgary, Montréal, and Halifax, we represent domestic, multinational, new-economy and traditional enterprises at every stage in development.



#### **Careers in Mass Spectrometry**

Tony Bristow (On behalf of the British Mass Spectrometry Society) Wednesday, 5:45 pm to 7:00 pm, Room 201

For the mass spectrometrist, career pathways are very diverse. These can be in various industrial environments (both within and outside a scientific discipline), academia, with the instrument manufacturers and in many other areas of research. To illustrate the wide variety of career options, and debate the future requirements for the "expert" user, mass spectrometrists from diverse backgrounds will provide short presentations describing their career paths. This has been a very popular and successful workshop at previous IMSC meetings and again promises to deliver high impact and thought provoking discussions at IMSC 2016. We look forward to seeing you there.

#### Trent Conference on Mass Spectrometry Workshop Prof. Travis Fridgen Monday to Wednesday, 5:45 pm to 7:00 pm, Room 202

The Trent Conference on Mass Spectrometry is a graduate student centered event that allows students to present their work to their peers in an informal setting. For 32 years the meeting has provided a rich educational and training experience for students in all areas of Mass Spectrometry. The 33rd installment will take place as a workshop at the IMSC. Graduate students wishing to make a 15 min oral presentation should email Prof. Travis Fridgen to have their name, affiliation (with supervisor) and presentation title logged. While open to all, the preference will be given to those not already presenting at IMSC 2016.



### Seminars

#### Waters Lunch Seminars:

Room 202, North Building, Metro Toronto Convention Centre

Monday, August 22 12:30 pm to 1:30 pm

David Heywood, Waters Corporation
Making large scale Omics workflows routine

The analysis of complex biological samples in support of "Omics" style workflows challenges current analytical systems. In this seminar we will discuss the role of ion mobility and informatics which have been developed to increase coverage and streamline biomarker identification in a robust, reproducible and accessible manner.

Tuesday, August 23 12:30 pm to 1:30 pm

#### Xavier Ortiz Almirall, Ministry of the Environment and Climate Change

Towards an automated untargeted method for microcystins analysis using two dimensional liquid chromatography and ion mobility/quadrupole time of flight mass spectrometry

Microcystins are cyclic heptatpeptide hepatotoxins produced by certain species of cyanobacteria (blue-green algae) found in freshwater environments. These secondary metabolites are toxic to higher organisms, causing human sickness or even death in some cases. Even though only one particular variant is currently regulated under the Ontario Safe Drinking Water Act (microcystin-LR,  $1.5~\mu g/L$ ) and there is only a handful of microcystin standards available in the market, over 90 different microcystins variants have been reported to date. For this reason, it is important to develop non-targeted methods for the analysis of these compounds. The present study describes an automated method for the analysis of microcystins by two dimensional liquid chromatography/quadrupole time of flight mass spectrometry (2D-LC/QTOF-MS) using a Waters Acquity I-Class and Waters Xevo G2-XS. Moreover, uncompleted chromatographic separation of all microcystins variants was further achieved by ion mobility mass spectrometry'

An automated method for microcystins extraction and clean up from water samples was developed using 2D-LC in the *trap* and *elute* configuration was used: a large volume of water sample (500 µl) was directly injected and trapped in the first column. After that, microcystins were desorbed in reverse flow and injected to the analytical column, prior to mass spectrometry analysis.

When the QTOF-MS was operated in high resolution full scan mode (RP  $\approx$  25.000), the instrument proved to be very sensitive for microcystin-LR (50 fg on column with S/N > 10). Combined with the 2D-LC, the system could detect 100 pg/L of microcistyn-LR in water with S/N>10. Mass accuracy (< 1 ppm) allowed assigning elemental compositions for unknown compounds with confidence. MS/MS mode monitoring the characteristic microcystin ion at m/z=135.0804 was useful to provide quantitative results of targeted compounds in complex samples.



For a more comprehensive characterization of complex algal bloom samples, ion mobility was used to distinguish the different microcystin variants based on their cross-section. This new dimension of separation allowed the identification of some congeners that could not be separated by means of chromatography or mass spectrometry alone. Advanced acquisition methods such as Data Dependant Acquisition (DDA) and Data Independent Acquisition (DIA) were successfully employed to elucidate new microcystin variants in real samples that have not been reported in literature yet.

Wednesday, August 24 12:30 pm to 1:30 pm

#### **TBD**

#### Molecular visualization - current and future perspectives on Mass Spectrometry Imaging

In this lunchtime session, Waters will discuss the latest developments in Mass Spectrometry imaging. We will present the data from both our internal and collaborative research programs, and look at the utility of Mass spec imaging across both preclinical and clinical research.

#### Waters Breakfast Seminars

Waters Hospitality Suite

Tuesday, August 23 7:00 am to 8:00 am

Dr. Roger Linington, Simon Fraser University

Integration of High-Content Screening and Untargeted Metabolomics for Comprehensive Functional Annotation of Natural Product Libraries

Traditional natural products discovery using a combination of live/dead screening followed by iterative bio-assay-guided fractionation affords no information about compound structure or mode of action until late in the discovery process. This leads to high rates of rediscovery and low probabilities of finding compounds with unique biological and/or chemical properties. By integrating image-based phenotypic screening in HeLa cells with high-resolution untargeted metabolomics analysis, we have developed a new platform, termed Compound Activity Mapping, which is capable of directly predicting the identities and modes of action of bioactive constituents for any complex natural product extract library. This new tool can be used to rapidly identify novel bioactive constituents and provide predictions of compound modes of action directly from primary screening data.

This approach inverts the natural products discovery process from the existing 'grind and find' model to a targeted, hypothesis-driven discovery model where the chemical features and biological function of bioactive metabolites are known early in the screening workflow, and lead compounds can be rationally selected based on biological and/or chemical novelty. Advantages of employing integrated Big Data approaches to natural products discovery will be presented, as well as current challenges and limitations associated with these emerging technologies.



Waters Hospitality Suite

Wednesday, August 24 7:00 am to 8:00 am

#### Patty Sun, Waters Corporation

ionKey [LC/MS] HT- improvements for LC/MC integration

As microflow LC-MS systems continue to evolve, an increasing number of users are looking into applying microflow technologies to various scientific fields. In order to satisfy the wide-ranged needs and provide flexibility in this growing market, the ionKey/MS HT products are introduced as the expansion of the current ionKey/MS offer by adding a series of new features. During the initial launch of the ionKey/MS HT product family, following iKey separation devices are released: 300  $\mu$ m ID and 5 cm BEH 130Å PsT C18, 1.7  $\mu$ m, and HSS T3 100Å, 1.8  $\mu$ m.

In this presentation, we will discuss the new features of the ionKey/MS HT product family and the benefits of applying 300  $\mu$ m ID iKey to certain applications. Sensitivity gain and reduced matrix effects are the well-known benefits of micro-scale LC/MS. However, the throughput of microflow LC/MS systems has been a challenge for laboratories performing routine analyses with large number of samples. The 300  $\mu$ m ID iKey devices packed with the sub 2.0  $\mu$ m particles achieve the sensitivity gain, throughput, and UPLC grade separation power by using higher flow rates and shorter cycle times.

#### **Bruker Lunch Seminars**

Room 206 ABCD, North Building, Metro Toronto Convention Centre

**Monday, August 22** 12:30 pm to 1:30 pm

Jeffrey N. Agar, Associate Professor and Barnett Institute Fellow, Depts. of Chemistry and Pharm. Sci., Northeastern University

Tracking the Dark Metabolome with a Novel Isotopic Fine Structure Enabled Metabolic Labeling Strategy

**Tuesday, August 23** 12:30 pm to 1:30 pm

Mel Park, Bruker Daltonics, Director of Research Ion Mobility Mass Spectrometry Coming of Age

Dr. Sven Meyer, Senior R&D Scientist OMIC's Solutions A New Dimension to QTOF Technology in the Analytical Lab



# LECO Lunch Seminar

Room 206 EF, North Building, Metro Toronto Convention Centre

**Tuesday, August 23** 12:30 pm to 1:30 pm

Susan D. Richardson, Arthur Sease Williams Professor of Chemistry University of South Carolina A Novel GC-TOF-MS: Quantifying Priority Unregulated Disinfection By-Products with the Sensitivity of SIM while acquiring Full Range Mass Spectra for Unknown Identification

# Agilent Lunch Seminar

Room 203, North Building, Metro Toronto Convention Centre

**Tuesday, August 23** 12:30 pm to 1:30 pm

Philip Britz-McKibbin: Associate Professor, Cystic Fibrosis Canada Researcher Improving Sample Throughput, Costs and Data Comparability in Mass Spectrometry using Multiplexed Separations

Separation science plays a key role in enhancing the selectivity, sensitivity and robustness of mass spectrometry (MS)-based metabolomic studies. However, low sample throughput and complicated data processing remain major bottlenecks to biomarker discovery when performing untargeted metabolite profiling. Herein, we introduce multi segment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) as a multiplexed separation platform that takes advantage of customized serial injections to enhance sample throughput and data fidelity with quality assurance. MSI-CE-MS offers a cost effective approach for greatly expanding the productivity of MS-based chemical analyses while offering an accelerating data workflow for biomarker discovery in metabolomics.

For Research Use Only. Not for use in diagnostic procedures.

Christine Des Rosiers Ph.D., Director, Metabolomics Platform, Montreal Heart Institute (MHI), Professor, Department of Nutrition & Biochemistry, Université de Montréal Using metabolomics to translate genetic discoveries in personalized medicine approach: Lessons from the iGenoMed Consortium in inflammatory bowel disease

Metabolomics - the most recent addition to the "omics" disciplines - offer a means to measure thousands of low molecular weight compounds from any cell, tissue or body fluid. This provides a global view of alterations in metabolic pathways induced by a given perturbation, whether resulting from a gene mutation or disease onset. Recent developments in technologies have enabled the application of metabolomics in the clinics in a high-through-put manner together with other omics. There are, however, numerous challenges and issues, which need to be taken into account for the successful application of metabolomics to disease biomarker discovery particularly in the setting of large cohort studies integrating other omics data. This presentation



will illustrate how we are tackling these challenges in the context of a multidisciplinary personalized medicine project on inflammatory bowel diseases (IDB) as part of the iGenoMed Consortium (http://www.medgeni.org/node/1), which exploits known IBD genetic risk factors to develop a tests for response to therapy. For Research Use Only. Not for use in diagnostic procedures.

# Thermo Lunch Seminars

Room 205, North Building, Metro Toronto Convention Centre

Monday, August 22 12:30 pm to 1:30 pm

TBA

# Protein Structure Analysis with Cross-Linking and Top Down MS

Chemical cross-linking combined with mass spectrometry (CX-MS) and Top Down mass spectrometry are powerful methods to probe the structure of proteins, complexes and interactions. The high resolution and mass accuracy of Orbitrap technology, in combination with enhanced fragmentation modes (e.g., HCD, ETD, EtHCD) and MS<sup>n</sup> modalities, allow completely unique and effective methods to probe protein structure. New reagents and software facilitate sample preparation and data interpretation to make these capabilities available to all labs. This seminar will feature the latest work on protein structure elucidation, protein characterization and protein-protein interaction networks.

**Tuesday, August 23** 12:30 pm to 1:30 pm

# **TBA**

# Complete Characterization of Biologics: mAbs and ADCs

Peptide mapping, subunit top/middle down analysis, and intact native and denatured analysis: The new Thermo Scientific™ Q Exactive™ BioPharma solution can do it all. Use the high resolution and mass accuracy of Orbitrap technology to generate exemplary data and Thermo Scientific™ BioPharma Finder™ software to analyze sequence variance, sites of modification, carbohydrate structure, etc. Verify these findings at the subunit level with top/middle down sequence analysis. Get a full picture of biologic heterogeneity, including glycosylation, linkers, drug conjugates, etc., with denatured and native intact analysis. This seminar will introduce the Q Exactive BioPharma solution and showcase examples of comprehensive characterization of biologic drugs.



# Wednesday, August 24 12:30 pm to 1:30 pm

# **TBA**

# Advances in Accurate, High-Throughput Quantitative Proteomics

The ability to perform accurate protein quantification at low levels lets scientists unravel the complexity of protein interactions and track protein abundance changes in a wide variety of samples. When combined with multiplexing capabilities, quantitative proteomics provides a deep and comprehensive understanding of the molecular mechanisms underlying biological processes and disease states. Thermo Scientific™ TMT™ isobaric mass tag labeling combined with Orbitrap high resolution accurate mass (HRAM) mass spectrometry (MS) enable greater multiplexing capacity, resulting in increased depth of quantitative proteomic analysis across larger numbers of samples. The improved sensitivity and accuracy achieved with Orbitrap HRAM MS and synchronous precursor selection (SPS)-based MS3 technology on the Thermo Scientific™ Orbitrap Tribrid™ MS systems provide a unique, unmatched capability to accurately measure the most subtle changes in low-abundance proteins. In this seminar, we will discuss multiplexed quantitative proteomics and present real-world applications from leading research laboratories.



# Oral Program

Saturday A		
-Saturday, A	ugust 20, 2016	
9:00 AM - 5:00 PM	Short course - Fundamentals in MS - Day 1 David Sparkman & Jürgen Gross	Room 201
9:00 AM - 5:00 PM	Short course - Advanced interpretation CID mass spectra LC/MS/MS - Day 1 Robert D. Voyksner	Room 202
9:00 AM - 5:00 PM	The NSERC CREATE training program in mass spectrometry-enabled science and engineering (York University)	Room 203
	Career Paths for Mass Spectrometry in Academia	
Sunday, Aug	gust 21, 2016	
9:00 AM - 5:00 PM	Short course - Fundamentals in MS - Day 2 David Sparkman & Jürgen Gross	Room 201
9:00 AM - 5:00 PM	Short course - Advanced interpretation CID mass spectra LC/MS/MS - Day 2 Robert D. Voyksner	Room 202
9:00 AM - 5:00 PM	The NSERC CREATE training program in mass spectrometry-enabled science and engineering (York University)	Room 203
	Career Paths for Mass Spectrometry in Industry	
5:00 PM - 6:00 PM	Plenary lecture - Mass spectrometry imaging in the service of human health Richard N. Zare, Department of Chemistry, Stanford University	Hall A, Level 300
6:00 PM - 6:30 PM	Opening ceremony	Hall A, Level 300
6:30 PM - 8:30 PM	Opening reception	Exhibits Hall B Level 300
Monday, Au	gust 22, 2016	
8:30 AM - 9:15 PM	Plenary Lecture - Native MS in structural biology:	Hall A, Level 300
	characterization of non-covalent complexes by SID/IMMS or SID/HRMS Vicki Wysocki, Ohio State University	Level 300
9:30 AM - 12:00 PM		Room 201
	Vicki Wysocki, Ohio State University  Metabolomics I	
12:00 PM	Vicki Wysocki, Ohio State University  Metabolomics I Chairs: Matej Orešič & Guowang Xu  Unexpected characteristics and artificial changes of body fluids: crucial factors in clinical metabolomics	
12:00 PM 9:30 AM	Vicki Wysocki, Ohio State University  Metabolomics I Chairs: Matej Orešič & Guowang Xu  Unexpected characteristics and artificial changes of body fluids: crucial factors in clinical metabolomics Dr. Rainer Lehmann, University Hospital Tuebingen / Central Laboratory  New advances in high-performance chemical isotope labeling LC-MS for metabolomics	Room 201
12:00 PM 9:30 AM 10:00 AM	Vicki Wysocki, Ohio State University  Metabolomics I Chairs: Matej Orešič & Guowang Xu  Unexpected characteristics and artificial changes of body fluids: crucial factors in clinical metabolomics Dr. Rainer Lehmann, University Hospital Tuebingen / Central Laboratory  New advances in high-performance chemical isotope labeling LC-MS for metabolomics Dr. Liang Li, University of Alberta  Interpreting LC-MS/MS-spectra from primary metabolites for tandem MS-based <sup>13</sup> C-fluxon	Room 201
12:00 PM 9:30 AM 10:00 AM 10:30 AM	Vicki Wysocki, Ohio State University  Metabolomics I Chairs: Matej Orešič & Guowang Xu  Unexpected characteristics and artificial changes of body fluids: crucial factors in clinical metabolomics Dr. Rainer Lehmann, University Hospital Tuebingen / Central Laboratory  New advances in high-performance chemical isotope labeling LC-MS for metabolomics Dr. Liang Li, University of Alberta  Interpreting LC-MS/MS-spectra from primary metabolites for tandem MS-based <sup>13</sup> C-fluxo Mr. Jannick Kappelmann, Research Center Juelich  Extending a high quality reference tandem mass spectral library for more comprehensive ridentification	Room 201  omics  metabolite



	TVIOLIDAY
9:30 AM - 12:00 PM	Proteomics of the PTMs Chair: Pierre Thibault Room 202
9:30 AM	Electron transfer dissociation (ETD) mass spectrometry and studies of the nucleocytosolic O-GlcNAc PTM Dr. Al Burlingame, University of California San Francisco
10:00 AM	Deciphering PTM cross-talk by middle-down protein analysis using ETD MS/MS Ole Jensen, University of Southern Denmark
10:30 AM	SUMO system interactome Brian Raught, University of Toronto
11:00 AM	Discovery of novel PTMs mediated by bacterial effectors Dr. Xiaoyun Liu, Peking University
11:20 AM	A mass spectrometry-based novel chemical method to specifically and globally analyze cell surface glycoproteins Dr. Ronghu Wu, Georgia Institute of Technology
11:40 AM	Quantitative analysis of induced reversible cysteine oxidation in an atherosclerotic model via modified biotin switch assays Dr. Juergen Kast, University of British Columbia
9:30 AM - 12:00 PM	Gaseous biomolecules: conformations, energetics and reactions Chair Rebecca Jockusch Room 203
9:30 AM	The structure of duplex nucleic acids in the gas phase Dr. Valérie Gabelica, Inserm, France
10:00 AM	An infrared spectroscopy approach to follow beta-sheet formation in peptide amyloid assemblies Mr. Waldemar Hoffmann, Freie Universitaet Berlin
10:30 AM	New developments in 2D UV-MS cold ion spectroscopy of biomolecules Dr. Oleg Boyarkine, EPFL
11:00 AM	Mass spectrometry fragmentation methods (BIRD, SORI-CID, IRMPD): powerful techniques to study physical chemistry of guanine quadruplexes Mr. Mohammad Azargun, Memorial University
11:20 AM	Electron photodetachment, an efficient relaxation mechanism for electronically excited nucleic acids anions?  Dr. Alexandre Giuliani, Synchrotron SOLEIL
11:40 AM	Probing the gaseous structure of a β-hairpin peptide with hydrogen/deuterium exchange (HDX) and electron capture dissociation (ECD)  Ms. Rita Straus, NSERC CREATE York University and University of Toronto
9:30 AM - 12:00 PM	Ultra high resolution MS & Petroleomics Chair: Karl Jobst
9:30 AM	Petroleomics and environmental monitoring: a more detailed view using FTICR MS  Dr. Mark Barrow, University of Warwick
10:00 AM	Characterization of the Gulf of Mexico Deepwater Horizon oil spill and natural oil seeps by FT-ICR MS Dr. Vlad Lobodin, National High Magnetic Field Laboratory
10:30 AM	Orbitrap GC-MS: one year on dr Alexander Makarov, Thermo Fisher Scientific
11:00 AM	Characterizations of heavy petrochemical fractions: high temperature GCxGC with HR-TOFMS detection and thermal analysis-photo ionization TOFMS  Dr. Ralf Zimmermann, University Rostock and Helmholtz Zentrum München
11:20 AM	The use of high resolution SpiralTOF MS and mass defect analysis for the characterization of coals and complex polymeric samples dr Thierry Fouquet, National Institute of Advanced Industrial Science and Technology (AIST), Japan
11:40 AM	Performance limits in ultrahigh resolution FT ICR mass spectrometry and the main limiting factors Dr. Evgeny Nikolaev, Institute of Energy Problems of Chemical Physics Russian Acad. Sciences



# Monday

9:30 AM - 12:00 PM	Advances in analytical separations for MS Chair: Oleg Krokhin	Room 206A-D
9:30 AM	Slicing proteomics to unveil the human proteome Dr. Yasushi Ishihama, Kyoto University	
10:00 AM	Method and software workflow for integrating paired CE-MS and LC-MS bottom- from SDS-PAGE pre-fractionated samples Dr. Yassene Mohammed, Center for Proteomics and Metabolomics, Leiden University	• •
10:30 AM	On-line coupling of field-flow fractionation with mass spectrometry for lipoprotein metalloproteins Dr. Myeong Hee Moon, Yonsei University	ns and
11:00 AM	Supercritical fluid chromatography coupled to high resolution mass spectrometry and quantification of lipids Dr. David Touboul, CNRS ICSN	for dereplication
11:20 AM	Analysis of derivatized glycans using differential mobility spectrometry Dr. J. Larry Campbell, SCIEX	
11:40 AM	Optimal selection of separation chemistry for 3D-LC-MS/MS in bottom-up protector. Oleg Krokhin, University of Manitoba	omics
12:00 PM - 3:00 PM	Lunch Seminars, Poster Sessions	
1:00 PM - 3:00 PM	Authors of Odd Number Posters Present Advanced chromatographic methods in environmental analysis Advances in analytical separations for MS Ambient ionization methods Biomolecular structure: covalent labeling and crosslinking Chemical proteomics Clinical proteomics Emerging and persistent environmental contaminants FAIMS/DMS and new developments in IMS instrumentation Gas phase ion chemistry and spectroscopy Gaseous biomolecules: conformations, energetics and reactions IMS developments in MS: computations, collision cross sections & complex mixtures Integrated omics Lipidomics Metabolomics Proteomics of PTMs Quantitative targeted proteomics Ultra high resolution mass spectrometry and petroleomics	
3:00 PM -	Lipidomics I	Room 201

3:00 PM - 5:30 PM	Lipidomics I Chair: Jeff Smith, Markus Wenk
3:00 PM	New ion-mobility and ion-activation strategies for lipid structure elucidation Dr. Stephen Blanksby, Queensland University of Technology
3:30 PM	Healthy plasma lipidome Dr. Andrej Shevchenko, MPI of Molecular Cell Biology and Genetics
4:00 PM	Natural variation of blood plasma lipids in healthy Asian individuals Markus Wenk, National University of Singapore
4:30 PM	TrEnDi using isotopically-labelled diazomethane to increase sensitivity and selectivity of PE, PC and PS derived from complex biological samples Mr. Carlos Canez, Carleton University
4:50 PM	Accurate quantification of polyunsaturated glycerophospholipids by shotgun lipidomics Dr. Kai Schuhmann, MPI CBG Dresden, Germany
5:10 PM	Broad separation of lipid isomers using high-definition differential ion mobility spectrometry and a range of ionizing species  Mr. Andrew Bowman, Wichita State University



	Menay _
3:00 PM - 5:30 PM	Integrated Omics Room 202 Chair: Liang Li
3:00 PM	IR MALDESI: a novel molecular microscopy method Dr. David Muddiman, North Carolina State University
3:30 PM	Integrated omics approach centered on MS-based metabolomics to decipher mechanism implicated in human diseases Dr. Guowang Xu, Dalian Institute of Chemical Physics, CAS
4:00 PM	Integrated proteomic datasets for biomarker discovery and verification of bladder cancer Dr. Yi-Ting Chen, Chang Gung University
4:30 PM	Increasing arginine production in <i>C. glutamicum</i> by rational strain design using a combination of metabolomics and proteomics  Dr. Aiko Barsch, Bruker Daltonics
4:50 PM	Combined metabolomic and proteomic studies of DOCK8-Hyper IgE syndrome Dr. Anas Abdel Rahman, King Faisal Specialist Hospital and Research Center
5:10 PM	Rapid identification of mechanisms of action through systems biology Dr. Akos Vertes, George Washington University
3:00 PM - 5:30 PM	Biomolecular structure: covalent labeling and crosslinking Chairs: Christoph Borchers & David Schreimer  Room 203
3:00 PM	XL-FASP: a new integrated cross-linking workflow to study extra large membrane protein complexes dr Julia Chamot-Rooke, Institut Pasteur, CNRS
3:30 PM	XPlex: a multi residue cross-linking strategy for protein structure determination dr Fabio Gozzo, Unicamp
4:00 PM	Functional group selective derivatization for comprehensive shotgun lipidome analysis and multiplexed lipid quantitation Dr. Gavin Reid, University of Melbourne
4:30 PM	Structural mass spectrometry: novel tool to study transcription factor/DNA interaction Dr. Petr Novak, Institute of Microbiology
4:50 PM	Probing the time scale of FPOP (fast photochemical oxidation of proteins): radical reactions extend over tens of milliseconds  Mr. Siavash Vahidi, University of Western Ontario
5:10 PM	Surface accessibility and dynamics of macromolecular assemblies captured by covalent labelling mass spectrometry and molecular simulations Dr. Argyris Politis, King's College London
3:00 PM - 5:30 PM	Advanced chromatographic methods in environmental analysis  Chair: Eric Reiner  Room 205
3:00 PM	Cryogenic zone compression (CZC) and comprehensive two-dimensional gas chromatography (GC×GC) coupled to (HR)MS for measuring hyper-trace compounds Dr. Jef Focant, University of Liege
3:30 PM	Why is firefighting dangerous? characterization of mixed-halogenated dioxins and furans in fire debris using GCxGC-TOFMS and APGC-MS/MS Dr. Frank Dorman, Penn State Unversity
4:00 PM	Fishing halogenated environmental contaminants in biota based on isotopic pattern and mass defect provided by high resolution MS profiling Dr. Ronan Cariou, LABERCA-Oniris, France
4:30 PM	Advantages of comprehensive two-dimensional gas chromatography-high resolution time-of-flight mass spectrometry in petroleomics Mr. Jonathan Byer, LECO Corporation
4:50 PM	Quantitative profiling by SFC and UHPLC-MS/MS reveals metabolic phenotype of internal exposure to phthalates Dr. Zdenek Spacil, Masaryk University
5:10 PM	Applications of ambient ionization mass spectrometry and LC-MS/MS for studying multi-phase chemistry in indoor environments Dr. Shouming Zhou, University of Toronto



# ☐ Monday/Tuesday

3:00 PM - 5:30 PM	Ambient ionization methods Chair: Graham Cooks	Room 206 A-D	
3:00 PM	C-H bond silylation of aromatic heterocycles catalyzed by potassium t-butoxide in n Dr. Richard Zare, Department of Chemistry, Stanford University	nicrodroplets	
3:30 PM	Intrasurgical brain tumor diagnosis and surgical margin definition by desorption electrospray ionization-mass spectrometry Dr. R. Graham Cooks, Purdue University		
4:00 PM	Ambient MS based analytical platform for rapid identification of brain cancer tumor Dr. Evgeny Nikolaev, Institute of Energy Problems of Chemical Physics Russian Acad.		
4:30 PM	Nanospray desorption electrospray ionization (nano-DESI) imaging of biological systems. Julia Laskin, Pacific Northwest National Laboratory	ems	
4:50 PM	DESI-MS imaging of AMMOENG 130 in zebrafish Mr. Demian Ifa, York University		
5:10 PM	Development and characterization of an airborne laser-spark ion source for ambient ionization mass spectrometry Mr. Andreas Bierstedt, Federal Institute for Materials Research and Testing	desorption/	
5:45 PM - 7:00 PM	Workshops		
	You've got an idea; Now what? Torys, LLP	Room 201	
	Trent Conference	Room 202	
7:00 PM - 8:00 PM	Dinner Break		
8:00 PM - 11:00 PM	Corporate Hospitality Suites	700 Level, South Building MTCC	

		MTCC
Tuesday, Au	ıgust 23, 2016	
8:30 AM - 9:15 PM	Plenary lecture - Expanding the number of chemicals measured in environmental media: challenges for analytical mass spectrometry Derek Muir, Environment and Climate Change Canada	Hall A, Level 300
9:30 AM - 12:00 PM	Chemical proteomics Chairs: Juergen Kast, Gavin Reid	Room 201
9:30 AM	Charting the cellular interactome by proteome-wide cross-linking mass spectrometry Dr. Albert Heck, Utrecht University	
10:00 AM	Tracking drug action in living cells by thermal profiling of the proteome Dr. Mikhail Savitski, EMBL	
10:30 AM	Activity-based probes for selective penicillin-binding protein visualization Dr. Erin Carlson, University of Minnesota	
11:00 AM	Metal labelling as a detection functionality for tri-functional capture compounds (CCs) to protein targets of small molecules  Ms. Oleksandra Kuzmich, Humboldt Universität zu Berlin	o detect
11:20 AM	High-throughput identification of the protein targets of bioactive natural products Mr. Hongbo Guo, University of Toronto	
11:40 AM	Identification of the molecular target of a growth inhibiting compound in <i>Staphylococcus</i> a chemical proteomics strategy Ms. Elena Kunold, TU Munich	aureus using
9:30 AM - 12:00 PM	Quantitative targeted proteomics Chair: Xiaohong Qian	Room 202
9:30 AM	Extending the limits of deep DIA in human cell line and mouse brain tissue samples Dr. Lukas Reiter, Biognosys AG	



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10:00 AM	Mass spec western: target absolute quantification of proteins and post-translational modif Mr. Mukesh Kumar, MPI-CBG, Dresden, Germany	fications
10:30 AM	Comprehensive relative quantification of the cytochromes P450 by micro-LC and SWATH tion and data processing using cloud computing Dr. Sibylle Heidelberger, Sciex	<sup>®</sup> acquisi-
11:00 AM	A simplified approach to fast and accurate, high throughput targeted MS2 quantitation usi standards Dr. Romain Huguet, Thermo Fisher Scientific	ng internal
11:20 AM	Quantitation of residual proteins in an HSV-2 vaccine candidate using LC-MRM Dr. Andrew James, Sanofi Pasteur	
11:40 AM	Fundamental aspects and diagnostic potential of immunocapture in bottom-up LC-MS/MS Dr. Leon Reubsaet, Department of Pharmaceutical Chemistry, School of Pharmacy	3
9:30 AM - 12:00 PM	Gas phase ion chemistry and spectroscopy Chairs: Travis Fridgen & Philippe Maitre	Room 203
9:30 AM	Photoisomerization of molecular ions in a tandem ion mobility spectrometer Dr. Evan Bieske, evanjb@unimelb.edu.au	
10:00 AM	IRMPD spectroscopy of fragments from proline-analog-containing peptides Dr. John Poutsma, College of William and Mary	
10:30 AM	Infrared-driven chemistry on isolated transition metal clusters: catalytic reaction barriers f IR-MPD and BIRD Dr. Stuart Mackenzie, University of Oxford	rom
11:00 AM	Reactivity and spectroscopic features of key intermediates in Cisplatin drug chemistry Dr. Simonetta Fornarini, Università degli Studi di Roma La Sapienza	
11:20 AM	<b>Evaluation of the Sharpless epoxidation by ESI-MS and IRMPD spectroscopy</b> Dr. Thiago C. Correra, IQ-USP - Brazil	
11:40 AM	Observing proton transfer reactions inside the MALDI plume: experimental and theoretical into MALDI gas-phase processes  Mr. Mario Francesco Mirabelli, ETH Zurich	l insight
9:30 AM - 12:00 PM	Emerging and persistent environmental contaminants Chair: Sue Richardson	Room 205
9:30 AM	Exploring environmental chemical space through HR/AM mass spectrometry and cheminform the example of wastewater-derived organic micropollutants  Dr. Lee Ferguson, Duke University	ormatics:
10:00 AM	Orbitrap™ based gas chromatography-mass spectrometry to characterize semi-volatile and disinfection by-products in water  Dr. Cristina Postigo, Institute for Environmental Assessment and Water Research (IDAEA-CS)	
10:30 AM	New approaches for characterization of unknown precursors of disinfection byproducts in Dr. Xing-Fang Li, University of Alberta	water
11:00 AM	What's in a cloud? A semi-volatile GC/MS study Dr. Albert Lebedev, Lomonosov Moscow State University	
11:20 AM	Aqueous film forming foam (AFFF) components and related perfluoroalkyl and polyfluoroa substances (PFASs) in Canadian surface waters	ilkyl
	Ms. Lisa D'Agostino, University of Toronto	
11:40 AM	Ms. Lisa D'Agostino, University of Toronto  General strategies to increase the repeatability in environmental non-target screening by lichromatography-high resolution mass spectrometry  Mr. Tobias Bader, Zweckverband Landeswasserversorgung (and Leuphana University Lünebe	-
11:40 AM 9:30 AM - 12:00 PM	General strategies to increase the repeatability in environmental non-target screening by lichromatography-high resolution mass spectrometry  Mr. Tobias Bader, Zweckverband Landeswasserversorgung (and Leuphana University Lüneb	-



Tuesda	ау
10:00 AM	Improved isotopic labelling quantitation for large scale proteomic analyses using high field asymmetric waveform ion mobility spectrometry (FAIMS)  Mr. Eric Bonneil, IRIC-Université de Montréal
10:30 AM	Differential ion mobility and tandem mass spectrometric analysis of a series of chlorogenic acid isomers in fruit juice  Dr. Anas El-Aneed, College of Pharmacy and Nutrition, University of Saskatchewan
11:00 AM	Characterization of sphingolipids from plasma by LC-differential mobility spectrometry-MS/MS Dr. Sibylle Heidelberger, Sciex
11:20 AM	Protein structural studies using ion mobility MS and in-source ion activation techniques Dr. Ruwan Kurulugama, Agilent Technologies
11:40 AM	Ion mobility mass spectrometry coming of age Dr. Melvin Park, Bruker Daltonics, Inc
12:00 PM - 3:00 PM	Lunch Seminars, Poster Sessions
1:00 PM - 3:00 PM	Authors of Even Number Posters Present Advanced chromatographic methods in environmental analysis Advances in analytical separations for MS Ambient ionization methods Biomolecular structure: covalent labeling and crosslinking Chemical proteomics Clinical proteomics Emerging and persistent environmental contaminants FAIMS/DMS and new developments in IMS instrumentation Gas phase ion chemistry and spectroscopy Gaseous biomolecules: conformations, energetics and reactions IMS developments in MS: computations, collision cross sections & complex mixtures Integrated omics Lipidomics Metabolomics Proteomics of PTMs Quantitative targeted proteomics Ultra high resolution mass spectrometry and petroleomics

3:00 PM - 5:30 PM	Lipidomics II Chair: Jeff Smith & Markus Wenk	Room 201
3:00 PM	Lipidomics in biomedical research: weighing the pros and cons of a targeted vs. untargeted mass-spectrometry-based approach for biomarker discovery Christine Des Rosiers, Montreal Heart Institute	d
3:30 PM	SIMPLEX: a combinatorial multimolecular omics approach for systems biology Dr. Robert Ahrends, ISAS	
4:00 PM	Conformational atlas of lipid structure for directed characterization in lipidomics and mole phenomics Dr. John McLean, Vanderbilt University	ecular
4:30 PM	Discriminating isomeric (O-acyl)-hydroxy fatty acids (OAHFAs) by tandem mass spectrome Dr. David Marshall, Queensland University of Technology	etry
4:50 PM	Investigating the lipidomic dynamics of torpor through examination of hibernating squirre tissue and dehydrated frog leg tissue Ms. Katrin Blank, Carleton University	l liver
5:10 PM	High-throughput measurement of lipid turnover rate in HeLa cell based on metabolic heaver labeling  Ms. Byoungsook Goh, Gwangju Institute of Science and Technology	y water
3:00 PM - 5:30 PM	Clinical proteomics Roc Chair: Thomas Kislinger	om 202
3:00 PM	Decoding ligand receptor interactions Dr. Bernd Wollscheid, ETH Zurich	



	Tuesday 🔝	
3:30 PM	TBA Hanno Steen, Boston Children's Hospital	
4:00 PM	Identifying key stem cell-associated proteins in normal blood development and leukemia Dr. Erwin Schoof, Princess Margaret Cancer Centre, University Health Network	
4:30 PM	From systems biology towards a diagnostic tool for platelet function Dr. Albert Sickmann, ISAS	
4:50 PM	A novel mass spectrometry based assay for the diagnosis and typing of systemic amyloidosis Dr. Paul Boersema, ETH Zurich	
5:10 PM	Novel biomarkers for detecting recurrence of ovarian cancer by combining patient derived xenografts with N-glycosylation enrichment strategies  Mr. Ankit Sinha, Princess Margaret Cancer Centre	
3:00 PM - 5:30 PM	Noncovalent interactions: proteins, nucleic acids, and small molecules I  Chairs: John Klasen & Valerie Gabelica  Room 203	
3:00 PM	Native mass spectrometry of protein-protein and protein-drug complexes Dr. Joseph Loo, University of California, Los Angeles	
3:30 PM	Probing very high mass noncovalent assemblies with mass spectrometry Dr. Renato Zenobi, ETH Zurich	
4:00 PM	Understanding the stability of non-covalent complexes of macromolecules in charged droplets by molecular simulations Dr. Styliani (Stella) Consta, Department of Chemistry	
4:30 PM	The gas phase structures of self-assembled cyclotricatechylene cation-pi and anion-pi complexes Dr. Nicole Rijs, Karlsruhe Institute of Technology	
4:50 PM	A native MS study of RNA kissing complexes and their interaction with magnesium cations Ms. Clémence RABIN, INSERM U1212 - ARNA Lab	
5:10 PM	Mass spectrometry of non-covalent bound membrane proteins in nanodiscs with LILBID-MS Mr. Oliver Peetz, Goethe-University of Frankfurt	
3:00 PM - 5:30 PM	<b>Novel applications in sampling real time sample analysis by MS I-direct analysis</b> Room 205  Chair: Chris Gill	
3:00 PM	Microfabricated technologies for addressing molecular measurements: microchip CE-nESI and highly pressure mass spectrometry Dr. J. Michael Ramsey, University of North Carolina at Chapel Hill	
3:30 PM	Solid phase microextraction-transmission mode and direct analysis in real time: an efficient tool for fast analysis of contaminants in complex samples Dr. Emanuela Gionfriddo, University Of Waterloo	
4:00 PM	Using MS with molecular imprinting to develop new environmental monitoring tools Dr. Stefana Egli, Memorial University of Newfoundland	
4:30 PM	Direct SPME-ambient MS couplings: towards the non-chromatographic era Mr. Mario Francesco Mirabelli, ETH Zurich	
4:50 PM	Snap-shot monitoring of acoustically levitated containerless microreactions via ambient ionization mass spectrometry Ms. Elizabeth Crawford, Universität des Saarlandes	
5:10 PM	Photoionization-generated dibromomethane cation chemical ionization TOFMS for rapid and sensitive detection of volatile sulfur compounds Dr. Jichun Jiang, Dalian Institute of Chemical Physics, Chinese Academy of Sciences	



# Tuesday/Wednesday

3:00 PM - 5:30 PM	IMS developments in mass spectrometry: computations, collision cross sections, and complex mixtures Chair: Brandon Ruotolo	Room 206 A-D	
3:00 PM	New ambient MS and ion mobility MS approaches for multidimensional complex mixture analysis Dr. Facundo Fernandez, School of Chemistry and Biochemistry		
3:30 PM	Recent developments in gas molecule scattering approaches for collision cross section/mobility calculations in polyatomic gases  Dr. Chris Hogan, University of Minnesota		
4:00 PM	Applications of ion mobility separation with electron-based dissociation tandem mass Dr. Catherine Costello, Boston University School of Medicine	spectrometry	
4:30 PM	Native mass spectrometry and in-source collision-induced unfolding on a commercial tube ion mobility spectrometer Dr. Valérie Gabelica, Inserm, France	helium drift	
4:50 PM	lon mobility mass spectrometry uncovers the conformational states of a supercomple Dr. Argyris Politis, King's College London	x	
5:10 PM	Quantitative IM-MS for structural biology Justin LP Benesch, University of Oxford		
5:45 PM - 7:00 PM	Workshops		
	You've got a start-up; what is your IP play? Torys, LLP	Room 201	
	Trent Conference	Room 202	
7:00 PM - 8:00 PM	Dinner Break		
8:00 PM - 11:00 PM	Corporate Hospitality Suites	700 Level, South Building MTCC	

Wedneso	day, A	∖ugust	: 24, 2	2016
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8:30 AM - 9:15 PM	<i>Plenary lecture - Curt Brunnée Award:</i> Dr. Yury Tsybin, Spectroswiss	Hall A, Level 300
9:30 AM - 12:00 PM	Award lectures	Hall A, Level 300
9:45 AM	Thomson Medal Award Presentations & Lecture: Scott McLuckey, Purdue University	
10:30 AM	Thomson Medal Award Presentations & Lecture: Marcus Eberlin, University of Campinas	
11:15 AM	Rapid Communication in Mass Spectrometry Beynon Award Presentation (no lecture)	
11:30 AM	CSMS Lossing Award Presentation & Lecture: Mel Comisarow, University of British Columbia	
12:00 PM - 3:00 PM	Lunch Seminars, Poster Sessions	



# 1:00 PM - Authors of Odd Number Posters Present

3:00 PM AstroChemistry

Atomic MS in environmental applications Biomolecular structure: H,D-exchange Challenges in biopharmaceutical analysis

Environomics Glycomics

Imaging - applications Imaging - instrumentation

Innovations in mass spectrometry instrumentation

Mass spectrometric insights into catalysis New trends in mass spectrometry and medicine

Noncovalent interactions: proteins, nucleic acids, and small molecules

Novel applications in sampling and real time sample analysis by mass spectrometry

Novel high throughput techniques

Phosphoproteomics

Protein-protein complexes

Quantitation and Structural elucidation of metabolites and covalent adducts

Radical peptides Top-down proteomics

3:00 PM - 5:30 PM	Metabolomics II Chairs: Matej Orešič & Guowang Xu
3:00 PM	Metabolomic Investigation of inflammatory bowel disease phenotypes using GC×GC-HRTOFMS Dr. Jef Focant, University of Liege
3:30 PM	Mass spectrometric analyses in the identification of blood-based biomarkers of traumatic brain injury Dr. Tuulia Hyötyläinen, University of Örebro
4:00 PM	Inter-comparison of modern methods for isotopologue ratio analysis in metabolomics: trueness and uncertainty Dr. Stephan Hann, University of Natural Resources and Life Sciences - BOKU Vienna
4:30 PM	Characterization of the muscle metabolome: does oral bicarbonate function as an ergogenic aide in strenuous interval exercise?  Mr. Philip Britz-McKibbin, McMaster University
4:50 PM	A metabolomics approach for the authentication of herbal supplements using UPLC/QTof-MS Dr. Jimmy Yuk, Waters Corporation
5:10 PM	Metabolomic analysis of mouse embryonic fibroblast cells in response to acute starvation with and without Atg7 Dr. Yu Bai, Peking University
3:00 PM - 5:30 PM	Phosphoroproteomics Chair: Anne-Claude Gingras & Yasushi Ishihama Room 202
3:00 PM	Phosphotyrosine interaction proteomics decodes signaling network architecture by functional annotation of <i>in-vivo</i> phosphorylation sites Dr. Jesper Olsen, University of Copenhagen
3:30 PM	TBA Dr. Pedro Beltrao, EMBL-EBI
4:00 PM	An expanded toolkit to interrogate the human phosphoproteome Dr. Judit Villen, University of Washington
4:30 PM	Advanced (phospho)proteomics to uncover dynamics and pathway dependence in melanoma drug resistance uncovers novel companion targets Dr. Maarten Altelaar, Utrecht University
4:50 PM	Deconvolution of drug-specific phenotypes associated with nutrient transport using dynamic phosphoproteomics Dr. Pierre Thibault, Universite de Montreal/IRIC
5:10 PM	TBA Dr. Michael Moran, University of Toronto



# .... Wednesday

3:00 PM - 5:30 PM	Biomolecular structure: H,D-exchange Chairs: Lars Konnerman & Eric Forest	Room 203
3:00 PM	Differential HDX to probe ligand mediated receptor signaling Dr. Patrick Griffin, The Scripps Research Institute	
3:30 PM	Chaperonin-assisted protein folding Dr. John R. Engen, Northeastern University	
4:00 PM	Probing the conformation and ligand binding of neurotransmitter symporter (NSS) protein HDX-MS Dr. Kasper Rand, University of Copenhagen	s by
4:30 PM	Time-resolved hydrogen deuterium exchange (HDX) reveals the structural basis of amyloic inhibition by Alzheimer's drug candidates  Mr. Shaolong Zhu, MS-ESE York University - NSERC CREATE	dogenesis
4:50 PM	HDX-MS studies of human SIRT1 activation by STACs Dr. Han Dai, GlaxoSmithKline	
5:10 PM	Innovator and biosimilar infliximab: comparability assessment of the host cell proteins and higher order structure Dr. Henry Shion, Waters Corporation	d protein
3:00 PM - 5:30 PM	Environomics Chair: Eric Reiner	Room 205
3:00 PM	In vivo metabolomic approach to study developmental neurotoxicity of pesticides: explain cognitive and motor function effects with metabolomics Dr. Pim Leonards, VU University	ing
3:30 PM	The use of plasma and integrated OMICs approaches for environmental toxicology Dr. Denina Simmons, University of Waterloo	
4:00 PM	Environmental metabolomics in marine ecosystems: impact of viral lysis and predation on organic matter Dr. Krista Longnecker, Woods Hole Oceanographic Institution	marine
4:30 PM	Measurements of biomarkers of oxidative DNA damage in zebra mussels by GC-MS/MS to the impact of environmental contaminants on aquatic life Dr. Pawel Jaruga, National Institute of Standards and Technology	o evaluate
4:50 PM	Comprehensive chemistry and mutagenicity of disinfection by-products in swimming pool Dr. Susan Richardson, University of South Carolina	ls and spas
5:10 PM	Development of a highly-sensitive multi-mycotoxin LC-MS method in human plasma for estudies Dr. Dajana Vuckovic, Concordia University	exposure
3:00 PM - 5:30 PM	<b>Quantitation &amp; structural elucidation of metabolites &amp; covalent adducts</b> Roo Chair: Lekha Sleno	m 206 A-D
3:00 PM	Use of mass spectrometry to study drug covalent binding and idiosyncratic drug reactions Dr. Jack Uetrecht, University of Toronto	3
3:30 PM	Sensitive quantification of drug metabolites with and without authentic standards Dr. Filip Cuyckens, Janssen Pharmaceutical Companies	
4:00 PM	Structural mass spectrometry for molecular phenomics in systems, synthetic, and chemical Dr. John McLean, Vanderbilt University	al biology
4:30 PM	Investigation of triapine metabolism by application of electrochemistry and liquid chroma coupled to mass spectrometry (EC/LC/ESI-MS)  Ms. Karla Pelivan, Institute of Inorganic Chemistry, University of Vienna	tography
4:50 PM	ESI-MS/MS study of drug-conjugated dendrimers Dr. Aura Tintaru, Aix-Marseille Université, CNRS, Institut de Chimie Radicalaire-UMR7273	
5:10 PM	A novel approach for identification of biologically active phenolic compounds in hops mat hybrid quadrupole-orbitrap mass spectrometer Dr. Martin Dusek, Research Institute of Brewing and Malting	rices using



3:00 PM - 5:30 PM	JMS Student Awards	Room 206 E-F
3:00 PM	Observing proton transfer reactions inside the MALDI plume: experimental and the into MALDI gas-phase processes  Mario Francesco Mirabelli, ETH Zurich	oretical insight
3:30 PM	Fast quantitation of target analytes in complex matrices by solid phase microextract spectrometry (SPME-MS): recent developments and applications German Augusto Gómez-Ríos	ion-mass
4:00 PM	Collision cross section prediction of deprotonated phenolics in a travelling-wave ion spectrometer using molecular descriptors and chemometrics Gerard Bryan Gonzales, Ghent University	mobility
4:30 PM	New strategy for analysis of the splicing regulatory factors using high-resolution mas Toru Takarada	ss spectrometry
5:00 PM	EASI-MSI can be used in clinical analysis without loss chemical information? Pedro H. Vendramini, University of Campinas	
5:45 PM - 7:00 PM	Workshops	
	Careers in Mass Spectrometry	Room 201
	Trent Conference	Room 202
7:00 PM - 8:00 PM	Dinner Break	
8:00 PM - 11:00 PM	Corporate Hospitality Suites	700 Level, South Build- ing MTCC

Thursday, Au	ugust 25, 2016	
8:30 AM - 9:15 PM	Plenary lecture - The composition of comet 67P/Churyumov-Gerasimenko revealed by the mass spectrometers of the Rosetta mission Hervé Cottin, Université Paris-Est Cretail (Rosetta Mission)	Hall A, Level 300
9:30 AM - 12:00 PM	Top-down proteomics Chair: Neil Kelleher	Room 201
9:30 AM	High throughput top down proteomics utilizing ultra violet photo dissociation Dr. Philip Compton, Northwestern University	
10:00 AM	Top-down mass spectrometry of proteins and protein complexes as a tool for structural Dr. Joseph Loo, University of California, Los Angeles	biology
10:30 AM	<b>21 Tesla Fourier transform ion cyclotron resonance mass spectrometer for top-down pr</b> Dr. Christopher Hendrickson, National High Magnetic Field Laboratory	oteomics
11:00 AM	An optimized high-throughput top-down proteomics platform for improving diagnostic microbiology  Dr. Mathieu Dupré, Institut Pasteur	s in clinical
11:20 AM	Top-down sequencing by electron photodetachment dissociation (EPD) to locate ligand binding sites on G-quadruplexes Dr. Frederic Rosu, Univ. Bordeaux, CNRS ums3033	and cation
11:40 AM	A quantum chemical tool for the prediction of mass spectra and the identification of fra pathways: inter-side-chain interactions in peptides  Dr. Frank Blockhuys, University of Antwerp	gmentation
9:30 AM - 12:00 PM	Challenges in biopharmaceutical analysis Chair: Kevin Bateman	Room 202
9:30 AM	State-of-the art orthogonal chromatographic, electrophoretic and MS methods for mAk structural assessment at multiple levels Dr. Alain Beck, Centre d'Immunologie Pierre Fabre (CIPF)	os and ADCs



Thursd	ay
10:00 AM	LC/MS-based approaches to therapeutic protein quantitation to support discovery stage pharmacokinetic studies Dr. Daniel Spellman, Merck Research Laboratories
10:30 AM	Rapid characterization of biotherapeutic proteins by size-exclusion chromatography coupled to native mass spectrometry  Mr. Markus Haberger, Roche Diagnostics GmbH
11:00 AM	Investigating the differential photosensitivity of tryptophan in a model trp-cage peptide Ms. Leslie Welch, Genentech a Member of the Roche Group
11:20 AM	Towards an automated approach to characterizing the metabolism of biotherapeutic drugs Dr. Jayne Kirk, Waters
11:40 AM	Analytical approaches for quantification of surrogate mAbs in rodent biological matrices using LC-MS Dr. John Mehl, Bristol-Myers Squibb
9:30 AM - 12:00 PM	AstroChemistry Chairs: Paul Mayer & Christine Joblin
9:30 AM	Characterization of PAH content and distribution in cosmic dust analogues Dr. Hassan Sabbah, University Paul Sabatier - IRAP/CNRS
10:00 AM	Mass spectrometry in space: highlights of the Rosetta mission Dr. Andre Bieler, University of Bern
10:30 AM	Experimental and theoretical studies of ionic reactions of astrochemical relevance Dr. Zhechen Wang, University of Colorado at Boulder
11:00 AM	$H/H_2$ loss of dibenzopyrene isomer cations: combining linear ion trap measurements and density functional theory calculations  Mrs Sarah Rodriguez, Institut de Recherche en Astrophysique et Planétologie (IRAP)
11:20 AM	Probing surface-induced dissociation of exospheric neutrals using an ultra-fast rotor reactor and GC-MS analysis Dr. Daniel Austin, Brigham Young University
11:40 AM	Reaction dynamics of ionized PAHs Dr. Paul M Mayer, University of Ottawa
9:30 AM - 12:00 PM	Novel applications in sampling & real time sample analysis by MS II-  Continuous on-line monitoring  Chair: Erik Krogh
9:30 AM	Real-time analysis with a transportable high-resolution PTR-FTICR-MS Dr. Essyllt Louarn, Paris Sud University
10:00 AM	Rapid evaporative ionization mass spectrometry – the ultimate tool for real-time analysis? Dr. Zsolt Bodai, Imperial College London
10:30 AM	New mass spectrometric tools to study the flavor formation during the roasting process of coffee beans and nuts in real time Dr. Ralf Zimmermann, University Rostock and Helmholtz Zentrum München
11:00 AM	Kinetic analysis of chemical reactions using electrospray ionization mass spectrometry Dr. Scott McIndoe, University of Victoria
11:20 AM	Multi-sample monitoring on the Mini 12 mass spectrometer Mr. Christopher Pulliam, Purdue University
11:40 AM	Condensed phase membrane introduction mass spectrometry (CP-MIMS): direct, online, measurements of non-volatile analytes in complex aqueous samples Dr. Chris Gill, Applied Environmental Research Laboratories - Vancouver Island University
9:30 AM - 12:00 PM	Imaging - instrumentation Room 206A-D Chair: Damian Ifa
9:30 AM	Laser ablation atmospheric pressure photoionization mass spectrometry imaging. Instrumentation and applications Dr. Tiina Kauppila, University of Helsinki



10:00 AM	An ion funnel based MALDI-MSI interface for Orbitrap mass spectrometers Dr. Shane Ellis, M4I Institute
10:30 AM	Infrared laser ablation microdissection for imaging mass spectrometry Dr. Kermit Murray, Louisiana State University
11:00 AM	Improvements in AP-SMALDI Orbitrap mass spectrometry imaging of biological tissue Dr. Bernhard Spengler, Justus Liebig University Giessen
11:20 AM	Molecular imaging of tissue sections by matrix-free nanophotonic laser desorption ionization mass spectrometry with ion mobility separation Dr. Bindesh Shrestha, Waters Corp
11:40 AM	Liquid extraction surface analysis (LESA) combined with nano-liquid chromatography (nLC) for analyte determination from biological surfaces Dr. Daniel Eikel, Advion Inc.
12:00 PM - 3:00 PM	Lunch Seminars, Poster Sessions
1:00 PM - 3:00 PM	Authors of Even Number Posters Present AstroChemistry Atomic MS in environmental applications Biomolecular structure: H,D-exchange Challenges in biopharmaceutical analysis Environomics Glycomics Imaging - applications

Imaging - instrumentation Innovations in mass spectrometry instrumentation Mass spectrometric insights into catalysis New trends in mass spectrometry and medicine Noncovalent interactions: proteins, nucleic acids, and small molecules Novel applications in sampling and real time sample analysis by mass spectrometry Novel High throughput techniques

Phosphoproteomics Protein-protein complexes

Quantitation and structural elucidation of metabolites and covalent adducts

Radical peptides Top-down proteomics

3:00 PM - 5:30 PM	Glycomics Room 201 Chair: Pauline Rudd
3:00 PM	New MS tools for the discovery and characterization of protein-glycan interactions Dr. John Klassen, University of Alberta
3:30 PM	Glycomics in a wind tunnel - ion mobility-mass spectrometry of isomeric glycans and glycopeptides Dr. Kevin Pagel, Freie Universitaet Berlin
4:00 PM	Glycomics, proteomics and glycoproteomics of glioblastoma Dr. Joseph Zaia, Boston University School of Medicine
4:30 PM	Synthetic glycopeptides are unique tools for functional glycoproteomics Mr. Kathirvel Alagesan, Max Planck Institute of Colloids and Interfaces
4:50 PM	Development of N-and O- glycan workflows utilising a novel UPLC-mass detection system for biotherapeutic drug products.  Dr. Mark Hilliard, NIBRT
5:10 PM	One sample, one pot and the whole glycome: towards a system to study disorders of protein glycosylation Ms. Kirsty Skeene, University of York, UK



# \_\_\_\_ Thursday

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3:00 PM - 5:30 PM	Novel high throughput techniques  Chair: John Janiszewski  Room 202
3:00 PM	Combining rapid isomer separations and physicochemical property measurements with differential mobility spectrometry Dr. Scott Hopkins, University of Waterloo
3:30 PM	Direct liquid extraction approaches to sample analysis Dr. Gary Van Berkel, Oak Ridge National Laboratory
4:00 PM	The perils, principles, and practice of high-throughput mitochondrial metabolic flux measurements Dr. Richard Kibbey, Yale University School of Medicine
4:30 PM	A novel high-throughput lipidomics platform and its applications to study drug polypharmacology Dr. Jiejun Wu, Janssen R&D US LLC
4:50 PM	Bidimensional FT-ICR MS: unravelling structural information from a complex sample without separation Dr. Christian Rolando, Université Lille 1, Sciences et Technologie
5:10 PM	Picodroplet mass spectrometry for miniaturized high throughput analysis of synthetic biology microbial clones Dr. Xin Li, Sphere Fluidics Limited
3:00 PM - 5:30 PM	Noncovalent interactions: proteins, nucleic acids, and small molecules II  Chairs: John Klassen & Valerie Gabelica  Room 203
3:00 PM	Behavior of intrinsically disordered regions in protein complexes Dr. Satoko Akashi, Yokohama City University
3:30 PM	Simultaneous analysis of enzyme structure and activity by kinetic capillary electrophoresis and mass spectrometry Dr. Maxim Berezovski, University of Ottawa
4:00 PM	Construction of accurate supramolecular DNA structures based on mass spectrometric analysis Dr. Xinhua Guo, College of chemistry, Jilin University
4:30 PM	Native state mass spectrometry in natural product and fragment-based drug discovery against malaria protein targets Ms. Liliana Pedro, Eskitis Institute for Drug Discovery, Griffith University
4:50 PM	Structure and dynamics of RNA binding to the non-canonical RNA recognition motif (RRM2) in the human La protein Ms. Kerene Brown, NSERC CREATE York University and University of Toronto
5:10 PM	Exploring the dynamics and function of the flexible domain of Human Histone Deacetylase 2 using mass spectrometry Ms. Zoja Nagurnaja, University College London
3:00 PM - 5:30 PM	Radical peptides Chairs: K.W. Michael Siu & Ivan K. Chu
3:00 PM	Ground and excited-state dissociations of biomolecular cation-radicals Dr. Frantisek Turecek, University of Washington
3:30 PM	Photo-electron transfer dissociation of peptides for zwitterion identification Dr. Ryan Julian, UC Riverside
4:00 PM	Structure and reactivity of metal ion adducts of cysteine-containing peptide radicals Dr. Victor Ryzhov, Northern Illinois University
4:30 PM	Reactions of hydroxyl radical and cysteine disulfide derivatives reveal mechanistic detail in radical induced disulfide cleavage Dr. Yu Xia, Purdue University
4:50 PM	<b>TEMPO-assisted free radical initiated peptide sequencing (FRIPS) mass spectrometry</b> Dr. Han-bin Oh, Sogang University
5:10 PM	Radical-mediated peptide tyrosine nitration Dr. Ivan CHU, University of Hong Kong



	Thurso	lay/Friday 🔝
3:00 PM - 5:30 PM	Imaging - applications Chair: Pierre Chaurand & Peter Hoffmann	Room 206 A-D
3:00 PM	High resolution mapping of N-glycans in FFPE prostate cancer tissues using MALDI-I MALDI-TOF mass spectrometry imaging Dr. Richard Drake, Medical University of South Carolina	TICR and rapid
3:30 PM	Bringing mass spectrometry imaging from pathologist bench to patient bedside: from guided surgery Dr. Isabelle Fournier, University of Lille - France	n diagnosis to
4:00 PM	Mass spectrometry imaging of proteins, lipids and metals in human and mouse chron encephalopathy tissues Dr. Catherine Costello, Boston University School of Medicine	ic traumatic
4:30 PM	Laser mass spectrometry imaging of cuticular lipids from insects using etched silver s Mr. Andreas Schnapp, University of Münster	ubstrates
4:50 PM	Lipid profiling using integrative mass spectrometry imaging (MSI) for nonalcoholic fat (NAFLD) in human liver biopsies Ms. Klara Scupakova, M4I Institute, University of Maastricht	ty liver disease
5:10 PM	Drug delivery quantitation in single cells with sub micrometric spatial resolution TOF Mr. Anthony Castellanos, Florida International University	-SIMS
7:30 PM to 11:30 PM	Banquet Constitution Hall, Metro Toronto Convention Centre, North Building	Room 105-106 Level 100
Friday, Augu	ıst 26, 2016	
8:30 AM - 9:15 PM	Plenary lecture - Single cell analysis with electrospray mass spectrometry Xinrong Zhang, Tsinghua University	Hall A, Level 300
9:30 AM - 12:00 PM	Mass spectrometric insights into catalysis Chairs: Scott McIndoe & Maria Schlengen	Room 201
9:30 AM	Structure and reactivity of phenyl-hydroxycarbene studied in the gas phase: hydroge room temperature Dr. Mathias Schäfer, University Cologne, Department of Chemistry	n tunneling at
10:00 AM	Listening in on reaction intermediates in solution Dr. Jana Roithova, Charles University in Prague	
10:30 AM	Threshold CID measurements probe organic and organometallic reaction mechanism Dr. Peter Chen, ETH Zürich	S
11:00 AM	A New approach for revealing superatomic cores in transition metal complexes by ES Mr. Dmitry Eremin, Zelinsky Institute of Organic Chemistry	I-MS/MS
11:20 AM	Investigating the peroxidase reaction mechanism of human cytochrome c (cyt c) Ms. Rinky Parakra, University of Otago	
11:40 AM	Catalytic reaction mechanism elucidation via real time mass spectrometric analysis Dr. Scott McIndoe, University of Victoria	
9:30 AM - 12:00 PM	New trends in mass spectrometry and medicine Chair: Natalie Agar	Room 202
9:30 AM	Illuminating the chemistry of human skin surface Amina Bouslimani	
10:00 AM	Mass spectrometry in systems medicine: towards the molecular operating theatre Dr. Ron Heeren, M4I, Maastricht University	
10:30 AM	Gas chromatography-differential mobility spectrometry for bedside diagnosis and sur fungal pneumonia Sophia Koo, Harvard University	rveillance of
11:00 AM	Mass spectrometric profiling of biomarkers in exhaled breath for medical diagnosis at medicine Dr. Renato Zenobi, ETH Zurich	nd personalized



Friday	
11:20 AM	Direct detection of endogenous microRNAs and their post-transcriptional modifications in cancer serum by capillary electrophoresis-mass spectrometry Dr. Maxim Berezovski, University of Ottawa
11:40 AM	High throughput quantification of Tenofovir and Emtricitabine in human plasma using LDTD-MS/MS Mr. Jean Lacoursiere, Phytronix Technologies Inc.
9:30 AM - 12:00 PM	Protein-protein complexes Room 203 Chair: Albert Heck
9:30 AM	Charge detection mass spectrometry: instrumentation and application to virus structure and assembly Dr. Martin Jarrold, Indiana University
10:00 AM	Biophysics of clathrin adaptors and new opportunities for native MS in single particle imaging at XFELs  Dr. Charlotte Uetrecht, Heinrich Pette Institute/ European XFEL
10:30 AM	Chemical modification as a path to improved sequencing and structural analysis of proteins and protein complexes  Mr. Daniel Polasky, University of Michigan - Ann Arbor
11:00 AM	Uncovering the complexity of protein complexes: A modified Q Exactive Plus Orbitrap instrument for multi-level analysis of protein complexes  Dr. Michal Sharon, Weizmann Institute of Science
11:20 AM	A platform to discovery protein complexes in biology samples  Mr. Zhongming Hu, NSERC CREATE, York University, University of Toronto
11:40 AM	Molecular simulation study of the dissociation rate and mechanisms of protein complexes in droplets Dr. Styliani (Stella) Consta, Department of Chemistry
9:30 AM -	Atomic MS in environmental applications Room 205
12:00 PM	Chair: Jack Cornett
9:30 AM	Chair: Jack Cornett  Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver  Dr. X. Chris Le, University of Alberta
	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver
9:30 AM	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of <sup>90</sup> Sr using thermal ionization mass spectrometry
9:30 AM 10:00 AM	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of 90Sr using thermal ionization mass spectrometry Dr. Sarata Sahoo, National Institute of Radiological Sciences  Determination of Cd and Te in metal materials and geochemical samples by dynamic reaction cell-inductively coupled plasma mass spectrometry
9:30 AM 10:00 AM 10:30 AM	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of 90 Sr using thermal ionization mass spectrometry Dr. Sarata Sahoo, National Institute of Radiological Sciences  Determination of Cd and Te in metal materials and geochemical samples by dynamic reaction cell-inductively coupled plasma mass spectrometry Dr. Jingyu Hu, NCS Testing Technology Co., Ltd.  Laser-assisted sample introduction for nanoparticle characterization using ICP MS
9:30 AM 10:00 AM 10:30 AM 11:00 AM	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of 90 Sr using thermal ionization mass spectrometry Dr. Sarata Sahoo, National Institute of Radiological Sciences  Determination of Cd and Te in metal materials and geochemical samples by dynamic reaction cell-inductively coupled plasma mass spectrometry Dr. Jingyu Hu, NCS Testing Technology Co., Ltd.  Laser-assisted sample introduction for nanoparticle characterization using ICP MS Dr. Jan Preisler, Masaryk University  Isotopic signature of selected rare earth elements for nuclear activities profiling using cloud point extraction and ICP-MS/MS
9:30 AM 10:00 AM 10:30 AM 11:00 AM 11:20 AM	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of 90Sr using thermal ionization mass spectrometry Dr. Sarata Sahoo, National Institute of Radiological Sciences  Determination of Cd and Te in metal materials and geochemical samples by dynamic reaction cell-inductively coupled plasma mass spectrometry Dr. Jingyu Hu, NCS Testing Technology Co., Ltd.  Laser-assisted sample introduction for nanoparticle characterization using ICP MS Dr. Jan Preisler, Masaryk University  Isotopic signature of selected rare earth elements for nuclear activities profiling using cloud point extraction and ICP-MS/MS Dr. Dominic Lariviere, Laval University  Proper quantification of scandium by ICP-MS/MS: the challenge
9:30 AM  10:00 AM  10:30 AM  11:00 AM  11:20 AM  11:40 AM  9:30 AM -	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of 90Sr using thermal ionization mass spectrometry Dr. Sarata Sahoo, National Institute of Radiological Sciences  Determination of Cd and Te in metal materials and geochemical samples by dynamic reaction cell-inductively coupled plasma mass spectrometry Dr. Jingyu Hu, NCS Testing Technology Co., Ltd.  Laser-assisted sample introduction for nanoparticle characterization using ICP MS Dr. Jan Preisler, Masaryk University  Isotopic signature of selected rare earth elements for nuclear activities profiling using cloud point extraction and ICP-MS/MS Dr. Dominic Lariviere, Laval University  Proper quantification of scandium by ICP-MS/MS: the challenge Ms. Laurence Whitty-Léveillé, Université Laval  Innovations in mass spectrometry instrumentation  Room 206A-D
9:30 AM 10:00 AM 10:30 AM 11:00 AM 11:20 AM 11:40 AM 9:30 AM - 12:00 PM	Complementary mass spectrometry and chromatography techniques enabling the characterization of arsenic metabolites in chicken meat and liver Dr. X. Chris Le, University of Alberta  Novel method for determination of 90 Sr using thermal ionization mass spectrometry Dr. Sarata Sahoo, National Institute of Radiological Sciences  Determination of Cd and Te in metal materials and geochemical samples by dynamic reaction cell-inductively coupled plasma mass spectrometry Dr. Jingyu Hu, NCS Testing Technology Co., Ltd.  Laser-assisted sample introduction for nanoparticle characterization using ICP MS Dr. Jan Preisler, Masaryk University  Isotopic signature of selected rare earth elements for nuclear activities profiling using cloud point extraction and ICP-MS/MS Dr. Dominic Lariviere, Laval University  Proper quantification of scandium by ICP-MS/MS: the challenge Ms. Laurence Whitty-Léveillé, Université Laval  Innovations in mass spectrometry instrumentation Chair: Scott Tanner  Ion boosters, superchargers, chemical modifiers – ion chemistry at work. But how?



		Friday 📋
11:00 AM	Matrix-assisted laser desorption ionization distance-of-flight mass spectrometry Dr. Steven Ray, State University of New York at Buffalo	
11:20 AM	Echo-MS: a versatile platform for ultrafast mass spectrometry analysis in drug discovery Dr. Martin Bachman, AstraZeneca	
11:40 AM	Direct enantiomer selective mass spectrometry of multi-component chiral mixtures by M Dr. Maurice Janssen, MassSpecpecD BV	IS-PECD
12:00 PM - 12:15 PM	Closing ceremony and presentation by IMSC 2018	Hall A, Level 300
12:15 PM - 1:00 PM	Farewell reception	Exhibits Hall B, Level 300



# **Posters**

# Advanced chromatographic methods in environmental analysis

#### M-T-001

Ozone-induced DNA damage: a pandora box of oxidatively modified DNA bases

Dr. Guru Swamy Madugundu, PERFORM Centre, Concordia University

# M-T-002

Chemical speciation of secondary organic aerosol using electrospray ionization-ion mobility time of flight mass spectrometer

Mr. Jianhuai (Jackie) Ye, University of Toronto

#### M-T-003

Sequential ultrasonic extraction of a Chinese coal and characterization of nitrogen-containing compounds in the extracts using HPLC/ESI-TOF-MS

Dr. Xing Fan, China University of Mining and Technology

## M-T-004

Screening for dioxin-like compounds in sediment using modified QuEChERS and a GC-qTOF mass spectrometer with atmospheric pressure chemical ionization

Mr. Liad Haimovici, Ontario Ministry of the Environment

# M-T-005

Phytosterols and phytoestrogens of red propolis determined by GC-MS

Ms. Begoña Gimenez-Cassina Lopez, UNICAMP

#### M-T-006

An accurate analysis of the internal concentration of pesticide in whole larvae tissue of Japanese medaka using LC-QqQ-MS without clean-up step

*Mr. Hattan Alharbi*, Toxicology Graduate Program at University of Saskatchewan

# Advances in analytical separations for MS

### M-T-007

Kinetic study of azobenzene E/Z isomerization using ion mobilitymass spectrometry

Dr. Salomé Poyer, University of Evry - LAMBE

#### M-T-008

**Using differential mobility spectrometry to study chiral compounds**Dr. J. Larry Campbell, SCIEX

#### M-T-009

**Utilising unusual ionisation and SFC to solve a taxing problem**Dr. John Langley, University of Southampton

#### M-T-010

High throughput non-depletive SPME method for LC-MS/MS determination of free and total concentrations of multi-residue in small sample volumes

Dr. Ezel Boyaci, University of Waterloo

# M-T-011

Metabolic distributions of vitamin D metabolites in dried blood spots after chemical derivatization and LC-MS/MS

Ms. Miriam Mueller, Institute of Bioanalytical Chemistry

# M-T-012

Can ASAP Provide a quantitative screen for rapid detection of drugs in saliva?

Ms. Julie Herniman, University of Southampton

#### M-T-013

lonisation enhancement through use of a supercritical fluid and a novel ionisation technique

Dr. John Langley, University of Southampton

#### M-T-014

Digital microfluidic immunoprecipitation for the microscale targeted analysis of proteins from biological samples using mass spectrometry

*Mr. Brendon Seale*, NSERC CREATE York University and University of Toronto



# Multimode gradient HPLC-MS method for metabolomics and environmental monitoring

Dr. Marc Suter, Eawag

### M-T-016

An automated method for microcystins analysis using twodimensional liquid chromatography-quadrupole time-of-flight mass spectrometry (2DLC-QTOFMS).

Dr. Xavier Ortiz, Ontario Ministry of the Environment and Climate Change

## M-T-017

CE-nanoESI-MS for Untargeted proteomic characterization of small neuron populations

Mr. Sam Choi, George Washington University

#### M-T-018

Optimal selection of separation chemistry for 3D-LC-MS/MS in bottom-up proteomics

Dr. Oleg Krokhin, University of Manitoba

### M-T-019

Expanded analytical capability through the application of open access UHPSFC-APPI-MS

Ms. Julie Herniman, University of Southampton

# M-T-020

Solid-phase microextraction low temperature plasma mass spectrometry for the direct and rapid analysis of complex mixtures Mr. Morphy Dumlao, School of Chemistry, University of New

South Wales

# M-T-021

Ultra-fast analysis of allergens using capillary electrophoresis coupled to mass spectrometry and ultraviolet photodissociation

Mr. Ken Miller, Thermo Fisher Scientific

### M-T-022

Cellular metabolomic analysis using photo-controlled probes coupled with ambient mass spectrometry

Dr. Lin Wang, Beijing University of Technology

### M-T-023

Rapid LC method development for multiple drug classes by using a new four-channel LC

Dr. Pengxiang Yang, Thermo Scientific

# M-T-024

The detection of allergens in foods using 2D-LC-MS/MS

Dr. Sophie Thurlow, LGC

### M-T-025

Effect of mobile phase pH: implications for the LC-MS/MS bioanalysis of vitamin D –sulfate compounds

Ms. Nur Sofiah Abu Kassim, The University of Queensland

### M-T-026

Identification of Dechloranes by gas chromatography coupled to tandem mass spectrometry with atmospheric pressure chemical ionization (GC-APCI-MS/MS)

Dr. Ronan Cariou, LABERCA-Oniris, France

#### M-T-027

Determination of phthalates in baby food by gas chromatographymass spectrometry

Ms. Adriana Godoy, University of Campinas

### M-T-028

A multi-class drug and metabolite screen of 231 analytes by LC-MS/MS

Mr. Justin Steimling, Restek Corporation

### M-T-029

Harnessing the efficiency of  $N_2$  as GC carrier gas with an atmospheric pressure MS source

Mr. Adam Ladak, Waters

### M-T-030

Comprehensive profiling of various platycosides in Platycodi radix by UPLC-QTOF/MS

Dr. DaeYoung Lee, Department of Herbal Crop Research, National Institute of Horticultural and Herbal Science, Rural Development Administration

# M-T-031

A Novel nanoLC-MRM workflow for analyzing deoxycholic acid (DOC)-solubilized protein digests from biological samples

Mr. Luc Tessier, National Research Council

### M-T-032

Automated protein digestion on a RTC-PAL system directly coupled to nano-LC-MS<sup>2</sup>

Dr. Andrea Vojs Stanova, University of Bern

### M-T-033

High-performance separation techniques in combination with high-resolution mass spectrometry in the study of MHGF-68

Dr. Magdalena Zimnicka, Comenius University in Bratislava, Faculty of Natural Sciences, Department of Analytical Chemistry



# Diversity of peptide diastereoisomers examined by ion mobility mass spectrometry (IM-MS)

*Dr. Magdalena Zimnicka*, Institute of Organic Chemistry Polish Academy of Sciences

#### M-T-035

# Detection and semi-quantitative determination of designer benzodiazepines in serum using LC-MS<sup>n</sup>

Mrs Laura Maria Huppertz, Institute of Forensic Medicine, Medical Center – University of Freiburg, Faculty of Medicine, University of Freiburg, Germany

#### M-T-036

Quantitation of Synthetic cannabinoids in serum: a comprehensive and sensitive multiplex assay for 99 compounds by LC-MS/MS

Dr. Andrea Kiehne, Bruker Daltonik GmbH

#### M-T-037

Comprehensive two-dimensional gas chromatography (GC×GC) with simultaneous TOFMS and flame ionization detector analysis of petroleum products

Mr. Joe Binkley, LECO Corporation

#### M-T-038

Determination of the antibiotic residues in meat by optimized liquid chromatography tandem mass spectrometry

Ms. Hye Young Park, Ministry of food and drug safety

## M-T-039

Improving the sensitivity for an immunocapture LC-MS assay of Infliximab in rat plasma using trap-and-elute MicroLC-MS

Dr. Johnny Cardenas, SCIEX

#### M-T-040

A sensitive two dimensional LC-MS approach for the characterization of free drug impurities in antibody-drug conjugates

Dr. Alexander Muck, Waters Corp.

#### M-T-041

Comparison of two protein precipitation methods for vitamin D LC/MS assay of human serum

Ms. Nur Sofiah Abu Kassim, The University of Queensland

# Ambient ionization methods

# M-T-042

ASAP and DART mass spectrometry analysis for the understanding of polymers degradation mechanisms

Diane Lebeau, Den-Service d'Etude du Comportement des Radionucléides (SECR), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France

#### M-T-043

Application of ambient mass spectrometry to high-throughput detection of drugs binding to proteins

Dr. Jin Ouyang, College of Chemistry, Beijing Normal University

#### M-T-044

Imaging volatile and semi-volatile compounds by low-temperature plasma MS

Dr. Robert Winkler, CINVESTAV Unidad Irapuato

#### M-T-045

An ambient ionization toolbox: comparison of helium and argon DART with complementary ambient ionization methods

Dr. Robert (Chip) Cody, JEOL USA, Inc.

#### M-T-046

The assessment of volatile organic compounds in foods using APCI-MS and chemometric methods

*Dr. Mathew Turner*, Centre for Analytical Science, Loughborough University

#### M-T-047

Characterization of the oxidation products of Shengli lignite using mass spectrometers with "hard", "soft" and ambient ion sources

Dr. Xing Fan, China University of Mining and Technology

#### M-T-048

Integrating digital microfluidic sample preparation with desorption atmospheric pressure photoionization-mass spectrometry

Mr. Gowtham Sathyanarayanan, University of Helsinki

# M-T-049

Development of a flowing atmospheric pressure afterglow (FAPA) ionisation source to extend the capability of ion trap and Orbitrap mass spectrometry

Dr. Christopher Williams, EPSRC NMSF

# M-T-050

Negative ion generation in the FAPA source: formation processes and auxiliary gas addition effect

Dr. Jaime Orejas, University at Buffalo



# DESI-HRMS leaf analysis for classification and characterization of mycorrhizal rosemary plants

Ms. Raquel Seró Llor, University of Barcelona

### M-T-052

Identification of organotin compounds in a molluscicide product by DESI-HRMS

Ms. Raquel Seró Llor, University of Barcelona

## M-T-053

pH effects on electrospray ionization efficiency

Mr. Jaanus Liigand, University of Tartu

#### M-T-054

Rapid determination of pharmacokinetic profiles of caffeine and its metabolites collected on skin by ambient mass spectrometry

Dr. Jentaie Shiea, National Sun Yat-Sen University, Taiwan

# Biomolecular structure: covalent labeling and crosslinking

#### M-T-055

A single approach to quantify protein-protein, protein-RNA interactions and posttranslational modifications

Dr. Florian Richter, Goethe University, Medical School

# M-T-056

MALDI mass spectrometry and HCCA labeling as a powerful tool for peptide quantitation in biology

Mr. Maxime ROSSATO, University of Montpellier

### M-T-057

Multidimensional mass spectrometry of peptides and proteins conjugated with poly(ethylene glycol)

Dr. Chrys Wesdemiotis, The University of Akron

#### M-T-058

Biochemistry of redox regulation of apoptosis signal-regulating kinase 1: identification and isolation of disulfide-linked intermediates

Mr. Johannes Weijman, Department of Biochemistry, University of Otago, NZ

#### M-T-059

Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer

Mr. Julian Saba, Thermo Fisher Scientific

### M-T-060

Formaldehyde versus established cross-linkers in examining a transient protein complex using mass spectrometry

Dr. Juergen Kast, University of British Columbia

# Chemical proteomics

#### M-T-061

Venom composition's study from genus Lonomia caterpillars, using SDS-PAGE and HPLC-MS/MS

Mr. Danny Alejandro Díaz Moscoso, Los Andes University

#### M-T-062

Proteomic analyses of Nm23-H1/NDPKA activator induced cellular responses in triple negative breast cancer cells

Dr. Jae-Jin Lee, EWHA woman's univ

#### M-T-063

Characterization of formaldehyde-induced modifications in diphtheria toxoid

Mr. Joost Uittenbogaard, Intravacc

# Clinical proteomics

### M-T-064

Quantifying signalling pathway activity from tissue lysates using immuno-MALDI

*Mr. Robert Popp*, University of Victoria - Genome BC Proteomics Centre

#### M-T-065

Alternative proteins: the hidden world of potential biomarkers *Dr. Julien Franck*, University of Lille

### M-T-066

Performance and Bioanalytical applicability of MALDI-compatible protein chips prepared by ambient ion soft landing

Dr. Petr Novak, Institute of Microbiology

#### M-T-067

Functionalized surfaces for direct immuno-affinity mass spectrometry - detection of haptoglobin phenotypes

Dr. Petr Pompach, Institute of Biotechnology

# M-T-068

Towards a new diagnostic tool for human urinary tract infection using LCMS data independent acquisition (DIA) analysis and specific spectral libraries

Mrs Florence Roux-Dalvai, CHU Quebec Research Center



Novel automated quantitative microproteomics approaches for analyzing minute sample amounts in tumour heterogeneity

Dr. Erik de Graaf, Fondazione Pisana per la Scienza

### M-T-070

Droplet-based liquid extraction for spatially-resolved microproteomics analysis from tissue sections

Mr. Maxence Wisztorski, Univ. Lille, INSERM U1192, PRISM

#### M-T-071

Novel therapeutic targets of spinal cord injury based on spatiotemporal proteomics analysis

Dr. Michel Salzet, University of Lille - France

#### M-T-072

The discovery of HDL-associated protein biomarkers to predict stroke

Dr. Chao-Jung Chen, Graduate institute of integrated medicine, China Medical University

# M-T-073

Fully automated sample preparation of whole blood for TDM and diagnostics procedures by LC/MS/MS using a commercial autosampler with tool change

Dr. Lucas Luethy, CTC Analytics AG

# M-T-074

Epitope identifiication and affinity characterization of human alpha-Galactosidase A to a monoclonal antibody by SPR-affinity mass spectrometry

*Mr. Zdenek Kukacka*, Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry

#### M-T-075

Mass spectrometry and computational approach for proteomic characterization of amniotic fluid in polyhydramnios pregnancies

*Dr. Ruta Navakauskiene*, Institute of Biochemistry, Vilnius University

#### M-T-076

Rapid discrimination of Aspergillus section Fumigati based on ribosomal protein profiling observed by MALDI-TOFMS

*Dr. Hiroaki Sato*, National Institute of Advanced Science and Technilogy (AIST)

### M-T-077

Proteomic analyses of mouse kidney with systemic lupus erythematosus using mass spectrometry and ion mobility drifttime dependent collision energies

Dr. Kleitos Sokratous, The Cyprus Institute of Neurology & Genetics, Nicosia, Cyprus

#### M-T-078

Detection of Bordetella pertussis protein pertactin using parallelreaction monitoring compared to Western Blot Analysis

Dr. Patrick Chong, Public Health Agency of Canada

### M-T-080

A quantitative approach using LC-MS in Hepatitis C Virus NS2-3 protease autolysis inhibition

Mr. Maxime Sansoucy, Université du Québec à Montréal

#### M-T-081

Differential proteomic analysis reveals characteristic protein expression changes in traumatic brain injury

Dr. Ganna Shevchenko, Uppsala University

# Emerging and persistent environmental contaminants

### M-T-082

Towards an extended application of MALDI-MS in archaeology and artworks: traces of the past in the mass spectra

Ivana K. Levy, CONICET-UMYMFOR, Consejo Nacional de Investigaciones Científicas y Técnicas, Unidad de Microanálisis y Métodos, Físicos aplicados a la química Orgánica, Ciudad de Buenos Aires, Argentina

# M-T-083

Comparative assessment of perfluoroalkyl substances (PFASs) levels in drinking water supplies of three South African cities

Adegbenro Daso, adegbenrop@gmail.com

#### M-T-084

Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry

Dr. Joe Anacleto, Bruker

#### M-T-085

A validated high resolution mass spectrometry method for the quantification of T-2 and HT-2 toxins in cereals

Dr. Bryan McCullough, LGC Ltd.

#### M-T-086

Development of extraction and LC-MS/MS methods for the quantitation of finasteride, levonorgestrel and melengestrol acetate in water and sediment

Dr. Naomi Stock, Water Quality Centre



An LC-MS/MS study of glyphosate and aminomethylphosphonic acid in soil and the reactivities of mono- to triply-deprotonated glyphosate

Dr. Raymond March, Trent University

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Monitoring of Baltic Sea sediments for sea-dumped chemical warfare agents using GC-MS/MS and LC-MS/MS

Mr. Martin Söderström, University of Helsinki

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Mr. Andre Schreiber, SCIEX

### M-T-090

Data independent acquisition-digital archiving mass spectrometry (DIA-DA MS) with next-generation sequencing for profiling fungal contaminated silage

Ms. Megan Kelman, Western University

### M-T-091

Identification and quantitation of underivatized glyphosate and other polar pesticides in water and beer samples using LC-MS/MS

Mr. Andre Schreiber, SCIEX

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Reading of accurate mass spectra to find anthropogenic substances in the environment

Dr. Atsushi Yamamoto, Tottori University of Environmental Studies

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Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS

Dr. Joe Anacleto. Bruker

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Identification of potential biomarkers of exposure to diundecyl phthalate

Dr. Manori Silva, Centers for Disease Control and Prevention

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A targeted quantitative LC-MS/MS method for 431 positive and negative ion pesticides in a single analysis

Dr. Laurie Allan, Bruker Ltd.

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Evaluation of atmospheric pressure ionization techniques for the determination of fluorotelomer alcohols and perfluorinated sulfonamides

Mr. Juan Francisco Ayala Cabrera, University of Barcelona

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Mammalian metabolism of the C-P bond in perfluorinated phosphinates (PFPiAs) and identification of resulting metabolites Ms. Shira Joudan, University of Toronto

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Phytochelatin production and sequestration of heavy metals as a detoxification pathway in Chara australis for use in phytoremediation

Mr. Jerod Hurst, University of Buffalo

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Mr. Adam Ladak, Waters

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Fast pesticide residue analysis using a novel benchtop time-offlight mass spectrometer

Mr. Jonathan Byer, LECO Corporation

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UHPLC-HRMS determination of palytoxin and ovatoxins from Ostreopsis cf. ovata, a marine microalgae blooming in a Northwestern Mediterranean beach

Ms. Encarna Moyano, University of Barcelona

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Using of a high resolution mass spectrometry for the identification of electrochemical degradation products of selected drugs

Ms. Monika Radicova, Comenius University in Bratislava, Faculty of Natural Sciences, Department of Analytical Chemistry

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A multi-year study of VOC emissions at a waste disposal facility using mobile LPCI-MS and APCI-MS instruments

Dr. Robert Healy, Ontario Ministry of the Environment and Climate Change

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A rapid and robust method for determination of 35 phthalates in influent, effluent and biosolids in wastewater treatment plants Mehran Alaee, Tommy Bisbicos



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Dr. Jerry Zweigenbaum, Agilent Technologies, Inc.

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Mr. Stephen Walker, University Waterloo

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Measuring ion-solvent binding energies with DMS

Mr. Johnathan Steffen, University of Waterloo

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Ms. Sibylle Pfammatter, IRIC - Université de Montréal

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An ion mobility screening approach for the detection of toxicologically relevant substances

Dr. Jeff Goshawk, Waters

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*Dr. Haiyang Li,* Dalian Institute of Chemical Physics, Chinese Academy of Sciences

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Glycan composition and charge state influence upon collision cross sections of high mannose N-linked glycopeptides

Ms. Abby Gelb, University of Nebraska-Lincoln

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Ms. Anne Bruinen, M4I - Maastricht University

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Dr. Daniel Beach, National Research Council Canada

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Peak broadening observations in APLI-IMS: detailed studies and explanation by three effects

Mr. Marvin Ihlenborg, Christian-Albrechts-Universität zu Kiel

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Ms. Jacquelyn Jhingree, Manchester Institute of Biotechnology, University of Manchester

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Dr. Ewa Jurneczko, University of Manchester

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Waters IMS raw data peptide feature identification

Mr. Chenyu Yao, University of Waterloo

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Automatic CCS and MS/MS library creation and application for large scale metabolic profiling

Mr. David Heywood, Waters Corporation

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Numerical simulation of time-of-flight analyzers

Dr. Andrey Trubitsyn, Ryazan State Radio Engineering University

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Simulation of transportation of ions by the electric field in gas in the case of gas flow and differential pressure

Dr. Victor Gurov, Ryazan State Radio Engineering University

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Multisectional monopolar mass-analyzer

Dr. Mikhail Dubkov, Ryazan State Radio Engineering University

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Dr. John Fjeldsted, Agilent Technologies

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Ion mobility mass spectrometry for polymer ions: arrival time distribution symmetry along the ion series

Dr. Julien De Winter, University of Mons



Mechanism of protein supercharging by Sulfolane and m-NBA: molecular dynamics simulations of the electrospray process

Mrs Haidy Metwally, University of Western Ontario

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Device for simultaneous energy, angular and mass analysis of flows of ions emitted by the solid state surface

Dr. Victor Gurov, Ryazan State Radio Engineering University

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Dr. Kazunari Takaya, Rikkyo university

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High resolution trapped ion mobility mass spectrometry analysis of isomeric compounds

Dr. Sven Meyer, Bruker Daltonik GmbH

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Dr. Mikhail Dubkov, Ryazan State Radio Engineering University

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Dr. Sven Meyer, Bruker Daltonik GmbH

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Dr. Andrey Trubitsyn, Ryazan State Radio Engineering University

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Dr. Simonetta Fornarini, Università degli Studi di Roma La Sapienza

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Dr. Thiago C. Correra, IQ-USP - Brazil

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Dr. Anzor Mikaia, National Institute of Standards and Technology

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Dr. Frederic Rosu, Univ. Bordeaux. CNRS ums3033

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Mr. Patrick Jäger, Karlsruhe Institute of Technology

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*Dr. Farid Benkaci-Ali*, University of Sciences and Technology Houari Boumediene, Faculty of Chemistry, Laboratory of Functional Organic Analysis,

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Dr. C K Andy Siu, City University of Hong Kong

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Dr. Michael Burt, University of Oxford

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Dr. Paul Gates, University of Bristol

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Dr. Terry Mcmahon, University of Waterloo

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Mr. Jocky Kung, University of Toronto

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Dr. Jana Roithova, Charles University in Prague

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*Mr. Jakob Hitzenberger*, Friedrich-Alexander University Erlangen-Nuremberg



**Reactions in gas-phase, solution-phase and electrospray ionization** *Mr. Ryan Bain*, Purdue University

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Ms. Yasaman Jami Alahmadi, Memorial University of NL

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Ms. Suzie Douix, Synchrotron Soleil

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Mr. Bryan Linford, Memorial University

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Mr. Matthew Kusinski, University of Toronto

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Dr. Travis Fridgen, Memorial University of Newfoundland

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**Scattering resonance fingerprints in CID mass spectra of PAHs?** *Mr. Eduardo Solano*, University of Ottawa

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Reaction of  $[(\eta 5-C5H5)-M]+(M = Mn, Fe, Co)$  with dichloromethane in the gas-phase: c-c bond formation and production of MCI2

Dr. Anna Troiani, Sapienza Rome University, Italy

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Ms. Sarah Seulen, Christian-Albrechts-Universität zu Kiel

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Dr. Anzor Mikaia, National Institute of Standards and Technology

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Mr. Brian Lam, NSERC CREATE York University and University of Toronto

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Dr. Jingpei Cao, China University of Mining & Technology

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Ms. Yating Wang, NSERC CREATE York University and University of Toronto

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Mr. Herbert Dias, USP - Univesity of São Paulo

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Role of charge position - radical fragmentation reactions from azobenzene derivatives containing diethylamino groups

Mr. Martin Clemen, Christian-Albrechts-Universität zu Kiel

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Dr. Elina Kalenius, University of Jyväskylä

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Mr. Jun Hong Tan, Health Sciences Authority

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Mrs Anniina Kiesilä, University of Jyväskylä



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Dr. Takemichi Nakamura, RIKEN CSRS, Molecular Structure Characterization

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Dr. Jürgen H. Gross, Heidelberg University

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Mr. Gabriel Gaiffe, Université Pierre et Marie Curie

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Chain-end and backbone analysis of poly(N-isopropylacrylamide)s by sequential electron transfer dissociation and collisionally activated dissociation

Mr. Selim Gerislioglu, The University of Akron

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Ms. Sydney Wellman, NSERC CREATE York University and University of Toronto

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Dr. Adel lakubov, Chemistry Department, Irkutsk State University

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Mr. Corentin Decroo, Umons

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Dr. Martin Czar, Eidgenössische Technische Hochschule Zürich

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Mr. Paolo Benigni, Florida International University

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Dr. Magnus Palmblad, Leiden University Medical Center

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HematoBeeTest project: identifying patterns of honeybee immune response by Biotyper-like mass spectrometry, in the context of bee health monitoring

Dr. Sebastien Voisin, Association Plateforme BioPark d'Archamps

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Comprehensive molecular profiling of 3D cardiac and liver cells in the context of toxicogenomics

Dr. Nathalie Selevsek, ETH Zurich

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Dr. Magnus Palmblad, Leiden University Medical Center

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Dr. Sebastien Voisin, Association Plateforme BioPark d'Archamps

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Dr. Olaf Jahn, Proteomics Group, Max-Planck-Institute of Experimental Medicine

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Mr. Maroun El Khoury, Thermo Fisher Scientific



Integrated approach of metabolomics and transcriptomics to reveals regulatory network of potato pigmentation

Dr. Myung Hee Nam, Korea Basic Science Instiyute

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Mr. Maroun El Khoury, Thermo Fisher Scientific

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Dr. Steven Husson, University of Antwerp

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Ms. Débora Sant'Ana, McGill University

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Dr. David Peake, Thermo Fisher Scientific

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Mr. Qi Tang, University of Waterloo

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Dr. Zoe Hall, University of Cambridge

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Ms. Kaija Schäpe, Justus-Liebig-University of Giessen

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Ms. Gilian Thomas, Carleton University

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Dr. Jeffrey Agar, Northeastern University

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Dr. Jiejun Wu, Janssen R&D US LLC

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Solution phase charge inversion of methylated phosphatidylcholine for the identification of fatty acyl components via collision induced dissociation

Mr. Sam Shields, Carleton University

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Mr. Juan Aristizabal Henao, University of Waterloo

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Dr. Roy Martin, Waters

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Ms. Helene Mobbs, Department of Biochemistry, University Cambridge

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Targeted lipidomic analysis of complex lipids in mouse synaptosomes by hydrophilic interaction liquid chromatographytandem mass spectrometry

Mr. Nicolas DEPRETRE, ChemoSens - INRA (France)

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Dr. Raquel Mary Rodrigues Peres, CAISM/UNICAMP

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Mr. Gerson Dirceu Lopez Muñoz, University of los Andes



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Mrs Anik Forest, Montreal Heart Institute

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Dr. Jackie Mosely, Durham University

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Mr. Olivier Berdeaux, ChemoSens - INRA (France)

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Sample preparation and analysis of gangliosides and phospholipids from human plasma by liquid chromatography coupled to mass spectrometry

Ms. Estelle Sibille, ChemoSens - INRA (France)

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Dr. Alexandra Furtos, University of Montreal

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Dr. Myung Hee Nam, Korea Basic Science Instiyute

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Dr. Damila Morais, Unicamp

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Dr. Brigitte Simons, SCIEX

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Dr. Brigitte Simons, SCIEX

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Dr. David Peake, Thermo Fisher Scientific

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Dr. Andrew Baker, Waters Corporation

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Dr. Heiko Neuweger, Bruker Daltonik GmbH

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Mr. Mitch Johnson, University of Missouri

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Dr. Stephen Stein, NIST

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Mass spectrometry metabolomics approach reveals the metabolic side effects of dexamethasone

Mrs Abeer Malkawi, Jordan University of Science and Technology

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*Mrs Ghazaleh Moghaddam,* Université du Québec à Montréal, Chemistry Department

#### M-T-216

Metabolomics to study the "war" between plants and insects systemic defense induction and post-ingestive rearrangement of plant toxins in insects.

Dr. Heiko Neuweger, Bruker Daltonik GmbH

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A novel benchtop time of flight GC/MS system for high performance analysis of human urine

Mr. David Alonso, LECO Corporation

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Can glutathione species be used as biomarkers for environmental metal exposure in fish?

*Dr. Stefanie Maedler,* Ontario Ministry of the Environment and Climate Change



# Characterization of new secondary metabolites of Penicillium using isotopic labeling and HPLC-HRMS

Dr. Emilien Jamin, MetaboHUB-MetaToul-AXIOM

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Mass spectrometry-based targeted metabolomics of serum in Greek-Cypriot women reveals favorable health effects of gene-Mediterranean diet interactions

Mrs Maria Kakkoura, The Cyprus Institute of Neurology and Genetics, Nicosia, Cyprus

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Enabling high-confidence human endogenous metabolite identification via high-resolution MS/MS retention-time library Dr. Verena Tellstroem, Bruker Daltonics

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Dr. Aiko Barsch, Bruker Daltonics

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Mr. Aaron Boice, Agilent Technologies

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Determination of potential diagnostic urinary biomarkers of asthma and COPD using a novel DIL-HPLC-MS/MS method

*Ms. Mona Hamada*, College of Pharmacy and Nutrition, University of Saskatchewan

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Semi quantitative LC-SRM workflow for the analysis of over 100 polyphenols in pulse crops

Dr. Randy Purves, University of Saskatchewan

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A step forward in GC-HRAM-MS based metabolomics - a novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance

Dr. Verena Tellstroem, Bruker Daltonics

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Ms. Elisa Ollikainen, Faculty of Pharmacy, University of Helsinki

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Ms. Adriana Godoy, University of Campinas

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Ms. Nathaly Reyes-Garces, University of Waterloo

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LC-MS/MS analysis of compounds involved in de novo pyrimidine biosynthesis in Solanum lycopersicum

Ms. Paula Galeano, Universidad de los Andes

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Ms. Encarna Moyano, University of Barcelona

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Ms. Mary Piotrowski, Pfizer

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Dr. Riya Christina Menezes, Max Planck Institute for Chemical Ecology

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Dr. Daisuke Miura, Kyushu University

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Ms. Hanan Elsayed, College of Pharmacy, University of Saskatchewan

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Mr. Lorne Fell, LECO Corporation



# Evaluation of the derivatization of organic thiols with N-substituted maleimides

Mrs Mariana Russo, Concordia University

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Intact trichomes single-cells analysis: metabolite profiling with internal electrode capillary pressure probe electrospray ionization MS

*Dr. Rosa Erra-Balsells*, Departamento de Quimica Organica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires

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# Metabolomics by LC-ESI-QTOF-MS in NOD/SCID mice under chemotherapy treatment: potential biomarkers of leukemia

Mr. Gustavo Henrique Bueno Duarte, ThoMSon Mass Spectrometry Laboratory

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# Vitreous humour: real-time analysis of opiates using Exactive FTMS

*Mr. Júlio César Santos Júnior*, Department of Clinical Pathology, School of Medical Sciences, State University of Campinas — UNICAMP

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# Metabolite profiling related with dysmenorrhea in Korean female subjects

Dr. Min Ho Cha, Korea Institute of Oriental Medicine

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### A novel targeted metabolomic approach in plant hormone analysis

Mr. Jan Šimura, Laboratory of Growth Regulators & Department of Chemical Biology and Genetics, Centre of the Region Haná for Biotechnological and Agricultural Research, Faculty of Science, Palacký University & Institute of Experimental Botany ASCR

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Dr. Yuqin Dai, Agilent Technologies

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*Dr. Kristyna Flokova*, Laboratory of Plant Physiology, Wageningen University

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Mr. Fabio Santos, University of Campinas

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Mrs Mi Kyeong Lee, Department of Food Technology and Services, Eulji University

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Application of dimetallic complex for mass spectrometric analysis of phosphate-containing metabolites

Dr. Fedor Kryuchkov, University of Bergen

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Mass spectrometry based proteomics and metabolomics of early dental plaque from caries-free Indian subjects

Ms. Nivedita Bhattacharya, CSIR-National Chemical Laboratory, India

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Dr. Richard B. Cole, Sorbonne Universités, UPMC Univ Paris 06

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Dr. Florian Richter, Goethe University, Medical School

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Dr. Gordon Nicol, MilliporeSigma

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Ms. Katherine Schumacher, University of Nebraska



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Mr. Frederic Lamoliatte, Institute for Research in Immunology and Cancer, University of Montréal

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Ms. In-kang Song, Ewha womans university

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Mr. Julian Saba, Thermo Fisher Scientific

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Dr. Tomoya Kinumi, National Metrology Institute of Japan (NMIJ)/ AIST

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Mr. David Heywood, Waters Corporation

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Targeting cancer-related proteoforms uncovered with proteogenomics

Ms. Marialaura Dilillo, Fondazione Pisana per la Scienza

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Dr. Simon Lauter, Bruker Daltonics Germany

### M-T-260

SWATH analysis of plasma from age-related macular degeneration (AMD) patients

Dr. Catherine Botting, University of St Andrews

### M-T-261

Improvements in LFQ for reproducible quantification of proteomic experiments: how DDA outperforms DIA

Mr. Ken Miller, Thermo Fisher Scientific

### M-T-262

Development of a targeted proteomic assay for rapid detection of Shiga toxins (Stx) 1 and 2 in Shiga toxin-producing E. coli (STEC) bacterial cultures

Ms. Leanne Scharikow, Public Health Agency of Canada

### M-T-263

Evaluation of a novel tandem quadrupole mass spectrometer for quantitative peptides analysis using a multi-point internal standard calibration method

Dr. Roy Martin, Waters

## M-T-264

**An automated workflow for absolute quantitation of large therapeutic proteins in biological samples using intact LC-HRMS** *Dr. Lyle Burton.* Sciex

#### M-T-265

A new method for Label-free quantification in the Proteome Discoverer framework

Mr. Bernard Delanghe, Thermo Fisher Scientific

# Ultra high resolution mass spectrometry and petroleomics

#### M-T-266

Convenient visualization of high resolution MS/MS spectra of synthetic polysiloxane ions using Kendrick mass defect analysis Dr. Thierry Fouquet, National Institute of Advanced Industrial Science and Technology (AIST), Japan

### M-T-267

A combination of on-plate degradation and Kendrick mass defect analysis for characterization of high molecular-weight polyesters by MALDI spiral-TOFMS

Dr. Kanae Teramoto, JEOL Ltd.

#### M-T-268

Photoionization as a soft ionization source for comprehensive twodimensional GC (GCxGC) and high-resolution TOFMS

Dr. John Dane, JEOL USA, Inc.

# M-T-269

GCxGC-HRTOFMS Analysis of base oils with chemical ionization, field ionization and photoionization

Mr. Koji Okuda, JEOL USA, Inc.



#### AstroChemistry

#### W-T-001

The discuss of the development of gas analyzer in space exploration

*Mr. Rongxin Yan*, Beijing Institute of Spacecraft Environment Engineering

#### W-T-002

Exploration and analysis of space atmosphere composition at 499 km sun-synchronous orbit

Dr. Meiru Guo, Lanzhou Institute of Physics

#### Atomic MS in environmental applications

#### W-T-003

Measuring actinides by accelerator mass spectrometry

Dr. Jack Cornett, University of Ottawa

#### W-T-004

Trace multi-elements detection for aerosol particles by using inductively coupled plasma high resolution time-of-flight mass spectrometer

Dr. Hiroyuki Hagino, Japan Autmobile Research Institute

#### W-T-005

High precision Plutonium (Pu) isotope analysis of environmental samples with a double-focusing multi collector inductively coupled plasma mass spectro

Dr. Inhee Choi, Korea Institute Of Nuclear Safety

#### Biomolecular structure: H,D-exchange

#### W-T-006

Microfluidic-enabled time-resolved hydrogen deuterium exchange mass spectrometry (TRHDX-MS) for equilibrated and kinetic epitope mapping

Dr. Bin Deng, York University

#### W-T-007

Improving digestion efficiency of problematic membrane proteins in hydrogen/deuterium exchange compatible workflows

*Mr. Ingvar Moller,* Department of Health and Medical Sciences, University of Copenhagen

#### W-T-008

Conformational differences of the monoclonal antibody Herceptin® demonstrated by Native TWIM-MS, DTIM-MS and HDX-MS

Ms. Rosie Upton, University of Manchester

#### W-T-009

The role of conformational dynamics in differing activity and substrate specificity amongst isozymes of glutathione S-transferase

*Mr. Nicole McGregor*, NSERC CREATE York University and University of Toronto

#### W-T-010

Structural differences between Diphtheria toxin and a detoxified single-point mutant CRM197 revealed by HDX-MS

Dr. Peter Liuni, Sanofi Pasteur/York University

#### W-T-011

Investigating allosteric hotpots and drug binding affinity of TEM-1  $\beta$ -lactamase using TRESI-HDX-MS

Ms. Ruth Knox, NSERC CREATE York University and University of Toronto

#### W-T-012

Functional and HDX-MS analysis of the Type 4 secretion system protein TraF from the Escherichia coli F-plasmid

Ms. Cristina Lento, MS-ESE York University - NSERC CREATE

#### W-T-013

Towards the measurement comparability of protein structural analysis

Ms. Kate Groves, LGC and University of Leeds

#### W-T-014

Dual-spray hydrogen deuterium exchange (HDX) reactions: a new method of probing protein structure

Mr. Bihac Mazigh, University of Ottawa

#### Challenges in biopharmaceutical analysis

#### W-T-015

Structural characterization of antibody-drug conjugates by a combination of intact, middle-up and bottom-up techniques using sheathless CE-MS

Dr. Yannis-Nicolas Francois, LSMIS- University of Strasbourg

#### W-T-016

Monitoring the critical quality attributes of antibody drug conjugates (ADCs) as part of biosimilar development: case studies of T-DM1

Dr. Henry Shion, Waters Corporation



# Selenium labelling combined with LC-ICP-MS, a new methodology in pharmacology to measure protein-ligand interactions

*Dr. Christine Enjalbal*, Université de Montpellier, Institut des Biomolécules Max Mousseron

#### W-T-018

# Selective and cooperative ligand binding to telomeric DNA G-quadruplex targets

Mr. Adrien Marchand, Inserm, ARNA Lab

#### W-T-019

## Ionization efficiency of oligopeptides and small hydrophilic molecules in ESI/MS

Mrs Piia Liigand, University of Tartu

#### W-T-020

# An LC/ESI-IM-MS/MS assay for identification and quantification of host cell proteins in therapeutic monoclonal antibodies

Dr. Min Du, Waters Corporation

#### W-T-021

### Software for monoclonal antibody protein sequencing with LC-MS/MS

Dr. Bin Ma, University of Waterloo

#### W-T-022

# Fully automated on-line extraction procedure using DBS In-Tips with RTC-LC-MS/MS

Dr. Sylvain Letarte, Phytronix Instruments inc.

#### W-T-023

Giving ion mobility to the masses: what collisional-cross section values can do for glycan analysis of biotheraputic monoclonal antibodies

Dr. William Alley, Waters

#### W-T-024

Rapid and simple flow injection analysis-tandem (FIA-MS/MS) mass spectrometric method for the quantification of melphalan in drug delivery systems

Mr. Waleed Mohammed Saeid, Drug Design & Discovery Research Group, College of Pharmacy & Nutrition, University of Saskatchewan

#### W-T-025

# HILIC-LC-MS/MS investigation of the intracellular fate of gemini surfactants designed for gene delivery

Mr. McDonald Donkuru, University of Saskatchewan

#### W-T-026

# Glycoform separation and characterization of Cetuximab variants by middle-up off-line CE-UV/ESI-MS

Dr. Yannis-Nicolas Francois, LSMIS- University of Strasbourg

#### W-T-027

MRM3 versus differential mass spectrometry (DMS) in background noise reduction for complex matrices like human plasma

Ms. Deborah Michel, University of Saskatchewan

#### W-T-028

Development of new sustainable cosmetic products using standardized Artemisia annua L. extract monitored by electrospray ionization mass spectrometry

*Dr. Rosana Alberici*, Thomson Mass Spectrometry Laboratory-UNICAMP

#### W-T-029

Investigating the differential photosensitivity of Tryptophan in a model trp-cage peptide

Ms. Leslie Welch, Genentech a Member of the Roche Group

#### W-T-030

Determination of rat synovial fluid lavage dilution factor using urea as dilution biomarker

Mrs Wei Sun, Sanofi

#### W-T-031

HR-MS characterization of Glc-Gal-Hyl-, O-xylosylation, phosphorylation, and O-linked glycosylation in GLP1-Fc expressed in CHO cells

Mr. Chris Spahr, Amgen, Inc.

#### W-T-032

Extending quantitative capabilities within forensic toxicology using standard addition and UPLC-QTOF-MS

Ms. Sydney Wellman, NSERC CREATE York University and University of Toronto

#### W-T-033

Full characterization of heterogeneous antibodies under denaturing and native/native-like conditions on a hybrid quadrupole-orbitrap mass spectrometer

Dr. Jonathan Josephs, Thermo Fisher Scientific

#### W-T-034

Complete characterization of a cysteine-linked antibody-drug conjugate using a hybrid quadrupole-orbitrap mass spectrometer with high mass range

Dr. Jonathan Josephs, Thermo Fisher Scientific



#### **Environomics**

#### W-T-035

The role of mass spectrometry in a multimodal investigation into how nitrogen sources govern carbon partitioning within a phototrophic consortium

Dr. Christopher Anderton, Pacific Northwest National Laboratory

#### W-T-036

Evaluating changes in the molecular structures of photoirradiated aquatic dissolved organic matter using ultra high resolution mass spectrometry

Dr. Celine Gueguen, Trent University

#### W-T-037

Expression of glutathione S-transferases in the developing zebrafish embryo - a targeted proteomic approach

Ms. Alena Tierbach, Eawag

#### W-T-038

Determination of association oxidative stress biomarker in metal oxides nanomaterial handling workers using on-line solid phase LC-MS/MS

Dr. Hui-Ling Lee, Department of Chemistry, Fu Jen Catholic University

#### W-T-039

A multi-method assessment of photoirradiated dissolved organic matter

Mr. Sohidul Islam, Trent University

#### W-T-040

Identification of mercury dissolved organic matter complexes by high resolution mass spectrometry

Mr. Vaughn Mangal, Trent University

#### W-T-041

Targeted and untargeted analysis of pesticides in fish oil using an ion mobility enabled Q-TOF mass spectrometer

Dr. Andrew Baker, Waters Corporation

#### **Glycomics**

#### W-T-042

lgCarbKB: a glycomics and glycoproteomics focused immunoglobulin knowledge base

*Mr. Kathirvel Alagesan*, Max Planck Institute of Colloids and Interfaces

#### W-T-043

Combination of reductive isotope labeling, exoglycosidase digestions and chromatographic separation for glycomics

Dr. Jianjun Li, National Research Council of Canada

#### W-T-044

Functional carbon surface for structural characterization of disaccharides by matrix-assisted laser desorption/ionization-mass spectrometry

Mrs Mei-Chun Tseng, Institute of Chemistry Academia Sinica

#### W-T-045

Probing carbohydrate isomerism through transition metal ion adduction, gas-phase ion chemistry, and collision-induced dissociation

Ms. Katherine Schumacher, University of Nebraska

#### W-T-046

Glycomic profiling of human hyaluronidase 1

Ms. Abby Gelb, University of Nebraska-Lincoln

#### W-T-047

Tandem mass spectrometry determination of the structure of a heterogeneous mixture of Lipid As isolated from the LPS of Aeromonas liquefaciens SJ-19a

Mrs Mervt Almostafa, Memorial University

#### W-T-048

Analysis of human Glycoproteins with different LC-MS/MS and NMR techniques

Ms. Melissa Bärenfänger, Institute of Organic Chemistry, University of Hamburg

#### W-T-049

LC-MS glycan fingerprinting for the species and serotype-specific determination of bacterial endotoxins

Dr. Anna Karen Laserna, National University of Singapore

#### W-T-050

Novel UPLC-IMS-MS method for identification of hyaluronan oligosaccharides

Dr. Martina Hermannova, Contipro a.s.

#### W-T-051

Comparison of different soft ionization matrices in matrix-assisted laser desorption ionization (MALDI)

Ms. Chuping Lee, Institute of Atomic and Molecular Sciences, Academia Sinica



#### Imaging - applications

#### W-T-052

A molecular insight of the song learning behaviour of zebra finch (Taeniopygia guttata) songbirds during ontogeny with mass spectrometry imaging

Dr. Nina Ogrinc Potocnik, M4I Institute, Maastricht University

#### W-T-053

Tissue mass spectrometry imaging (tMSI) of biomarkers for Niemann-Pick disease

Dr. Petra Oliva, Sanofi Genzyme

#### W-T-054

Metabolomic imaging mass spectrometry of high-risk metastasizing uveal tumors classified upon BAP1 mutational status

Mrs Nasim Bararpour, Centre universitaire romand de médecine légale, Lausanne - Genève (CURML)

#### W-T-055

**A** molecular map of non-alcoholic fatty liver disease progression Dr. Zoe Hall, University of Cambridge

#### W-T-056

imzML: flexibility and exchangeability for mass spectrometry imaging data processing

*Dr. Nicolas Desbenoit,* Chair of Bioanalytical Science and Food Analysis, University of Bayreuth, Bayreuth, Germany

#### W-T-057

Metal-assisted LDI for high resolution imaging MS of neutral lipids from thin tissue sections

Dr. Pierre Chaurand, Université de Montréal

#### W-T-058

Demonstration of enhanced ion mobility separation of derivatised isobaric steroids by DESI and MALDI TOF mass spectrometry

Mr. Michael Batey, Waters Corporation

#### W-T-059

Multimodal mass spectrometry imaging analysis of N-linked glycans and proteins from a single tissue section

Mr. Bram Heijs, Leiden University Medical Center

#### W-T-060

Rapid detection of necrosis in breast cancer with desorption electrospray ionization mass spectrometry

Dr. Arash Zarrine-Afsar, Department of Medical Biophysics

#### W-T-061

Mapping peptide hormones in mouse brain and pituitary using MALDI imaging mass spectrometry

Dr. Brandi West, University of Auckland

#### W-T-062

NanoSIMS for probing intracellular distribution of a isotopically labelled ruthenium (II) anti-cancer drug

*Mr. Ronald Fook Seng Lee*, Ecole Polytechnique Federale de Lausanne

#### W-T-063

Quantitative imaging mass spectrometry (q-IMS) of tyrosine kinase inhibitor in mouse tissues

Dr. Shuichi Shimma, Osaka University

#### W-T-064

Atmospheric pressure mass spectrometry imaging and its application in studying biological samples

Dr. Filip Kaftan, Max Planck Institute for Chemical Ecology

#### W-T-065

Imaging mass spectrometry of rat brain tissue using matrixenhanced surface-assisted laser desorption/ionization with sputter-deposited platinum film

Mr. Satoshi Hamada, Nissan Chemical Industries, LTD.

#### W-T-066

Imaging phospholipid fatty acid composition in different rat brain disease states using DESI and high resolution mass spectrometry Mr. Joseph Kennedy, Prosolia

#### W-T-067

Molecular imaging of gangliosides to investigate lysosomal storage diseases using mass spectrometry imaging with ion mobility separation

Dr. Bindesh Shrestha, Waters Corp.

#### W-T-068

Near infrared fluorescence (NIRF) guided MALDI mass imaging of hypoxia region in tumor tissue

Dr. Jooyeon Oh, ASTA Inc.

#### W-T-069

Surface analysis of murchison meteorite with MALDI stigmatic imaging mass spectrometer

Dr. Jun Aoki, Osaka University

#### W-T-070

An investigation of DESI imaging at varying acquisition rates with real time display for optimized tissue imaging

Mr. Michael Batey, Waters Corporation



Laser ablation atmospheric pressure photoionization (LAAPPI) for ambient mass spectrometry imaging of low polarity compounds in animal tissue

Mr. Juha-Pekka Hieta, University of Helsinki

#### W-T-072

Dense accumulation of adenosine in the outer stripes of outer medulla in murine kidney identified by microscopic MALDIimaging mass spectrometry

Dr. Akiko Kubo, Keio University

#### W-T-073

Dsorption electrospray ionization mass spectrometry imaging (DESI-MSI) for unravel of biomarkers of neuroplasticity in pain and stress

Dr. Anna Maria Fernandes, ThoMSon Mass Spectrometry Laboratory

#### W-T-075

The key point extraction technique for amniotic fluid proteome characterization

Dr. Ruta Navakauskiene, Institute of Biochemistry, Vilnius University

#### Imaging - instrumentation

#### W-T-076

Cool-MALDI: matrix-free mass spectrometric imaging of metabolites in snap-frozen tissue sections using IR-laser ablation and UV-laser postionization

Mr. Jens Soltwisch, Institut for Hygiene, University of Muenster

#### W-T-077

Back to basics - revisiting sprayer design for desorption electrospray ionisation mass spectrometry imaging (DESI-MSI) of biological tissues

Ms. Jocelyn Tillner, Imperial College

#### W-T-078

Effect of excitation laser beam diameter and tissue type on the phospholipid ion signal intensities obtained by MALDI-MS imaging in oversampling mode

*Mr. Marcel Wiegelmann,* Biomedical mass spectrometry, University of Münster, Germany

#### W-T-079

Elemental and molecular imaging of tumour tissues treated with a combination of Sunitinib and Evofosfamide with ToF-SIMS

Mr. Florian Brenner, Vienna University of Technology

#### W-T-080

Sub-micron imaging and identification of molecular chemistry in materials and biological research by TOF-SIMS parallel imaging MS/MS

Dr. John Hammond, Physical Electronics USA

#### W-T-081

An investigation of MALDI imaging with higher speed sample stage "rastering" from an ion mobility enabled Q-TOF mass spectrometer

Ms. Emmanuelle Claude, Waters Corporation

#### W-T-082

MALDI FT-ICR imaging: double the performance or double the samples using quadrupolar detection

Dr. Shannon Cornett, Bruker

#### W-T-083

MSI-directed LCM of the same tissue section: quantitative proteome analysis of regions with distinct MSI profiles

Dr. Rima Ait-Belkacem, Fondazione Pisana per la Scienza ONLUS

#### W-T-084

Mapping rough terrain - laser ablation electrospray ionization (LAESI) of non-flat, biological samples

Mr. Benjamin Bartels, IMPRS

#### W-T-085

A next-generation ultrafast detector for imaging mass spectrometry: the pixel imaging mass spectrometry (PImMS) sensor

Dr. Jason Lee, University of Oxford

# Innovations in mass spectrometry instrumentation

#### W-T-086

Point-of-care analysis of lipids in biological samples using miniature mass spectrometry systems

Dr. Zheng Ouyang, Tsinghua University

#### W-T-087

Development of a heavy ion mass spectrometer incorporating a linear ion trap – part I

Dr. Mark Bier, Carnegie Mellon University

#### W-T-088

 $2\omega$ -FT-ICR mass spectrometry with quadrupolar detection

Dr. Gökhan Baykut, Bruker Daltonik GmbH



#### "The ETD-like fragmentation for small molecules"

Dr. Romain Huguet, Thermo Fisher Scientific

#### W-T-090

Real-time monitoring of surface reactions of biomolecules by means of cluster-induced desorption/ionization mass spectrometry

Dr. Michael Durr, Justus Liebig University Giessen

#### W-T-091

Advancements in increasing resolution in multi reflecting TOF mass spectrometry with folded flight path

Dr. Viatcheslav Artaev, LECO Corporation

#### W-T-092

Negative ion behavior in pulse-heating ion source mass spectrometry

Dr. Xi Luo, Japan advanced institute of science and technology

#### W-T-093

Non uniform sampling (NUS) for bidimensional (2D) FT-ICR MS: how many points we can skip and what resolution we can achieve in a given time?

Dr. Christian Rolando, Université Lille 1, Sciences et Technologies

#### W-T-094

Multiply charged peptides and proteins from liquid matrices using laser spallation at UV/VIS and near-IR wavelengths and rapid evaporative ionization

*Ms. Annika Koch,* University of Münster, Biomedical Mass Spectrometry

#### W-T-095

The improvement of mass resolution, collision induced dissociation efficiency and low mass cutoff by octopole field in linear quadrupole ion trap mass

Dr. Chuan-Fan Ding, Department of Chemistry, Fudan University

#### W-T-096

Multi-reflection time-of-flight mass analyzer for rare earth isotopic geochemistry

*Dr. Ping Chen*, Dalian Institute of Chemical Physics, Chinese Academy of Sciences

#### W-T-097

Accelerated organic reactions in microdroplets: phenomena and fundamentals

Dr. R. Graham Cooks, Purdue University

#### W-T-098

Development of a high sensitivity source for matrix-assisted ionization in vacuum (MAIV) and approaches to fundamental studies

*Dr. I-Chung Lu*, Department of Chemistry, Wayne State University

#### W-T-099

Non-volatile mobile phase compatible LC/MS

Dr. Binghe Gu, The Dow Chemical Company

#### W-T-100

Online biosensor- mass spectrometry for epitope identification and affinity quantification of protein- ligand interactions

Dr. Michael Przybylski, Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry

#### W-T-101

The Electrostatic linear ion trap: a compact, low-power, fourier transform mass spectrometer with tandem MS capabilities

Mr. Eric Dziekonski, Purdue University

#### W-T-102

**Multiplexed Targeted assays using ion trap waveform isolation**Dr. Philip Remes, Thermo Fisher Scientific

#### W-T-103

Evidence for laser-induced redox-reactions between added trifluoroacetate salts and substrate material during polystyrene/DCTB MALDI

Mr. Guido Zeegers, ETH Zürich

#### W-T-104

Improving the resolution of LILBID mass-spectrometry

Dr. Jan Hoffmann, Group of Jun.-Prof. Morgner

#### W-T-105

Sub-picogram detection and identification of analytes in complex matrices using a novel GC-TOFMS

Mr. Matthew Soyk, LECO Corporation

#### W-T-106

Electron induced activation: a mean for inner shell spectroscopy of ions

Dr. Alexandre Giuliani, Synchrotron SOLEIL

#### W-T-108

Development of a novel nano separation device for robust and accurate gradient delivery with intelligent diagnostics

Dr. Simon Lauter, Bruker Daltonics Germany



**lonization efficiency on silicon-based, micro-fabricated electrospray nozzles for micro flow LC-ESI-MS applications** *Dr. Daniel Eikel,* Advion Inc.

#### W-T-110

Analysis of steroids in human urine by gas chromatographycapillary photoionization-tandem mass spectrometry

Ms. Päivi Pöhö, Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki

#### W-T-111

Exploring collision induced dissociation of coronene cation  $C_{24}H_{12}^{\dagger}$  in a linear quadrupole ion trap driven by rectangular voltage RF waveforms

Dr. Christine Joblin, University Toulouse 3 / CNRS, IRAP

#### W-T-112

Calculation of stability diagrams and quadrupole mass filter performance for general digital waveforms

Dr. David Langridge, Waters Corporation

#### W-T-113

Molecule identifier software for improved sample identification by GC-MS

Dr. Aviv Amirav, Tel Aviv University

#### W-T-114

LC-MS with cold EI - the new system and recent applications

Dr. Alexander Fialkov, Tel Aviv University

#### W-T-115

Development of a MEMS gas analyzer and mass spectrometer using a highly efficient CNT field ionizer/electron source

*Mr. Philipp Laufer,* Technische Universität Dresden - Institute for Aerospace Engineering

#### W-T-116

Optimization and applications of low-flow APCI and APPI mass spectrometry with microfabricated heated glass nebulizer

*Dr. Josef Cvačka*, Institute of Organic Chemistry and Biochemistry, Prague

#### W-T-117

Cluster analysis by means of low temperature plasma Fourier transform ion cyclotron resonance mass spectrometry (LTP-FT-ICR-MS) and Cassinian ion trap

Mr. Björn Raupers, Institute of pysical chemistry, University of Kiel

#### W-T-118

Seconds per sample with Echo-DART-MS: acoustic loading of a mass spectrometer for high-throughput label-free screening Dr. Martin Bachman, AstraZeneca

#### W-T-119

A computational study of a multi capillary inlet system using gas dynamics and ion optical simulations

Dr. Dimitris Papanastasiou, Fasmatech Science & Technology

#### W-T-120

Atomic force microscope tip enhanced laser ablation mass spectrometry

Dr. Kermit Murray, Louisiana State University

#### W-T-121

Low power consuming handheld portable ion trap mass spectrometer

Dr. Seung Yong Kim, Korea Basic Science Institute

#### W-T-122

Complex protein digest analyses using ion mobility drift time directed quadrupole wide-band isolation for improved peptide coverage

Dr. Ruwan Kurulugama, Agilent Technologies

#### W-T-123

Utilising a novel, data independent, mode of acquisition on a QTof instrument in combination with a scanning quadrupole mass filter for lipid analysis

Dr. Jayne Kirk, Waters

#### W-T-124

Dual polarity mixing source

Dr. Sharon Curtis, John Holmes Mass Spec Facility Ottawa

#### W-T-125

Mass spectrometry of peptides using a combination of thin-layer chromatography and desorption/ionization induced by neutral SO<sub>2</sub> clusters

Dr. Michael Durr, Justus Liebig University Giessen

#### W-T-126

GC-MS with cold EI and its unexpected benefits

Dr. Aviv Amirav, Tel Aviv University

#### W-T-127

Thermal desorption direct analysis in real-time mass spectrometry (TD-DART-MS)

Mr. Robert Goguen, IonSense



#### FTMS based on the ion orbiting frequency

Dr. Li Ding, SRL (Europe) Ltd.

#### W-T-129

The method for correcting mass spectral interference of  ${\rm CO_2}^+$  from  ${\rm N^+}$  signal and its application in simultaneous analysis of O and N in metals

Dr. Xuejing Shen, NCS Testing technology Co., Ltd

#### W-T-130

The analysis of two-dimensional distribution of trace elements in a micro area by LA-ICP-MS

Ms. Zilan Xiao, NCSTestingTechnology Co., Ltd

#### W-T-131

#### Time dependent desorption process in MALDI

*Mr. Hou-Yu Lin*, Institute of Atomic and Molecular Sciences Academia Sinica

#### W-T-132

A compendium of food and beverage comparisons with a novel benchtop GC-TOFMS system

Mr. Lorne Fell, LECO Corporation

#### W-T-133

A solution for determination of high-concentration aromatic compounds in finished gasolines satisfying ASTM D5769 using a new benchtop GC-TOFMS

Mrs Christina Kelly, LECO Corporation

#### W-T-134

Characterization of ZnO nanoparticles using superconducting tunnel junction cryodetection MS

Mr. Logan Plath, Carnegie Mellon University

#### W-T-135

A novel benchtop GC-TOFMS for fast targeted allergen screening and non-targeted characterization for personal care products

Mr. Bernie Yeung, LECO Corporation

#### W-T-136

Time of flight SIMS quantification of bromine based insecticide in mosquito netting

Dr. Chuanzhen Zhou, Analytical Instrumentation Facility at NCSU

#### W-T-137

Predicting concentrations of small molecules without standard substances in LC/ESI/MS via ionization efficiency scales

Dr. Anneli Kruve, University of Tartu

#### W-T-138

Accurate analysis of small molecules with conventional HCCA (α-cyano-4-hydoxycinnamic acid) MALDI-TOF-MS

Mr. Jian Jun Li, University of Calgary

#### W-T-139

The distinction of cis and trans fatty acids in food products with a novel benchtop time of flight GC-MS system

Mr. Bernie Yeung, LECO Corporation

#### W-T-140

Comparison of weird and wild" jelly bean flavors using HS SPME - gas chromatography - mass spectrometry"

Mr. Joe Binkley, LECO Corporation

#### W-T-141

Multidimensional mass spectrometry to characterize by-products generated during MALDI of polystyrenes synthesized by controlled radical polymerization

Mr. Christophe Chendo, Aix-Marseille Université – CNRS, UMR 7273, Institut de Chimie Radicalaire, Marseille – France

#### W-T-142

Battling fuel-washing: identification of Accutrace S10 in diesel samples using a new benchtop GC-TOF MS system

Mrs Christina Kelly, LECO Corporation

#### W-T-143

Illicit-substance mass spectral libraries: data quality control measures

*Dr. William Wallace*, National Institute of Standards and Technology

#### Mass spectrometric insights into catalysis

#### W-T-144

A mechanistic investigation of the Hiyama cross-coupling reaction using ESI-MS

Ms. Natalie Dean, University of Victoria

#### W-T-145

Combined spectroscopic-mass spectrometric methodology for the study of homogeneous catalytic reactions

Mr. Eric Janusson, University of Victoria

#### W-T-146

Ion/molecule chemistry of isomeric (multi-)metal complexes using ESI-TWIMS-MS

Dr. Nicole Rijs, Karlsruhe Institute of Technology



# New trends in mass spectrometry and medicine

#### W-T-147

In-depth study of the molecular events underlying mGluR-LTD by combining pulsedSILAC/AHA labeling and phosphoproteomics: implications for ASD

Mrs Renske Penning, Utrecht University

#### W-T-148

Stratifying asthma disease in the U-BIOPRED severe asthma project: large-scale MSE and TDA to define sub-phenotype biomarker fingerprints

Dr. James Schofield, University of Southampton, UK

#### W-T-149

Simultaneous detection of xenon and krypton in equine plasma by gas chromatography / tandem mass spectrometry for doping control

Dr. Wai Him Kwok, Racing Laboratory, The Hong Kong Jockey Club

#### W-T-150

Mapping the spatial distribution of cassette-dosed drugs in tissue sections applying a targeted DESI-MSI approach

Mr. Andreas Dannhorn, Imperial College London

#### W-T-151

High resolution mass spectrometry for genomics-driven microbial drug discovery

Dr. Lijiang Song, University of Warwick

#### W-T-152

Monitoring the oligomerization of beta-amyloid (1-42) and its inhibition with LILBID mass-spectrometry

Mr. Tobias Lieblein, Goethe-University Frankfurt

#### W-T-153

Analytic directed synthesis system for the manufacture of pharmaceuticals

Mr. Michael Wleklinski, Purdue University

#### W-T-154

Making ESI-MS/MS newborn screening simplier and much less expensive

*Mrs Andréia Porcari*, ThoMSon Mass Spectrometry Laboratory, Institute of Chemistry, University of Campinas, UNICAMP, Campinas, SP, Brazil

#### W-T-155

Protein mass spectra database for rapid identification of fieldcaught phlebotomine sand flies

Dr. Petr Halada, Institute of Microbiology AVCR

#### W-T-156

Determination of methotrexate (MTX) and its main metabolites by LC-UHR-QTOF in human serum of leukemia patients with high-dose administration

Dr. Arnd Ingendoh, Bruker Daltonics

#### W-T-157

Protein mass spectrometry and DNA Aptamers reveal biomarkers of human monocyte

Mr. Shahrokh Ghobadloo, University of Ottawa

#### W-T-158

Application of GC-MS/MS with isotope dilution for the discovery of inhibitors of DNA glycosylases as potential drugs in cancer therapy

Dr. Pawel Jaruga, National Institute of Standards and Technology

#### W-T-159

Real time SESI-MS analysis of exhaled breath identifies altered metabolic signature in chronic obstructive pulmonary disease Mr. Lukas Bregy, ETH Zurich

#### W-T-160

Exploring microfluidics for ultrasensitive proteomic analysis of laser-capture microdissected fresh frozen tissues

Ms. Marialaura Dilillo, Fondazione Pisana per la Scienza

#### W-T-161

Adherence to cardiovascular pharmacotherapy assessed by quantitative LC-HRMS analysis of dried blood spots

Dr. Sangeeta Tanna, De Montfort University

#### W-T-162

Development and validation of LC-MS/MS method for quantification of rifampicin, amoxicillin and faropenem in plasma and application in clinical study

Dr. Daryl Hee, National University of Singapore

#### W-T-163

Intrasurgical brain tumor diagnosis and surgical margin definition by desorption electrospray ionization-mass spectrometry

Dr. R. Graham Cooks, Purdue University

#### W-T-164

Mass spectrometry application in a real case of acute intoxication after alternative natural therapy treatment

Dr. Damila Morais, Unicamp



# Isotope effects in stability of MS analyte/internal standard ratio measurements

Dr. Geoffrey Rule, ARUP Laboratories

#### W-T-166

Exploring microfluidics for ultrasensitive proteomic analysis of laser-capture microdissected fresh frozen tissues

Mr. Davide Pellegrini, NEST, Scuola Normale Superiore

# Noncovalent interactions: proteins, nucleic acids, and small molecules

#### W-T-168

Deciphering G-quadruplex DNA folding landscape with mass spectrometry, ion mobility and circular dichroism

Mr. Adrien Marchand, Inserm, ARNA Lab

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DNA oligonucleotide fragmentation in tandem mass spectrometry experiments

Mrs Stefanie Ickert, Federal Institute for Materials Research and Testing

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Gas-phase complexation of  $\alpha$ -/ $\beta$ -cyclodextrins with amino acids studied by ion mobility-mass spectroscopy and molecular dynamics simulations

Dr. Chuan-Fan Ding, Department of Chemistry, Fudan University

#### W-T-171

Ligand induced conformation and stability change of G-quadruplexes formed by the BRCA1 gene promoter

Dr. Jiang Zhou, Peking University

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Behavior of intrinsically disordered regions in protein complexes

Dr. Satoko Akashi, Yokohama City University

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Construction of accurate supramolecular DNA structures based on mass spectrometric analysis

Dr. Xinhua Guo, College of chemistry, Jilin University

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Simultaneous analysis of enzyme structure and activity by kinetic capillary electrophoresis and mass spectrometry

Dr. Maxim Berezovski, University of Ottawa

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Host-guest complexes probed by mass spectrometry: bridging the gap between the solution and the gas phase

Dr. Pascal Gerbaux, University of Mons

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Exploring the dynamics and function of the flexible domain of human histone deacetylase 2 using mass spectrometry

Ms. Zoja Nagurnaja, University College London

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Native state mass spectrometry in natural product and fragmentbased drug discovery against malaria protein targets

Ms. Liliana Pedro, Eskitis Institute for Drug Discovery, Griffith University

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Direct interfacing of imaging SPR with MALDI MS

Ms. Ulrike Anders, ETH Zurich

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A liquid chromatography-tandem mass spectrometry method for quantitative analysis of curcumin and curcumin metabolites in human plasma

*Dr. Guru Swamy Madugundu*, PERFORM Centre, Concordia University

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Structure and dynamics of RNA binding to the non-canonical RNA recognition motif (RRM2) in the human La protein

Ms. Kerene Brown, NSERC CREATE York University and University of Toronto

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RED-LCMS as an orthogonal technique for high throughput fragment based drug discovery

Dr. Besnik Bajrami, Broad Institute of MIT and Harvard

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New strategy for analysis of the splicing regulatory factors using high-resolution mass spectrometry

Mr. Toru Takarada, Kobe Pharmaceutical University

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Studying non-covalent interactions with nano ESI-MS: an insight into the allosteric mechanism of M2 pyruvate kinase isoform (PKM2)

Mrs Agni Faviola Mika Gavriilidou, ETH Zurich



Dual-spray reactions: a new method of synthesizing inorganic complexes within the electrospray source

Mr. Shaan Rashid, University of Ottawa

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Proteomic analysis of integral membrane proteins in different larval tissues from the poplar leaf beetle Chrysomela populi

Dr. Natalie Wielsch, Max Planck Institute for Chemical Ecology

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Tandem mass spectrometric analysis of novel positively charged peptide-modified gemini surfactants

Ms. Mays Al-Dulaymi, University of Saskatchewan

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Investigation of halogen bonded supramolecular capsules by ESI-MS and IM-MS

Ms. Ulrike Warzok, Freie Universität Berlin

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Implication of tau-metal interactions in Alzheimer's diseases; investigation by ESI-MS and IMS-MS

Mrs Soha Ahmadi, University of Toronto

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Dr. Jiang Zhou, Peking University

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Insight into the noncovalent associations of folinic acid and pemetrexed with native cyclodextrins using mass spectrometry-based techniques

*Dr. Magdalena Zimnicka*, Institute of Organic Chemistry Polish Academy of Sciences

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Comparison of LC-MS and SFC-MS analytical strategies for the characterization of modified transfer RNA

Mr. Vincent Guerineau, CNRS ICSN

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Dr. Meital Kupervaser-Cohen, Weizmann Institute of Science

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**Differential mobility spectrometry of protonated nucleobases**Ms. Ahdia Anwar, University of Waterloo

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Coupling solid phase micro-extraction (SPME) to mass spectrometry via an open-port probe (OPP) sampling interface Dr. Chang Liu, SCIEX

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Emerging applications in biochemical profiling and imaging atmospheric pressure mass spectrometry

Dr. Mariam ElNaggar, Prosolia

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Real time monitoring of photoreactions performed within levitated droplets by LA-DBD-MS

*Mrs Aleksandra Michalik-Onichomowska*, Bundesanstalt für Materialforschung und -prüfung (BAM)

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Analysis of squalene oxidation on human skin by paper spray mass spectrometry

Dr. Pu Wei, Purdue University

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A novel benchtop time of flight GC/MS system for high throughput qualitative and quantitative analysis of drugs of abuse in human urine

Mr. David Alonso, LECO Corporation

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Utilizing new reverse search library program and DART-MS for targeted screening of food and supplements for adulterants Mr. Frederick Li, IonSense, Inc.

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Medical swab analysis using desorption electrospray ionization mass spectrometry (DESI-MS) – a novel, non-invasive approach for mucosal diagnostics

Ms. Pamela Pruski, Imperial College London

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Spatially resolved analysis of symbiotic soybean-rhizobia interactions by laser ablation-electrospray ionization mass spectrometry

Dr. Christopher Anderton, Pacific Northwest National Laboratory



Mobile membrane introduction mass spectrometry for real-time geo-spatial resolution of atmospheric trace organics

Dr. Erik Krogh, Applied Environmental Research Labs, Department of Chemistry

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Temperature-regulated thermal desorption and pyrolysis coupled with direct analysis in real time mass spectrometry (DART)

Dr. Robert (Chip) Cody, JEOL USA, Inc.

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Metabolic phenotyping of cell lines by rapid evaporative ionization mass spectrometry

Ms. Emmanuelle Claude, Waters Corporation

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Real time detection of fish fraud using rapid evaporative ionisation mass spectrometry (REIMS)

Dr. Olivier Chevallier, Queen's University Belfast

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Fast identification of counterfeit medicines – a comparison of two MS systems

Dr. Graham Lawson, De Montfort University

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The effect of sampling pipeline on the measure gas partial pressure with mass spectrometer in molecule flow

*Mr. Rongxin Yan*, Beijing Institute of Spacecraft Environment Engineering

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Mr. Jeremy Gauthier, Memorial University of Newfoundland

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Ms. Juhyun Lee, Korea Institute of Nuclear Safety

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Mr. Koji Okuda, JEOL USA, Inc.

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Open probe fast GC-MS - real time analysis with separation

Dr. Alexander Fialkov, Tel Aviv University

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Fresh approaches to the analysis of small polar N-nitrosamines in water using MIP-DESI-MS

Dr. Christina Bottaro, Department of Chemistry, Memorial University

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Polymer inclusion membranes with condensed phase membrane introduction mass spectrometry (CP-MIMS): improved analytical response time and sensitivity

Dr. Chris Gill, Applied Environmental Research Laboratories - Vancouver Island University

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Dr. David Cox, SCIEX

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Dr. Michael Easterling, Bruker Daltonics

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Measurement of Estradiol in human serum by LC-MS/MS using a novel estrogen-specific derivatization reagent

Mrs Reena Desai, Anzac Research Institute, Sydney, Australia

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Generic sample extraction workflow for analysis of complete drugs of abuse panel by LDTD-MS/MS (screening) and LC-MS/MS (confirmation)

Mr. Alex Birsan, Phytronix Technologies Inc.

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Now a reality: sub second quantitative mass spectrometry analysis with Acoustic sample deposition and fiber coupled LDTD-MS/MS

Dr. Pierre Picard, Phytronix Technologies Inc

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Direct insertion probe coupled to a high resolution time of flight mass spectrometer for rapid targeted and non-targeted analysis of drugs of abuse

Mr. David Borton, LECO Corporation



# Non-aqueous capillary electrophoresis-electrospray ionization mass spectrometry on thiol-ene-based microchips

*Ms. Sari Tähkä*, Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki, Finland

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#### 2D-patterning technique for analysis of post-translationally modified proteins using LC-MS with different chromatographic separations

*Mr. Akira Tarui,* School of Materials Science, Japan Advanced Institute of Science and Technology

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# Ultra high throughput screening by MALDI-TOF MS in drug discovery – exceeding one million samples per week

Dr. Sergei Dikler, Bruker Daltonics Inc.

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#### Long term test on a new four-channel HPLC

Dr. Byungchul Cha, Thermo Fisher Scientific

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# A continuous flow sampling interface for high-throughput SPME-MS/MS analysis of in-vitro ADME samples

Mr. John Janiszewski, Pfizer Inc.

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# Microscale isolation of cytokinins by magnetic microparticle-based immunopurification

Dr. Ondrej Novak, Laboratory of Growth Regulators, IEB & UP Olomouc

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# Screening of $\alpha\nu\beta\delta$ antagonists using ultrafiltration-liquid chromatography-mass spectrometry

Mr. Nkazimulo Tshuma, University of Nottingham

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Mrs Sahar Ghiasikhou, ETH Zurich

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# Enzymatic assay development using novel MALDI high-throughput screening system

Dr. Sergei Dikler, Bruker Daltonics Inc.

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A high-throughput LC/MS biochemical assay for monitoring activity of the early wall teichoic acid pathway gene product TarO

Mr. Paul Tawa, Merck & Co

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# High throughput microflow LC/MS: sensitivity gains on a practical timescale

Dr. Michael Donegan, Waters Corp

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Dr. Sara Smith, MilliporeSigma

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Dr. Mariette Matondo, Institut Pasteur

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Ms. Linsey Raaijmakers, Utrecht University

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# Proteomic and phosphoproteomic analysis of cell response to photon and particle irradiation

Mr. Martin Winter, German Cancer Research Center

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# High sensitivity and high throughput phosphoproteomics with micro-scale TMT labeling

*Mr. Kosuke Ogata*, Graduate School of Pharmaceutical Sciences, Kyoto University

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#### Analysis of protein pyrophosphorylation by CID and EThcD mass

Dr. Eberhard Krause, Leibniz-Institut für Molekulare Pharmakologie Berlin

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Dr. Finn Holding, Astex Pharmaceuticals

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Phosphoproteomic pipeline for the identification of non-genomic signaling pathways activated by contaminant exposure in aquatic species

Dr. Tara Sabo-Attwood, University of Florida



#### Protein-protein complexes

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New developments in intact mass analysis of proteins and protein complexes

Dr. Chris Becker, Protein Metrics Inc.

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Epitope binning by hydrogen deuterium exchange mass spectrometry: Understanding epitope-driven effects

Dr. Chris Morgan, Sanofi Genzyme

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A novel two-dimensional (2-D) proteomic platform for proteomewide protein-protein interaction studies

Dr. Reza Pourhaghighi, University of Toronto

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Slightly bigger is better: protein interaction analysis with 100um ID columns

Mr. Brett Larsen, LTRI

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Dr. Jim Kapron, Bruker

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Mr. Quentin Dutertre, Philip Morris

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Dr. Atsuko Takeuchi, Kobe Pharmaceutical University

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*Dr. Wolfram Engst*, German Institute of Human Nutrition Potsdam- Rehbrücke (DIfE)

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Ms. Fadwa Benkessou, Karolinska Institutet

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Dr. Sarah Theiner, Insitute of Analytical Chemsitry, University of Vienna

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Dr. John Cahill, Oak Ridge National Laboratory

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Dr. Kyoung-Moon Han, NIFDS, MFDS, Republic of Korea

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Thermal degradation of sulfamethoxazole during food cooking

Dr. Laurent Debrauwer, Axiom Platform - UMR 1331 INRA Toxalim - Toulouse - France

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Dr. Sylvie Chevolleau, Axiom platform - UMR 1331 Toxalim INRA Toulouse - France

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Data and prediction driven convergent analysis for metabolite identification in drug discovery

Dr. Richard Lee, Advanced Chemistry Development, Inc. (ACD/Labs)

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Dr. Kai Chi Lau, MS-ESE York University - NSERC CREATE

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Mr. Bai Han Wu, NSERC CREATE York University and University of Toronto



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Dr. Cheuk Kuen Lai, MS-ESE York University - NSERC CREATE

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Dr. Albert Lebedev, Lomonosov Moscow State University

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Mr. Paul Fayad, Thermo Fisher Scientific

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Proteomic and metabolomic analysis of wort: differentiation of malting barley cultivars

Dr. Martin Dusek, Research Institute of Brewing and Malting

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Characterization of virulent Bacillus cereus species using top-down proteomics

Mr. Christian Malosse, Institut Pasteur

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Profiling of intact proteins in the CSF of Alzheimer's disease patients

Mr. Victor Fursey, Bruker Daltonics Inc

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Dr. Rima Ait-Belkacem, Fondazione Pisana per la Scienza ONLUS

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Dr. Chad Weisbrod, Thermo Fisher Scientific

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Ms. Julie Cautereels, University of Antwerp

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Dr. Olena Masui, MS-ESE York University - NSERC CREATE

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Identification of novel cysteine-containing peptides in tropical ant venoms using 3D mass mapping

Mr. Luuk van Oosten, Heidelberg University

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Method for clinical application of MALDI imaging driven top-down microproteomics for discovery of tumor biomarkers

Mr. Vivian Delcourt, Université Lille 1 INSERM U-1192 PRISM -Université Sherbrooke





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