

# **19<sup>th</sup> International Mass Spectrometry Conference**

## **PROGRAMME**



**IMSC2012  
KYOTO**

**Kyoto International Conference Center**  
**Saturday 15<sup>th</sup> September – Friday 21<sup>st</sup> September 2012**



**19th IMSC**



**Organizers  
of the 19<sup>th</sup> International Mass Spectrometry Conference**



**International Mass Spectrometry Foundation**



**Mass Spectrometry Society of Japan**



**Science Council of Japan**

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## Welcome Address from the Chair of the 19<sup>th</sup> IMSC

**Yoshinao Wada**

Chair of the 19<sup>th</sup> International  
Mass Spectrometry Conference



On behalf of the Mass Spectrometry Society of Japan (MSSJ) and the Local Organizing Committee it is my great pleasure to welcome all delegates to the 19<sup>th</sup> IMSC in Kyoto, Japan.

It is a particular honor to stage this landmark event in Kyoto. The first IMSC held outside of Europe demonstrates the mass spectrometry community to be a global body.

The MSSJ was established in 1953, and held international meetings on mass spectrometry twice: “International Mass Spectrometry Conference (Japan)” on September 9-12, 1969 and “Biological Mass Spectrometry (BMS)” on September 20-24, 1992. In 1967 during the 4<sup>th</sup> IMSC in Berlin, Professor Ogata (Osaka University) discussed holding the IMSC in Japan with executives of four countries (UK, France, Germany and USA), but it did not come off due to the IMSC tradition and the long distance. Consequently, the meeting in 1969 was regarded as an “intermediate” between the 4<sup>th</sup> (Berlin) and 5<sup>th</sup> (Brussels) IMSCs. Twenty years later, Professor Matsuo (Osaka University) took a different approach, in which he recognized the importance of biological applications to mass spectrometry and added “Biological” to the name for the second meeting. The International Organizing Committee of the BMS’92 was held in Amsterdam during the 12<sup>th</sup> IMSC (1991). The venue of these meetings was here at the Kyoto International Conference Center.

The applications of mass spectrometry especially in the biological field have continued to grow and are a high stage of development, especially in the current post-genome era. In addition, the role of mass spectrometry is expanding in other fields and purposes: e.g. security and safety as well as curiosity about the uncharted territory of space. It should be stressed as well that the development of core technology is essential for mass spectrometry to meet these demands. The program committee has tried to reflect the developments of the fundamentals in physics and chemistry in the programme. Here, we have eight Plenary and Tutorial Lectures and 45 scientific sessions with Keynote Lectures in this abstract book.

Recovery from the 2008 financial recession has been slow and the world economy is facing many problems such as those in Europe. Japan is also struggling to recover from the stall in our economy triggered by the magnitude 9.0 earthquake in March 11, 2011, and the nuclear reactor accident that followed. The organizing committee was afraid of a severe impact of these problems on the preparation for this conference and participation at this meeting. However, at the time of printing this booklet, we were relieved that we already had 1,400 registered delegates, a total of 1,042 papers for 233 oral and 809 poster presentations, and 46 corporate registrations for exhibition and advertisement.

A conference of this size could not take place without the cooperation and support of many individuals, organizations and companies. The Science Council of Japan co-hosts this conference with MSSJ and provides sizable financial support. Moreover, the 19<sup>th</sup> IMSC is thus accorded high status among the international meetings held in Japan this year. Next, I would like to convey special thanks to a number of mass spectrometric companies, listed in this booklet. Without their financial support this conference could not have been arranged. The organizing committee is grateful to the Executive Board of the International Mass Spectrometry Foundation (IMSF) as well as to scientists from many countries for their help in arranging the scientific sessions.

The MSSJ has chosen Kyoto as the venue for this meeting. It is not only renowned as the former capital and cultural heart of Japan, but also for its place at the cutting edge of mass spectrometry research.

Welcome and enjoy the science and your stay in Kyoto.

## Welcome Address from the President of the International Mass Spectrometry Foundation

**Marcos N Eberlin**

IMSF President

We are making Mass Spectrometry history here in Kyoto at our 19<sup>th</sup> International Mass spectrometry Conference!



For the first time ever, an IMSC is being held outside Europe. This is an extraordinary accomplishment for our society in its endeavor to become a fully international forum for the worldwide advance of the science and practice of MS through the promotion and dissemination of MS knowledge to everyone and everywhere. Our international conferences, which starting from Kyoto are held now biannually, are the main means for IMSF to achieve its goals; hence the importance of hosting IMSC across the different continents.

On behalf of the IMSF board and all of our ca. 40 affiliate MS societies, I therefore very enthusiastically welcome all the ca. 2000 IMSF participants to the city of Kyoto for the historical 19<sup>th</sup> IMSC. We are also glad to announce here in Kyoto several key IMSF actions to improve education and dissemination of MS knowledge. For example, the creation of MSpedia ([www.internationalmspedia.com](http://www.internationalmspedia.com)), an interactive website which has the goal to become the most authoritative source of free, web-based multi-lingual information about MS. This initiative has been generously sponsored by Waters Corporation. Also, IMSF will be selecting the site to host the inaugural international MS school in 2013. The IMSF funding for speakers to attend affiliate MS conferences has also been implemented and the South African Association for MS (SAAMS) has been the first to be sponsored. This program is designed to help spread the “MS-word” to under-resourced areas.

It is also my great pleasure to congratulate Dr. Ruedi Aebersold (nominated by the Swiss Group for Mass Spectrometry); Dr. Alexander Markarov (nominated by the British Society for Mass Spectrometry); and Dr. František Tureček (nominated by the Czech Society for Mass Spectrometry) who have been selected by IMSF affiliate societies to receive the Thomson medal for outstanding achievements in MS and for distinguished service to international MS, and Dr. Zheng Ouyang from Purdue University for who will receive the Curt Brunée award, generously sponsored by Thermo Fisher Scientific and made to a young mass spectrometrist for outstanding contributions to the development of MS instrumentation.

For an even brighter future of MS, it is also a privilege for me, as the IMSF president, to congratulate the five young mass spectrometrists: Zoe Hall (University of Oxford), Nicolas Dietl (Technische Universität Berlin), Fan Chen (ETH Zürich), David Marshall (University of Wollongong) and Daniel G. Beach (University of Guelph) for being selected to receive the Journal of Mass Spectrometry Award generously sponsored by Wiley. We also congratulate the 26 students from all over the world who have received IMSF travel scholarships to help them attend the Kyoto Conference.

I also want to deeply thank Prof. Yoshinao Wada for the presidency and all his colleagues from the Japanese MS Society for participating in the organizing committee and for all their efforts that have resulted in a very-well organized conference full of MS novelties and both scientific and social excitement. Congratulations also to all of you who have contributed to the 19<sup>th</sup> IMSC; very well done indeed! Enjoy the conference, I am sure you will have a most enjoyable and rewarding time in Kyoto. And by the end of the week, please start planning your attendance at the 20<sup>th</sup> IMSC to be held in Geneva in 2014.

## Previous, Current and Future IMSCs

1 <sup>st</sup> Meeting	London, UK	1958	11 <sup>th</sup> Meeting	Bordeaux, France	1988
2 <sup>nd</sup> Meeting	Oxford, UK	1961	12 <sup>th</sup> Meeting	Amsterdam, The Netherlands	1991
3 <sup>rd</sup> Meeting	Paris, France	1964	13 <sup>th</sup> Meeting	Budapest, Hungary	1994
4 <sup>th</sup> Meeting	Berlin, Germany	1967	14 <sup>th</sup> Meeting	Tampere, Finland	1997
5 <sup>th</sup> Meeting	Brussels, Belgium	1970	15 <sup>th</sup> Meeting	Barcelona, Spain	2000
6 <sup>th</sup> Meeting	Edinburgh, UK	1973	16 <sup>th</sup> Meeting	Edinburgh, UK	2003
7 <sup>th</sup> Meeting	Florence, Italy	1976	17 <sup>th</sup> Meeting	Prague, Czech Republic	2006
8 <sup>th</sup> Meeting	Oslo, Norway	1979	18 <sup>th</sup> Meeting	Bremen, Germany	2009
9 <sup>th</sup> Meeting	Vienna, Austria	1982	19 <sup>th</sup> Meeting	Kyoto, Japan	2012
10 <sup>th</sup> Meeting	Swansea, UK	1985	20 <sup>th</sup> Meeting	Geneva, Switzerland	2014

### Important Addresses:

Chair of the 19<sup>th</sup> International Mass Spectrometry Conference

Prof. Dr. Yoshinao Wada

Department of Molecular Medicine

Osaka Medical Center and Research Institute for Maternal and Child Health.

840 Murodo-cho, Izumi

Osaka 594-1101, Japan

Phone: +81 725 57 4105

Fax: +81 725 57 3021

E-mail: imsc@mch.pref.osaka.jp

19<sup>th</sup> IMSC Venue:

Kyoto International Conference Center (ICC Kyoto)

Takaragaike, Sakyo-ku

Kyoto 606-0001, Japan

Phone: +81 75 705 2001 (Sep. 15~21) / +81 75 705 1234

Fax: +81 75 705 1100

E-mail: ask@icckyoto.or.jp

Conference Secretariat:

c/o Congress Corporation

3-6-13 Awajimachi, Chuo-ku

Osaka 541-0047, Japan

Phone: +81 6 6229 2555

Fax: +81 6 6229 2556

E-mail: imsc2012@congre.co.jp

## IMSF Governing, IMSF Executive and Local Organizing Committees

### International Mass Spectrometry Foundation (IMSF)

#### Executive Committee

Marcos N Eberlin (Brazil)	President
John C Traeger (Australia)	Past President
Catherine E Costello (United States of America)	Vice President (Society)
Yoshinao Wada (Japan)	Vice President (Conference)
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Jen-tiae Shiea (Taiwan)	Region B Representative
Paul M Mayer (Canada)	Region C Representative

### International Mass Spectrometry Foundation (IMSF) - Affiliates

Argentina	Gabriela M Cabrera	Japan	Ryuichi Arakawa
Australia/New Zealand	Stephen Blanksby	Korea	Kyuseok Song
Austria	Gunter Allmaier	The Netherlands	Christian H Grun
Belgium	Jan Van Boxclaer	Norway	Einar Uggerud
Brazil	Fabio Gozzo	Peoples Republic of China	Jin-Ying Li
Canada	Michael Siu	Poland	Piotr Stefanowicz
Croatia	Mario Cindric	Portugal	Maria Helena Florencio
Czech Republic	Michal Holcapek	Romania	Zaharie Moldovan
Denmark	Steen Pontoppidan	Russia	Albert Lebedev
Egypt	Ezzat Selim	Singapore	Manfred Raida
Finland	Tiina Kauppila	Slovakia	Vladimir Kovacik
France	Olivier Laprévote	Slovenia	Helena Prosen
Germany	Juergen Grotzmeyer	South Africa	Egmont Rohwer
Hellenic	Anthony Tsarbopoulos	Spain	Damia Barcelo
Hong Kong	Terence Chuen-wai Poon	Sweden	Jonas Bergquist
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India	Suresh Aggarwal	Taiwan	Yu-Ju Chen
Ireland	Edward Malone	Ukraine	Marina Kosevich
Israel	Tsippy Tamiri	United Kingdom	Susan Crosland
Italy	Gianluca Giorgi	United States of America	Scott McLuckey

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**Local Organizing Committee**

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Yoshinao Wada ————— Chair  
Koichi Tanaka ————— Co-Chair  
Michisato Toyoda ————— Secretary  
Takemichi Nakamura ————— Treasurer  
Toshifumi Takao ————— Scientific Programme  
Hiroshi Yamaoka ————— Social Programme  
Mitsuo Takayama ————— Fund-Raising  
Yasuo Mizooku ————— Company Support  
Kazuo Furusawa ————— Local Support

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**Scientific Programme Committee**

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Toshifumi Takao ————— Chair

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Satoko Akashi  
Satoka Aoyagi  
Ryuichi Arakawa  
Toshiyuki Azuma  
Takeshi Bamba  
Shigeo Hayakawa  
Kenzo Hiraoka  
Takafumi Hirata  
Yasushi Ishihama  
Morio Ishihara  
Akira Ishii  
Shigeki Kajihara  
Shinobu Kudoh  
Tsutomu Masujima  
Jiro Matsuo  
Hiroyuki Matsuzaki  
Fuminori Misaizu  
Keisuke Nagao  
Yasuhide Naito  
Takemichi Nakamura  
Toyofumi Nakanishi  
Takeshi Nakano  
Yoshiya Oda  
Tomoyuki Oe

**Overseas Members**

Hyun Joo An  
Stephen Blanksby  
Dominic T W Chan  
Ajai Chaudhary  
Richard B Cole  
Catherine E Costello  
Catherine Fenselau  
David Fenyö  
Jean Futrell  
Anastassios Giannakopoulos  
Peter Haglund  
Myung Soo Kim  
Jinying Li  
Joseph A Loo  
DaeWon Moon  
Evgeny N Nikolaev  
Bela Paizs  
Gavin E Reid  
Jentaie Shiea  
Seung-Koo Shin  
Jane Thomas-Oates  
Vicki H Wysocki  
Renato Zenobi  
Roman A Zubarev

**20<sup>th</sup> IMSC**

International Mass Spectrometry Conference  
Geneva, Switzerland  
August 24–29, 2014

**20<sup>th</sup> International Mass Spectrometry Conference****Geneva, Switzerland****August 24–29, 2014****Conference web site <http://www.imsc2014.ch/>**

The 20<sup>th</sup> International Mass Spectrometry Conference will be held in Geneva, Switzerland. It will be jointly organized by the Swiss Group for Mass Spectrometry (SGMS), the French Mass Spectrometry Society (SFSM) and the Division of Mass Spectrometry of the Italian Chemical Society (DSM). Geneva, in the French-speaking part of Switzerland, is a buoyant, international city with an excellent infrastructure. Many international organizations have their headquarters in Geneva, including the UN and the WHO. Located in the heart of Europe, close to the Swiss alps, and well connected to many destinations worldwide by air and train, Geneva is a popular city that hosts many international conferences. We proudly invite you to attend the 20<sup>th</sup> IMSC in Geneva!

**Venue**

The conference will be held at the newly renovated International Conference Centre in Geneva (CICG; [www.cicg.ch](http://www.cicg.ch)), a very modern, centrally located facility, which offers room for up to 2,200 persons.

**Scientific Program**

The program will consist of plenary lectures (including award lectures, and a couple of plenaries outside the area of mass spectrometry) and a technical program of 4 parallel sessions, grouped around 7 main topics that will reflect the latest developments in mass spectrometry. Keynote and contributed oral presentations will be complemented by workshops and poster sessions.

**Accommodations**

Geneva has a wide range of hotels – from five-star accommodations to an above average number of inexpensive accommodations for students and budget travelers that cost less than € 30 per night. 2,000 hotel rooms in all categories have already been tentatively reserved for 2014.

**Exhibition and Sponsorship**

An exhibition will be organized during IMSC2014. More detailed information will be available on the website or from the conference office in due time.

**Organizing Committee**

Marc Suter & Renato Zenobi (co-chairs). Ruedi Aebersold, Günter Allmaier, Silvia Catinella, Leopoldo Ceraulo, Julia Chamot-Rooke, Laurent Fay, Eric Forest, Gianluca Giorgi, Detlef Günther, Gerard Hopfgartner, Olivier Laprévote, Markus Stöckli.

**Conference Office**

the conference office will be in the hands of a professional conference organizer located in Geneva:

Symporg SA, Rue Rousseau 30, CH-1201 Genève, Switzerland  
([www.symporg.ch](http://www.symporg.ch)). Contact: M. Bertrand Joehr, [bjoehr@symporg.ch](mailto:bjoehr@symporg.ch))

## THOMSON MEDAL

The International Mass Spectrometry Foundation will present the 2012 **Thomson Medals** at the 19<sup>th</sup> International Mass Spectrometry Conference, Kyoto.

The winners are:

- Prof. Ruedi Aebersold
- Dr. Alexander Makarov
- Prof. František Tureček

The award ceremony and lectures will be held in the Main Hall on Wednesday, 19<sup>th</sup> September, 08:00 (ceremony) and on Thursday, 20<sup>th</sup> September, 17:10 (lectures).

**Ruedi Aebersold** is the Professor in Molecular Systems Biology the ETH (Swiss Federal Institute of Technology) Zurich, Switzerland and the University of Zurich. He received his undergraduate and PhD degrees in cell biology from the Biozentrum at the University of Basel, Switzerland. He trained as a postdoctoral fellow at Caltech with Lee Hood and had his first faculty appointment at the University of British Columbia in Vancouver, Canada. In 1993 he moved to the University of Washington and in 2000 he co-founded, with Lee Hood and Alan Aderem, the Institute for Systems Biology in Seattle. In 2004 he assumed his present position at ETH Zurich and the University of Zurich in Switzerland. He serves on the advisory boards of a number of academic and private sector organizations.



His research is focused on the development and application of mass spectrometric techniques to study the proteome, the ensemble of proteins expressed by a cell or tissue. Specifically, his group has been interested in the quantitative analysis of the proteome, in developing publicly accessible, open source computational tools and data resources for the statistically sound analysis of large scale proteomics datasets, on the development of targeted mass spectrometric methods for the reproducible analysis of clinical samples and on the use of chemical reagents and mass spectrometry to probe to structure of protein complexes.

Prof. Ruedi Aebersold is the recipient of several awards for his research, including the ASBMB Herbert Sober award (2009) the Otto Naegeli Prize (2009), the ABRF Award (2008), the FEBS Buchner Medal (2006), the HUPO Achievement Award (2005), the ASMS Biemann medal (2002) and the 2003 World Technology award. He is a member of EMBO and has published more than 500 scientific papers.

**Alexander A Makarov** is Director of Research in Life Sciences Mass Spectrometry business of Thermo Fisher Scientific in Bremen, Germany since 2007. He obtained his MSc in Technical Physics from Moscow Physics-Engineering Institute (MPEI), Russia in 1989 and his PhD in Physics and Mathematics with Prof. A.A. Sysoev in 1992 in the same institution.



After two years in a post-doc position in Warwick University, UK, he joined a small high-tech company HD Technologies in Manchester, UK. There he has started his work on the Orbitrap mass analyzer. Following the acquisition of HD Technologies by Thermo Electron Corporation in 2000, Alexander has provided scientific leadership of the Orbitrap research and development which led to the commercial release of LTQ Orbitrap tandem mass spectrometer in 2005. Since then he continues to provide scientific guidance on further extensions of this instrument family as well as a new Exactive/ Q Exactive family of instruments. His research focuses on the strategic goal of bringing Orbitrap-based mass spectrometry into new analytical applications.

Dr. Makarov has been the recipient of several awards for his research, including Heinrich-Emmanuel Merck award (2007), Gold medal of Russian Mass Spectrometry Society (2007), Award of American Society of Mass Spectrometry for Distinguished Contribution in Mass Spectrometry (2008), Curt Brunner research award of International Society for Mass Spectrometry (2009), Science and Technology Award of Human Proteome Organization (2011) and others. He is among authors of more than 40 papers and more than 50 patents and patent applications.

**František Tureček** is Professor of Chemistry at University of Washington, Seattle. He received a BS in Chemistry from Charles University, Prague, where he also obtained an M.S. and a Ph.D. in Organic Chemistry. In 1977-1987 he was Research Scientist at the J. Heyrovsky Institute of Physical Chemistry and Electrochemistry in Prague, Czechoslovakia. In 1987 he left Czechoslovakia, and after 11 months in a refugee camp in Austria he rejoined Fred McLafferty at Cornell University as a Post-Doctoral Associate and Lecturer. In 1990 joined the faculty at University of Washington where he chaired the Analytical Chemistry Division (1992-2007). His research interests range from fundamental topics of ion chemistry and reaction mechanisms through instrumentation and development of new analytical techniques to applications of mass spectrometry in diagnostics and newborn screening.



Prof. Tureček is author of over 360 scientific papers, over 20 review articles and book chapters, and 3 books, among them the 4th Edition of Interpretation of Mass Spectra. He served as Secretary and on several committees of the American Society for Mass Spectrometry and is an Honorary Member of the Czech Society of Mass Spectrometry. He is one of the founding Editors of Journal of Mass Spectrometry and has served on editorial and advisory boards of several journals.

## CURT BRUNNÉE AWARD sponsored by ThermoFisher Scientific

This award is generously sponsored by ThermoFisher Scientific and is presented 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 award**”.

The award ceremony and lecture will be held in the Main Hall on Wednesday, 19<sup>th</sup> September, 08:00 (ceremony) and 08:30 (lecture).

**The winner is: Dr. Zheng Ouyang**

**Zheng Ouyang** is currently an Associate Professor in the Weldon School of Biomedical Engineering at Purdue University in West Lafayette, Indiana, USA. He started as an engineering student in Automatic Control at Tsinghua University in Beijing, China and obtained a bachelor’s and a master’s degree from the Department of Automation. He then went to the University of West Virginia in Morgantown, West Virginia, USA to study Raman spectroscopy and received his 2nd master’s degree in Physical Chemistry. In 1997, he went to Purdue University to explore Mass Spectrometry and received his Ph. D in Analytical Chemistry in 2002. He stayed at Purdue as a postdoctoral fellow and later a research scientist and joined the Department of Biomedical Engineering as an assistant professor in 2007.



Dr. Ouyang has a broad interest in developing instrumentation and applications for mass spectrometry. He has established and maintained a research group consisting of students and researchers with knowledge and complementary skills in Engineering, Physics, and Chemistry. His main achievements in research include the electromagnetic and hydrodynamic simulation methods for ion transfer and mass analysis, algorithms and methods for signal and data processing, ion trap mass analyzers and arrays of simple geometries, discontinuous atmospheric pressure interface for miniature vacuum systems, low temperature plasma probe and paper spray ionization for direct chemical analysis, and miniature MS analysis systems for chemical analysis and biomedical diagnosis.

Dr. Ouyang has published more than 90 research papers and received several awards including the Wallace H. Coulter Foundation Early Career Translational Research Award in Biomedical Engineering, China National Natural Science Foundation Award for Distinguished Oversea Young Scholars, USA National Science Foundation Early Career Award, and the American Society for Mass Spectrometry Research Award.

## 5<sup>th</sup> Journal of Mass Spectrometry Awards Symposium

The **Journal of Mass Spectrometry** Award Symposium is held every 3 years on the occasion of the International Mass Spectrometry Conference. The fifth symposium will take place in conjunction with the 19<sup>th</sup> International Mass Spectrometry Conference in the Room B-1 on Thursday, 20<sup>th</sup> September, at 09:00.

The winners of the Postgraduate Awards are:

### **Fan Chen**

ETH Zurich, Switzerland:

**Integral Membrane Proteins by High-mass MALDI-MS: Direct Access to the Stoichiometry of their Complexes and to Posttranslational Modifications**

### **Nicolas Dietl**

Technical University Berlin, Germany:

**Great Insights from a Small System: Structure and Reactivity of  $[VPO_4]^{·+}$  in comparison with  $[V_2O_4]^{·+}$**

### **Zoe Hall**

University of Oxford, UK:

**Charge-State Dependent Compaction and Dissociation of Protein Complexes: Insights from Ion Mobility and Molecular Dynamics**

### **David Marshall**

University of Wollongong, Australia:

**Odd Products from Even-electron Ions: Exploiting Charge-remote Bond Homolysis to Compare Bond Dissociation Energies**

### **Daniel Beach \***

University of Guelph, Canada

**Quantitative Capabilities of Non-Target Analysis of Urine Using ESI-FAIMS-MS/MS**

(\* not attending Symposium)

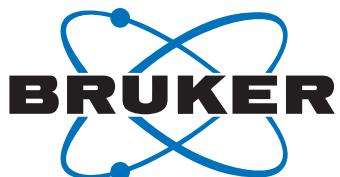
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## Platinum Medal Sponsors



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## Gold Medal Sponsor



## Silver Medal Sponsors



## Local Support Societies and Organizations

The Chemical Society of Japan  
The Pharmaceutical Society of Japan  
The Japan Society for Analytical Chemistry  
The Japanese Biochemical Society  
Japan Society for Bioscience, Biotechnology, and Agrochemistry  
Japanese Society for Food Hygiene and Safety  
The Japanese Society for the Study of Xenobiotics  
Atomic Energy Society of Japan  
The Japan Society of Applied Physics  
The Atomic Collision Society of Japan  
Japan Society for Environmental Chemistry  
The Japan Institute of Metals  
The Surface Science Society of Japan  
The Ceramic Society of Japan  
Japanese Society for Biomedical Mass Spectrometry  
The Japan Society of Plasma Science and Nuclear Fusion Research  
The Society of Polymer Science, Japan  
The Japan Society of Calorimetry and Thermal Analysis  
The Spectroscopical Society of Japan  
The Vacuum Society of Japan  
The Society for Biotechnology, Japan  
Japan Analytical Instruments Manufacturers' Association  
Japan Human Proteome Organization

Kyoto Prefecture  
Kyoto City  
Kyoto Chamber of Commerce and Industry  
Kyoto Convention Bureau  
Kyoto Prefectural Board of Education  
The Kyoto Shimbun Newspaper Co., Ltd.

The Kato Memorial Bioscience Foundation  
Suntory Institute for Bioorganic Research

Matrix Science K. K.  
JCL Bioassay Corporation  
DAINIHON JOCHUGIKU Co.,Ltd.  
DAIICHI SANKYO COMPANY, LIMITED  
Taisho Pharmaceutical Co., Ltd.  
Ajinomoto Co., Inc.

Commemorative Organization for the Japan World Exposition '70

## List of Exhibitors

Company	Booth	Company Room
AB SCIEX	B	Room H
Advion, Inc.	5	
Agilent Technologies, Inc.	A	Room G
Antec	37	
APRIORI CORPORATION	38	
Biologica Co.	39	
Biotage JAPAN, Ltd.	4	
Bruker	E	Room J
CTC Analytics AG	2,3	
Fujitsu Limited	36, 43	
GL Sciences Inc.	49	
Hakuto Co., Ltd.	14	
HAMAMATSU PHOTONICS K.K.	45	
Hitachi, Ltd. Central Research Laboratory	7	
HORIBA,Ltd.	10,11	
Hudson Surface Tech	15,16	
INFOCOM CORPORATION	27	
IONICON Analytik GmbH	9	
IONICS Mass Spectrometry	38	
IonSense, Inc. / AMR, Inc.	48	
JCL Bioassay Corporation	50	
JEOL Ltd.	C	Room K
LECO Corporation	41	
LMS Co. Ltd.	42	
Matrix Science K.K.	29	
MS NOISE	6	
Nihon Pall Ltd.	44	
PEAK SCIENTIFIC JAPAN KK	12,13	
PHOTONIS USA	25,26	
Phytronix Technologies Inc.	28	
Polymer Factory Sweden AB	46	
Shimadzu Corporation	F	Room I
SYSTEM INSTRUMENTS CO., LTD	8	
Thermo Fisher Scientific	17~24	
ULVAC-PHI, Inc.	1	
VRS	30	
Waters Corporation	D	Room F
YMC Co., Ltd.	40	
Zivak Technologies	47	

## List of Publications' Exhibitors

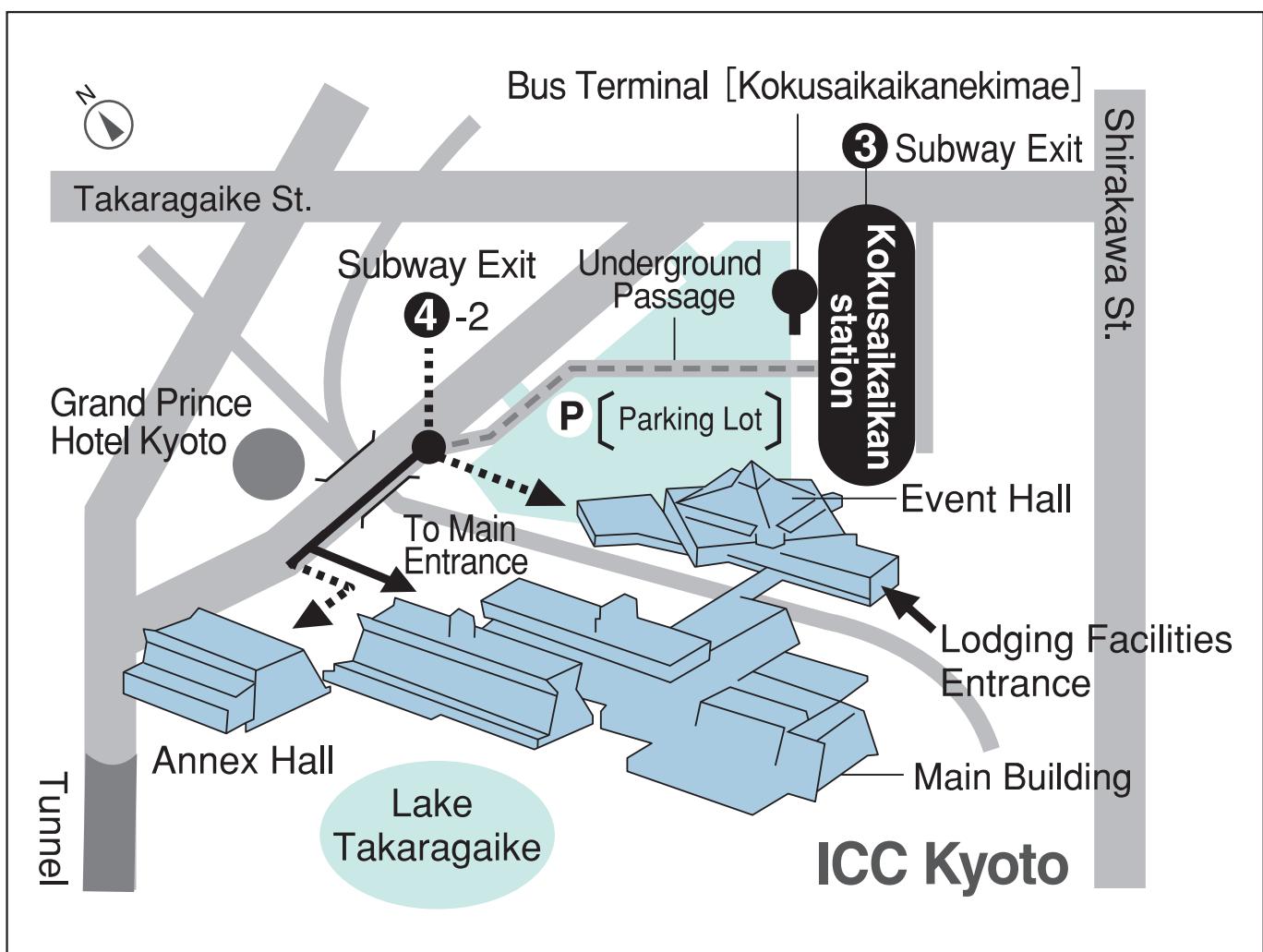
Company	Table
AAAS/Science	H
IM Publications LLP	I
Imtakt Corporation	E
Merck Ltd.,Japan	A
Mass Spectrometry Data Center, National Institute of Standards and Technology	D
The Mass Spectrometry Society of Japan / International Academic Printing Co., Ltd	G
NetWell Corporation	J
SGE Analytical Science Pty Ltd	F
Wiley	B&C

## Conference Venue

### Kyoto International Conference Center (ICC Kyoto)



### ICC Kyoto Area Map



## General Information

### Conference Regulations

- Smoking is prohibited in the conference venue.
- Cell phones must be turned off during oral sessions.
- No photography and/or recording is allowed in any sessions, including posters.
- The placement of advertising in the conference venue is strictly prohibited unless approved by the conference organizers.
- No organized activities (even off-site) other than those approved by the conference organizers are allowed during conference week (15:30 on Sunday through 14:00 on Friday).
- Hardware, terminals, accessories, or any items for commercial advertisement may be displayed only in exhibit booths and corporate meeting rooms.

### Official Conference Language

The official conference language is English. Simultaneous translation is not provided.

### Registration Desk

#### The Registration Desk open hours:

Saturday, 15 <sup>th</sup> September	09:30-17:00
Sunday, 16 <sup>th</sup> September	09:30-19:00
Monday, 17 <sup>th</sup> September	
Tuesday, 18 <sup>th</sup> September	07:30-18:00
Wednesday, 19 <sup>th</sup> September	
Thursday, 20 <sup>th</sup> September	
Friday, 21 <sup>st</sup> September	07:30-10:00

On-site registration ONLY AVAILABLE hours below (JPY cash or credit card is acceptable):

Sunday, 16 <sup>th</sup> September	09:30-19:00
Monday, 17 <sup>th</sup> September	
Tuesday, 18 <sup>th</sup> September	07:30-18:00
Wednesday, 19 <sup>th</sup> September	
Thursday, 20 <sup>th</sup> September	07:30-16:00

The registration desk is located on Main Entrance.

### Badges

The name badge must be worn and clearly displayed by each registered participant and accompanying person at all times during the conference. All participants will receive the badge upon registration. Access to the conference venue will not be granted without a proper name badge. If a participant loses or forgets to bring the name badge, a fixed handling fee of JPY 5,000 will be charged for a new name badge.

## Registration Coverage

	Conference bag	19 <sup>th</sup> IMSC programme	Abstract CD-ROM	Scientific programme	Exhibition	Opening Ceremony, Welcome Mixer & ARIGATO & SAYONARA
Regular	✓	✓	✓	✓	✓	✓
Student	✓	✓	✓	✓	✓	✓
Accompanying Person						✓

Accompanying persons are admitted to the Opening / Closing Ceremonies, Opening Plenary, Welcome Mixer and ARIGATO & SAYONARA ONLY. Accompanying persons will not be provided Conference bags.

## Presentation Guidelines

### – Oral Presentation

#### Length of presentations:

Plenary / Tutorial 45 minutes (introduction and 40 min talk)

Keynotes 40 minutes (introduction, 30 min talk, Q&A)

Other orals 20 minutes (15 min talk, Q&A)

Please adhere strictly to the start and finish times of the presentation. You should arrive in the session room 30 minutes before the start of your session.

## Computer Data Projection

In order to avoid trouble arising from software incompatibility, the organizing committee recommends speakers to use their own laptop computer with an analog VGA (mini D-SUB 15 pin) connector for data projection. Please bring the AC 100V power adaptor for your computer. A VGA cable will be available to use.

Please bring your computer or USB flash drive with you to the session room 30 minutes before the start of your session and make sure you have tested your data projection in advance. Please visit the Speaker Preview Room one day before if you are using a USB flash drive. (See below for more details)

Please turn off the sleep-mode and screen saver of your computer prior to your presentation. The computer must be kept powered-on and AC 100V power supplied throughout the session to avoid any trouble.

All the meeting rooms are equipped with one projector that can be connected to either your laptop or a conference PC (for USB flash drive users). The data on the USB flash drive must be compatible with either the English version Power Point (2007, 2010) or Adobe Reader (ver. 10) on the Windows 7 conference PC.



## Speaker Preview Room

Please check the compatibility of your data with the conference projection system in advance to ensure that your presentation can be correctly displayed. Speakers are fully responsible for the functionality of their presentations. If you bring a USB flash drive containing your presentation, please visit the Speaker Preview Room one day before. The Speaker Preview Room is Room 104 on the 1st floor.

A technician in the Speaker Preview Room (Room 104 on the 1<sup>st</sup> floor) may assist you to solve problems that you may have with your presentation.

### Opening Hours:

Sunday, 16 <sup>th</sup> September	13:00-17:00
Monday, 17 <sup>th</sup> September	08:00-17:00
Tuesday, 18 <sup>th</sup> September	
Wednesday, 19 <sup>th</sup> September	07:30-18:00
Thursday, 20 <sup>th</sup> September	

### – Poster Presentations

There will be poster sessions from Monday to Thursday. Authors of odd-numbered posters will present during the first core time (11:10 to 12:20), authors of even-numbered posters will present during the second core time (13:30 to 14:40). Authors must be present at their posters during the core time. Authors have to wear a “presenter badge”. Presenter badges are available at the poster reception desk located at the entrance to the Event hall. Poster boards are labeled with the number corresponding to the last three digit of presentation number in the Final Program. All posters must be set up before 08:00 from Monday through Thursday.

Mounting time is from 7:30 to 8:00 and removal time is 17:00 to 17:30 from Monday through Thursday. After removal time organizers are not responsible for returning posted material to the authors.

Poster board specification: 1.80 m wide and 1.2 m high. Pushpins should be attached to the poster board for you to use and are also available at the poster reception desk.

Poster Mounting time	7:30-8:00
Poster Core Time	Odd-number
	Even-number
Poster Removing time	17:00-17:30

## Exhibition

The exhibition will take place in the Event Hall and Room C-1.

### Exhibition Opening Hours:

Sunday, 16 <sup>th</sup> September	13:00-18:00
Monday, 17 <sup>th</sup> September	
Tuesday, 18 <sup>th</sup> September	
Wednesday, 19 <sup>th</sup> September	09:00-18:00
Thursday, 20 <sup>th</sup> September	

## Conference Proceedings

The plenary and keynote lectures will be published shortly after the meeting in "Advance in Mass Spectrometry vol.19" as a special issue of an open access journal "*Mass Spectrometry*".  
(<http://mass-spectrometry.jp>)

## Workshops

Workshops are scheduled 17:15-19:15 on Monday, Tuesday and Wednesday. For details, please see the Workshop pages in this programme book.

## Corporate Luncheon Seminars

Corporate luncheon seminars are scheduled 12:20-13:30 on Monday, Tuesday, Wednesday and Thursday. For more information, see the Company Luncheon Seminars' pages in this programme book.

Company	Date	Venue
AB SCIEX	Monday, 17 <sup>th</sup> September Tuesday, 18 <sup>th</sup> September Wednesday, 19 <sup>th</sup> September Thursday, 20 <sup>th</sup> September	Room A
Advion	Tuesday, 18 <sup>th</sup> September	Room E
Agilent Technologies	Monday, 17 <sup>th</sup> September Wednesday, 19 <sup>th</sup> September	Room E
AMR	Thursday, 20 <sup>th</sup> September	Room D
Bruker	Wednesday, 19 <sup>th</sup> September Thursday, 20 <sup>th</sup> September	Main Hall Room E
JEOL	Monday, 17 <sup>th</sup> September	Room D
Thermo Fisher Scientific	Tuesday, 18 <sup>th</sup> September	Main Hall
SHIMADZU	Monday, 17 <sup>th</sup> September Thursday, 20 <sup>th</sup> September Tuesday, 18 <sup>th</sup> September Wednesday, 19 <sup>th</sup> September	Main Hall Room D
Waters	Monday, 17 <sup>th</sup> September Tuesday, 18 <sup>th</sup> September Wednesday, 19 <sup>th</sup> September Thursday, 20 <sup>th</sup> September	Room B-1

## Corporate Meeting Rooms

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Meeting rooms may be open 15:00-18:00 on Sunday and open all day Monday through Friday.  
Meeting rooms are located in 1<sup>st</sup> floor and 2<sup>nd</sup> floor of ICC Kyoto.

The following companies offer a meeting room as indicated:

AB Sciex	Room H
Agilent Technologies	Room G
Bruker	Room J
JEOL	Room K
SHIMADZU	Room I
Waters	Room F

## Coffee Breaks

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Soft drinks may be available after the morning oral sessions and before the afternoon oral sessions.

## Lunch

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Lunch is not included in the registration fee.

## Social Activities

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- **Welcome Mixer**, Sunday, 16<sup>th</sup> September, 18:30-20:00, Swan in ICC Kyoto. Conference name badge is required.
- **Conference Banquet**, Thursday, 20<sup>th</sup> September, 18:30-21:00, Grand Prince Hotel Kyoto. Banquet fee is not included in the registration. Banquet ticket printed on name badge is required. *Tickets are already sold out.*
- **ARIGATO & SAYONARA**, Friday, 21<sup>st</sup> September, 13:00-13:45, Swan in ICC Kyoto. Conference name badge is required.

## Information Board

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Information of conference programme, society meetings, Lost and Found items etc. will be displayed on the information boards, located entrance/registration area on the 1<sup>st</sup> floor.

## Internet Connections / International Phones

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Wireless LAN connection is available in Main Lounge, Main Lobby and at the entrance of Event hall (see page 27). Business center with internet connection and international telephone service are located on the 1<sup>st</sup> floor.

## First Aid

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If you need first aid, please contact the registration desk.

## Cloakroom

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The cloakrooms are located near the main Entrance. Valuables cannot be checked in the Cloakroom.

### Opening Hours:

Sunday, 16 <sup>th</sup> September	13:00-21:00
Monday, 17 <sup>th</sup> September	
Tuesday, 18 <sup>th</sup> September	07:30-20:00
Wednesday, 19 <sup>th</sup> September	
Thursday, 20 <sup>th</sup> September	
Friday, 21 <sup>st</sup> September	07:30-15:00

## Certificate of Attendance / Presentation

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A certificate of attendance and/or presentation will be issued at registration desk.

## Insurance

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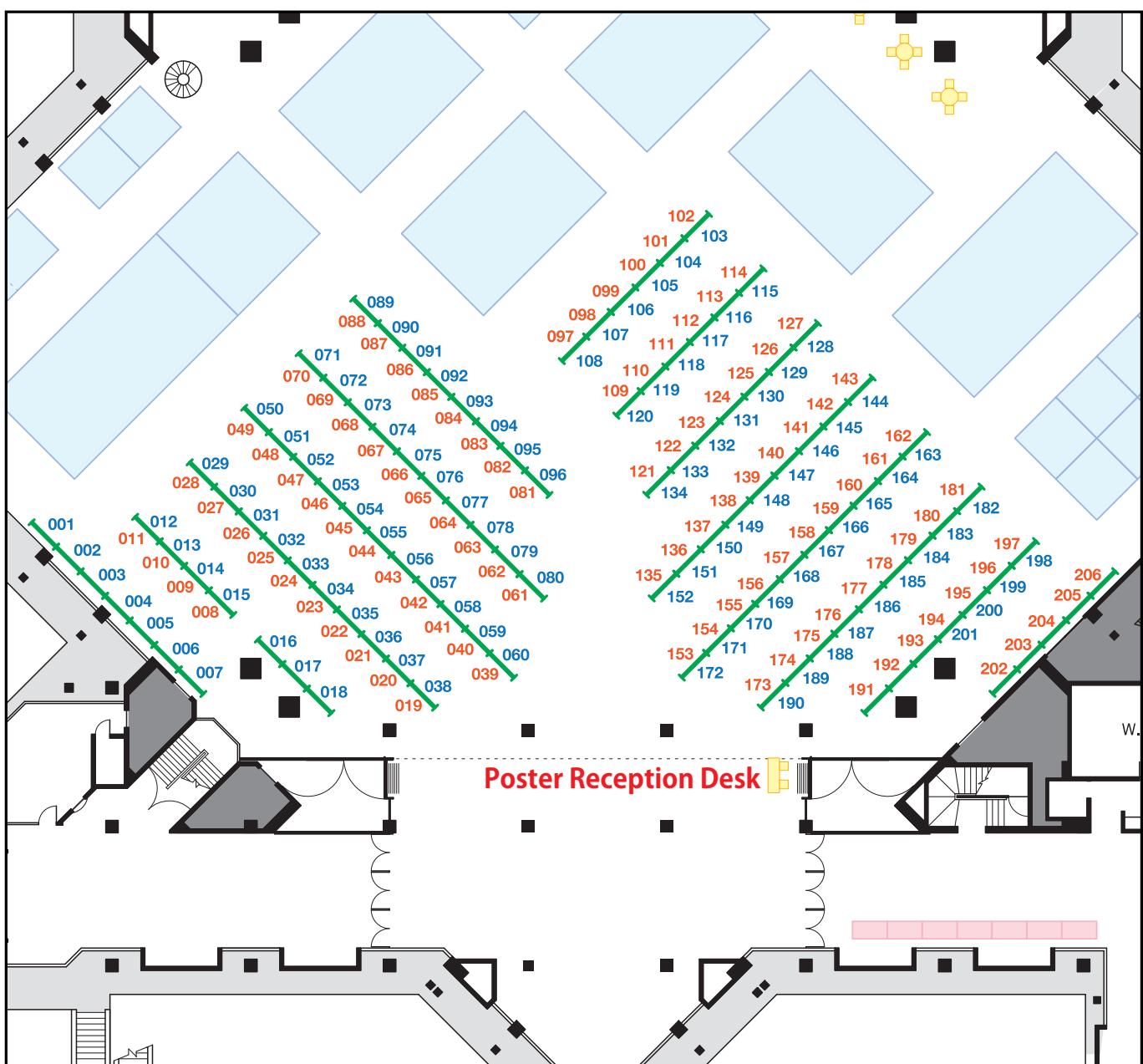
The conference organizers cannot accept liability for personal injuries sustained, or for loss or damage of properties belonging to conference participants (or their accompanying persons), either during or as result of the conference.

Please check validity of your insurance.

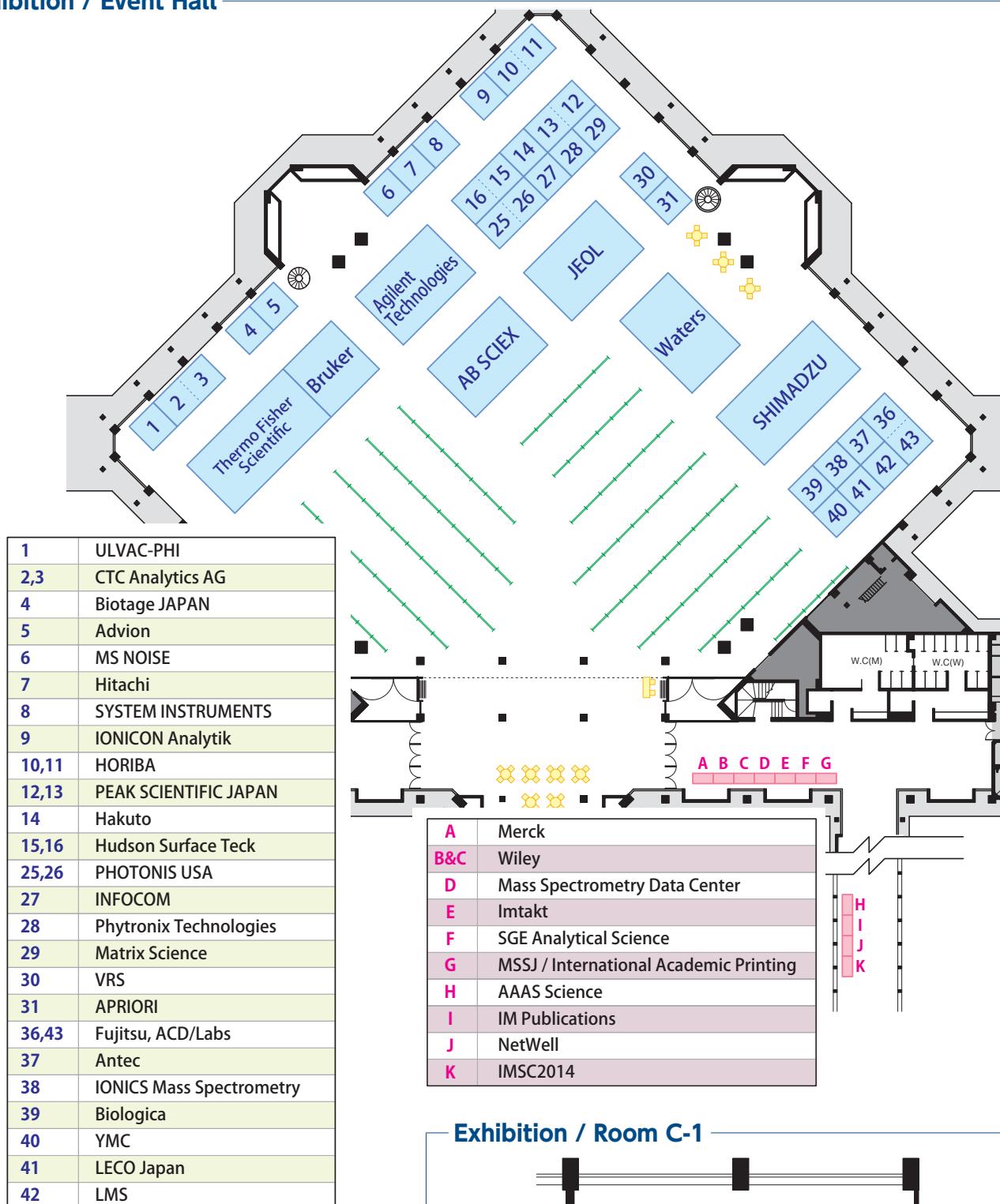
## Venue Floor Plans



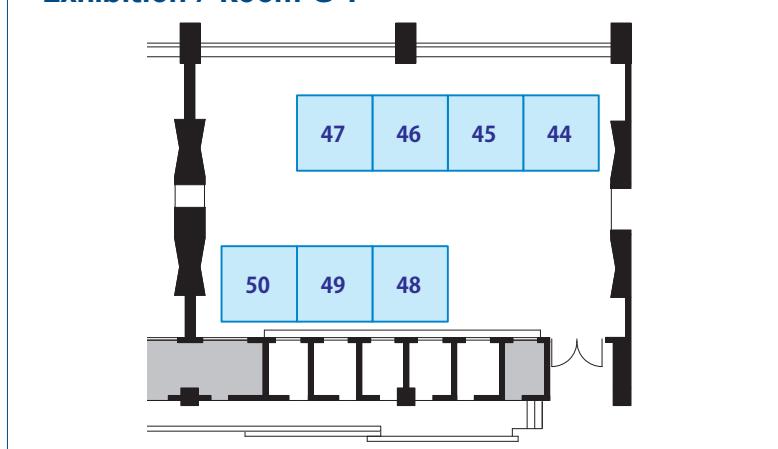
## Poster Presentation / Event Hall



## Exhibition / Event Hall



## Exhibition / Room C-1

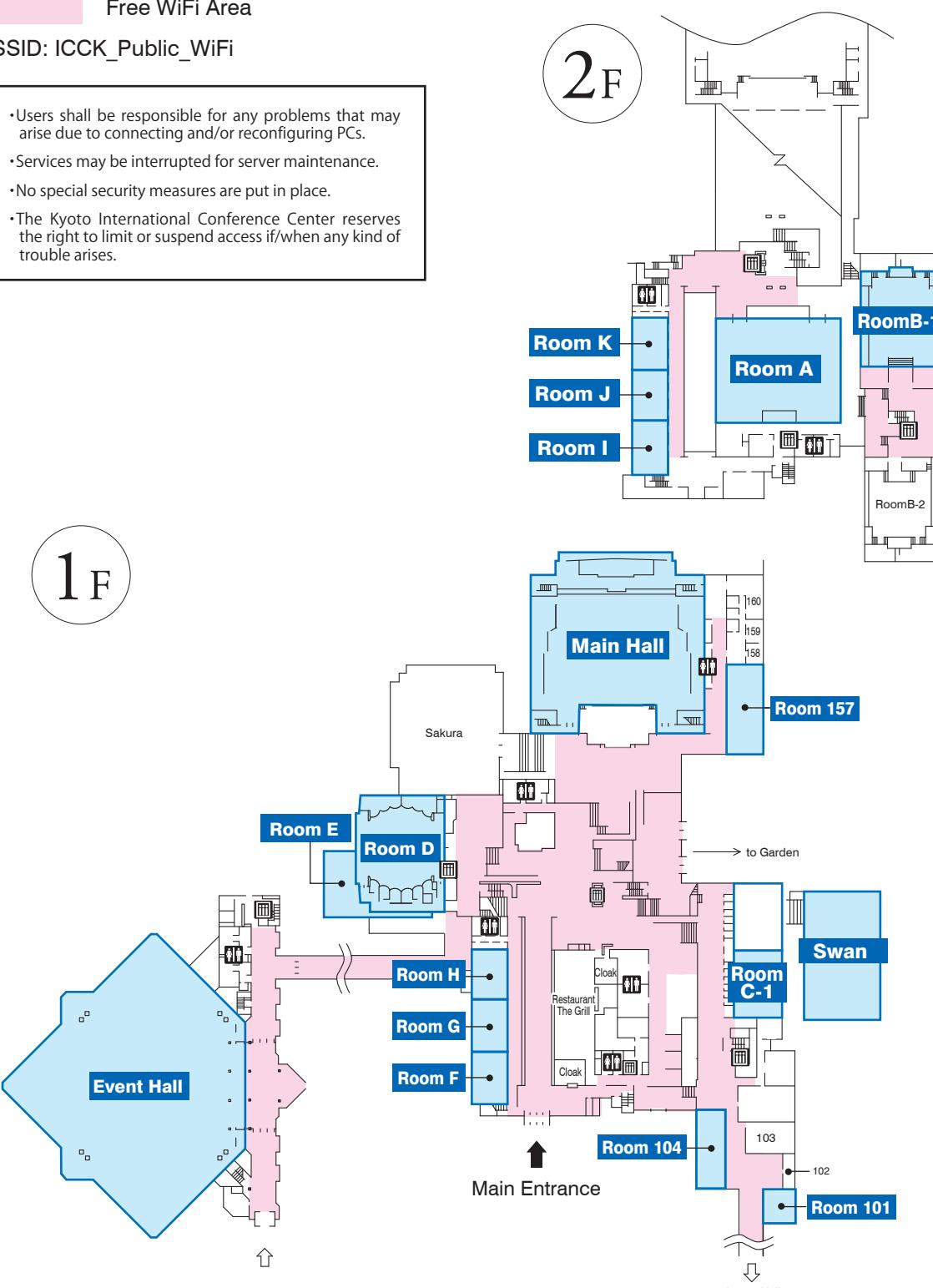


## Wifi Map

Free WiFi Area

SSID: ICCK\_Public\_WiFi

- Users shall be responsible for any problems that may arise due to connecting and/or reconfiguring PCs.
- Services may be interrupted for server maintenance.
- No special security measures are put in place.
- The Kyoto International Conference Center reserves the right to limit or suspend access if/when any kind of trouble arises.



**To Banquet**  
(Grand Prince Hotel Kyoto)

## Week at a glance

## Timetable

Saturday, 15<sup>th</sup> September

Main Hall	Room A	Room 103	Room C-1	Room C-2	
10:00	10:00-17:00	10:00-17:00	10:00-17:00	10:00-17:00	
11:00					
12:00					
13:00					
14:00	14:00-16:00  <b>Open Lectures for General Public (in Japanese)</b>	<b>Users' Day (AB SCIEX)</b>	<b>Short Course</b> Fragmentation Methods, Their Fundamentals and Application in Proteomics Roman A Zubarev	<b>Short Course</b> Introduction to Imaging Mass Spectrometry Mitsutoshi Setou	<b>Short Course</b> Fundamentals of Mass Spectrometry O David Sparkman & Jürgen Gross
15:00					
16:00					
17:00					
18:00					
19:00					

**Sunday, 16<sup>th</sup> September**

Main Hall	Room A	Room C-2	Swan
10:00	10:00-15:00	10:00-15:00	
11:00			
12:00			
13:00	<b>Users' Day</b> (SHIMADZU)	<b>Short Course</b> <b>Fundamentals of Mass Spectrometry</b> O David Sparkman & Jürgen Gross	
14:00			
15:00			
16:00	15:30-16:15 <b>Tutorial (Plenary)</b> <b>Lecture 1</b> Nico M M Nibbering		
16:15-17:00			
17:00	16:15-17:00 <b>Tutorial (Plenary)</b> <b>Lecture 2</b> Michael L Gross		
17:00-17:30			
18:00	<b>Opening Ceremony</b>		
17:30-18:15			
18:00	<b>Plenary Lecture 1</b> Hiroyuki Hamada		
19:00			18:30-20:00 <b>Welcome Mixer</b>

**13:00–18:00 Exhibition (Event Hall & Room C-1)**

**Monday, 17<sup>th</sup> September**

Life Sciences Instrumentation	Medical Sciences Ionization	Fundamentals	Isotope Ratio MS Environment / Microorganism
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Main Hall	Room A	Room B-1	Room D	Room E	Event Hall
					7:30-8:00 <b>Mounting Posters</b>
8:00 8:00-8:45 <b>Plenary Lecture 2</b> David E Clemmer					
9:00 9:00-11:00 <b>Session 1</b> Developments in Tandem Mass Spectrometry - Hybrid Instrumentation "The whole is greater than the sum of its parts" (Aristotle). Chair: Morio Ishihara Keynote: Alexander A Makarov	9:00-11:00 <b>Session 2</b> Advances in Methods and MS Instrumentation for Biomolecule Characterization Chair: Vicki H Wysocki Keynote: Andrea Sinz	9:00-11:00 <b>Session 3</b> Structures and Dynamics of Atomic and Molecular Clusters Chair: Fuminori Misaizu Keynote: Knut R Asmis	9:00-11:00 <b>Session 4</b> Imaging-I Chair: Mitsutoshi Setou Keynote: Ron Heeren	9:00-11:00 <b>Session 5</b> Advances in Spray Ionization Techniques Chair: Charles N McEwen Keynote: Kentaro Yamaguchi	Poster Viewing Time
10:00					
11:00					11:10-12:20 <b>Poster Core Time (Odd-number)</b>
12:00					
13:00 12:20-13:30 <b>Luncheon Seminar</b> (SHIMADZU)	12:20-13:30 <b>Luncheon Seminar</b> (AB SCIEX)	12:20-13:30 <b>Luncheon Seminar</b> (Waters)	12:20-13:30 <b>Luncheon Seminar</b> (JEOL)	12:20-13:30 <b>Luncheon Seminar</b> (Agilent Technologies)	Poster Viewing Time
14:00					13:30-14:40 <b>Poster Core Time (Even-number)</b>
15:00 15:00-17:00 <b>Session 6</b> Novel Approaches in Proteomics Analysis Chair: Roman Zubarev Keynote: Joshua J Coon	15:00-17:00 <b>Session 7</b> New Ionization Methods and Related Topics for the Next Generation Chair: Kenzo Hirooka Keynote: Robert Cody	15:00-17:00 <b>Session 8</b> Collision Dynamics and Spectroscopy Using Ion Storage Rings and Traps Chair: Haruo Shiromaru Keynote: Steen Brøndsted Nielsen	15:00-17:00 <b>Session 9</b> Imaging-II Chair: Jiro Matsuo Keynote: Nick Winograd	15:00-17:00 <b>Session 10</b> Ion Mobility Spectroscopy Based on Instrument & Theoretical Development Chair: Toshiki Sugai Keynote: Alexandre A Shvartsburg	Poster Viewing Time
16:00					
17:00					17:00-17:30 <b>Removing Posters</b>
18:00 17:15-19:15 <b>3<sup>rd</sup> Asian-Oceanic MS Conference (AOMSC3) Day-1</b>	17:15-19:15 <b>Workshop 1</b> Mass Spectrometry of Polymers and Industrial Materials Organizer: Hiroaki Sato	17:15-19:15 <b>Workshop 2</b> Hydrogen/Deuterium Exchange Mass Spectrometry Organizer: Yoshitomo Hamuro, Rachel Garlish	17:15-19:15 <b>(Reserved for MSSJ Local Meeting)</b>		
19:00					

**9:00–18:00 Exhibition (Event Hall & Room C-1)  
(17:15–) Company Events and others (Room F, G, H, I, J, K)**

**Tuesday, 18<sup>th</sup> September**

Life Sciences Instrumentation	Medical Sciences Ionization	Fundamentals	Isotope Ratio MS Environment / Microorganism
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Main Hall	Room A	Room B-1	Room D	Room E	Event Hall
					7:30-8:00 <b>Mounting Posters</b>
8:00 8:00-8:45 <b>Plenary Lecture 3</b> Albert J R Heck					
9:00 <b>Session 11</b> Glycomics: From Disease Markers to Therapeutic Antibody Products Chair: Hyun-joo An Keynote: Carlito Lebrilla	9:00-11:00 <b>Session 12</b> On-site Mass Spectrometry -Miniaturized Instruments and Allied Technologies- Chair: Shuichi Shimma Keynote: Zoltán Takáts	9:00-11:00 <b>Session 13</b> Accelerator Mass Spectrometry Chair: Hiroyuki Matsuzaki Keynote: Peter Steier	9:00-11:00 <b>Session 14</b> Ion-surface Collisions: Collision-induced Dissociation and Soft Landing Chair: Jean Furell Keynote: Julia Laskin	9:00-11:00 <b>Session 15</b> Mass Spectrometry for Nuclear Applications and Safety Chair: Nobuo Takaoka Keynote: Yongzhong Ouyang	Poster Viewing Time
10:00					11:10-12:20 <b>Poster Core Time (Odd-number)</b>
11:00					
12:00					
13:00 12:20-13:30 <b>Luncheon Seminar</b> (Thermo Fisher Scientific)	12:20-13:30 <b>Luncheon Seminar</b> (AB SCIEX)	12:20-13:30 <b>Luncheon Seminar</b> (Waters)	12:20-13:30 <b>Luncheon Seminar</b> (SHIMADZU)	12:20-13:30 <b>Luncheon Seminar</b> (Adion)	Poster Viewing Time
14:00					13:30-14:40 <b>Poster Core Time (Even-number)</b>
15:00 15:00-17:00 <b>Session 16</b> Glycoanalytical Technology for Systems Glycobiology and Functional Glycomics Chair: Jane Thomas-Oates Keynote: Pauline M Rudd	15:00-17:00 <b>Session 17</b> Non-Covalent Ion-Molecule Interactions Chair: Seung-Koo Shin Keynote: Peter B Armentrout	15:00-17:00 <b>Session 18</b> Advances in Resolution and Accuracy of Isotope Ratio Analyses Chair: Takaaki Hirata Invited: Jochen Vogl	15:00-17:00 <b>Session 19</b> Mass Spectrometric Diagnosis Chair: Toyofumi Nakanishi Keynote: Renato Zenobi	15:00-17:00 <b>Session 20</b> The Ion formation and Dissociation Mechanisms in MALDI Chair: Myung Soo Kim Keynote: Richard Knochenmuss	Poster Viewing Time
16:00					
17:00					17:00-17:30 <b>Removing Posters</b>
18:00 17:15-19:15 <b>3<sup>rd</sup> Asian-Oceanic MS Conference (AOMSC3) Day-2</b>	17:15-19:15 <b>Workshop 3</b> Careers in Mass Spectrometry Organizer: Tony Bristow	17:15-19:15 <b>Workshop 4</b> Mass++ and MassBank: Tools for Data Processing and Database on PC Organizer: Satoshi Tanaka, Takaaki Nishioka	17:15-19:15 <b>(Reserved for MSSJ Local Meeting)</b>		
19:00					

**9:00–18:00 Exhibition (Event Hall & Room C-1)  
(17:15–) Company Events and others (Room F, G, H, I, J, K)**

**Wednesday, 19<sup>th</sup> September**

Life Sciences Instrumentation	Medical Sciences Ionization	Fundamentals	Isotope Ratio MS Environment / Microorganism
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Main Hall	Room A	Room B-1	Room D	Room E	Event Hall
					7:30-8:00 <b>Mounting Posters</b>
8:00 8:00-8:30 <b>Thomson Medal and Curt Brunée Award Ceremony</b>					
8:30-8:50 <b>Curt Brunée Award Lecture</b>					
9:00 9:00-11:00 <b>Session 21</b> Platform Technology for Metabolomics Chair: Yoshiya Oda Keynote: Annie Evans	9:00-11:00 <b>Session 22</b> Instrumentation Developments in Mass Spectrometric Imaging Chair: Anastassios Giannakopoulos Keynote: Bernhard Spengler	9:00-11:00 <b>Session 23</b> Gas Phase Fragmentation Mechanisms of Biomolecular Radicals Chair: Shigeo Hayakawa Keynote: Richard A J O'Hair	9:00-11:00 <b>Session 24</b> Regulated Bioanalysis Chair: Shinobu Kudoh Keynote: Tatsuo Kurokawa	9:00-11:00 <b>Session 25</b> New Approaches to Defining the Diversity of Glycans Chair: Catherine E Costello Keynote: Jane Thomas-Oates	Poster Viewing Time
10:00					
11:00					11:10-12:20 <b>Poster Core Time (Odd-number)</b>
12:00					
13:00 12:20-13:30 <b>Luncheon Seminar</b> (Bruker)	12:20-13:30 <b>Luncheon Seminar</b> (AB SCIEX)	12:20-13:30 <b>Luncheon Seminar</b> (Waters)	12:20-13:30 <b>Luncheon Seminar</b> (SHIMADZU)	12:20-13:30 <b>Luncheon Seminar</b> (Agilent Technologies)	Poster Viewing Time
14:00					13:30-14:40 <b>Poster Core Time (Even-number)</b>
15:00 15:00-17:00 <b>Session 26</b> Lipidomics : Recent New Techniques and Applications Chair: Stephen Blanksby Keynote: Gavin E Reid	15:00-17:00 <b>Session 27</b> Progress in Microbiology Chair: Catherine Fenselau Keynote: Jeremy K Nicholson	15:00-17:00 <b>Session 28</b> IR Spectroscopy of Gas-phase Ions Chair: Dietmar Kuck Keynote: Philippe Maitre	15:00-17:00 <b>Session 29</b> The Advances in Biological Mass Spectrometry in Drug Discovery and Development: Current State of the Art and Challenges Chair: Ajai Chaudhary Keynote: Ragu Ramanathan	15:00-17:00 <b>Session 30</b> Data Processing and Informatics for SIMS Chair: DaeWon Moon Keynote: David Castner	Poster Viewing Time
16:00					
17:00					17:00-17:30 <b>Removing Posters</b>
18:00					
19:00					

**9:00–18:00 Exhibition (Event Hall & Room C-1)  
(17:15–) Company Events and others (Room F, G, H, I, J, K)**

**Thursday, 20<sup>th</sup> September**

						Life Sciences Instrumentation	Medical Sciences Ionization	Fundamentals Environment / Microorganism	Isotope Ratio MS
Main Hall	Room A	Room B-1	Room D	Room E	Event Hall				
						7:30-8:00			
8:00	8:00-8:45 <b>Plenary Lecture 4</b> Hisayoshi Yurimoto					<b>Mounting Posters</b>			
9:00	9:00-11:00 <b>Session 31</b> Native Mass Spectrometry and Structural Biology Chair: Satoko Akashi Keynote: Joseph A Loo	9:00-11:00 <b>Session 32</b> Formation and Dissociation of Peptide Radical Ions Chair: Dominic T W Chan Keynote: Roman A Zubarev	9:00-11:00 <b>Session 33</b> JMS Award Symposium Chair: Richard M Caprioli (Editor-in-Chief, JMS)	9:00-11:00 <b>Session 34</b> MS Informatics for Identification and Characterization Chair: Shigeki Kajihara Keynote: David Fenyö	9:00-11:00 <b>Session 35</b> Environment I Chair: Peter Haglund Keynote: Terry Bidleman	<b>Poster Viewing Time</b>			
10:00						11:10-12:20			
11:00						<b>Poster Core Time (Odd-number)</b>			
12:00									
13:00	12:20-13:30 <b>Luncheon Seminar</b> (SHIMADZU)	12:20-13:30 <b>Luncheon Seminar</b> (AB SCIEX)	12:20-13:30 <b>Luncheon Seminar</b> (Waters)	12:20-13:30 <b>Luncheon Seminar</b> (AMR INCORPORATED)	12:20-13:30 <b>Luncheon Seminar</b> (Bruker)	<b>Poster Viewing Time</b>			
14:00						13:30-14:40			
15:00	15:00-17:00 <b>Session 36</b> Advances in Ion Mobility Mass Spectrometry Chair: Joseph A Loo Keynote: Michael T Bowers	15:00-17:00 <b>Session 37</b> Challenges in High Resolution and High Accuracy Mass Measurement Mass Spectrometry Chair: Evgeny Nikolaev Keynote: Alan G Marshall	15:00-17:00 <b>Session 38</b> Mass Spectrometry for Metabolic Diseases Chair: Makoto Yoshino, Seiji Yamaguchi	15:00-17:00 <b>Session 39</b> MS Informatics for Quantitation Chair: David Fenyö Keynote: Jürgen Cox	15:00-17:00 <b>Session 40</b> Environment II Chair: Takeshi Nakano Keynote: Peter Haglund	<b>Poster Viewing Time</b>			
16:00						17:00-17:30			
17:00	17:10-18:10 <b>Thomson Medal Award Lectures</b>					<b>Removing Posters</b>			
18:00									
19:00						<b>Grand Prince Hotel Kyoto</b>			
						18:30-21:00			
						<b>Banquet</b>			
<b>9:00–18:00 Exhibition (Event Hall &amp; Room C-1)</b>									

**Friday, 21<sup>st</sup> September**

Life Sciences	Medical Sciences	Fundamentals	Isotope Ratio MS
Instrumentation	Ionization	Environment	Environment / Microorganism

Main Hall	Room A	Room B-1	Room D	Room E	Swan
8:00	8:00-8:45 <b>Plenary Lecture 5</b> Richard M Caprioli				
9:00	9:00-11:00 <b>Session 41</b> Chemistries of Trapped Ions and their Applications to Biological Mass Spectrometry Chair: Gavin E Reid Keynote: Scott A McLuckey	9:00-11:00 <b>Session 42</b> New Developments in Instruments and Detectors Chair: Takaya Sato Keynote: Evgeny N Nikolaev	9:00-11:00 <b>Session 43</b> Novel Proteomics Methodologies Chair: Yasushi Ishihama Keynote: Michael J MacCoss	9:00-11:00 <b>Session 44</b> Ambient Ionization Chair: Jentae Shiea Keynote: Kenzo Hiraoka	9:00-11:00 <b>Session 45</b> Cell Biology / Cellular Pathways Chair: Renato Zenobi Keynote: Tsutomu Masujima
10:00					
11:00	11:15-11:45 <b>IMSC 2014 Geneva Presentation</b>				
12:00	11:45-12:30 <b>Plenary Lecture 6</b> R Graham Cooks				
13:00	12:30-13:00 <b>Closing Ceremony</b>				13:00-13:45 <b>ARIGATO &amp; SAYONARA</b>
14:00					

Sunday, 16<sup>th</sup> September

Afternoon

**Tutorial Lecture**

15:30 – 16:15

Main Hall

**Tutorial Lecture 1: Nico M M Nibbering**Chair: Ryuichi Arakawa  
Kansai University, Japan**TL1-1530** Selected examples of gas-phase ion chemistry studies.15:30 – 16:15  
Nico M M Nibbering  
Vrije Universiteit, Amsterdam, The Netherlands**Tutorial Lecture**

16:15 – 17:00

Main Hall

**Tutorial Lecture 2: Michael L Gross**Chair: Yoko Ohashi  
RIKEN, Japan**TL2-1615** “Can Mass Spectrometry Play a Role in Protein Biophysics and Structural Biology?”16:15 – 17:00  
Michael L Gross, D Rempel, H Zhang, D Hambly, B Gau, J Chen, R Huang, J Zhang, L Jones, M Zhu  
Washington University, St Louis, MO, USA**Plenary Lecture**

17:30 – 18:15

Main Hall

**Plenary Lecture 1: Hiroyuki Hamada**Chair: Koichi Tanaka  
SHIMADZU Corp., Japan**PL1-1730** Applied Conventional Technology- Look at Tradition for Our Future-17:30 – 18:15  
Hiroyuki Hamada  
Kyoto Institute of Technology, Kyoto, Japan

Monday, 17<sup>th</sup> September

Morning

**Plenary Lecture**

08:00 – 08:45

Main Hall

**Plenary Lecture 2: David E Clemmer**Chair: Peter J Derrick  
Massey University, New Zealand**PL2-0800 Development of Next Generation Ion Mobility/Mass Spectrometry Techniques**08:00 – 08:45  
David E Clemmer  
Indiana University Department of Chemistry/Bloomington, IN/United States**Oral Session**

09:00 – 11:00

Main Hall

**Session 1: Developments in Tandem Mass Spectrometry - Hybrid Instrumentation  
“The whole is greater than the sum of its parts” (Aristotle).**Chair: Morio Ishihara  
Osaka University, Japan**S01-0900 [Keynote Lecture] Orbitrap-based hybrid mass spectrometers: synergy of analyzers**Alexander A Makarov  
ThermoFisher Scientific, Bremen, Germany**S01-0940 High Mass Resolution MALDI TOF MS/MS With A Curved Field Reflectron (Or The CFR Comes Of Age)**Andrew R Bowdler, Ian Brookhouse  
Kratos Analytical Ltd, Manchester, UK**S01-1000 High resolution, high aperture, high sensitivity TOF mass-spectrometers with expanded functionalities**Aldan A Sapargaliyev<sup>3</sup>, Igor F Spivak-Lavrov<sup>2</sup>,  
Yerbol A Sapargaliyev<sup>1,3</sup><sup>1</sup>Scientific Center “REB”, <sup>2</sup>Aktobe State University, Aktobe, Kazakhstan,<sup>3</sup>Scientific Center REB, Almaty, Kazakhstan**S01-1020 On the way to the holy grail of CID (20 keV and C12 precursor ion): from MALDI-LinTOF/CF-RTOF- to MALDI-SpiralTOF/offset parabolic-RTOF-MS**Guenter Allmaier<sup>1</sup>, Ernst Pittenauer<sup>1</sup>, Pavel Rehulka<sup>2</sup>,  
Akihiko Kusai<sup>3</sup><sup>1</sup>Vienna University of Technology, Vienna, Austria, <sup>2</sup>University of Defence, Hradec Kralova, Czech Republic, <sup>3</sup>JEOL (Europe), Croissy-sur-Seine, France**S01-1040 Identification of trace level process related impurities of small molecule Irbesartan, an angiotensin II receptor antagonist through MSMS analysis**Saravanan Subramaniam, Raman Palvannanathan,  
Rampriya Uthayakumar, Govindarajan Chandramohan,  
Mohan Kasi, Arvind Thyagarajan, Manohar Venkat  
Indian Institute of Chromatography & Mass Spectrometry

**Monday, 17<sup>th</sup> September**

**Morning**

**Mon**

## Oral Session

09:00 – 11:00

Room A

### Session 2: Advances in Methods and MS Instrumentation for Biomolecule Characterization

Chair: Vicki H Wysocki  
Ohio State University, USA

- S02-0900** [Keynote Lecture] Chemical Cross-Linking and Mass Spectrometry: A Fruitful Combination for Protein 3D-Structure Analysis

Andrea Sinz  
Martin-Luther University Halle-Wittenberg, Halle, Germany

- S02-0940** Applications of online- bioaffinity- mass spectrometry to structure and affinity determination of neurodegenerative proteins from brain material

Stefan Slamnoiu<sup>1</sup>, Camelia Vlad<sup>1,2</sup>, Adrian Moise<sup>1</sup>, Mihaela Stumbaum<sup>1,2</sup>, Thomas Gronewold<sup>2</sup>, Markus Perpeet<sup>2</sup>, Michael Przybylski<sup>1</sup>

<sup>1</sup>Laboratory of Analytical Chemistry and Biopolymer Structure Analysis, Department of Chemistry, University of Konstanz, Germany

<sup>2</sup>SAW Instruments GmbH, Bonn, Germany

- S02-1000** Pinpointing individual sites that change conformation in large protein complexes by H/D exchange and ETD-MS

Song Hongjian<sup>1</sup>, Jeff M Brown<sup>2</sup>, Steven D Pringle<sup>2</sup>, Michael Morris<sup>2</sup>, Kasper D Rand<sup>1</sup>

<sup>1</sup>Laboratory for Biomacromolecular Analysis, Advanced Drug Analysis Section, Department of Pharmacy, University of Copenhagen, Denmark, <sup>2</sup>Waters MS Technologies Centre, Manchester, UK.

- S02-1020** What happens on the histone multimers in the gas phase?

Kazumi Saikusa<sup>1</sup>, Sotaro Fuchigami<sup>1</sup>, Kyohei Takahashi<sup>1</sup>, Yuuki Asano<sup>1</sup>, Aritaka Nagadoi<sup>1</sup>, Hiroaki Tachiwana<sup>2</sup>, Hitoshi Kurumizaka<sup>2</sup>, Mitsunori Ikeguchi<sup>1</sup>, Yoshifumi Nishimura<sup>1</sup>, Satoko Akashi<sup>1</sup>

<sup>1</sup>Yokohama City University, Yokohama, Japan, <sup>2</sup>Waseda University, Tokyo, Japan

- S02-1040** Dibasic Site-Specific Proteolysis for Improved Bottom-Up and Middle-Down Proteomics

Unige A Laskay<sup>1</sup>, Upir Oxana<sup>1</sup>, Luca Fornelli<sup>1</sup>, Kozhinov N Anton<sup>1</sup>, Michel Monod<sup>2</sup>, Goran Mitulovic<sup>3</sup>, Yury O Tsypin<sup>1</sup>

<sup>1</sup>Ecole Polytechnique Federale de Lausanne Switzerland, <sup>2</sup>Centre Hospitalier Universitaire Vaudois, Lausanne, Switzerland, <sup>3</sup>Medical University Vienna, Austria

## Oral Session

09:00 – 11:00

Room B-1

### Session 3: Structures and Dynamics of Atomic and Molecular Clusters

Chair: Fuminori Misaiju  
Tohoku University, Japan

- S03-0900** [Keynote Lecture] Recent Advances in the Vibrational Spectroscopy of Mass-Selected Gas Phase Cluster Ions

Knut R Asmis  
Fritz-Haber-Institut der MPG, Berlin, Germany

- S03-0940** Laser desorption supersonic jet spectroscopy of neurotransmitter molecules and partial peptides of their receptors

Shun-ichi Ishiuchi, Masaaki Fujii  
Tokyo Institute of Technology, Yokohama, Japan

- S03-1000** The 'sticky business' of cleaning gas-phase membrane proteins: a detergent oriented perspective

Antoni J Borysik, Carol V Robinson  
University of Oxford

- S03-1020** Adsorption, Activation and Reaction of Molecules on Size-Selected Metal Cluster Ions

Masahiko Ichihashi<sup>1</sup>, Shinichi Hirabayashi<sup>2</sup>

<sup>1</sup>Toyota Technological Institute, Ichikawa, Japan, <sup>2</sup>Genesis Research Institute, Inc. Ichikawa, Japan

- S03-1040** Formation, Characterization and Reactivity of a Gaseous Adduct of Carbon Dioxide to Magnesium(I),  $\text{HOMgCO}_2$ -

Héloïse Dossmann (Soldi-Lose)<sup>2</sup>, Carlos Afonso<sup>3</sup>, Denis Lesage<sup>2</sup>, Jean-Claude Tabet<sup>2</sup>, Einar Uggerud<sup>1</sup>

<sup>1</sup>University of Oslo, <sup>2</sup>Pierre and Marie Curie University (Paris VI), <sup>3</sup>University of Rouen

Monday, 17<sup>th</sup> September

Morning

**Oral Session**

09:00 – 11:00

Room D

**Session 4: Imaging-I**

Chair: Mitsutoshi Setou

Hamamatsu University School of Medicine, Japan

- S04-0900** [Keynote Lecture] Imaging molecular signals with multimodal imaging mass spectrometry  
09:00 – 09:40

Ron M Heeren

FOM-Institute AMOLF

- S04-0940** Single cell level mass spectrometry imaging for plant metabolites  
09:40 – 10:00

Young-Jin Lee<sup>1,2</sup><sup>1</sup>Iowa State University, Ames, USA/<sup>2</sup>Iowa, Ames Laboratory-USDOE, Ames, USA/Iowa

- S04-1000** Molecular Imaging of Cells and Tissues with Continuous Cluster Ion Beams  
10:00 – 10:20

Jiro Matsuo<sup>1,2</sup>, Takaaki Aoki<sup>1,2</sup>, Toshio Seki<sup>1,2</sup><sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>JST, CREST

- S04-1020** Spatial Resolution of Metabolites during Barley Grain Development by Imaging Mass Spectrometric Analysis  
10:20 – 10:40

Manuela Peukert<sup>1</sup>, Andrea Matros<sup>1</sup>, Ales Svatos<sup>2</sup>, Hans-Peter Mock<sup>1</sup>  
<sup>1</sup>IPK Gatersleben, Germany, <sup>2</sup>MPI Jena, Germany

- S04-1040** Mass spectrometry imaging (MALDI-TOF/TOF) of drugs in a brain mouse model of Parkinson disease  
10:40 – 11:00

David Touboul<sup>1</sup>, Hanane Kadar<sup>1</sup>, Gael Le Douaron<sup>2</sup>, Majid Amar<sup>3</sup>, Bruno Figadère<sup>2</sup>, Laurent Ferrié<sup>2</sup>, Rita Raisman-Vozani<sup>3</sup>, Alain Brunelle<sup>1</sup>  
<sup>1</sup>ICSN CNRS, Gif-sur-Yvette, France, <sup>2</sup>UMR-8076 (BioCIS) Laboratoire de Pharmacognosie, Châtenay -Malabry, France, <sup>3</sup>INSERM UMR-S 975, CNRS UMR 7225, UPMC, CRIMC, Paris, France

**Oral Session**

09:00 – 11:00

Room E

**Session 5: Advances in Spray Ionization Techniques**Chair: Charles N McEwen  
University of the Sciences, USA

- S05-0900** [Keynote Lecture] Cold-Spray Ionization Mass Spectrometry  
09:00 – 09:40

Kentaro Yamaguchi

Tokushima Bunri University, Kagawa, Japan

- S05-0940** Mass Spectrometric Analyses of Isomeric Sugars, Lipids and their Conjugates: Introduction to “Charge-Localization Isomers”  
09:40 – 10:00

Yoko Ohashi<sup>1,2</sup>, Masayuki Kubota<sup>3</sup>, Takashi Hirano<sup>2</sup><sup>1</sup>RIKEN, Wako, Japan, <sup>2</sup>The Univ. of Electro.-Comm., Chofu, Tokyo, Japan,<sup>3</sup>ThermoFisher Sci. Co., Yokohama, Kanagawa, Japan

- S05-1000** “Supercharging” and “Subcharging” Proteins and Protein Complexes to Explore Electrospray Ionization  
10:00 – 10:20

Rachel R Loo, Rajeswari Lakshmanan, Jiang Zhang,  
Joseph A Loo  
University of California-Los Angeles, Los Angeles, CA/USA

- S05-1020** Ionization Methods Requiring as little as the vacuum of the Mass Spectrometer to Produce Highly-Charged Ions from Surfaces or Solutions  
10:20 – 10:40

Sarah Trimpin  
Wayne State University, Detroit, MI

- S05-1040** Rapid Characterization of Chemicals in Plant via Direct Electrospray Probe Coupling with Mass Spectrometry  
10:40 – 11:00

Hung Su, Chu-Nian Cheng, Min-Zong Huang, Jentae Shiea  
National Sun Yat-Sen University, Kaohsiung, Taiwan

**Monday, 17<sup>th</sup> September**

**Afternoon**

Mon

## Oral Session

15:00 – 17:00

Main Hall

### Session 6: Novel Approaches in Proteomics Analysis

Chair: Roman A Zubarev  
Karolinska Institutet, Sweden

**S06-1500 [Keynote Lecture] Instant Spectral Assignment for Rapid, High-Throughput Targeted Proteomics**

15:00 – 15:40 Derek J Bailey, Amelia C Peterson, Christopher M Rose, Michael S Westphall, Joshua J Coon  
University of Wisconsin-Madison/Madison, Wisconsin/USA

**S06-1540 Miniaturised Chemical Proteomics to Profile Clinically-relevant Kinase Inhibitors in Tumour Core Biopsies**

15:40 – 16:00 Ivo Chamrad<sup>2</sup>, Uwe Rix<sup>3</sup>, Manuela Gridling<sup>1</sup>, Katja Parapatics<sup>1</sup>, Andre C Mueller<sup>1</sup>, Alexey Stukalov<sup>1</sup>, Giulio Superti-Furga<sup>1</sup>, Eric B Haura<sup>3</sup>, Keiryn L Bennett<sup>1</sup>  
<sup>1</sup>CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, <sup>2</sup>Palacky University, Olomouc, Czech Republic, <sup>3</sup>H. Lee Moffitt Cancer Center and Research Institute, Tampa, Florida, USA

**S06-1600 Combining ribosome profiling (ribosome captured mRNA sequencing) and mass spectrometry into an unprecedentedly comprehensive protein identification strategy.**

16:00 – 16:20 Gerben Menschaert<sup>1</sup>, Petra Van Damme<sup>1,2</sup>, Jeroen Crappe<sup>1</sup>, Geert Baggerman<sup>3,4</sup>, Wim Van Criekinge<sup>1</sup>  
<sup>1</sup>Ghent University, Ghent, Belgium, <sup>2</sup>VIB (Flemish Institute for Biotechnology), Ghent, Belgium, <sup>3</sup>Antwerp University CFP (Center For Proteomics), Antwerp, Belgium, <sup>4</sup>VITO, Mol, Belgium

**S06-1620 Top-down mass spectrometry for comprehensive quantitative proteomics**

16:20 – 16:40 Ljiljana Pasa-Tolic, Shawna M Hengel, Si Wu, Zhixin Tian, David Stenoien, Rui Zhao, Nikola Tolic, Joshua T Aldrich, Da Meng, Ronald J Moore, Errol W Robbinson  
Pacific Northwest National Laboratory

**S06-1640 In silico Compensation of Instrumental Response Fluctuations Improves Label-free Quantification of High-Resolution Proteomics Data**

16:40 – 17:00 Yaroslav Lyutvinskiy<sup>1</sup>, Hongqian Yang<sup>1</sup>, Dorothea Rutishauser<sup>1</sup>, Hilkka Soininen<sup>2</sup>, Roman Zubarev<sup>1</sup>  
<sup>1</sup>Karolinska Institutet, Stockholm, Sweden, <sup>2</sup>University of Eastern Finland, Kuopio, Finland

## Oral Session

15:00 – 17:00

Room A

### Session 7: New Ionization Methods and Related Topics for the Next Generation

Chair: Kenzo Hiraoka  
University of Yamanashi, Japan

**S07-1500 [Keynote Lecture] What is the Opposite of Pandora's Box? Direct Analysis, Ambient Ionization, and a New Generation of Atmospheric Pressure Ion Sources.**

Robert B Cody  
JEOL USA, Inc.

**S07-1540 Temperature Dependence of Proton Transfer for Biomolecular Ions with Electrospray Ionization**

15:40 – 16:00 Shinji Nonose, Kazuki Yamashita, Ayako Sudo, Keishi Machida, Kanako Yokoyama, Minami Kawashima, Takashige Mori, Yuto Ohshima  
Yokohama City University, Yokohama, Japan

**S07-1600 Design and Development of A Novel Nuclear Magnetic Resonance Detection for the Mass-selected Gas-Phase Ions by "Magnetic Resonance Acceleration" Technique**

16:00 – 16:20 Kiyokazu Fuke<sup>1,2</sup>, Masahide Tona<sup>1</sup>, Akimasa Fujihara<sup>2</sup>, Haruki Ishikawa<sup>3</sup>

<sup>1</sup>Kobe University, Kobe, Japan, <sup>2</sup>Osaka Prefecture University, Osaka, Japan, <sup>3</sup>Kitasato University, Kanagawa, Japan

**S07-1620 New prospects for post-ionization mass spectrometry using ultrafast laser pulses**

16:20 – 16:40 Alessia Longobardo<sup>2</sup>, Alisdair Macpherson<sup>2</sup>, John Vickerman<sup>1</sup>, Nick Lockyer<sup>1,2</sup>

<sup>1</sup>Manchester Interdisciplinary Biocentre, University of Manchester, Manchester, UK, <sup>2</sup>Photon Science Institute, University of Manchester, Manchester, UK

**S07-1640 Desorption/ionization induced by neutral clusters as matrix-free, soft, and efficient ion source for ion-trap mass spectrometry of biomolecules**

16:40 – 17:00 Markus Baur<sup>1</sup>, Bong-Jun Lee<sup>1</sup>, Christoph R Gebhardt<sup>2</sup>, Michael Durr<sup>1</sup>

<sup>1</sup>University of Applied Sciences Esslingen, Esslingen, Germany, <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany

**Monday, 17<sup>th</sup> September**

**Afternoon**

## Oral Session

15:00 – 17:00

Room B-1

### Session 8: Collision Dynamics and Spectroscopy Using Ion Storage Rings and Traps

Chair: Haruo Shiromaru  
Tokyo Metropolitan University, Japan

- S08-1500** [Keynote Lecture] Spectroscopy of firefly luciferin and oxyluciferin anions in vacuo. Color tuning by a micro-environment?  
15:00 – 15:40

Steen Brøndsted Nielsen

Aarhus University, Aarhus, Denmark

- S08-1540** Electronic and photonic collision experiments on molecular ions with an electrostatic storage ring at KEK  
15:40 – 16:00

Tetsumi Tanabe<sup>1,3</sup>, Manabu Saito<sup>2</sup>, Koji Noda<sup>3</sup>,  
Evgeni B Starikov<sup>4</sup>

<sup>1</sup>High Energy Accelerator Research Organization (KEK), Tsukuba, Japan,  
<sup>2</sup>Kyoto Prefectural University, Kyoto, Japan, <sup>3</sup>National Institute of Radiological Sciences, Chiba, Japan, <sup>4</sup>Chalmers University of Technology, Gothenburg, Sweden

- S08-1600** Cold chemical reactions between sympathetically cooled molecular ions and slow polar molecules  
16:00 – 16:20

Kunihiro OKADA<sup>1</sup>, Takahiro FURUKAWA<sup>1</sup>,  
Masanari ICHIKAWA<sup>1</sup>, Michiharu WADA<sup>2</sup>, Hans SCHUESSLER<sup>3</sup>  
<sup>1</sup>Sophia University, Tokyo, Japan, <sup>2</sup>RIKEN, Saitama, Japan, <sup>3</sup>Texas A&M University, Texas, USA

- S08-1620** Development of a portable electrostatic ion storage ring in TMU  
16:20 – 16:40

Jun Matsumoto, Haruo Shiromaru  
Tokyo Metropolitan University, Tokyo, Japan

- S08-1640** Investigation of a novel apparatus which combines ion trap - laser cooling technique with ICP-MS for trace isotope analysis  
16:40 – 17:00

Masanori Kitaoka, Yuta Yamamoto, Takuma Yoshida,  
Kyunghun Jung, Shuichi Hasegawa  
The University of Tokyo, Tokyo, Japan

## Oral Session

15:00 – 17:00

Room D

### Session 9: Imaging-II

Chair: Jiro Matsuo  
Kyoto University, Japan

- S09-1500** [Keynote Lecture] Nanoscale Chemical Imaging of Biomaterials with Cluster SIMS  
15:00 – 15:40

Nicholas Winograd

Penn State University

- S09-1540** TOF-SIMS imaging analysis of atherosclerotic aortic sinuses and gastric cancer tissues  
15:40 – 16:00

Eun-Soo Lee<sup>1,2</sup>, Ji-Won Park<sup>1,2</sup>, Se-Hwa Kim<sup>1</sup>, Hyun Kyong Shon<sup>1</sup>,  
Sohee Yoon<sup>1</sup>, JuYeon Oh<sup>1</sup>, Tae Geol Lee<sup>1,2</sup>, Hark Kyun Kim<sup>3</sup>,  
Daehee Hwang<sup>4</sup>, DaeWon Moon<sup>1,2</sup>

<sup>1</sup>Center for Nano-Bio Technology, Korea Research Institute of Standards and Science, Daejeon, 305-340, Korea, <sup>2</sup>Department of Nano and Bio Surface Science, University of Science and Technology, Daejeon, 305-350, Korea,

<sup>3</sup>National Cancer Center, Goyang, Republic of Korea, <sup>4</sup>School of Interdisciplinary Bioscience and Bioengineering, POSTECH, Pohang, Republic of Korea

- S09-1600** Diagnostic application of Imaging Mass Spectrometry  
16:00 – 16:20

Mitsutoshi Setou<sup>1</sup>, Kiyoshi Ogawa<sup>2</sup>, Akiko Kubo<sup>3</sup>, Ikuko Yao<sup>4</sup>,  
Masaaki Matsuura<sup>5</sup>

<sup>1</sup>Hamamatsu University School of Medicine, <sup>2</sup>Shimadzu, <sup>3</sup>Keio University, <sup>4</sup>Kansai Medical University, <sup>5</sup>Japanese foundation for cancer research

- S09-1620** High-throughput analysis for metabolic dynamics and in situ metabolite imaging by MALDI mass spectrometry  
16:20 – 16:40

Daisuke Miura<sup>1</sup>, Yoshinori Fujimura<sup>1</sup>, Shin-ichi Yamaguchi<sup>2</sup>,  
Noriyuki Ojima<sup>2</sup>, Mitsuru Shindo<sup>1</sup>, Hiroyuki Wariishi<sup>1</sup>

<sup>1</sup>Kyushu University, <sup>2</sup>Shimadzu Co., Kyoto, Japan

- S09-1640** Imaging of metabolites in plants and insects with high resolution AP-MALDI MSI  
16:40 – 17:00

Dhaka R Bhandari, Andreas Roempf, Bernhard Spengler  
Justus Liebig University Giessen, Giessen, Germany

Monday, 17<sup>th</sup> September

Afternoon

## Oral Session

15:00 – 17:00

Room E

**Session 10: Ion Mobility Spectroscopy Based on Instrument & Theoretical Development**Chair: Toshiki Sugai  
Toho University, Japan

- S10-1500** [Keynote Lecture] Pushing the frontier of  
15:00 – 15:40 high-definition ion mobility spectrometry  
using FAIMS

Alexandre A Shvartsburg, Gordon A Anderson, Richard D Smith  
Pacific Northwest National Laboratory

- S10-1540** Mobility of atomic and small molecular  
15:40 – 16:00 ions in cooled helium gas for  
investigation on interaction potentials  
and collision dynamics

Hajime Tanuma<sup>1</sup>, Ryosuke Isawa<sup>1</sup>, Jun-ichi Yamazoe<sup>1</sup>,  
Shiro Matoba<sup>2</sup>

<sup>1</sup>Tokyo Metropolitan University, Tokyo, Japan, <sup>2</sup>Japan Atomic Energy Agency, Takasaki, Japan

- S10-1600** Novel analytical approaches enabled by  
16:00 – 16:20 ultra-fast chip-based FAIMS separation  
coupled to mass spectrometry

Michael Ugarov<sup>1</sup>, Yuqin Dai<sup>1</sup>, Michael Flanagan<sup>1</sup>,  
Michelle Romm<sup>2</sup>, Vaughn Miller<sup>2</sup>  
<sup>1</sup>Agilent Technologies, Santa Clara, USA, <sup>2</sup>Agilent Technologies, Wakefield, USA

- S10-1620** Real-Time 2D separation with LC-DMS-  
16:20 – 16:40 TOF-MS: Increasing the Selectivity of  
High Resolution MS in Qualitative and  
Quantitative Analysis

J C Yves Le Blanc, Larry Campbell, Nic Bloomfield,  
Alexander V Loboda, Brad Schneider, Igor V Chernushevich  
AB SCIEX, Concord, Canada

- S10-1640** Isomer-selected photodissociation of  
16:40 – 17:00 carbon and silicon cluster ions with ion  
mobility mass spectrometry using a  
double reflectron time-of-flight mass  
spectrometer

Kiichiro Koyasu, Ryoichi Moriyama, Tomohiro Ohtaki,  
Jun Hosoya, Fuminori Misaizu  
Tohoku University, Sendai, Japan

Monday, 17<sup>th</sup> September

## Poster Session

Core Time : 11:10 - 12:20 (Odd number),  
13:30 - 14:40 (Even number)

Event Hall

## Session 1

**Developments in Tandem Mass Spectrometry - Hybrid Instrumentation "The whole is greater than the sum of its parts" (Aristotle).**

**PMo-001 Boundary Activated Dissociation in a Low Pressure Linear Ion Trap in the presence of Nonlinear DC Fields**  
11:10 – 12:20

mircea guna  
AB SCIEX, Concord, ON, Canada

**PMo-002 ECD in an RF-Free Electromagnetostatic Cell on a Triple Quadrupole Mass Spectrometer**  
13:30 – 14:40

Yu Chu Lin<sup>1</sup>, Samuel Bennett<sup>1</sup>, Valery G Voinov<sup>1,2</sup>,  
Douglas F Barofsky<sup>1</sup>  
<sup>1</sup>Oregon State University, Corvallis, Oregon, U.S.A., <sup>2</sup>Pacific Institute of Bioorganic Chemistry, Vladivostok, Rusia

**PMo-003 A rapid and sensitive liquid chromatography tandem mass spectrometry method for quantification of etoposide and etoposide chatechol in cerebrospinal fluid**  
11:10 – 12:20

Hsiao-Wei Liao<sup>1,2</sup>, Yen-Shen Lu<sup>3</sup>, Ching-Hung Lin<sup>3</sup>,  
Ching-Hua Kuo<sup>1,2</sup>  
<sup>1</sup>National Taiwan University, Taipei, Taiwan, <sup>2</sup>School of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan, <sup>3</sup>Department of Oncology, National Taiwan University Hospital, Taipei, Taiwan

**PMo-004 Qualitative analysis of impurities in enalapril using liquid chromatography-ion trap time of flight hybrid mass spectrometry**  
13:30 – 14:40

FENG JI, QI Y LI, JING DONG  
Shimazu Co., Beijing, China

**PMo-005 Qualitative Analysis of Gossypol, Free Gossypol, and Gossypol Derivatives in Cottonseeds By Electrospray Ionization Tandem Mass Spectrometry**  
11:10 – 12:20

Luying Zhou<sup>1</sup>, Lai Chen<sup>2</sup>, Jinting Yao<sup>1</sup>, Hongyuan Hao<sup>1</sup>,  
Hengtao Dong<sup>1</sup>, Qiang Li<sup>1</sup>  
<sup>1</sup>Shimadzu (China) Co., Ltd., Shanghai, China, <sup>2</sup>Shanghai Ocean University

**PMo-006 Evaluation of the higher sensitive LC/ MS/MS incorporates novel desolvation technologies to achieve low femto-gram LOQ**  
13:30 – 14:40

Shinjiro Fujita, Natsuyo Asano, Kazuo Mukaibatake  
Shimadzu Corporation, Kyoto, Japan

**PMo-007 Determination and pharmacokinetics of di-(2-ethylhexyl) phthalate in rats by ultra performance liquid chromatography with tandem mass spectrometry**  
11:10 – 12:20

Wan-Ling Chang-Liao<sup>1</sup>, Lie-Chwen Lin<sup>1,2</sup>, Tung-Hu Tsai<sup>1,3</sup>

<sup>1</sup>National Yang-Ming University, Taipei, Taiwan, <sup>2</sup>National Research Institute of Chinese Medicine, <sup>3</sup>Taipei City Hospital, Taipei, Taiwan

**PMo-008 Pharmacokinetics of Di-isonyl Phthalate in Freely Moving Rats by UPLC-MS/MS**  
13:30 – 14:40

Mei-Ling Hou<sup>1</sup>, Tung-Hu Tsai<sup>1,2</sup>

<sup>1</sup>Institute of Traditional Medicine, School of Medicine, National Yang-Ming University, Taipei, Taiwan, <sup>2</sup>Department of Education and Research, Taipei City Hospital, Taipei, Taiwan

**PMo-009 Pharmacokinetics of dibutyl phthalate by ultra performance liquid chromatography with tandem mass spectrometry in rats**  
11:10 – 12:20

Li-Wen Chang<sup>1</sup>, Tung-Hu Tsai<sup>1,2</sup>

<sup>1</sup>National Yang-Ming University, Taipei, Taiwan, <sup>2</sup>Taipei City Hospital, Taipei, Taiwan

**PMo-010 Separation of polar solutes by hydrophilic methacrylate-based monolithic columns via capillary electrochromatography coupled with UV-Vis and mass spectrometry detection.**  
13:30 – 14:40

Yung-Han Shih, Ching-Yi Wu, Cheng-Lan Lin, Pei-Zhu Liang,  
Hsi-Ya Huang  
Chung Yuan Christian University, ChungLi, Taiwan

## Session 2

**Advances in Methods and MS Instrumentation for Biomolecule Characterization**

**PMo-011 The CORrelation Ion-Neutral Time Of Flight Mass Spectrometry (COIN-TOF MS)**  
11:10 – 12:20

Victor Buridon<sup>1</sup>, Cecile Teyssier<sup>1</sup>, Hassan Abdoul-Carime<sup>1</sup>,  
Bernadette Farizon<sup>1</sup>, Michel Farizon<sup>1</sup>, Tilmann D Mark<sup>2</sup>

<sup>1</sup>Universite de Lyon 1, Institut de Physique Nucleaire Lyon, Villeurbanne, France, <sup>2</sup>Institut für Ionenphysik und Angewandte Physik, Leopold Franzens Universität, Technikerstrasse 25, A-6020 Innsbruck, Austria

**PMo-012 Automatic Disulfide Bond Assignment Using a1 Ion Screening by Mass Spectrometry for Structural Characterization of Protein Pharmaceuticals**  
13:30 – 14:40

Sheng-Yu Huang<sup>2</sup>, Yu-Ting Hsieh<sup>1</sup>, Chun-Hao Chen<sup>1</sup>,  
Chao-Chi Chen<sup>2</sup>, Wang-Chou Sung<sup>3</sup>, Min-Yuan Chou<sup>4</sup>,  
Sung-Fang Chen<sup>1</sup>

<sup>1</sup>National Taiwan Normal University, Taipei, Taiwan, <sup>2</sup>Mithra Biotechnology Inc., Taiwan, <sup>3</sup>National Health Research Institutes, Taiwan, <sup>4</sup>Industrial Technology Research Institute, Taiwan

Monday, 17<sup>th</sup> September

Mon

**PMo-013** Determination of chloramphenicol in biological samples by gas chromatography-mass spectrometry11:10 – 12:20  
Suh-Jen J Tsai, Hsiu-Hua Huang, Pei-Yin Hsieh, Che-Wei Chang  
Providence University, Taichung, Taiwan**PMo-014** Combining quantum mechanical and MS analysis to understanding the source of H<sup>+</sup> during APPI of PAH dissolved in toluene13:30 – 14:40  
Arif Ahmed, Chell Ho Choi, Kim Sunghwan  
Kyungpook National University, Daegu, Korea**PMo-015** Transformation of the Green Fluorescence Protein upon transfer from solution to the gas phase.11:10 – 12:20  
Vladimir Frankevich, Konstantin Barylyuk, Pavil Sagulenka, Renato Zenobi  
Swiss Federal Institute of Technology, Zurich, Switzerland**PMo-016** Elucidation of CID and ETD based MS/MS Fragmentation for Analysis of Doubly Derivatized Steroids13:30 – 14:40  
Yu-Min Juang, Tzu-Fang She, Chien-Chen Lai  
Institute of Molecular Biology, National Chung Hsing University, Taichung, Taiwan**PMo-018** Identification of protein ligands by FT-ICR-MS/MS13:30 – 14:40  
Adam A Dowle, Abbas Maqbool, Gavin H Thomas, Jerry Thomas  
University of York**PMo-019** Absolute Internal Mass Calibration with Carbon Soot Ions for High Resolution MALDI 15T FT-ICR Mass Spectrometry11:10 – 12:20  
Choi Myoung Choul, Kyu Hwan Park, Hyun Sik Kim, Se Gyu Lee  
Korea Basic Science Institute, Ochang, Korea**PMo-020** Identification of epitopes recognized by monoclonal antibodies raised against the meningococcal factor H binding protein13:30 – 14:40  
Agnese Falieri<sup>1,2</sup>, Sebastien Brier<sup>2</sup>, Laura Santini<sup>2</sup>, Silvana Savino<sup>2</sup>, Marzia Monica Giuliani<sup>2</sup>, Mikkel Nissum<sup>2</sup>, Mariagrazia Pizza<sup>2</sup>, Vega Massignani<sup>2</sup>, Nathalie Norais<sup>2</sup><sup>1</sup>University of Siena, Siena, Italy, <sup>2</sup>Novartis Vaccines and Diagnostics, Siena, Italy**PMo-021** Variable Temperature Ion Mobility Mass Spectrometry of Multimeric Protein Complexes11:10 – 12:20  
Kamila J Pacholarz, Perdita E Barran  
University of Edinburgh, Edinburgh, United Kingdom**PMo-022** Full H/D Exchange for Improving Small Molecule and Peptide Identification with Electrospray Ionization13:30 – 14:40  
Sebastian Tittebrandt<sup>1</sup>, Bernhard Spengler<sup>2</sup>, Wolf D Lehmann<sup>1</sup>  
<sup>1</sup>German Cancer Research Institute, Heidelberg, Germany, <sup>2</sup>Institute for Inorganic and Analytical Chemistry, University Giessen, Germany**PMo-023** SALDI-MS of oligopeptide using gold nanorods on ITO plates.11:10 – 12:20  
Masanori Fujii<sup>1</sup>, Naotoshi Nakashima<sup>1,2,3</sup>, Yasuro Niidome<sup>1,2</sup>  
<sup>1</sup>Kyushu University, Fukuoka, Japan, <sup>2</sup>WPI I2CNER, <sup>3</sup>JST-CREST**PMo-024** Collision/Reaction cell for ICP-MS - a new Concept for an improved removal of low masses13:30 – 14:40  
Lothar Rottmann, Jung Gerhard, Tomoko Vincent  
Thermo Fisher Scientific, Bremen, Germany**PMo-025** Applications of online- bioaffinity- mass spectrometry to structure and affinity determination of neurodegenerative proteins from brain material11:10 – 12:20  
Stefan Slamnoiu<sup>1</sup>, Camelia Vlad<sup>1,2</sup>, Adrian Moise<sup>1</sup>, Mihaela Stumbaum<sup>1,2</sup>, Thomas Gronewold<sup>2</sup>, Markus Perpeet<sup>2</sup>, Michael Przybylski<sup>1</sup><sup>1</sup>Laboratory of Analytical Chemistry and Biopolymer Structure Analysis, Department of Chemistry, University of Konstanz, Germany, <sup>2</sup>SAW Instruments GmbH, Bonn, Germany**PMo-027** Determination of Opiates in Dried Blood Spots using Novel Flow-through Technology coupled to LC/MS/MS11:10 – 12:20  
Kenneth Lewis<sup>2</sup>, Dennis NAGTALON<sup>1</sup>  
<sup>1</sup>Agilent Technologies, <sup>2</sup>OpAns**PMo-029** Optimization of serum N-linked glycan profiling using MALDI-TOF mass spectrometry11:10 – 12:20  
Yongha In<sup>1,2</sup>, Heysun Maeng<sup>1,2</sup>, Sun Young Ahn<sup>1,2</sup>, Chang Won Park<sup>1,2</sup>, Yangsun Kim<sup>1,2</sup><sup>1</sup>HUDSON SURFACE TECHNOLOGY, FORT LEE, NJ, USA, <sup>2</sup>APPLIED SURFACE TECHNOLOGY INC., SUWON, KOREA**PMo-030** Analysis of Panax ginseng extracts by comprehensive Two-Dimensional Ultra High Performance Liquid Chromatography coupled with IT-TOF13:30 – 14:40  
Tatsunari Yoshida<sup>1</sup>, Shin-ichi Yaguchi<sup>2</sup>, Tsutomu Nishine<sup>1</sup>, Hirohisa Mikami<sup>1</sup><sup>1</sup>Shimadzu Co., GADC, Japan, <sup>2</sup>Shimadzu Co., MSBU, Japan**PMo-031** Influence of Sample Preparation Techniques on the Sensitive Detection of Peptides by MALDI-MS11:10 – 12:20  
YUSAKU HIOKI, Hiroki Kuyama, Chikako Hamana, Kohei Takeyama, Koichi Tanaka  
Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, Japan**PMo-032** Development of modified micro-array MALDI plates with carboxylated dopamine for the analysis of small molecules.13:30 – 14:40  
Duhee Park<sup>1,2</sup>, Hyunjung Seo<sup>1,2</sup>, Chang Won Park<sup>1,2</sup>, Yangsun Kim<sup>1,2</sup><sup>1</sup>Applied surface technology Inc., Suwon, Korea, <sup>2</sup>Hudson Surface Technology, Inc., Fort Lee, NJ, USA

Monday, 17<sup>th</sup> September**PMo-033 Bonded Zwitterionic Stationary Phases and Mass Spectrometric Detection for Bioanalysis**

11:10 – 12:20 Patrik Appelblad, Wen Jiang, Jonsson Tobias, Petrus Hemstrom  
Merck SeQuant, Umea, Sweden

**PMo-034 Quantitative Analysis of Free and Total Thyroid Hormones in Serum With and Without Online Sample Cleanup using LC/MS/MS**

13:30 – 14:40 Rory Doyle, Kevin McCann  
AGILENT TECHNOLOGIES

**PMo-035 Selective introduction of 4-amidinobenzyl moiety into peptide N-terminus for straightforward de novo sequencing**

11:10 – 12:20 Toru Yoshikawa, Masahiro Miyashita, Hisashi Miyagawa  
Kyoto University, Kyoto, Japan

**PMo-036 Extractive electrospray ionization mass spectrometry (EESI-MS) for sensitive detection of iodine-129**

13:30 – 14:40 Zhongchen Wu<sup>1</sup>, Yafei Zhou<sup>2</sup>, Bin Jia<sup>2</sup>, Huanwen Chen<sup>2</sup>  
<sup>1</sup>Shandong University at Weihai, Weihai city, China/<sup>2</sup>East China Institute of Technology, Nanchang city, China/Jiangxi

**PMo-037 De novo peptide sequencing facilitated by N-terminal charge derivatization with high proton affinity**

11:10 – 12:20 Yoichiro Nihashi, Hiroyuki Awane, Masahiro Miyashita, Hisashi Miyagawa  
Kyoto University, Kyoto, Japan

**PMo-038 Efficient and rapid multienzymatic limited digestion (MELD) method for complete protein characterization and bottom-up de novo sequencing**

13:30 – 14:40 Gabriel Mazzucchelli<sup>1</sup>, Tyler A Zimmerman<sup>1</sup>, Marie-Alice Meuwis<sup>1</sup>, Nicolas Smargiasso<sup>1</sup>, Michel Deguelde<sup>1</sup>, Dominique Baiwir<sup>1</sup>, Laurent Leclercq<sup>2</sup>, Edwin De Pauw<sup>1</sup>  
<sup>1</sup>University of Liege, Liege, Belgium, <sup>2</sup>Johnson & Johnson Pharmaceutical R&D, Beerse, BELGIUM

**PMo-039 ANALYSIS OF 8 KINDS OF ESTROGENS IN ENVIRONMENTAL WATER BY ULTRA HIGH PERFORMANCE LIQUID CHROMATOGRAPH HYBRID TRIPLE QUADRUPOLE MASS SPECTROMETER**

11:10 – 12:20 hongyuan Hao, Jinting Yao, Luying Zhou, Hengtao Deng, Qiang Li  
Shimadzu (China) Co., LTD. Shanghai, China

**PMo-040 Identification of metabolic pathways related to xylose fermentation performance in recombinant yeast by metabolome analysis**

13:30 – 14:40 Hitoshi MITSUNAGA<sup>1</sup>, Danang Waluyo<sup>1</sup>, Haruyo Hatanaka<sup>2</sup>, Takeshi Bamba<sup>1</sup>, Eiichiro Fukusaki<sup>1</sup>  
<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>Suntory Business Expert Limited.

**PMo-041 Study using synthetic organic acids in Thermo Finnigan LTQ Orbitrap APCI. Application to the acidic fraction, from Brazilian marine oil.**

11:10 – 12:20 Luzia Koike<sup>1</sup>, Eugenio V Santos Neto<sup>2</sup>, Rosane A Fontes<sup>2</sup>, Rosane N Castro<sup>3</sup>

<sup>1</sup>Campinas State University - Campinas- Brazil- southeast, <sup>2</sup>Petrobras R&D Center, Rio de Janeiro, RJ., <sup>3</sup>Federal University of Rio de Janeiro, RJ.

**PMo-042 Standard Samples to Establish Benchmark Metrics and Enable Optimization of Quantitative Proteomics Methods**

13:30 – 14:40 Sean L Seymour<sup>2</sup>, Xu Wang<sup>1</sup>, Brian Williamson<sup>1</sup>, Ignat Shilov<sup>2</sup>, John F MacNamara<sup>1</sup>, Christie L Hunter<sup>2</sup>, Fadi A Abdi<sup>1</sup>

<sup>1</sup>AB SCIEX Framingham MA, <sup>2</sup>AB SCIEX Foster City CA

**PMo-043 Improvement in Mass Measurement Accuracy and Resolving Power Using a New Compensated Fourier Transform Ion Cyclotron Resonance Cell**

11:10 – 12:20 Nobuyuki Shimura<sup>1</sup>, Magnus Palmblad<sup>2</sup>, Jens Fuchser<sup>3</sup>, Yuri E M Van Der Burgt<sup>2</sup>, M Goekhan Baykut<sup>3</sup>, André M Deelder<sup>2</sup>

<sup>1</sup>Bruker Daltonics K.K., Yokohama, Japan, <sup>2</sup>Leiden University Medical Center, Leiden, Netherlands, <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany

**Session 3****Structures and Dynamics of Atomic and Molecular Clusters****PMo-044 Gas phase ion-molecule reactions of C2H5+ and C2H3+ with C2H2 using low-temperature drift tube mass spectrometer**

13:30 – 14:40 Kenichi Iwamoto, Haruto IKUTA  
Osaka Prefecture University, Osaka, Japan

**PMo-045 Assembly Modulated Metallosupramolecular Polymer Formation Observed by CSI-MS and Other Analytical Methods**

Masatoshi Kawahata<sup>1</sup>, Kadzuya Hirata<sup>2</sup>, Hiroshi Danjo<sup>2</sup>, Kentaro Yamaguchi<sup>1</sup>

<sup>1</sup>Tokushima Bunri University, Kagawa, Japan, <sup>2</sup>Konan University, Kobe, Japan

**PMo-046 Clusters of Water, Acetonitrile and Azeotropic Mixtures in Gas and Liquid Phases Studied by Liquid-ionization Tandem Mass Spectrometry**

13:30 – 14:40 Masahiko Tsuchiya<sup>1</sup>, Haruhiko Fukaya<sup>2</sup>, Yoshiaki Kurita<sup>3</sup>  
<sup>1</sup>Yokohama National University, Yokohama, Japan, <sup>2</sup>Tokyo University of Pharmacy, <sup>3</sup>Housei University

Monday, 17<sup>th</sup> September

Mon

- PMo-047** ICP-MS and IR techniques used in metal detection and control of some new synthetized materials with bioactive potential  
11:10 – 12:20

NICOLETA C VEDEANU<sup>1</sup>, Ramona Stanescu<sup>2</sup>,  
Dana Alina Magdas<sup>3</sup>, Cezara Voica<sup>3</sup>

<sup>1</sup>"IULIU HATIEGANU" UNIVERSITY OF MEDICINE AND PHARMACY, CLUJ-NAPOCA, ROMANIA, <sup>2</sup>Babes-Bolyai University, Faculty of Physics, RO-400084, Cluj-Napoca, Romania, <sup>3</sup>National Institute for Research and Development for Isotopic and Molecular Technologies, RO-400293, Cluj-Napoca, Romania

- PMo-048** Size-dependent structures of zinc oxide cluster ions studied by ion mobility mass spectrometry  
13:30 – 14:40

Kunihiro Komatsu, Kiichiro Koyasu, Fuminori Misaizu  
Tohoku University, Sendai, Japan

- PMo-049** Photodissociation dynamics of mass-selected cluster ions examined by fragment-ion imaging  
11:10 – 12:20

Hiroshi Hoshino, Yoshihiro Yamakita, Yoshitomo Suzuki,  
Masataka Saito, Kiichiro Koyasu, Fuminori Misaizu  
Tohoku University, Sendai, Japan

## Session 4

### Imaging I

- PMo-050** Chemical digestion for imaging mass spectrometry  
13:30 – 14:40

Junpei Naito, Shuya Satoh, Hiroyuki Hashimoto  
Canon Inc., Tokyo, Japan

- PMo-051** Enhanced peptide molecular imaging by depositing ice in Time-of-Flight Secondary Ion Mass Spectrometry  
11:10 – 12:20

Naofumi Aoki, Manabu Komatsu, Masafumi Kyogaku,  
Hiroyuki Hashimoto  
Canon Inc., Tokyo, Japan

- PMo-052** Direct and indirect imaging of secondary metabolites and enzymatic reactions in plant material by Desorption Electrospray Ionization  
13:30 – 14:40

Bir Li<sup>3</sup>, Nanna Bjarnholt<sup>2</sup>, Camilla Knudsen<sup>2</sup>, Janina Thunig<sup>3</sup>,  
Steen H Hansen<sup>3</sup>, Christian Janfelt<sup>1,3</sup>

<sup>1</sup>University of Copenhagen, Copenhagen, Denmark, <sup>2</sup>Dept. of Plant Biology and Biotechnology, University of Copenhagen, Copenhagen, Denmark,  
<sup>3</sup>Dept. of Pharmacy, Center for Advanced Drug Analysis, University of Copenhagen, Copenhagen, Denmark

- PMo-053** Sub-Micrometer Imaging of Lipids and Trace Elements in Various Cells with ToF-SIMS and Laser-SNMS  
11:10 – 12:20

Heinrich F Arlinghaus<sup>1</sup>, Felix Draude<sup>1</sup>, Sebastian Galla<sup>1</sup>,  
Andreas Pelster<sup>1</sup>, Martin Koersgen<sup>1</sup>, Jutta Tentschert<sup>2</sup>,  
Harald Jungnickel<sup>2</sup>, Andrea Haase<sup>2</sup>, Andreas Luch<sup>2</sup>,  
Tanja Schwerdtle<sup>3</sup>, Johannes Muethling<sup>4</sup>

<sup>1</sup>Institute of Physics, University of Muenster, Muenster, Germany, <sup>2</sup>German Federal Institute of Risk Assessment, Department of Product Safety, Berlin, Germany, <sup>3</sup>Institute of Food Chemistry, University of Muenster, Muenster, Germany, <sup>4</sup>Institute of Hygiene, University of Muenster, Muenster, Germany

- PMo-054** The potential use of reactive DESI to assess oxidative stress in the cell culture  
13:30 – 14:40

Anna Bodzon-Kulakowska, Piotr Suder, Tomasz Cichon,  
Jerzy Silberring  
AGH University of Science and Technology, Krakow, Poland

- PMo-055** Higher sensitivity sub-micron spatial resolution TOF-SIMS bio-molecular imaging using interleaved Gas Cluster Ion Beam (GCIB) sputtering  
11:10 – 12:20

Itsuko Ishizaki<sup>1</sup>, John S Hammond<sup>2</sup>, Takuya Miyayama<sup>1</sup>,  
Gregory L Fisher<sup>2</sup>

<sup>1</sup>ULVAC-PHI, Inc., Kanagawa, Japan, <sup>2</sup>Physical Electronics USA, Chanhassen, MN, USA

- PMo-056** Drug and metabolites study in whole body animal by High Definition MALDI imaging  
13:30 – 14:40

Thanai Paxton<sup>1</sup>, Motoji Oshikata<sup>1</sup>, Emmanuelle Claude<sup>2</sup>,  
Lars Bendahl<sup>3</sup>, Ian Edwards<sup>2</sup>, Paul Murray<sup>2</sup>, Johannes P Vissers<sup>2</sup>  
<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>Waters Corporation, Manchester, UNITED KINGDOM, <sup>3</sup>H. Lundbeck A/S, Dk-2500 Valby, DENMARK

- PMo-057** DESI-MS imaging of differences between physiological and morphine-treated rat brains.  
11:10 – 12:20

Piotr Suder<sup>1</sup>, Anna Bodzon-Kulakowska<sup>1</sup>, Anna Drabik<sup>1</sup>,  
Joanna Ner<sup>1</sup>, Ewelina Paszynska<sup>1</sup>, Jolanta H Kotlinska<sup>2</sup>  
<sup>1</sup>AGH University of Science and Technology, Krakow, Poland, <sup>2</sup>Medical University of Lublin, Lublin, Poland

- PMo-058** High-resolution TOF-SIMS Imaging reveals Multi-layered Barrier Structure of the Stratum Corneum of Skin  
13:30 – 14:40

Akiharu Kubo<sup>1</sup>, Itsuko Ishizaki<sup>2</sup>, Akiko Kubo<sup>1</sup>, Hiroshi Kawasaki<sup>1</sup>,  
Yoshiharu Ohashi<sup>2</sup>, Masayuki Amagai<sup>1</sup>

<sup>1</sup>Keio University, Tokyo, Japan, <sup>2</sup>ULVAC-PHI, Chigasaki, Japan

- PMo-059** Quantitative MALDI Imaging of a Peptide Pharmaceutical for Drug Distribution Studies  
11:10 – 12:20

Nozomi Takai, Yukari Tanaka, Ayahisa Watanabe  
Shionogi & Co., Ltd., Osaka, Japan

- PMo-060** Investigation of Zeolite Matrix for Analysis of Pharmacokinetics Using Imaging Mass Spectrometry with Laser Desorption/Ionization  
13:30 – 14:40

Naoki Moriguchi<sup>1</sup>, Hisanao Hazama<sup>1</sup>, Tatsuya Fujino<sup>2</sup>,  
Kunio Awazu<sup>1</sup>

<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>Tokyo Metropolitan University, Tokyo, Japan

- PMo-061** Imaging the Penetration Behaviour of Topically Applied Drugs into Skin by Desorption Electrospray Ionization Mass Spectrometry  
11:10 – 12:20

Janina Thunig<sup>1</sup>, Rasmus Mortensen<sup>2</sup>, Louise Bastholm-Jensen<sup>2</sup>,  
Steen H Hansen<sup>1</sup>, Christian Janfelt<sup>1</sup>

<sup>1</sup>Department of Pharmaceutics and Analytical Chemistry, University of Copenhagen, Copenhagen, Denmark, <sup>2</sup>New Products, LEO Pharma A/S, Ballerup, Denmark

## Monday, 17<sup>th</sup> September

**PMo-062** Platinum Vapor Deposition Surface-Assisted Laser Desorption/Ionization for Mass Spectrometry Imaging of Small Molecules  
 13:30 – 14:40

Tomoyuki Ozawa<sup>1,2</sup>, Hirotaka Hisatomi<sup>2</sup>,  
 Tetsuro Higashisokawa<sup>2</sup>, Hideya Kawasaki<sup>2</sup>, Ryuichi Arakawa<sup>2</sup>  
<sup>1</sup>Nissan Chemical Industries Ltd., Funabashi, Japan, <sup>2</sup>Kansai University, Osaka, Japan

**PMo-063** Comparison of MALDI Imaging modalities using a Peptide Gel matrix for stem cell implantation  
 11:10 – 12:20

Duncan M Forster<sup>1</sup>, Adam Mcmahon<sup>1</sup>, Catherine Merry<sup>1</sup>,  
 Omar Belgacem<sup>2</sup>  
<sup>1</sup>The University of Manchester, Manchester, United Kingdom, <sup>2</sup>Shimadzu, Manchester, United Kingdom

**PMo-064** NALDI-IMAGING OF TUMORS: PHOSPHOETANOLAMINE EFFECT ON THE LIPID PROFILE OF A MELANOMA MODEL  
 13:30 – 14:40

Alessandra Tata<sup>1</sup>, Anna Maria A P Fernandes<sup>1</sup>,  
 Vanessa G Santos<sup>1</sup>, Rosana M Alberici<sup>1</sup>, Carlos A Parada<sup>2</sup>, Wellington Braguini<sup>2</sup>, Luciana Veronez<sup>2</sup>, Gabriela Silvia Bisson<sup>2</sup>, Felipe H Z Reis<sup>3</sup>, Luciane C Alberici<sup>3</sup>, Marcos N Eberlin<sup>1</sup>  
<sup>1</sup>Thomson Mass Spectrometry Laboratory, Institute of Chemistry, University of Campinas-UNICAMP, 13084-971, Campinas, SP, Brazil, <sup>2</sup>Departamento de Enfermagem Materno-Infantil e Saude Publica, Escola de Enfermagem de Ribeirao Preto, SP, Brazil, <sup>3</sup>Departamento de Fisica e Quimica, Faculdade de Ciencias Farmaceuticas de Ribeirao Preto, Universidade de Sao Paulo, Ribeirao Preto, SP, Brazil.

**PMo-065** An optimized organ fixation technique for imaging and quantitative mass spectrometry for high energy phosphate-metabolites  
 11:10 – 12:20

Sugiura Yuki<sup>1,2</sup>, Makoto Suematsu<sup>1</sup>  
<sup>1</sup>Keio University, Tokyo, Japan, <sup>2</sup>Precursory Research for Embryonic Science and Technology (PRESTO)

**PMo-066** A novel method to observe cell surface protein GRP78 expression by time of flight-secondary ion mass spectrometer (TOF-SIMS)  
 13:30 – 14:40

Hsiao-Ting Hsieh<sup>2,3</sup>, Tsui-Yun Lo<sup>1</sup>, Fu-Der Mai<sup>1,2,3</sup>  
<sup>1</sup>Department of Biochemistry, School of Medicine, Taipei Medical University, Taipei, Taiwan, <sup>2</sup>Graduate Institute of Medical Science, Taipei Medical University, Taipei, Taiwan, <sup>3</sup>Biomedical Mass Imaging Research Center, Taipei Medical University, Taipei, Taiwan

**PMo-067** Imaging Mass Spectrometry of Plant Tissue Slices: Comparison of MALDI-TOF MSI and MALDI-FTICR MSI  
 11:10 – 12:20

Katsutoshi Takahashi<sup>1</sup>, Daisuke Miura<sup>2</sup>  
<sup>1</sup>Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, <sup>2</sup>Kyushu University, Fukuoka, Japan

**PMo-068** MALDI-MS Imaging Atlas of Mouse Development  
 13:30 – 14:40

Takashi Nirasawa<sup>1</sup>, Masaya Ikegawa<sup>2</sup>  
<sup>1</sup>Bruker Daltonics K.K., Yokohama, Japan, <sup>2</sup>Kyoto Prefectural University of Medicine, Kyoto, Japan

**PMo-069** MALDI imaging of desalted rat brain sections reveals the up- and down-regulation of phospholipids by ischemia  
 11:10 – 12:20

HAY-YAN J WANG<sup>1</sup>, HSUAN-WEN WU<sup>1</sup>, PING-JU TSAI<sup>1,2</sup>, CHENG BIN LIU<sup>1,3</sup>

<sup>1</sup>Department of Biological Sciences, National Sun Yat-Sen University, Kaohsiung, Taiwan, <sup>2</sup>Department of Surgery, Yuan's General Hospital, Kaohsiung, Taiwan, <sup>3</sup>Department of Obstetrics and Gynecology, Veterans General Hospital-Kaohsiung, Kaohsiung, Taiwan

**PMo-070** Visualization of Transdermal Drug Delivery by 2D-DESI Mass Spectrometry ---- a Novel Approach to Generate Pseudo Cross-sectional Skin Images  
 13:30 – 14:40

Akira Motoyama<sup>1,2</sup>, Keishi Kihara<sup>1</sup>, Yuichiro Mori<sup>1</sup>, Mitsuo Takayama<sup>2</sup>

<sup>1</sup>Shiseido Co., Ltd, Yokohama, Japan, <sup>2</sup>Yokohama City University, Yokohama, Japan

**PMo-071** Chemical sensor arrays for application in mass spectrometry on surfaces and tissues  
 11:10 – 12:20

Martina Lorey<sup>1</sup>, Rabah Soliymani<sup>1</sup>, Jari Yli-Kauhaluoma<sup>2</sup>, Marc Baumann<sup>1</sup>

<sup>1</sup>Protein Chemistry Unit, University of Helsinki, Helsinki, Finland, <sup>2</sup>Division of Pharmaceutical Chemistry, University of Helsinki, Helsinki, Finland

**PMo-072** The Sausage Omelette: Breakfast of (IMS) Champions or a Novel Quantitation Tool for Small Molecule Imaging?  
 13:30 – 14:40

Shannon Cornett<sup>1</sup>, Katherine Kellersberger<sup>1</sup>, Mark R Groseclose<sup>2</sup>, David S Wagner<sup>2</sup>, Stephan Castellino<sup>2</sup>

<sup>1</sup>Bruker Daltonics, Billerica, MA, USA, <sup>2</sup>GlaxoSmithKline, Research Triangle Park, NC, USA

**PMo-073** To Digest or Not to Digest, That's the Question  
 11:10 – 12:20

Martin Schuerenberg<sup>1</sup>, Christine Luebbert<sup>1</sup>, Rainer Paape<sup>1</sup>, Janine Rattke<sup>1</sup>, Axel Walch<sup>2</sup>, Sandra Rauser<sup>2</sup>, Michael Becker<sup>1</sup>

<sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany, <sup>2</sup>Helmholtz Center Munich, Neuherberg, Germany

**PMo-074** Rapid assessment of drug and metabolite distribution in whole animal tissues via accurate mass imaging  
 13:30 – 14:40

Arnd Ingendoh<sup>1</sup>, Cristine Quiason<sup>2</sup>, Katherine Kellersberger<sup>1</sup>, Brian Dean<sup>2</sup>, Sheerin Shahidi-Latham<sup>2</sup>

<sup>1</sup>Bruker Daltonik GmbH, <sup>2</sup>Genentech Inc., South San Francisco, CA

**PMo-075** Development of MALDI-MS Imaging of Metabolite and Protein in a Single Tissue Section  
 11:10 – 12:20

Ayumi Yamaguchi, Daisuke Miura, Yoshinori Fujimura, Hiroyuki Wariishi  
 Kyushu University, Fukuoka, Japan

**PMo-076** Automated Tissue State Assignment for High Resolution FTMS MALDI Imaging Data  
 13:30 – 14:40

Paul Speir<sup>1</sup>, Jens Fuchser<sup>2</sup>, Soeren Deininger<sup>2</sup>, Michael Becker<sup>2</sup>, Katherine Kellersberger<sup>1</sup>

<sup>1</sup>Bruker Daltonics, Inc., <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany

Monday, 17<sup>th</sup> September

Mon

**PMo-077** An Investigation of Spatiotemporal Metabolic Behaviors in Response to Pathological Progress using Multiple Mass Spectrometry Techniques

11:10 – 12:20 Miho Irie, Yoshinori Fujimura, Daiki Setoyama, Mayumi Yamato, Daisuke Miura, Hiroyuki Wariishi Kyushu University, Fukuoka, Japan

**PMo-078** Imaging Hair Analyses for Drugs: A New Perspective to Investigate Drug Use History

13:30 – 14:40 Tooru Kamata<sup>1</sup>, Noriaki Shima<sup>1</sup>, Akihiro Miki<sup>1</sup>, Kei Zaitsu<sup>1</sup>, Munehiro Katagi<sup>1</sup>, Michiaki Tatsumi<sup>1</sup>, Toyofumi Nakanishi<sup>2</sup>, Takako Sato<sup>2</sup>, Hitoshi Tsuchihashi<sup>2</sup>, Koichi Suzuki<sup>2</sup>  
<sup>1</sup>Forensic Science Laboratory, Osaka, Japan, <sup>2</sup>Osaka Medical College, Osaka, Japan

**PMo-079** Easy ambient sonic-spray ionization mass spectrometry imaging (EASI-MSI).

11:10 – 12:20 Dragos Lostun<sup>1</sup>, Mario F Mirabelli<sup>1,2</sup>, Tanam S Hamid<sup>1</sup>, Alexander Chramow<sup>1</sup>, Demian R Ifa<sup>1</sup>  
<sup>1</sup>York University, Toronto, ON, Canada, <sup>2</sup>University of Calabria, Cosenza, Italy

**PMo-080** Optimization of conditions for acetylcholine detection in the nerve tissue sections by imaging mass spectrometry

13:30 – 14:40 Ikuko Yao<sup>1,2</sup>, Yuki Sugjura<sup>2,3</sup>, Nobuhiro Zaima<sup>3</sup>, Mitsutoshi Setou<sup>3</sup>, Seiji Ito<sup>1</sup>  
<sup>1</sup>Kansai Medical University, Osaka, Japan, <sup>2</sup>Precursory Research for Embryonic Science and Technology (PRESTO), Tokyo, Japan, <sup>3</sup>Hamamatsu University School of Medicine, Hamamatsu, Japan

**PMo-081** MALDI-IMS - The challenge of on-tissue digestion, a comparison of different protocols to improve imaging experiments

11:10 – 12:20 Hanna C Diehl, Julian Elm, Judith Baronner, Helmut E Meyer, Corinna Henkel  
Medizinisches Proteom Center, Ruhr University Bochum, Germany

**PMo-082** Molecular detection of breast cancer-related phosphatidylinositol by high-resolution imaging mass spectrometry

13:30 – 14:40 Masahiro Kawashima<sup>1</sup>, Noriko Fukao<sup>2</sup>, Minoru Suzuki<sup>2</sup>, Taka-aki Sato<sup>2</sup>, Koichi Tanaka<sup>2</sup>, Nobuko Kawaguchi-Sakita<sup>1</sup>, Masahiro Sugimoto<sup>1</sup>, Takayuki Ueno<sup>1</sup>, Kazuya Terasawa<sup>3</sup>, Gozo Tsujimoto<sup>3</sup>, Kazuharu Shimizu<sup>3</sup>, Masakazu Toi<sup>1</sup>  
<sup>1</sup>Department of Breast Surgery, Graduate School of medicine, Kyoto University, Kyoto, JAPAN, <sup>2</sup>Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, JAPAN, <sup>3</sup>Department of Cancer Omics Research, World-Leading Drug Discovery Research Center, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, JAPAN

**PMo-083** Oxygen defect chemistry proposed by zinc and antimony images in the dense tin dioxide ceramics by means of NanoSIMS 50

11:10 – 12:20 Isao Sakaguchi, Ken Watanabe, Hajime Haneda, Naoki Ohashi, Shunichi Hishita  
National Institute for Materials Science, Tsukuba, Japan

**PMo-084** MALDI Imaging of Metabolites Reconstructed by CE-MS Based Quantitative Analysis

13:30 – 14:40 Tsuyoshi Nakanishi<sup>1</sup>, Takako Hishiki<sup>2,3</sup>, Shigeki Kajihara<sup>1</sup>, Kiyoshi Ogawa<sup>1</sup>, Makoto Suematsu<sup>2,3</sup>

<sup>1</sup>Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>School of Medicine, Keio University, Tokyo, Japan, <sup>3</sup>JST ERATO Suematsu Gas Biology Project, Tokyo, Japan

**Session 5**

## Advances in Spray Ionization Techniques

**PMo-085** New nano ESI source development for increased performance nanoLC-MS with plug-and-spray configuration

11:10 – 12:20 Reiko Kiyonami<sup>2</sup>, Peter Soendergaard<sup>1</sup>, Christian Ravnsborg<sup>1</sup>, Vlad Zabrouskov<sup>2</sup>

<sup>1</sup>Thermo Fisher Scientific Odense Denmark, <sup>2</sup>Thermo Fisher Scientific San Jose CA

**PMo-086** Electrostatic Spray Ionization and Microchips Emitter for On-Line MS Monitoring of Chemical and Electrochemical Reactions

13:30 – 14:40 Liang QIAO<sup>1</sup>, Romain SARTOR<sup>1</sup>, Elena TOBOLKINA<sup>1</sup>, Dmitry MOMOTENKO<sup>1</sup>, Mathieu ODIJK<sup>2</sup>, Pekka PELJO<sup>3</sup>, Hubert GIRault<sup>1</sup>

<sup>1</sup>ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE, SWITZERLAND,

<sup>2</sup>UNIVERSITY OF TWENTE, ENSCHEDE, NETHERLANDS, <sup>3</sup>DEPARTMENT OF CHEMISTRY, AALTO UNIVERSITY, ESPOO, FINLAND

**PMo-087** Miniaturized Peptide Sample Pretreatment Platform for Indirect Spray Analysis

11:10 – 12:20 Hoi Sze Yeung, Tak-Wah Dominic Chan  
The Chinese University of Hong Kong, Hong Kong SAR, China

**PMo-088** Novel off-line electrospray ion source with a disposable needle

13:30 – 14:40 Hideki Hasegawa, Hiroyuki Satake, Masao Suga, Yuichiro Hashimoto  
Hitachi Ltd., Central Research Laboratory, Kokubunji, Japan

**PMo-089** Movement of Ions and Charged Droplets from Atmospheric Region into the Gas Dynamic Interface

11:10 – 12:20 Natalia Fomina<sup>1</sup>, Nikolai Gall<sup>2</sup>, Sergey Masyukevich<sup>1</sup>, Alexandra Kretinina<sup>1</sup>, Lidia Gall<sup>1</sup>, Alexander Bazhenov<sup>3</sup>, Sergey Bulovich<sup>4</sup>

<sup>1</sup>The Institute for Analytical Instrumentation RAS, Saint-Petersburg, Russia, <sup>2</sup>A. F.Ioffe Physico-Technical Institute of RAS, St.Petersburg, Russia, <sup>3</sup>All Russian Scientific Research Institute for Geology and Mineral Resources named of I. S.Gramberg, St. Petersburg, Russia, <sup>4</sup>Saint-Petersburg State Polytechnical University St.Petersburg, Russia

**PMo-090** An introduction of a novel atmospheric pressure Micro/Nano-ESI ion source

13:30 – 14:40 Reza Javahery<sup>1</sup>, Hui Qiao<sup>1</sup>, Brett Larsen<sup>2</sup>, Lorne E Taylor<sup>2</sup>, Lisa Cousins<sup>1</sup>

<sup>1</sup>IONICS Mass Spectrometry, Toronto, Canada, <sup>2</sup>Samuel Lunenfeld Research Institute, Mount Sinai Hospital, Toronto, Canada

Monday, 17<sup>th</sup> September

Mon

- PMo-091** Electrospraying, Movement and Evaporation of Charged Droplets Using Rotating Gas Flows and Transverse Ion Extraction  
11:10 – 12:20

Sergey Masyukevich<sup>1</sup>, Nikolai Gall<sup>2</sup>, Natalia Fomina<sup>1</sup>, Mihail Lapushkin<sup>2</sup>, Alexandra Kretinina<sup>1</sup>  
<sup>1</sup>Institute for Analytical Instrumentation, Saint-Peterburg, Russia, <sup>2</sup>A.F.Ioffe Physico-Technical Institute of Russian Academy of Sciences, St. Petersburg, Russia

## Session 6

### Novel Approaches in Proteomics Analysis

- PMo-092** A reference method for the SI-traceable quantification of somatropin in human serum using an isotopically labeled protein internal standard  
13:30 – 14:40

Caroline E Pritchard<sup>1</sup>, Milena Quaglia<sup>2</sup>, Alison E Ashcroft<sup>3</sup>, Gavin O'Connor<sup>2</sup>  
<sup>1</sup>LGC, London, UK & University of Leeds, Leeds, UK, <sup>2</sup>LGC, London, UK, <sup>3</sup>Astbury Centre for Structural and Molecular Biology, University of Leeds, Leeds, UK

- PMo-093** Large-scale LC-MS-based Profiling of Soluble Protein Complexes  
11:10 – 12:20

Cuihong WAN<sup>1</sup>, Pierre C Havugimana<sup>1</sup>, Andrew Lugowski<sup>1</sup>, Kathy Foltz<sup>2</sup>, Andrew Emili<sup>1</sup>  
<sup>1</sup>University of Toronto, Toronto, Canada, <sup>2</sup>University of California Santa Barbara, California, USA

- PMo-094** Mass spectrometry-based sequencing of protein C-terminal peptide using alpha-carboxyl group specific derivatization and COOH capturing  
13:30 – 14:40

Chihiro Nakajima, Hiroki Kuyama, Koichi Tanaka  
Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, Japan

- PMo-095** Identification of proteins with different expression profiles related to Nasal Polyps in Aspirin Intolerant Asthma(AIA) using MALDI-TOF/MS  
11:10 – 12:20

Yukie Tanaka<sup>1</sup>, Dai Susuki<sup>2</sup>, Shigeharu Fujieda<sup>2</sup>, Yutaka Fujii<sup>1</sup>  
<sup>1</sup>Department of Molecular Biology and Chemistry, University of Fukui, Fukui, Japan, <sup>2</sup>Department of Otorhinolaryngology Head & Neck Surgery, University of Fukui, Fukui, Japan

- PMo-096** Specific Racemization of a Cysteine Residue in the Hinge Region of Immunoglobulin Gamma 1 during Storage  
13:30 – 14:40

Masato Amano<sup>1</sup>, Naoki Kobayashi<sup>1</sup>, Takashi Nakazawa<sup>2</sup>, Susumu Uchiyama<sup>3</sup>, Kiichi Fukui<sup>3</sup>  
<sup>1</sup>Daiichi Sankyo, Hiratsuka, Japan, <sup>2</sup>Nara Women's University, Nara, Japan, <sup>3</sup>Osaka University, Osaka, Japan

- PMo-097** Identification and affinity characterization of carbohydrate-binding epitopes in human Galectin-9 and rat Galectin-5 by proteolytic Excision-MS and bioaffinity analysis  
11:10 – 12:20

Frederike Eggers<sup>1</sup>, Adrian Moise<sup>1</sup>, Sabine Andre<sup>2</sup>, Hans-Joachim Gabius<sup>2</sup>, Michael Przybylski<sup>1</sup>

<sup>1</sup>University of Konstanz, Konstanz, Germany, <sup>2</sup>Ludwig-Maximilians-University, Munich, Germany

- PMo-098** Differentiation of isobaric residues in SPITC-derivatized tryptic peptides using MS/MS technique in a novel Curved Field Reflectron.  
13:30 – 14:40

yuzo yamazaki, Keisuke Shima  
Shimadzu Corporation, Kyoto, Japan

- PMo-099** Study of hydrogen-induced cleavage of peptides with MALDI-ISD and sonolytic hydrolysis  
11:10 – 12:20

Motoshi Sakakura, Mitsuo Takayama  
Yokohama City University, Yokohama, Japan

- PMo-100** Electrochemically Assisted Reduction of Disulfide Bonds of Peptides and Proteins With On-Line Mass Spectrometric Detection  
13:30 – 14:40

Martin Eysberg, Agnieszka Kraj, Hendrik-Jan Brouwer, Nico Reinhoud, Jean-Pierre Chervet  
Antec, Zoeterwoude, the Netherlands

- PMo-101** Isotope dilution LC-ESI/MS/MS method for the determination of phenylthiohydantoin (PTH)-amino acids derived from Edman degradation products of proteins  
11:10 – 12:20

Ryo Satoh, Takaaki Goto, Seon Hwa Lee, Tomoyuki Oe  
Tohoku University

- PMo-102** Mechanistic Study on Non-enzymatic Isomerization of N-terminal Amino Acids by Endogenous Aldehydes  
13:30 – 14:40

Ryo Kajita, Takaaki Goto, Seon Hwa Lee, Tomoyuki Oe  
Tohoku University, Sendai, Japan

- PMo-103** Peptide fragmentation upon low and high energy CID in ESI and MALDI mass spectrometry: A statistical approach  
11:10 – 12:20

Christine Enjalbal, Mathieu Dupre, Sonia Cantel, Jean Martinez  
University of Montpellier 2

- PMo-104** Rapid Asp-selective Acid Hydrolysis for Proteomic Workflows  
13:30 – 14:40

Joe R Cannon, Catherine Fenselau  
University of Maryland, College Park, MD United States

- PMo-105** Optimization of matrix preparation methods for MALDI-ISD of protein  
11:10 – 12:20

Ryunosuke Iimuro, Mitsuo Takayama  
Yokohama City University, Yokohama, Japan

## Monday, 17<sup>th</sup> September

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**PMo-106 Comparative Proteomic Analysis of Virulence Variations in *Xanthomonas Campestris* pv. *Campestris* Strain 17, 11 and P20H**

Tao-Shan Chang, Chien-Chen Lai

National Chung Hsing University, Taichung, Taiwan/Institute of Molecular Biology College of Life Science

**PMo-107 Proteomic Evidences for Starch Biosynthetic Pathway in Rice Endosperm**

Chih-Wei Liu, Chien-Chen Lai

Institute of Molecular Biology, National Chung Hsing University, Taiwan

**PMo-108 MALDI-TOF-MS-based proteomics for urinary biomarker discovery in gamma-irradiated mouse**

Keita KIRIYAMA, Susumu YOSHIOKA, Daisuke IIZUKA,

Hidehiko KAWAI, Shunsuke IZUMI

Hiroshima University, Hiroshima, Japan

**PMo-109 LDI-MS on nanostructured materials for sensitive and efficient protein digest characterization**

Mathieu Dupre<sup>1</sup>, Sonia Cantel<sup>1</sup>, Yannick Coffinier<sup>2</sup>,

Rabah Boukherroub<sup>2</sup>, Jean Martinez<sup>1</sup>, Christine Enjalbal<sup>1</sup>

<sup>1</sup>University of Montpellier, Montpellier, France, <sup>2</sup>University of Lille, Lille, France

**PMo-110 Evaluation of peptide adsorption-controlled liquid chromatography-mass spectrometric (PAC-LC-MS) method to quantify peptides in biological fluids**

Ryoya Goda<sup>1</sup>, Ryo Yokoyama<sup>2</sup>, Nobuhiro Kobayashi<sup>1</sup>

<sup>1</sup>Daiichi Sankyo, Co., Ltd., Tokyo, Japan, <sup>2</sup>KK AB Sciex, Tokyo, Japan

**PMo-111 Comparative proteomics of CD133-positive liver cancer stem cells**

Sheng-Ta Tsai<sup>1,2</sup>, Chih-Chiang Tsou<sup>3</sup>, Wan-Yu Mao<sup>1</sup>,

Wei-Chao Chang<sup>1</sup>, Wen-Lian Hsu<sup>3</sup>, Chia-Ning Shen<sup>1,2</sup>,

Chung-Hsuan Chen<sup>1,2,4,5</sup>

<sup>1</sup>Genomics Research Center, Academia Sinica, Nankang, Taipei, Taiwan,

<sup>2</sup>Institute of Biochemistry & Molecular Biology, National Yang-Ming University, Taipei, Taiwan, <sup>3</sup>Institute of Information Science, Academia Sinica, Nankang, Taipei, Taiwan, <sup>4</sup>Department of Chemistry, National Taiwan University,

<sup>5</sup>Institute of Atomic & Molecular Sciences, Academia Sinica

**PMo-112 Quantitative proteomics approach with isotope dimethyl labeling for protein pathway analysis using high resolution mass spectrometry**

Ping Sui, Konstantin Artyomenko, Jonas Bergquist

Uppsala University, Uppsala, Sweden

**PMo-113 MS-based proteogenomics and comparative proteomics help to identify novel key proteins in organisms with newly sequenced genomes**

Rainer Cramer<sup>1</sup>, Laurence V Bindschedler<sup>1</sup>, Dana M Gheorge<sup>2</sup>, Liam J McGuffin<sup>1</sup>, Celia J Smith<sup>1</sup>, Clara M Pliego Prieto<sup>2</sup>, Pietro D Spanu<sup>2</sup>

<sup>1</sup>University of Reading, UK, <sup>2</sup>Imperial College London, UK

**PMo-114 MALDI msn analysis of protein oxidation in major diseases**

Lina Sellami<sup>1</sup>, Claude Villard<sup>1</sup>, Kamel Mabrouk<sup>1</sup>, Therese Schembri<sup>1</sup>, Didier Gigmes<sup>1</sup>, Matthew Openshaw<sup>2</sup>, Omar Belgacem<sup>2</sup>, Daniel Lafitte<sup>1</sup>

<sup>1</sup>Aix Marseille Universite, Marseille, France, <sup>2</sup>Shimadzu, Manchester, United Kingdom

**PMo-115 Quantitative Proteomics Using a Quadrupole-Orbitrap Mass**

**Spectrometer (Q-Exactive): Application to the Analysis of Clinical Samples**

Bruno Domon, Sebastien Gallien, Elodie Duriez  
Luxembourg Clinical Proteomics Center CRP-Sante Luxembourg

**PMo-116 Using Selected Reaction Monitoring to determine cell and drug specific profiles of caspase cleaved substrates in apoptosis**

Kazutaka Shimbo<sup>1,2</sup>, Gerald W Hsu<sup>2</sup>, Huy Nguyen<sup>2,3</sup>, Sami Mahrus<sup>2</sup>, Jonathan C Trinidad<sup>2</sup>, Alma L Burlingame<sup>2</sup>, James A Wells<sup>2,3</sup>

<sup>1</sup>Institute for Innovation, Ajinomoto Co., Inc., Kawasaki, Japan, <sup>2</sup>Department of Pharmaceutical Chemistry, University of California, San Francisco, San Francisco, CA, <sup>3</sup>Department of Cellular and Molecular Pharmacology, University of California, San Francisco, San Francisco, CA

**PMo-117 Rapid enzyme digestion system consisting of microwave and air bubble-mediated cooling.**

Hyunjung Seo<sup>1</sup>, Dong Min Kim<sup>1,2</sup>, Chang Won Park<sup>1,2</sup>, Yangsun Kim<sup>1,2</sup>

<sup>1</sup>HUDSON SURFACE TECHNOLOGY, FORT LEE, NJ, USA, <sup>2</sup>APPLIED SURFACE TECHNOLOGY INC., SUWON, KOREA

**PMo-118 Biomarker Discovery and Validation with Nonglycosylated Tryptic Peptides from N-linked Glycoproteins in Human Plasma**

Ju Yeon Lee<sup>1,2</sup>, Jin Young Kim<sup>1</sup>, Gun Wook Park<sup>1,4</sup>, Kyung-Hoon Kwon<sup>1</sup>, Yeong Hee Ahn<sup>1</sup>, Myeong Hee Moon<sup>2</sup>, Young Ki Paik<sup>3</sup>, Jong Shin Yoo<sup>1,4</sup>

<sup>1</sup>Korea Basic Science Institute, O-chang Campus, Chungcheongbukdo, Korea,

<sup>2</sup>Department of Chemistry, Yonsei University, Seoul, Korea, <sup>3</sup>Yonsei Proteome Research Center and Biomedical Proteome Research Center, Department of Biochemistry, Yonsei University, Seoul, Korea, <sup>4</sup>Graduate School of Science and Technology, Chungnam National University, Daejon, Korea

**PMo-119 The application of biomarker discovery for atopic dermatitis and normalized spectral index based label free quantitation**

Ki Na Yun<sup>1</sup>, Gun Wook Park<sup>1</sup>, Hye Kyoeng Min<sup>1</sup>, Jong Shin Yoo<sup>1</sup>, Seongmin Noh<sup>2</sup>, Chang Ook Park<sup>2</sup>, Kwang Hoon Lee<sup>2</sup>, Jing Young Kim<sup>1</sup>

<sup>1</sup>Korea Basic Science Institute, Ochang, Korea, <sup>2</sup>Brain Korea 21 Project for Medical Science, Yonsei University College of Medicine, Seoul, Korea

## Monday, 17<sup>th</sup> September

**PMo-120 Multidimensional LC-MALDI Workflow for High Sensitivity Detection of Low-Abundance Peptides from Complex Samples**

13:30 – 14:40  
 Shinichi Iwamoto<sup>1</sup>, Yusaku Hioki<sup>1</sup>, Ritsuko Tanimura<sup>1</sup>,  
 Yuki Ohta<sup>1</sup>, Takashi Shimada<sup>2</sup>, Koichi Tanaka<sup>1</sup>  
<sup>1</sup>Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>Life Science Research Center, Shimadzu Corporation, Tokyo, Japan

**PMo-121 LC-ESI/MS analysis of protein modifications derived from a mixture of 13-HPODE and [13C18]-13-HPODE**

11:10 – 12:20  
 Ryo Takahashi, Seon Hwa Lee, Takaaki Goto, Tomoyuki Oe  
 Tohoku University, Sendai, Japan

**PMo-122 Systematic investigation of peptide fragmentation processes in HCD on an Orbitrap instrument using a computer Expert System**

13:30 – 14:40  
 Annette Michalski, Neuhauser Nadin, Jurgen Cox,  
 Matthias Mann  
 Max-Planck-Institute of Biochemistry

**PMo-123 Intraocular Lens Adsorbome: a Proteomic Study of Adsorbed Proteins onto Acrylic Materials and Its Implication in Secondary Cataract**

11:10 – 12:20  
 Yi-Shiang Huang<sup>1,2</sup>, Virginie Bertrand<sup>1</sup>, Gabriel Mazzucchelli<sup>1</sup>,  
 Dimitriya Bozukova<sup>3</sup>, Christophe Pagnoulle<sup>3</sup>,  
 Marie-Christine Durrieu<sup>2</sup>, Edwin De Pauw<sup>1</sup>,  
 Marie-Claire De Pauw<sup>1</sup>  
<sup>1</sup>University of Liege, Liege, Belgium, <sup>2</sup>University of Bordeaux 1, Bordeaux, France, <sup>3</sup>Physiol, Liege, Belgium

**PMo-124 Analysis of SOD in cell line HepG2 by LC-nanospray-MS for screening natural antioxidants**

13:30 – 14:40  
 Shih-Ying Dai, Kuo-Lung Ku  
 National Chiayi University, Chiayi City, Taiwan

**PMo-125 Comparing and validating protein expression in multiple experimental conditions of antiviral immune response using clustering techniques on label-free LC-MS/MS data**

11:10 – 12:20  
 Aivett Bilbao<sup>1,2</sup>, Ying Zhang<sup>1</sup>, Dario Bottinelli<sup>3</sup>,  
 Bandar Alghanem<sup>1</sup>, Frederic Nikitin<sup>2</sup>, Markus Mueller<sup>2</sup>,  
 Frederique Lisacek<sup>2</sup>, Jeremy Luban<sup>3</sup>,  
 Caterina Strambio De Castillia<sup>3</sup>, Emmanuel Varesio<sup>1</sup>,  
 Gerard Hopfgartner<sup>1</sup>  
<sup>1</sup>Life Sciences Mass Spectrometry, School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, Geneva, Switzerland,  
<sup>2</sup>Proteome Informatics Group, Swiss Institute of Bioinformatics, Geneva, Switzerland, <sup>3</sup>Department of Microbiology and Molecular Medicine, University of Geneva, Geneva, Switzerland

**PMo-126 Identification of a modified amino acid residue in the heme protein using LC/MS/MS**

13:30 – 14:40  
 Jun Watanabe<sup>1</sup>, Yuki Ando<sup>2</sup>, Keiko Matsumoto<sup>1</sup>, Junko Iida<sup>1</sup>,  
 Shun Hirota<sup>2</sup>  
<sup>1</sup>Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>Nara Institute of Science and Technology, Nara, Japan

**PMo-127 Population proteogenomics: qualitative and quantitative analysis of SNP and protein markers for obesity from plasma proteome**

11:10 – 12:20  
 Nam Young Hong<sup>1</sup>, Jin Nyung Choi<sup>1</sup>, Sarah Yang<sup>2</sup>,  
 Joohon Sung<sup>2</sup>, Kwang Pyo Kim<sup>1</sup>

<sup>1</sup>Konkuk University, Seoul, Korea, <sup>2</sup>Seoul National University, Seoul, Korea

**PMo-128 Optimization of chemical derivatization of nitro-peptides for fluorous solid-phase extraction.**

13:30 – 14:40  
 Ji Hye Hong, Kyung-Cho Cho, Jeong Won Kang, Kwang Pyo Kim  
 Konkuk University, Seoul, Korea

**PMo-129 Quantification of biological drugs in plasma by liquid chromatography-tandem mass spectrometry.**

11:10 – 12:20  
 Nozomu Kato<sup>1</sup>, Takesada Shimura<sup>2</sup>, Atsuko Takeuchi<sup>4</sup>,  
 Hisahide Nishio<sup>3</sup>

<sup>1</sup>Kobe University, Japan / Mitsubishi Tanabe Pharma Co., Osaka, Japan,

<sup>2</sup>Mitsubishi Tanabe Pharma Co., Osaka, Japan, <sup>3</sup>Kobe University, Kobe, Japan, <sup>4</sup>Kobe Pharmaceutical University, Kobe, Japan

**PMo-130 Label-Free Semi-Quantitative Analysis of Histone Modification Dynamics using High-Resolution Mass Spectrometer**

13:30 – 14:40  
 Kazuki Yamamoto, Yoko Chikaoka, Takeshi Kawamura,  
 Takao Hamakubo, Tatsuhiko Kodama

Laboratory for System Biology and Medicine, Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo, Japan

**PMo-131 Simultaneous quantification of CYP1A2, 2D6, and 3A4 isoform proteins by liquid chromatography-tandem mass spectrometry using a single internal standard peptide.**

11:10 – 12:20  
 Nozomu Kato<sup>2</sup>, Tetsuya Narita<sup>1</sup>, Yasuhiro Yamada<sup>2</sup>,  
 Atsuko Takeuchi<sup>1</sup>, Hisahide Nishio<sup>2</sup>

<sup>1</sup>Kobe Pharmaceutical University, Kobe, Japan, <sup>2</sup>Kobe University, Kobe, Japan

**PMo-132 Testing of LC-MS/MS identification criteria for ricin protein**

13:30 – 14:40  
 Martin T Söderström, Paula Vanninen  
 VERIFIN, Department of Chemistry, University of Helsinki, Finland

**PMo-133 The Precision of Heavy-Light Peptide Ratios measured by MALDI-TOF Mass Spectrometry and its Application to LC-Free SISCAPA Protein Quantification**

11:10 – 12:20  
 Detlev Suckau<sup>1</sup>, Leigh Anderson<sup>2</sup>, Morteza Razavi<sup>2</sup>,  
 Terry Pearson<sup>2</sup>, Rainer Paape<sup>1</sup>

<sup>1</sup>Bruker Daltonik GmbH, <sup>2</sup>Andersson Forschung

**PMo-134 Production of Standards for Quantitative Proteomics and Phosphoproteomics with Focus on ICP-MS and ESI-MS**

13:30 – 14:40  
 Wolf D Lehmann  
 German Cancer Research Center (DKFZ)

## Monday, 17<sup>th</sup> September

Mon

**PMo-135 Exploring the dynamic range of label-free mass spectrometric quantification in complex samples**

11:10 – 12:20  
Stephanie Kaspar, Wolfgang Jabs, Markus Lubeck,  
Carsten Baessmann

Bruker Daltonik GmbH, Bremen, Germany

**PMo-136 Multiple Products Monitoring Using Q-Exactive Mass Spectrometer (Q-MpM)**

13:30 – 14:40  
Je-Hyun Baek, Eugene C Yi  
Molecular Medicine and Biopharmaceutical Sciences, Seoul National University, Seoul, Korea

**PMo-137 In-Source Decay for the high-throughput sequencing of animal toxins**

11:10 – 12:20  
Loic Quinton<sup>1</sup>, Michel Degueldre<sup>1</sup>, Nicolas Gilles<sup>2,3</sup>,  
Pierre Escoubas<sup>3</sup>, Edwin De Pauw<sup>1</sup>  
<sup>1</sup>Mass Spec Laboratory - University of Liège - BELGIUM, <sup>2</sup>CEA-IBITECS-SIMOPRO- Gif-sur-Yvette - FRANCE, <sup>3</sup>VenomeTech- Valbonne- FRANCE

**PMo-138 Screening and Quantitative Analysis of Specific Proteins in Clinical Samples by LC-ESI-MS/MS**

13:30 – 14:40  
Rieko Goto<sup>1</sup>, Yasushi Nakamura<sup>2</sup>, Shohei Shioyama<sup>1</sup>,  
Yukiko Nishida<sup>1</sup>, Tomonori Takami<sup>1</sup>, Tokio Sanke<sup>2</sup>  
<sup>1</sup>JCL Bioassay Corporation, Hyogo, Japan, <sup>2</sup>Wakayama Medical University, Wakayama, Japan

**PMo-139 Analysis of modified amyloid beta peptide by Mass Spectrometry**

11:10 – 12:20  
Akutsu Hiroaki, Tsumura Naomi, Funakoshi Hiroshi,  
Nakamura Masao  
Asahikawa Medical University, Asahikawa Japan

**PMo-140 The trial of lower background in using a nanoelectrospray (nano ES) interface**

13:30 – 14:40  
Toshie Takahashi<sup>1</sup>, Takashi Usui<sup>2</sup>  
<sup>1</sup>University of Tokyo, Tokyo, Japan, <sup>2</sup>Nikkyo Technos, Co., Ltd. Tokyo, Japan

**PMo-141 Fully automated chip-based nanoelectrospray combined with electron transfer dissociation for high throughput top-down proteomics**

CORINA FLANGEA<sup>1,2</sup>, CRISTINA MOSOARCA<sup>1,3</sup>, MARILENA MANEA<sup>4</sup>, CATALIN SCHIOPU<sup>1,5</sup>, EUGEN SISU<sup>5,6</sup>, ALINA D ZAMFIR<sup>1,2</sup>  
<sup>1</sup>Aurel Vlaicu University, Arad, Romania, <sup>2</sup>National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania, <sup>3</sup>West University Timisoara, Romania, <sup>4</sup>Zukunftskolleg, University of Konstanz, Germany, <sup>5</sup>Victor Babes University of Medicine and Pharmacy, Timisoara, Romania, <sup>6</sup>Chemistry Institute of Romanian Academy, Timisoara, Romania

**PMo-142 Analysis of nitroproteome in *S. cerevisiae* using chemical approach**

13:30 – 14:40  
Jeong Won Kang<sup>1</sup>, Na Young Lee<sup>2</sup>, Kyung-Cho Cho<sup>1</sup>, Sang-Hyun Park<sup>2</sup>, Kwang Pyo Kim<sup>1</sup>  
<sup>1</sup>Konkuk University, Seoul, Korea, <sup>2</sup>Seoul National University, Seoul, Korea

**PMo-143 Mass spectrometric and bioaffinity MS investigations of proteins involved in metabolic and age related diseases**

11:10 – 12:20  
Marius I Iurascu<sup>1</sup>, Claudia Cozma<sup>1</sup>, Michael Gross<sup>2</sup>, David Clemmer<sup>3</sup>, Michael Przybylski<sup>1</sup>

<sup>1</sup>University of Konstanz, Konstanz, Germany, <sup>2</sup>Washington University in St. Louis, MO, USA, <sup>3</sup>Indiana University, Bloomington, IN, USA

**PMo-144 Higher resolution improves top-down protein ID results on an Orbitrap mass analyzer for large (>40 kDa) proteins**

13:30 – 14:40  
Daisuke Higo<sup>1</sup>, David Horn<sup>2</sup>, Rosa Viner<sup>2</sup>, Seema Sharma<sup>2</sup>, Eduard Denisov<sup>3</sup>, Alexander Makarov<sup>3</sup>

<sup>1</sup>Thermo fisher scientific, Yokohama, Japan, <sup>2</sup>Thermo Fisher Scientific, San Jose, CA, <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, GERMANY

**PMo-145 HR/AM Targeted Peptide Quantification on Q Exactive: A Unique Combination of High Selectivity, High Sensitivity and High Throughput**

11:10 – 12:20  
Yi Zhang<sup>2,3</sup>, Makoto Takahata<sup>1</sup>, Zhiqi Hao<sup>2,3</sup>, Markus Kellmann<sup>2,3</sup>, Andreas Huhmer<sup>2,3</sup>

<sup>1</sup>Thermo Fisher Scientific K.K., Japan, <sup>2</sup>Thermo Scientific, San Jose, CA,

<sup>3</sup>Thermo Scientific, Bremen, Germany

## Session 7

### New Ionization Methods and Related Topics for the Next Generation

**PMo-146 Development of an Ion Source for the Analysis of Cuticular Hydrocarbons from Living Insects and Steps toward Comprehensive Hydrocarbon Analysis**

13:30 – 14:40  
Alexander Pirkl<sup>1</sup>, Ann-Christin Buelter<sup>1</sup>, Joanne Y Yew<sup>2,3</sup>, Klaus Dreisewerd<sup>1</sup>

<sup>1</sup>University of Muenster, Muenster, Germany, <sup>2</sup>Temasek Life Sciences Laboratory, Singapore, Singapore, <sup>3</sup>Department of Biological Sciences, National University of Singapore, Singapore

**PMo-147 Oligonucleotide analysis by nanoparticle-assisted laser desorption/ionization mass spectrometry**

11:10 – 12:20  
Shu TAIRA<sup>1</sup>, Daisaku KANEKO<sup>1</sup>, Yasuko KONISHI-KAWAMURA<sup>-2</sup>, Yuko ICHIYANAGI<sup>3</sup>

<sup>1</sup>JAPAN Advanced Institute of Science and Technology, <sup>2</sup>Ishikawa Prefectural University, <sup>3</sup>Yokohama National University

**PMo-148 Temperature Dependence of Proton Transfer and Conformation Change for Ubiquitin Ions**

13:30 – 14:40  
Minami Kawashima, Ayako Sudo, Takashige Mori, Yuto Ohshima, Keishi Machida, Kanako Yokoyama, Kazuki Yamashita, Shinji Nonose  
Yokohama City University, Yokohama, Japan

**PMo-149 Development of a Dual Pressure Operating Hollow Cathode Glow Discharge Ion Source for Detection of Explosives and Explosive-related Compounds**

11:10 – 12:20  
Md Ahsan Habib, Lee Chuin Chen, Satoshi Ninomiya, Kenzo Hiraoka  
University of Yamanashi, Kofu, Japan

## Monday, 17<sup>th</sup> September

### **PMo-150 A Novel Source Design for the Analysis of both Polar and Non-Polar Species**

13:30 – 14:40  
Steve M Smith<sup>1</sup>, Hilary Major<sup>1</sup>, Steve Bajic<sup>1</sup>, Anthony Bristow<sup>2</sup>, Andrew Ray<sup>2</sup>

<sup>1</sup>Waters Corporation, Manchester, UK, <sup>2</sup>AstraZeneca, Macclesfield, UK

### **PMo-151 Sheath-flow PESI for Dry Samples**

11:10 – 12:20

Md Obaidur Rahman, Yasuo Shida, Mridul Kanti Mandal, Satoshi Ninomiya, Lee Chuin Chen, Kenzo Hiraoka  
University of Yamanashi, Kofu, Japan

### **PMo-152 An Electron Impact Ion Source for a Miniature Mass spectrometer**

13:30 – 14:40  
yide zhao, meiru guo, liang wang, yuhua xiao, taiguo li  
Science and Technology on Vacuum & cryogenics Technology and Physics Laboratory, Lanzhou Institute of Physics, Lanzhou, China

### **PMo-153 Development of High Pressure Ion Sources with Operating Pressure Higher Than Atmospheric Pressure**

11:10 – 12:20  
Lee Chuin Chen, Matiur M Rahman, Mridul Kanti Mandal, Kenzo Hiraoka  
University of Yamanashi, Kofu, Japan

### **PMo-154 Conformation Change for Insulin and Insulin Chain B Ions; Temperature Dependence of Proton Transfer**

13:30 – 14:40  
Ayako Sudo, Keishi Machida, Kanako Yokoyama, Minami Kawashima, Takashige Mori, Yuto Ohshima, Kazuki Yamashita, Shinji Nonose  
Yokohama City University

### **PMo-155 Development of high sensitive low vacuum dielectric barrier discharge ionization method**

11:10 – 12:20  
Kazushige Nishimura<sup>1</sup>, Shun Kumano<sup>1</sup>, Masuyuki Sugiyama<sup>1</sup>, Masuyoshi Yamada<sup>1</sup>, Hidetoshi Morokuma<sup>2</sup>, Yuichiro Hashimoto<sup>1</sup>  
<sup>1</sup>Hitachi Ltd., Tokyo, Japan, <sup>2</sup>Hitachi High-Technologies Corp., Ibaraki-ken, Japan

### **PMo-156 High ion yields of carbohydrates from frozen solution by UV-MALDI**

13:30 – 14:40  
Chi-Wei Liang, Po-Jul Chang, Yu-Jiun Lin, Yuan T Lee, Chi-Kung Ni  
Academia Sinica, Taipei, Taiwan

### **PMo-157 ATMOSPHERIC PRESSURE PHOTOIONIZATION-MASS SPECTROMETRY OF ESTROGENIC COMPOUNDS**

11:10 – 12:20  
Oscar Nunez<sup>1</sup>, Paolo Lucci<sup>2</sup>, Encarnacion Moyano<sup>1</sup>, Maria Teresa Galceran<sup>1</sup>  
<sup>1</sup>University of Barcelona, Barcelona, Spain, <sup>2</sup>Pontificia Universidad Javeriana, Bogota, Colombia

### **PMo-158 Application of Electrospray Droplet Impact / SIMS to synthetic polymers**

13:30 – 14:40  
Rio Takaishi, Yuji Sakai, Satoshi Ninomiya, Kenzo Hiraoka  
Clean Energy Research Center, University of Yamanashi, Yamanashi, Japan

### **PMo-159 Development of high pressure (>1 atm) probe electrospray ionization mass spectrometry**

11:10 – 12:20  
Md Matiur Rahman, Lee Chuin Chen, Kenzo Hiraoka  
University of Yamanashi, Kofu, Japan

### **PMo-160 Development of an Atmospheric Pressure Laser Ionization Technique using a Novel 6 um-band Mid-Infrared Tunable Laser and Liquid Water Matrix**

Ryuji Hiraguchi, Hisanao Hazama, Kunio Awazu  
Osaka University, Osaka, Japan

### **PMo-161 Influence of source parameters on the detection and the fragmentation of aroma compounds using PTR-SRI-ToF MS**

Xaviera Pennanec<sup>1,2,3</sup>, Etienne Semon<sup>1,2,3</sup>, Jean-Luc Le Quere<sup>1,2,3</sup>  
<sup>1</sup>INRA, UMR1324 Centre des Sciences du Gout et de l'Alimentation, Dijon, France, <sup>2</sup>CNRS, UMR6265 Centre des Sciences du Gout et de l'Alimentation, Dijon, France, <sup>3</sup>Universite de Bourgogne, UMR Centre des Sciences du Gout et de l'Alimentation, Dijon, France

### **PMo-162 Expansion of an ionization technique in nonpolar solvents with cation tetrakis(3,5-bis(trifluoromethyl)-phenyl) borate**

13:30 – 14:40  
Atsushi Takamizawa<sup>1,2</sup>, Naoto Niizuma<sup>2</sup>, Takashi Korenaga<sup>2</sup>  
<sup>1</sup>Japan Science and Technology Agency (JST), Saitama, Japan, <sup>2</sup>Tokyo Metropolitan University, Tokyo, Japan

### **PMo-163 Gas chromatographic separation and accurate mass determination by low temperature plasma ionization API-QTOF-MS**

11:10 – 12:20  
Asger W Noergaard, Vivi Kofoed-Sørensen, Peder Wolkeff, Per A Clausen  
National Research Centre for the Working Environment, Denmark

### **PMo-164 Fast, High Throughput LC-MS/MS Method for Immunosuppressants Analysis Using Dual Probe Electrospray**

13:30 – 14:40  
Lisa Cousins, Heather Gamble, Hui Qiao, Frenny Ruparelia, George Scott, Sha Joshua Ye  
IONICS Mass Spectrometry, Toronto, Canada

### **PMo-165 Evaluation of Pt-deposited Porous Alumina Target Plate with MALDI Spiral-TOFMS**

11:10 – 12:20  
Takafumi Sato<sup>1</sup>, Kanae Teramoto<sup>1</sup>, Yoshihisa Ueda<sup>1</sup>, Tomohiko Tamura<sup>2</sup>, Moriyuki Hamada<sup>2</sup>, Ken-Ichiro Suzuki<sup>2</sup>, Yoshinao Wada<sup>3</sup>, Takashi Yanagishita<sup>4</sup>, Hideki Masuda<sup>4,5</sup>  
<sup>1</sup>JEOL Ltd., Tokyo, Japan, <sup>2</sup>NITE Biological Resource Center, Kisarazu, Japan, <sup>3</sup>Osaka Medical Center and Research Institute for Maternal and Child Health, Osaka, Japan, <sup>4</sup>Tokyo Metropolitan University, Tokyo, Japan, <sup>5</sup>Kanagawa Academy of Science and Technology, Sagamihara, Japan

### **PMo-166 New Version of Desorption Corona Beam Ionization Source and Applications**

13:30 – 14:40  
Yupeng Cheng, Junsheng Zhang, Joseph Ting, Wenjian Sun  
Shimadzu Research Laboratory (Shanghai) Co., Ltd, Shanghai, China

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## Monday, 17<sup>th</sup> September

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**PMo-167 Development of TLC/MS by LI-API and WAr-APPI (Photoionization in Argon Gas Contained Water) Method**

11:10 – 12:20  
yoshiyuki mochida, gennki kobayashi, futoshi matumoto  
Kanagawa University, Yokohama, Japan

**PMo-168 Charged-droplet beam source using vacuum electrospray of an ionic liquid for secondary ion mass spectrometry (SIMS)**

13:30 – 14:40  
Yukio Fujiwara, Naoaki Saito, Hidehiko Nonaka,  
Shingo Ichimura  
AIST, Tsukuba, Japan

**PMo-169 High Throughput Molecular Weight Confirmation of Pharmaceutical Compounds Using DART MS Analysis with Ultra-fast Polarity Switching**

Teruhisa Shiota<sup>1</sup>, Hirotaka Honda<sup>1</sup>, Jun Watanabe<sup>2</sup>, Kazuo Mukaibatake<sup>2</sup>, Junko Iida<sup>2</sup>, Tsubasa Ibushi<sup>3</sup>, Manabu Ueda<sup>2</sup>  
<sup>1</sup>AMR, Inc., Tokyo, Japan, <sup>2</sup>Shimadzu Corporation, Kyoto, Japan, <sup>3</sup>Shimadzu Techno Research, Kyoto, Japan

**PMo-170 Componential Analysis of Pepper of Various Origins Using DART-MS Using Ultra-fast Polarity Switching**

13:30 – 14:40  
FUMIHIKO USUI<sup>1</sup>, Teruhisa Shiota<sup>1</sup>, Manabu Ueda<sup>2</sup>, Kazuo Mukaibatake<sup>2</sup>, Junko Iida<sup>2</sup>, Tsubasa Ibushi<sup>3</sup>, Yasuhiko Bando<sup>1</sup>, Jun Watanabe<sup>2</sup>  
<sup>1</sup>AMR INCORPORATED Tokyo, Japan, <sup>2</sup>Shimadzu Corporation, Kyoto, Japan, <sup>3</sup>Shimadzu Techno Research, Kyoto, Japan

**PMo-171 Gas Chromatography/Ambient Ionization Mass Spectrometry (GC/AMS) for the Analysis of Long Chain n-Alkanes in Crude Oil**

11:10 – 12:20  
Jentiae Shiea<sup>1</sup>, Min-Zong Huang<sup>1</sup>, Yi-Tzu Cho<sup>2</sup>  
<sup>1</sup>RIKEN ASI, Wako, Japan, <sup>2</sup>Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan

**PMo-172 A Combined DSMC - CFD Approach for the Numerical Simulation of an Under-expanded Jet**

13:30 – 14:40  
Athanasios Zacharos<sup>2</sup>, Ioannis Nikолос<sup>3</sup>, Dimitris Papanastasiou<sup>2</sup>, Roger Giles<sup>1</sup>, Andrew Entwistle<sup>1</sup>, Emmanuel Raptakis<sup>2</sup>  
<sup>1</sup>Shimadzu Research Laboratory (EUROPE) LTD, <sup>2</sup>Fasmatech, Athens, GR, <sup>3</sup>Department of Production Engineering & Management, TUC, Chania, Crete, GR

**PMo-173 Proposal of the New Method for 3DAP Analysis of Biological Molecules Utilizing Photocatalyst and Mesoporous Materials**

11:10 – 12:20  
Masato Morita, Mahito Shimizu, Yuya Hanaoka, Masanori Owari  
The University of Tokyo, Tokyo, Japan

**PMo-174 High Sensitivity Spray Ionization Approaches at AP and Vacuum with Matrices or Solution With or Without Voltage or a Laser**

13:30 – 14:40  
Charles N McEwen<sup>1</sup>, Sarah Trimpin<sup>2</sup>

<sup>1</sup>University of the Sciences, <sup>2</sup>Wayne State University

**PMo-175 Fundamental Aspects of Solvent free Atmospheric Pressure Chemical Ionization and Laser Diode Thermal Desorption Ionization Source (LDTD)**

11:10 – 12:20  
Pierre Picard<sup>1</sup>, Real E Paquin<sup>2</sup>

<sup>1</sup>Phytronix Technologies Inc, Quebec, QC, Canada, <sup>2</sup>Universite Laval, Quebec, QC, Canada

**PMo-176 Photo-ionisation mass spectrometry for on-line monitoring: Technology and real-time monitoring applications such as characterisation of the coffee-roasting and cigarette-smoking process**

13:30 – 14:40  
Ralf Zimmermann<sup>1</sup>, Romy Hertz<sup>1</sup>, Matthias Bente<sup>2</sup>, Mohammad Saraji<sup>2</sup>, Thorsten Streibel<sup>1</sup>

<sup>1</sup>Joint Mass Spectrometry Centre of University Rostock and Helmholtz Zentrum München, Oberschleissheim/Rostock, Germany, <sup>2</sup>Photonion GmbH, Schwerin Germany

## Session 8

### Collision Dynamics and Spectroscopy Using Ion Storage Rings and Traps

**PMo-177 Design of Electrodynamic Ion Funnel-Stacked Ring Trap**

11:10 – 12:20  
Liulin Deng, T-W Dominic Chan  
The Chinese University of Hongkong, Hongkong

**PMo-178 Delayed electron emission and radiative cooling of stored molecular ions in TMU electrostatic ion storage ring**

13:30 – 14:40  
Toshiyuki Azuma<sup>1,2</sup>, Motoshi Goto<sup>1,3</sup>, Jun Matsumoto<sup>3</sup>, Haruo Shiromaru<sup>3</sup>, Takeshi Furukawa<sup>2</sup>, Takuya Majima<sup>2</sup>, Hajime Tanuma<sup>2</sup>, Tsuneto Kanai<sup>1</sup>, Erika Sundén<sup>4</sup>, Klavs Hansen<sup>4</sup>

<sup>1</sup>RIKEN, Wako, Japan, <sup>2</sup>Department of Physics, Tokyo Metropolitan University, Tokyo, Japan, <sup>3</sup>Department of Chemistry, Tokyo Metropolitan University, Tokyo, Japan, <sup>4</sup>Department of Physics, University of Gothenburg, Gothenburg, Sweden

**PMo-179 Development of a cryogenic ion storage ring in RIKEN**

11:10 – 12:20  
yoshinori enomoto, yuji nakano, takuya masunaga, toshiyuki azuma  
RIKEN, Wako, Japan

## Monday, 17<sup>th</sup> September

### Session 9

#### Imaging II

- PMo-180** Development of MALDI-MS-based imaging technique for visualizing the green tea polyphenol EGCG in mammalian tissues  
 13:30 – 14:40

Yoshinori Fujimura, Yoon Hee Kim, Takatoki Hagihara, Daichi Yukihira, Ayumi Yamaguchi, Miho Irie, Daisuke Miura, Hiroyuki Wariishi, Mitsu Shindo, Hirofumi Tachibana  
 Kyushu University, Fukuoka, Japan

- PMo-181** Development of micro-focusing electrospray droplet impact gun for SIMS analysis  
 11:10 – 12:20

YUJI SAKAI, RIO TAKAISHI, SATOSHI NINOMIYA, KENZO HIRAKAWA  
 University of Yamanashi, Kofu, Japan

- PMo-182** Dyeing Regions of Oxidative Hair Dyes in Human Hair Investigated by Nanoscale Secondary Ion Mass Spectrometry  
 13:30 – 14:40

Toru Kojima<sup>1</sup>, Hiromi Yamada<sup>1</sup>, Toshihiko Yamamoto<sup>1</sup>, Miyuki Takeuchi<sup>2</sup>, Yasuyuki Matsushita<sup>3</sup>, Kazuhiko Fukushima<sup>3</sup>  
<sup>1</sup>Hoyu Co., Ltd., Nagakute, Japan, <sup>2</sup>The University of Tokyo, Tokyo, Japan, <sup>3</sup>Nagoya University, Nagoya, Japan

- PMo-183** Bio-imaging with Swift Heavy Ion Beams  
 11:10 – 12:20

Toshio Seki<sup>1,2</sup>, Sho Shitomoto<sup>1</sup>, Shunichiro Nakagawa<sup>1</sup>, Takaaki Aoki<sup>2,3</sup>, Jiro Matsuo<sup>1,2</sup>  
<sup>1</sup>Kyoto University, Uji, Japan, <sup>2</sup>CREST, Tokyo, Japan, <sup>3</sup>Kyoto University, Kyoto, Japan

- PMo-184** Secondary Ion Emission with Methanol Gas Cluster Ion Beam Irradiation  
 13:30 – 14:40

Shunichiro Nakagawa<sup>1</sup>, Tosio Seki<sup>1,4</sup>, Takaaki Aoki<sup>3,4</sup>, Jiro Matsuo<sup>2,4</sup>

<sup>1</sup>Nuclear Engineering, Kyoto University, Uji, Japan, <sup>2</sup>Quantum Science and Engineering Center, Kyoto University, Uji, Japan, <sup>3</sup>Department of Electronic Science and Engineering, Kyoto University, Kyoto, Japan, <sup>4</sup>CREST, Japan Science and Technology Agency (JST), Tokyo, Japan

- PMo-185** Development of Electrostatic Quadrupole Lens for MeV-SIMS Imaging  
 11:10 – 12:20

Sho Shitomoto<sup>1</sup>, Toshio Seki<sup>1,2</sup>, Takaaki Aoki<sup>1,2</sup>, Jiro Matsuo<sup>1,2</sup>  
<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>CREST, Tokyo, Japan

- PMo-186** Evaluation of the Damage on a Polymer Sample Caused by Shave-off Section Processing  
 13:30 – 14:40

Teruhiko Tobe, Yoshihiro Morita, Atsuko Yamazaki, Makiko Fujii, Masanori Owari  
 The University of Tokyo, Tokyo, Japan

- PMo-187** Study on Depth Resolution Factor of Shave-off Depth Profiling  
 11:10 – 12:20

Makiko FUJII, Yuya HANAOKA, Tatsuya TAKETSUGU, Masanori OWARI  
 The University of Tokyo, Tokyo, Japan

- PMo-188** Tracing photosynthetic product accumulation in xylem cell wall using carbon isotope labeling  
 13:30 – 14:40

Miyuki Takeuchi, Akira Isogai  
 The university of Tokyo, Tokyo, Japan

- PMo-189** Acceleration of gluconeogenesis of the host liver bearing human colon cancer metastases revealed by microscopic imaging mass spectrometry  
 11:10 – 12:20

Akiko Kubo<sup>1</sup>, Mitsuyo Ohmura<sup>1</sup>, Tsuyoshi Nakanishi<sup>3</sup>, Shigeki Kajihara<sup>3</sup>, Kiyoshi Ogawa<sup>3</sup>, Makoto Suematsu<sup>1,2</sup>

<sup>1</sup>Keio University, Tokyo, Japan, <sup>2</sup>JST, ERATO Suematsu Gas Biology Project, Tokyo, Japan, <sup>3</sup>Shimadzu Corporation, Kyoto, Japan

- PMo-190** Early Detection of Gastric Cancer using ToF-SIMS Metabolomic Imaging  
 13:30 – 14:40

Yong-Chien Ling<sup>1</sup>, Shiou-Ling Lei<sup>1</sup>, Chun-Chao Chang<sup>2</sup>, Chia-Lang Fang<sup>3</sup>, Fu-Der Mai<sup>4</sup>

<sup>1</sup>Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan,

<sup>2</sup>Department of Internal Medicine, Taipei Medical University, Taipei, Taiwan,

<sup>3</sup>Department of Pathology, Taipei Medical University, Taipei, Taiwan,

<sup>4</sup>Biomedical Mass Imaging research Center, Taipei Medical University, Taiwan

### Session 10

#### Ion Mobility Spectroscopy Based on Instrument & Theoretical Development

- PMo-191** Separation and identification of Structural isomers of Methylpyrazole by Differential Mobility Spectrometry  
 11:10 – 12:20

Kazuhide Inoue<sup>1</sup>, Yasutohi Kawase<sup>1</sup>, Masazumi Yasumoto<sup>1</sup>, Seiji Horie<sup>1</sup>, Shigeru Yamada<sup>2</sup>, Ryoma Yamamoto<sup>2</sup>

<sup>1</sup>TAKARA BIO INC. Shiga, Japan, <sup>2</sup>K.K. AB SCIEX. Tokyo, Japan

- PMo-192** Investigation of an IMS-TOF MS with a laser based ionisation under atmospheric conditions  
 13:30 – 14:40

Marvin Ihlenborg, Tassilo Muskat, Juergen Grottemeyer  
 CAU Kiel, Kiel, Germany

- PMo-193** Separation of Isobaric Phosphopeptides using Differential Ion Mobility Spectrometry with Tandem Mass Spectrometry.  
 11:10 – 12:20

Chie Inagaki, Masato Aoshima, Takeshi Shibata, Shigeru Yamada, Sumie Ando  
 KK ABSIEX, Tokyo, Japan

- PMo-194** Integrative structure determination of protein assemblies using mass spectrometry, ion mobility and cross-linking.  
 13:30 – 14:40

Argyris Politis<sup>1</sup>, Zoe Hall<sup>1</sup>, Florian Stengel<sup>2</sup>, Ruedi Abersold<sup>2</sup>, Carol V Robinson<sup>1</sup>

<sup>1</sup>University of Oxford, <sup>2</sup>ETH Zurich

Monday, 17<sup>th</sup> September

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**PMo-195 Advances in Chip-based FAIMS/Triple Quadrupole MS: Instrumental Studies and Analytical Capabilities**11:10 – 12:20 Richard A Yost<sup>1</sup>, Christopher R Beekman<sup>1</sup>, Chia-Wei Tsai<sup>1</sup>, Michael Ugarov<sup>2</sup>, George Stafford<sup>2</sup><sup>1</sup>UNIVERSITY OF FLORIDA, Gainesville, Florida USA, <sup>2</sup>Agilent Technologies, Santa Clara, California USA**PMo-196 Selected Mobility Accumulation (SMA) in a Trapped Ion Mobility Mass Spectrometer (TIMS-MS)**

13:30 – 14:40 Ulrich Giessmann, Melvin A Park, Desmond Kaplan, Mark Ridgeway

Bruker Daltonics, Billerica, MA, USA

**PMo-197 Evaluation of the performance of microscale FAIMS for enhancement of quantitative analysis of metabolites and peptides**11:10 – 12:20 Robert W Smith<sup>2</sup>, Lauren Brown<sup>1</sup>, Danielle E Toutoungi<sup>1</sup>, James Reynolds<sup>2</sup>, Ashley Sage<sup>3</sup>, Anthony W Bristow<sup>4</sup>, Andrew Ray<sup>4</sup>, Daniel Weston<sup>5</sup>, Ian Wilson<sup>5</sup>, Billy Boyle<sup>1</sup>, Colin Creaser<sup>2</sup><sup>1</sup>Owlstone Ltd, <sup>2</sup>Loughborough University, Loughborough, United Kingdom,<sup>3</sup>Agilent Technologies, Stockport, United Kingdom, <sup>4</sup>AstraZeneca, Pharmaceutical Development, Macclesfield, United Kingdom, <sup>5</sup>AstraZeneca, DMPK Innovative Medicines, Alderley Park, United Kingdom**PMo-198 Development of Ion Trap Mobility Measurement System**

13:30 – 14:40 Toshiki Sugai, Yoshihiko Sawanishi, Masashi Shinozaki, Sho Osaka

Toho University, Funabashi, Japan

**PMo-199 Achieving High Resolution in a Benchtop Resistive Glass Drift Tube Ion Mobility Spectrometer**11:10 – 12:20 WILLIAM C NETOLICKY<sup>1</sup>, PAULA HOLMES<sup>1</sup>, FACUNDO FERNANDEZ<sup>2</sup>, JOE TICE<sup>3</sup>, BRIAN MUSSELMAN<sup>3</sup><sup>1</sup>Photonis USA, Sturbridge, USA, <sup>2</sup>Georgia Institute of Technology, Atlanta GA, USA, <sup>3</sup>IonSense Inc., Saugus MA, USA**Others****PMo-200 Direct detection of S-nitrosylated peptides with UV-MALDI MS using porphyrin and retinoic acid as a matrix additive**13:30 – 14:40 Makoto Watanabe<sup>1</sup>, Rie Yamamoto<sup>1</sup>, Shinichi Iwamoto<sup>1</sup>, Yuko Fukuyama<sup>1</sup>, Ritsuko Tanimura<sup>1</sup>, Shin-Ichirou Kawabata<sup>1</sup>, Taka-Aki Sato<sup>1</sup>, Shunsuke Izumi<sup>2</sup>, Koichi Tanaka<sup>1</sup><sup>1</sup>Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>Hiroshima University, Higashi-Hiroshima, Japan**PMo-201 Bactericidal effects of atmospheric ions formed in ambient corona discharges**

11:10 – 12:20 Rena Gonda, Yuya Yamakawa, Kanako Sekimoto, Mitsuo Takayama

Yokohama City University, Yokohama, Japan

**PMo-202 Thermal Activation of Methane: Why [Ti,O,H]<sup>+</sup> and [V,O,H]<sup>+</sup> are More Than the Sum of Their Atoms.**

13:30 – 14:40 Robert Kretschmer, Maria Schlangen, Helmut Schwarz

Technical University Berlin

**PMo-203 Measurements of Proton and Alkali Ion Affinities using CID Spectra of High Performance Tandem Mass Spectrometer**11:10 – 12:20 KIMIO ISA<sup>1</sup>, SHIGEKI MATSUMURA<sup>2</sup>, RYUJI NAKADA<sup>3</sup><sup>1</sup>Jin-Ai University, Echizen City, Japan, <sup>2</sup>Headquarters of Fukui Prefecture Police, Fukui City, Japan, <sup>3</sup>Fukui University, Fukui City, Japan

Tuesday, 18<sup>th</sup> September

Morning

**Plenary Lecture**

08:00 – 08:45

Main Hall

**Plenary Lecture 3: Albert J R Heck**Chair: Alma L Burlingame  
UCSF, USA**PL3-0800 A personal perspective on the role of mass spectrometry for protein analysis in proteomics and structural biology**Albert J R Heck<sup>1,2</sup><sup>1</sup>Utrecht University, Utrecht, The Netherlands, <sup>2</sup>Netherlands Proteomics Centre**PL3-0800 A personal perspective on the role of mass spectrometry for protein analysis in proteomics and structural biology**Albert J R Heck<sup>1,2</sup><sup>1</sup>Utrecht University, Utrecht, The Netherlands, <sup>2</sup>Netherlands Proteomics Centre**Oral Session**

09:00 – 11:00

Main Hall

**Session 11: Glycomics: From Disease Markers to Therapeutic Antibody Products**Chair: Hyun joo An  
ChungNam National University, Korea**S11-0900 [Keynote Lecture] Is high throughput glycomics possible?**

Carlito B Lebrilla

University of California, Davis

**S11-0940 Site specific characterization of O-GlcNAcylation on cytosolic and nuclear proteins using electron transfer dissociation mass spectrometry.**Alma L Burlingame<sup>1</sup>, Samuel Myers<sup>1</sup>, Jonathan C Trinidad<sup>1</sup>, Giselle Knudsen<sup>1</sup>, Barbara Panning<sup>1</sup>, Agnes Thalhammer<sup>2</sup>, Ralf Schoepfer<sup>2</sup>  
<sup>1</sup>UCSF, <sup>2</sup>University College, London**S11-1000 Carbonyl trapping activity of pyridoxal 5'-phosphate in vitro and in vivo**Roumyana Mironova<sup>1</sup>, Ivaylo Ivanov<sup>2</sup>, Valentin Lozanov<sup>3</sup>, Silvia Russeva<sup>3</sup>, Svetlana Simova<sup>4</sup>, Ivan Ivanov<sup>1</sup>, Toshimitsu Niwa<sup>5</sup><sup>1</sup>Institute of Molecular Biology Roumen Tsanev, Sofia, Bulgaria, <sup>2</sup>University of Sofia St. Kliment Ohridski, Sofia, Bulgaria, <sup>3</sup>Medical University, Sofia, Bulgaria, <sup>4</sup>Institute of Organic Chemistry with Centre of Phytochemistry, Sofia, Bulgaria, <sup>5</sup>Nagoya University Graduate School of Medicine, Nagoya, Japan**S11-1020 Bioinformatics Platform for the Glycan Marker Discovery by Mass Spectrometry**Jaehan Kim<sup>1</sup>, Hyunjoo An<sup>1</sup>, Carlito Lebrilla<sup>2</sup><sup>1</sup>Chungnam National University, Daejeon, Korea, <sup>2</sup>University of California, Davis, USA**S11-1040 Characterization of Elastin Degraded Peptides in Chronic Obstructive Pulmonary Disease (COPD)**Yong Y Lin<sup>1</sup>, Toyonobu Usuki<sup>2</sup><sup>1</sup>St.Luke-Roosevelt Hospital Center, Columbia University College of Physicians and Surgeons, <sup>2</sup>Faculty of Materials and Sciences, Sophia University

Tuesday, 18<sup>th</sup> September

Morning

## Oral Session

09:00 – 11:00

Room A

### Session 12: On-site Mass Spectrometry -Miniaturized Instruments and Allied Technologies-

Chair: Shuichi Shimma

National Cancer Center Research Institute, Japan

- S12-0900** [Keynote Lecture] In-vivo, Real-time Identification of Tissues in Human Surgical Environment by Rapid Evaporative Ionization Mass Spectrometry

Zoltan Takats<sup>1</sup>, Julia Balog<sup>2</sup>, James Kinross<sup>1</sup>, Christian Schafer<sup>1</sup>, Laura Muirhead<sup>1</sup>, Ottmar Golf<sup>4</sup>, Laszlo Sasi-Szabo<sup>3</sup>, Balazs Dezso<sup>3</sup>, Kirill Veselkov<sup>1</sup>

<sup>1</sup>Imperial College, London, UK, <sup>2</sup>Medimass Ltd., Budapest, Hungary, <sup>3</sup>University of Debrecen, Debrecen, Hungary, <sup>4</sup>Justus Liebig University, Giessen, Germany

- S12-0940** Miniaturization of a Toroidal Ion Trap Mass Analyzer Composed of Cylindrical Electrodes

09:40 – 10:00 Daniel E Austin, Nicholas Taylor, Jessica Higgs

Brigham Young University, Provo, Utah, USA

- S12-1000** Auto-sampling Explosives Trace Detection System using Mass Spectrometry

10:00 – 10:20 Yuichiro Hashimoto, Hisashi Nagano, Yasuaki Takada, Yasutaka Suzuki, Hideo Kashima, Masakazu Sugaya, Yasunori Doi, Koichi Terada, Minoru Sakairi Hitachi, Ltd. Central Research Laboratory

- S12-1020** Rapid Screening Chemicals in the Liquids and Solids via Mobile Ambient Mass Spectrometry (MAMS)

10:20 – 10:40 Min-Zong Huang, Chu-Nian Cheng, Hung Su, Jentae Shiea National Sun Yat-Sen University, Kaohsiung, Taiwan

- S12-1040** Development of portable vacuum ultraviolet single photon ionization mass spectrometer for trace measurement of volatile organic compounds

10:40 – 11:00 Yukio Yamamoto<sup>1</sup>, Hiroyuki Yamada<sup>2</sup>, Kenichi Tonokura<sup>1</sup>  
<sup>1</sup>The University of Tokyo, Chiba, Japan, <sup>2</sup>National Traffic Safety and Environmental Laboratory, Tokyo, Japan

## Oral Session

09:00 – 11:00

Room B-1

### Session 13: Accelerator Mass Spectrometry

Chair: Hiroyuki Matsuzaki  
The University of Tokyo, Japan

- S13-0900** Accelerator Mass Spectrometry - analysis of the rarest atom species for earth and environmental science

Peter Steier

University of Vienna, Faculty of Physics

- S13-0940** Small scale radiocarbon dating and its applications to understand Antarctic ice sheet

Yusuke Yokoyama<sup>1</sup>, Yosuke Miyairi<sup>1</sup>, Suga Hisami<sup>2</sup>, Matsuzaki Hiroyuki<sup>3</sup>, Ohkouchi Naohiko<sup>2</sup>

<sup>1</sup>University of Tokyo, Chiba, Japan, <sup>2</sup>JAMSTEC, Yokosuka, Japan, <sup>3</sup>University of Tokyo, Tokyo, Japan

- S13-1000** Beryllium 10 analysis for the Dome Fuji ice cores and cosmic-ray stratigraphy

Kazuho Horiuchi<sup>1</sup>, Shota Suguchi<sup>1</sup>, Kensuke Suda<sup>1</sup>, Tomoko Uchida<sup>2</sup>, Takahiro Aze<sup>3</sup>, Yusuke Yokoyama<sup>4</sup>, Yasuyuki Muramatsu<sup>5</sup>, Hiroyuki Matsuzaki<sup>4</sup>, Hideaki Motoyama<sup>6</sup>  
<sup>1</sup>Hirosaki University, Hirosaki, Japan, <sup>2</sup>IAA, Shirakawa, Japan, <sup>3</sup>Tokyo Institute of Technology, Tokyo, Japan, <sup>4</sup>The University of Tokyo, Tokyo, Japan, <sup>5</sup>Gakushuin University, Tokyo, Japan, <sup>6</sup>National Institute of Polar Research, Tokyo, Japan

- S13-1020** Quantifying soil formation and sediment yield in mountains watersheds using terrestrial cosmogenic nuclides

Yuki Matsushi<sup>1</sup>, Hiroyuki Matsuzaki<sup>2</sup>

<sup>1</sup>Kyoto University, Uji, Japan, <sup>2</sup>The University of Tokyo, Tokyo, Japan

- S13-1040** Iodine isotope system in environment: Natural system, anthropogenic system and influence from NPP accident

Hiroyuki Matsuzaki<sup>1</sup>, Maki Honda<sup>2</sup>, Yasuto Miyake<sup>1</sup>, Takeyasu Yamagata<sup>2</sup>, Hironori Tokuyama<sup>1</sup>, Yasuyuki Muramatsu<sup>3</sup>

<sup>1</sup>The University of Tokyo, Tokyo, Japan, <sup>2</sup>Nihon University, Tokyo, Japan,

<sup>3</sup>Gakushuin University, Tokyo, Japan

Tuesday, 18<sup>th</sup> September

Morning

## Oral Session

09:00 – 11:00

Room D

### Session 14: Ion-surface Collisions: Collision-induced Dissociation and Soft Landing

Chair: Jean H Futrell  
Pacific Northwest National Laboratory, USA

- S14-0900** [Keynote Lecture] Ion-Surface Collisions  
09:00 – 09:40 in Mass Spectrometry: Activation,  
Dissociation and Soft-Landing

Julia Laskin  
Pacific Northwest National Laboratory, Richland, WA, USA

- S14-0940** Surface-induced Dissociation of Non-  
covalent Macromolecular Complexes

Vicki H Wysocki<sup>1,2</sup>, Mowei Zhou<sup>1,2</sup>, Anne Blackwell<sup>2</sup>,  
Royston Quintyn<sup>1,2</sup>, Xin Ma<sup>1,2</sup>, Shai Dagan<sup>2</sup>  
<sup>1</sup>Ohio State University, Columbus, OH, USA, <sup>2</sup>University of Arizona, Tucson,  
AZ, USA

- S14-1000** Mimicking redox protein function by  
10:00 – 10:20 soft landing Co(Salen) ions on self-  
assembled monolayer surfaces

Wen-Ping Peng<sup>1</sup>, Grant Johnson<sup>2</sup>, Julia Laskin<sup>2</sup>  
<sup>1</sup>Department of Physics, National Dong Hwa University, Taiwan, <sup>2</sup>Pacific  
Northwest National Laboratory, Richland, WA

- S14-1020** Epitaxy and Nanostructure Growth by  
10:20 – 10:40 Electrospray Ion Beam Deposition:  
Nonvolatile Molecules, Peptides,  
Proteins

Stephan Rauschenbach<sup>1</sup>, Gordon Rinke<sup>1</sup>, Matthias Pauly<sup>1</sup>,  
Ludger Harnau<sup>2,3</sup>, Klaus Kern<sup>1,4</sup>  
<sup>1</sup>Max-Planck-Institute for Solid State Research, Stuttgart, Germany, <sup>2</sup>Max-  
Planck-Institute for Intelligent Systems, Stuttgart, Germany, <sup>3</sup>Institute for  
Theoretical and Applied Physics, Univ. Stuttgart, Germany, <sup>4</sup>Institut de  
Physique de la Matiere Condensee, Ecole Polytechnique Federale de  
Lausanne, Switzerland

- S14-1040** Soft and Reactive Landing of Ions for the  
10:40 – 11:00 Fabrication of Bioactive Metal Surfaces

Michael Volny, Joelle M Rolfs, Tim Elam, Frantisek Turecek  
University of Washington, Seattle, USA

## Oral Session

09:00 – 11:00

Room E

### Session 15: Mass Spectrometry for Nuclear Applications and Safety

Chair: Nobuo Takaoka  
Kyushu University, Japan

- S15-0900** [Keynote Lecture] Extractive  
09:00 – 09:40 Electrospray Ionization Mass  
Spectrometry for Uranium Chemistry  
Studies

Huanwen Chen, Mingbiao Luo, Saijin Xiao, Yongzhong Ouyang,  
Yafei Zhou, Xinglei Zhang  
East China Institute of Technology, Nanchang, P.R. China

- S15-0940** Importance of process blank in isotope  
09:40 – 10:00 ratio determination of uranium and  
plutonium in ultra trace levels

Sunyoung Lee, Young Geun Ha, Jong-Ho Park, Kyuseok Song  
Korea atomic energy research institute, Daejeon, Korea

- S15-1000** Fissionogenic noble gases anomaly  
10:00 – 10:20 associated with Fukushima-daiichi  
nuclear power plant disaster after the  
3.11 Northeast Japan Earthquake

Keiko Sato<sup>1</sup>, Hidenori Kumagai<sup>1</sup>, Naoyoshi Iwata<sup>2</sup>,  
Hironobu Hyodo<sup>3</sup>, Katsuhiko Suzuki<sup>1</sup>  
<sup>1</sup>IFREE, JAMSTEC, Yokosuka, Japan, <sup>2</sup>Faculty of Science, Yamagata University,  
Yamagata, Japan, <sup>3</sup>RINS, Okayama University of Science, Okayama, JAPAN

- S15-1020** Investigations of Different Sample  
10:20 – 10:40 Matrices in Uranium Abundance  
Analysis Using the MTE Methodology

Claudie K Black, Evelyn Zuleger, Joan Horta-Domench,  
Martin Vargas Zuniga  
Institute for Transuranium Elements, Joint Research Centre, European  
Commission, Karlsruhe, Germany

- S15-1040** Selective analysis of individual uranium  
10:40 – 11:00 particles with higher U-235 abundance  
by secondary ion mass spectrometry

Fumitaka Esaka, Chi-Gyu Lee, Masaaki Magara,  
Takaumi Kimura  
Japan Atomic Energy Agency, Ibaraki, Japan

Tuesday, 18<sup>th</sup> September

Afternoon

## Oral Session

15:00 – 17:00

Main Hall

### Session 16: Glycoanalytical Technology for Systems Glycobiology and Functional Glycomics

Chair: Jane Thomas-Oates  
University of York, UK

#### S16-1500 [Keynote Lecture] Glycoanalytical technologies for systems glycobiology, biomarker discovery & therapies

15:00 – 15:40 Radka Fahey, Eugene Dempsey, Karna Marino, Amanda McCann, Pauline M Rudd  
NIBRT - Ireland

#### S16-1540 A Rapid-Throughput Platform for Quantitation of Site-Specific Glycosylation with Differentiation of Structural Isomers

15:40 – 16:00 Serenus Hua<sup>1</sup>, Chloe Hu<sup>2</sup>, Charles C Nwosu<sup>2</sup>, John S Strum<sup>2</sup>, Carlito B Lebrilla<sup>2</sup>, Hyun Joo An<sup>1</sup>

<sup>1</sup>Chungnam National University, Daejeon, South Korea, <sup>2</sup>University of California, Davis, USA

#### S16-1600 Glycome Signature for Cancer Cell Identification

16:00 – 16:20 Hyun Joo An<sup>1</sup>, Lauren Dimapasoc<sup>2</sup>, Mary Saunders<sup>2</sup>, Seunghyup Jeong<sup>1</sup>, Jaehan Kim<sup>1</sup>, Kit Lam<sup>2</sup>, Carlito B Lebrilla<sup>2</sup>  
<sup>1</sup>ChungNam National University, <sup>2</sup>University of California, Davis

#### S16-1620 Enhancement of carbohydrate signal by diamond nanoparticles in MALDI-MS

16:20 – 16:40 Chieh-Lin Wu<sup>1</sup>, Chia-Chen Wang<sup>2</sup>, Yin-Hung Lai<sup>1</sup>, Yuan Tseh Lee<sup>1</sup>, Yi-Sheng Wang<sup>1,2</sup>  
<sup>1</sup>Academia Sinica, <sup>2</sup>National Yang-Ming University and Academia Sinica

#### S16-1640 Electron-based fragmentation approaches for glycans and glycoconjugates

Catherine E Costello, Joseph Zaia, Cheng Lin  
Boston University School of Medicine

## Oral Session

15:00 – 17:00

Room A

### Session 17: Non-Covalent Ion-Molecule Interactions

Chair: Seung-Koo Shin  
Pohang University of Science and Technology, Korea

#### S17-1500 [Keynote Lecture] The Thermochemistry of Non-Covalent Ion-Molecule

15:00 – 15:40 Peter B Armentrout  
University of Utah, Salt Lake City, USA

#### S17-1540 Atomic metal anions: one-step dehydrogenation and defluorination of linear and cyclic hydrocarbons, alcohols and their fluorinated analogues

15:40 – 16:00 Paul M Mayer<sup>1</sup>, Alex Munham<sup>1</sup>, Jeffery Butson<sup>1</sup>, Jaleh Halvachizadeh<sup>1</sup>, Dhiya Hassan<sup>1</sup>, Sharon Curtis<sup>1</sup>  
<sup>1</sup>University of Ottawa, Ottawa, Canada

#### S17-1600 Structural and Energetic Effects in the Molecular Recognition of Peptides and Proteins by 18-Crown-6: Threshold Collision-Induced Dissociation and Theoretical Studies

16:00 – 16:20 Mary T Rodgers, Ranran Wu  
Wayne State University

#### S17-1620 Cation and solvent effects on G-quadruplex nucleic acid structure: from the solution to the gas phase

16:20 – 16:40 Valerie Gabelica<sup>1</sup>, Adrien Marchand<sup>1</sup>, Rubén Ferreira<sup>2</sup>, Frédéric Rosu<sup>1</sup>, Hisae Tateishi-Karimata<sup>3</sup>, Daisuke Miyoshi<sup>3,4</sup>, Naoki Sugimoto<sup>3,4</sup>, Edwin De Pauw<sup>1</sup>

<sup>1</sup>University of Liege, Liège, Belgium, <sup>2</sup>Institute for Research in Biomedicine (IRB), Barcelona, Spain, <sup>3</sup>Frontier Institute for Biomolecular Engineering Research (FIBER), Konan University, Japan, <sup>4</sup>Faculty of Frontiers of Innovative Research in Science and Technology (FIRST), Konan University, Japan

#### S17-1640 Noncovalent Binding of Tetracationic Porphyrin to Thrombin-Binding Aptamer DNA Destabilizes the Guanine-Quadruplex Structure

16:40 – 17:00 Jongcheol Seo, Eun Sun Hong, Hye-Joo Yoon, Seung Koo Shin  
Pohang University of Science and Technology (POSTECH)

Tuesday, 18<sup>th</sup> September

Afternoon

**Oral Session**

15:00 – 17:00

Room B-1

**Session 18: Advances in Resolution and Accuracy of Isotope Ratio Analyses**Chair: Takafumi Hirata  
Kyoto University, Japan**S18-1500 [Keynote Lecture] Advances in Isotope Ratio Mass Spectrometry and Required Isotope Reference Materials**Jochen Vogl  
BAM Federal Institute for Materials Research and Testing, Berlin, Germany**S18-1540 An experimental study on stable isotopic fractionation of rare earth elements during the adsorption on iron and manganese oxides**Ryoichi Nakada<sup>1</sup>, Masaharu Tanimizu<sup>1,2</sup>, Yoshio Takahashi<sup>1,2</sup>  
<sup>1</sup>Hiroshima University, Higashi-Hiroshima, Japan, <sup>2</sup>Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Nankoku, Kochi**S18-1600 The influence of the extreme climate conditions on Romanian fruit juices isotopic composition**Dana Alina I Magdas<sup>1</sup>, Romulus Puscas<sup>1</sup>, Gabriela Cristea<sup>1</sup>, Nicoleta Vedeanu<sup>2</sup><sup>1</sup>National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, ROMANIA, <sup>2</sup>Iuliu Hatieganu "University of Medicine and Pharmacy", Biophysics Department, Cluj-Napoca, Romania**S18-1620 The Fe isotopic analysis using LAL-MC-ICPMS technique**Satoki Okabayashi<sup>1</sup>, Tetsuya Yokoyama<sup>2</sup>, Takafumi Hirata<sup>1</sup>  
<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Tokyo Institute of Technology**S18-1640 A novel technique for correction of instrumental mass bias in isotope ratio measurements**Gina Chew, Thomas Walczyk  
NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Singapore**Oral Session**

15:00 – 17:00

Room D

**Session 19: Mass Spectrometric Diagnosis**Chair: Toyofumi Nakanishi  
Osaka Medical College, Japan**S19-1500 [Keynote Lecture] Ambient Mass Spectrometry for Detecting Biomarkers in Breath**Renato Zenobi  
ETH Zurich**S19-1540 A Validation Assay for Cardiac Ischemia Biomarkers**Robert J Cotter<sup>1</sup>, Christine Jelinek<sup>1</sup>, Jennifer Van Eyk<sup>1</sup>, Kevin W Meyer<sup>2</sup>, David Taggart<sup>3</sup><sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD 21205, USA, <sup>2</sup>Perfinity Biosciences, West Lafayette, IN, USA, <sup>3</sup>John Radcliffe Hospital, Oxford, England**S19-1600 Diagnosis, analysis of pathogenesis and therapies for transthyretin form of amyloidosis**Yukio Ando  
Department of Diagnostic Medicine, Graduate School of Medical Sciences, Kumamoto, Japan**S19-1620 Cerebrospinal fluid proteomics: A new window for understanding human neurological disorders**Masaya Ikegawa  
Kyoto Prefectural University of Medicine**S19-1640 Digging deeper into Small Cell Lung Cancer. Can targeted LC-MS reveal tomorrow's diagnostic level?**Silje B Torsetnes<sup>1</sup>, Marianne S Nordlund<sup>2</sup>, Elisabeth Paus<sup>2</sup>, Trine G Halvorsen<sup>1</sup>, Leon Reubaet<sup>1</sup><sup>1</sup>University of Oslo, Oslo, Norway, <sup>2</sup>Central Laboratory - Radiumhospitalet, Oslo, Norway

Tuesday, 18<sup>th</sup> September

Afternoon

## Oral Session

15:00 – 17:00

Room E

## Session 20: The Ion formation and Dissociation Mechanisms in MALDI

Chair: Myung Soo Kim  
Seoul National University, Korea**S20-1500** [Keynote Lecture] MALDI and Related

15:00 – 15:40 Desorption / Ablation / Ionization Methods: A Solved Problem or Still a Mystery?

Richard Knochenmuss  
Tofwerk, Thun, Switzerland**S20-1540** Ion yield and laser shot number-

15:40 – 16:00 dependent variation of mass spectral pattern in MALDI of peptides; a thermal model for MALDI

Yong Jin Bae, Kyung Man Park, Sung Hee Ahn, Myung Soo Kim  
Seoul National University, Seoul, Korea**S20-1600** Plume Expansion Dynamics of Ionic

16:00 – 16:20 Liquid Matrices for Matrix-assisted Laser Desorption/Ionization

I-Chung Lu, Sheng Lee, Yuan T Lee, Chi-Kung Ni  
Academia Sinica, Taipei, Taiwan**S20-1620** New Insights in MALDI In-Source Decay

16:20 – 16:40 Process

Daiki Asakawa<sup>1,2</sup>, Nicolas Smargiasso<sup>1</sup>, Edwin De Pauw<sup>1</sup><sup>1</sup>University of Liege, Liege, Belgium, <sup>2</sup>Yokohama City University, Yokohama, Japan**S20-1640** CO<sub>2</sub>-Laser Atmospheric Pressure

16:40 – 17:00 Ionization of Acoustically Levitated Droplets

Arne Stindt<sup>1</sup>, Merwe Albrecht<sup>1</sup>, Ulrich Panne<sup>1,2</sup>, Jens Riedel<sup>1</sup><sup>1</sup>BAM Federal Institute for Materials Research and Testing, Berlin, Germany,<sup>2</sup>Humboldt-Universitaet zu Berlin, Department of Chemistry, Berlin, Germany

Tuesday, 18<sup>th</sup> September

## Poster Session

Core Time : 11:10 - 12:20 (Odd number),  
13:30 - 14:40 (Even number)

Event Hall

## Session 11

### Glycomics: From Disease Markers to Therapeutic Antibody Products

**PTu-001 Identification of Native N-linked Glycan Structures from Human Cancer Cell Using HPLC on a Microfluidic Chip and Time-of-Flight Mass Spectrometry**

Jong-Moon Park<sup>1</sup>, Kyeong-seob Lee<sup>4</sup>, Na-Young Han<sup>1</sup>,  
Eugene C Yi<sup>3,4</sup>, Hooken Lee<sup>1,2</sup>  
<sup>1</sup>Lee Gil Ya Cancer and Diabetes Institute, Incheon, Republic of Korea,  
<sup>2</sup>College of Pharmacy, Gachon University, Republic of Korea, <sup>3</sup>Dept of Molecular Medicine and Biopharmaceutical Sciences Seoul National University, College of Medicine, Republic of Korea, <sup>4</sup>Dept. of Molecular Medicine and Biopharmaceutical Sciences Graduate school of Convergence Science and Technology Seoul National University, Republic of Korea

**PTu-002 Development of Analytical Method of Keratan Sulfate Structure**

Shigeyasu Ito, Hiroshi Fujita, Toshikazu Minamisawa  
SEIKAGAKU CORPORATION, Tokyo, Japan

**PTu-003 Detection of the Heterogeneous O-Glycosylation Profile of MT1-MMP Expressed in Cancer Cells by a Simple MALDI-MS Method**

Takuya Shuo<sup>1</sup>, Naohiko Koshikawa<sup>1</sup>, Daisuke Hoshino<sup>1</sup>,  
Tomoko Minegishi<sup>1</sup>, Hiroko Ao-Kondo<sup>2</sup>, Masaaki Oyama<sup>2</sup>,  
Sadanori Sekiya<sup>3</sup>, Shinichi Iwamoto<sup>3</sup>, Koichi Tanaka<sup>3</sup>,  
Motoharu Seiki<sup>1</sup>  
<sup>1</sup>Division of Cancer Cell Research, Institute of Medical Science, University of Tokyo, Tokyo, Japan, <sup>2</sup>Medical Proteomics Laboratory, Institute of Medical Science, University of Tokyo, Tokyo, Japan, <sup>3</sup>Koichi Tanaka Mass Spectrom. Res. Lab., Shimadzu Corp., Kyoto, Japan

**PTu-004 Age-related Changes in the Composition and Structure of Glycan released from Mouse Skin Tissues**

Bum Jin Kim<sup>1</sup>, Inae Kang<sup>1</sup>, Su Hee Kim<sup>1</sup>, Sureyya Ozcan<sup>2</sup>,  
Lauren Dimapasoc<sup>2</sup>, Ik-Soon Jang<sup>3</sup>, Jong-Soon Choi<sup>3</sup>,  
Hyun Joo An<sup>1</sup>  
<sup>1</sup>Chungnam National University, Daejeon, Republic of Korea, <sup>2</sup>Department of Biochemistry, University of California Davis, Davis, CA95616, <sup>3</sup>Korea Basic Science Institute, 113 Gwangangno, Yuseong-gu, Daejeon, Korea

**PTu-006 An MSn platform for detailed characterisation of both the peptide and the glycan moieties and the peptide/glycan linkage in glycoproteins.**

Helen V Montgomery<sup>1</sup>, Matthew E Openshaw<sup>2</sup>,  
Omar Belgacem<sup>2</sup>, Masaki Murase<sup>3</sup>, Koichi Tanaka<sup>3</sup>  
<sup>1</sup>Shimadzu Koichi Tanaka Mass Spectrometry Research Laboratory, Manchester, UK, <sup>2</sup>Kratos Analytical Ltd, Manchester, UK, <sup>3</sup>Shimadzu Corp., Kyoto Japan

**PTu-007 Comparative Study of Protein Concentration, Glycoform Profile and Site Occupancy of a Glycoprotein with Multiple Glycosylation Sites and Complex Glycans**

Yi-Chun Ma, Guor-Rong Her  
National Taiwan University, Taipei, Taiwan

**PTu-008 Automated intact mass analysis for routine identity testing and quality tracking of recombinant monoclonal antibodies**

Yoshihiko Morishita<sup>1</sup>, Jette Wagtberg<sup>2</sup>, Christian Albers<sup>3</sup>,  
Laura Main<sup>3</sup>, Wolfgang Jabs<sup>3</sup>

<sup>1</sup>Bruker Daltonics K.K., <sup>2</sup>SympHogen A/S, Lyngby, Denmark, <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany

**PTu-009 Comprehensive Glycan Profiling of Exosomes Derived from Human Body Fluids for Disease Biomarker Discovery**

Seunghyup Jeong<sup>1</sup>, Do-Young Choi<sup>2</sup>, Pyong-Gon Moon<sup>3</sup>,  
Kwang Pyo Kim<sup>2</sup>, Moon Chang Back<sup>3</sup>, Hyun Joo An<sup>1</sup>

<sup>1</sup>Chungnam National University, Daejeon, South Korea, <sup>2</sup>Konkuk University, Seoul, South Korea, <sup>3</sup>Kyungpook National University, Daegu, South Korea

**PTu-010 Determination of core fucosylation in glycopeptides of monoclonal antibodies**

Toshiji Kudo<sup>1</sup>, Anja Resemann<sup>2</sup>, Ulrike Schweiger-Hufnagel<sup>2</sup>,  
Detlev Suckau<sup>2</sup>, Daniel Kolarich<sup>3</sup>

<sup>1</sup>Bruker Daltonics K.K., <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany, <sup>3</sup>Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Berlin, Germany

**PTu-011 Identification and structural analysis by chip-based nanoelectrospray mass spectrometry of novel brain-associated chondroitin/dermatan sulfate motifs**

ALINA D ZAMFIR<sup>1</sup>, CORINA FLANGEA<sup>1</sup>, ROXANA M GHILAI<sup>2</sup>,  
DANIELA G SEIDLER<sup>3</sup>

<sup>1</sup>Aurel Vlaicu University, Arad, Romania, <sup>2</sup>Victor Babes University of Medicine and Pharmacy, Timisoara, Romania, <sup>3</sup>University of Muenster, Germany

**PTu-012 Glycobiomarkers for atherosclerosis**

13:30 – 14:40

Oliver Ozohanics<sup>1</sup>, Lilla Turiak<sup>1</sup>, Anita Jeko<sup>1</sup>, Angel Puerta<sup>2</sup>,  
Jose Carlos Diez-Masa<sup>2</sup>, Mercedes de Frutos<sup>2</sup>, Karoly Vekey<sup>1</sup>,  
Laszlo Drahos<sup>1</sup>

<sup>1</sup>Research Centre for Natural Sciences Hungarian Academy of Sciences, Budapest, Hungary, <sup>2</sup>Institute of Organic Chemistry (CSIC), Juan de la Cierva 3 Madrid, 28006, Spain

**PTu-013 Top-Down Mass Spectrometric Analysis of Glycosylated and Phosphorylated Proteins**

Fujio Nishida<sup>1</sup>, Anja Resemann<sup>2</sup>, Lars Vorwerg<sup>2</sup>, Paul Kowalski<sup>3</sup>,  
Deltev Suckau<sup>2</sup>

<sup>1</sup>Bruker Daltonics K.K., Yokohama, Japan, <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany, <sup>3</sup>Bruker Daltonics, Inc., Billerica, MA, USA

Tuesday, 18<sup>th</sup> September

## Session 12

### On-site Mass Spectrometry -Miniaturized Instruments and Allied Technologies-

**PTu-014 Design and Testing of a Miniature Magnetic Sector Mass Spectrometer**

13:30 – 14:40  
meiru guo, liang wang, yide zhao, yuhua xiao, taiguo li  
 Science and Technology on Vacuum & cryogenics Technology and Physics Laboratory, Lanzhou Institute of Physics, Lanzhou, China

**PTu-016 Real-Time Monitoring of a Suzuki Reaction using a Hood-Based Compact Mass Spectrometer**

13:30 – 14:40  
Daniel Eikel, Jack Henion, Simon Prosser, Nigel Sousou, Collier Lee, Jamey Jones  
 Advion Inc., Ithaca, New York, USA

**PTu-017 Explosives Trace Detection by Mass Spectrometry: An Automated Particle Sampler for Collecting Explosives Particles Adhering to Passenger's Baggage**

11:10 – 12:20  
Hisashi Nagano, Yuichiro Hashimoto, Yasuaki Takada, Yasutaka Suzuki, Hideo Kashima, Masakazu Sugaya, Yasunori Doi, Koichi Terada, Minoru Sakairi  
 Hitachi,Ltd.,Central Research Laboratory,Tokyo,Japan

**PTu-019 Radio Frequency Mass Reflectrons with plane Discrete Electrodes**

11:10 – 12:20  
Alexander A Dyagilev, Eugeny Y Grachev, Vladimir V Zhuravlev, Eugeny V Mamontov  
 Ryazan State Radio Engineering University, Ryazan, Russia

**PTu-020 Development of Low Pressure Dielectric Barrier Discharge Ionization Source and Vacuumed Headspace Method for Portable Mass Spectrometer**

13:30 – 14:40  
Shun Kumano<sup>1</sup>, Masuyuki Sugiyama<sup>1</sup>, Masuyoshi Yamada<sup>1</sup>, Hideotoshi Morokuma<sup>2</sup>, Kazushige Nishimura<sup>1</sup>, Yuichiro Hashimoto<sup>1</sup>, Hiroyuki Inoue<sup>3</sup>  
<sup>1</sup>Hitachi, Ltd., Tokyo, Japan, <sup>2</sup>Hitachi High-Technologies Corp., Hitachinaka, Japan, <sup>3</sup>National Research Institute of Police Science, Kashiwa, Japan

**PTu-021 Broad range detection in a low field FTICR instrument**

11:10 – 12:20  
Joel Lemaire<sup>1</sup>, Vincent Kromer<sup>1</sup>, Gwendoline Jamet<sup>1</sup>, Clotilde Le Vot<sup>1</sup>, Essylt Louarn<sup>1</sup>, Michel Heninger<sup>1,2</sup>, Helene Mestdagh<sup>1</sup>  
<sup>1</sup>LCP CNRS-Universite Paris Sud, Orsay, France, <sup>2</sup>ALYXAN, Orsay, france

**PTu-022 Digital Linear Ion Trap in a Portable Mass Spectrometer**

13:30 – 14:40  
Zhengxu Huang<sup>2</sup>, Hui Mu<sup>1</sup>, Xiaoyu Meng<sup>1</sup>, Junsheng Zhang<sup>1</sup>, Lin Tao<sup>1</sup>, Gongyu Jiang<sup>1</sup>, Li Ding<sup>1</sup>, Xu Wu<sup>2</sup>, Zhen Zhou<sup>2</sup>, Wenjian Sun<sup>1</sup>, Zhong Fu<sup>2</sup>  
<sup>1</sup>Shimadzu Research Laboratory, Shanghai, China, <sup>2</sup>Kunshan Hexin Mass Spectrometry Technology Co., Ltd, Kunshan, China

**PTu-023 Photo ionisation time-of-flight mass spectrometry as a powerful tool for the on-line analysis of tobacco and wood combustion and pyrolysis**

11:10 – 12:20  
Christian Busch<sup>1</sup>, Thorsten Streibel<sup>1,2</sup>, Chuan Liu<sup>3</sup>, Kevin G McAdam<sup>3</sup>, Christian Radischat<sup>1</sup>, Ralf Zimmermann<sup>1,2</sup>  
<sup>1</sup>University of Rostock / Chair of Analytical Chemistry, Rostock, Germany, <sup>2</sup>Helmholtz Zentrum Muenchen / German Research Centre for Environmental Health, Neuherberg, Germany, <sup>3</sup>British American Tobacco / Group Research & Development Centre, Southampton, United Kingdom

**PTu-024 Development of a multi-turn time-of-flight mass spectrometer with an atmospheric ionization**

13:30 – 14:40  
Masanobu Nakazono<sup>1</sup>, Hiroki Andoh<sup>1</sup>, Shinichi Miki<sup>2</sup>, Michisato Toyoda<sup>1,2</sup>  
<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>MSI. TOKYO, Chofu, Japan

**PTu-025 Sample Gas Concentration and Pulsed Injection System for a Portable Ion Trap Mass Spectrometer**

11:10 – 12:20  
Hyun Sik Kim<sup>1</sup>, Seung Yong Kim<sup>1</sup>, Yong Hak Kim<sup>1</sup>, Mo Yang<sup>1</sup>, Minyoung Youn<sup>1</sup>, Yong-Moon Lee<sup>2</sup>  
<sup>1</sup>Korea Basic Science Institute, Ochang, Chungcheongbuk-do, 363-883 Korea, <sup>2</sup>Chungbuk National University,Cheongju, Chungcheongbuk-do, 361-763, Korea

## Session 13

### Accelerator Mass Spectrometry

**PTu-026 Various erosion rates of weathered soil surfaces of mountain ridges in Tohoku District, Japan using in-situ cosmogenic nuclides depth profile.**

13:30 – 14:40  
Kazuyo Shiroya<sup>1</sup>, Junichi Itoh<sup>1</sup>, Yusuke Yokoyama<sup>2</sup>, Hiroyuki Matsuzaki<sup>2</sup>  
<sup>1</sup>Geological Survey of Japan, AIST, Tsukuba, Japan, <sup>2</sup>University of Tokyo

**PTu-027 Estimation of Isotopic ratio of radioactive iodine (I-129/I-131) released from Fukushima Daiichi NPP accident**

11:10 – 12:20  
Yasuto Miyake<sup>1</sup>, Hiroyuki Matsuzaki<sup>1</sup>, Takeshi Fujiwara<sup>1</sup>, Takumi Saito<sup>1</sup>, Takeyasu Yamagata<sup>2</sup>, Maki Honda<sup>2</sup>, Yasuyuki Muramatsu<sup>3</sup>  
<sup>1</sup>The University of Tokyo, Tokyo, Japan, <sup>2</sup>Nihon Universityo, Tokyo, Japan,

<sup>3</sup>Gakushuin University, Tokyo, Japan

**PTu-028 Depth profile and migration of 129I concentration in soil at Abukuma, Fukushima**

13:30 – 14:40  
Maki Honda<sup>1</sup>, Hiroyuki Matsuzaki<sup>2</sup>, Takeyasu Yamagata<sup>1</sup>, Yoko Tuchiya<sup>2</sup>, Chuichiro Nakano<sup>2</sup>, Yuki Matsushi<sup>3</sup>, Hisao Nagai<sup>1</sup>, Yuji Maejima<sup>4</sup>  
<sup>1</sup>Nihon university, Tokyo, Japan, <sup>2</sup>The University of Tokyo, <sup>3</sup>Disaster Prevention Research Institute Kyoto University, <sup>4</sup>National Institute for Agro-Environmental Sciences

## Tuesday, 18<sup>th</sup> September

TUE

### PTu-029 Progresses in sample treatment for BAMs analysis

11:10 – 12:20  
 Minyoung Youn<sup>1</sup>, Seung Yong Kim<sup>1</sup>, Yong Hak Kim Kim<sup>1</sup>, Hyun Sik Kim<sup>1</sup>, Jae-Gook Shin<sup>2</sup>, Ji Hong Son<sup>2</sup>, Soo Kyung Bae<sup>2</sup>, Hyun Sic Chae<sup>3</sup>  
<sup>1</sup>Korea Basic Science Institute, Ochang, Chungcheongbuk-do, 363-883 Korea, <sup>2</sup>Inje University College of Medicine, Busan, 614-735 Korea, <sup>3</sup>Sans Frontier Technology, Daejeon, 305-510 Korea

## Session 14

### Ion-surface Collisions: Collision-induced Dissociation and Soft Landing

### PTu-030 Soft-sputtering of protein molecules using various gas cluster ion beams

13:30 – 14:40  
 Kousuke Moritani, Kosuke Goto, Issei Ihara, Norio Inui, Kozo Mochiji  
 University of Hyogo

### PTu-031 Sensitive Ionization of Non-Volatile Analytes Using Multiply Charged Primary Ions in Desorption Electrospray Ionization Mass Spectrometry

11:10 – 12:20  
 zhiquiang zhu, Qiliang Gong, Yafei Zhou, Ning Xu, Haiwei Gu, Huanwen Chen, Tenggao Zhu  
 Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology, Nanchang, Jiangxi Province, P. R.China

### PTu-032 The Gas Phase Mechanism of 2-Furaldehyde Formation from Pentose Sugars: A Mass Spectrometric and Theoretical Study

13:30 – 14:40  
 Federico Pepi<sup>1</sup>, Andreina Ricci<sup>2</sup>, Simona Piccolella<sup>2</sup>, Stefania Garzoli<sup>1</sup>, Rino Rago<sup>1</sup>, Alexandros Patsilinakos<sup>1</sup>, Pierluigi Giacomello<sup>1</sup>  
<sup>1</sup>University of Rome Sapienza, Rome, Italy, <sup>2</sup>Second University of Naples, Caserta, Italy

## Session 15

### Mass Spectrometry for Nuclear Applications and Safety

### PTu-033 SEPARATION AND MEASUREMENT OF URANIUM, PLUTONIUM AND NEODYMIUM IN SIMULATE SPENT NUCLEAR FUELS BY EXTRACTIONCHROMATOGRAPHY WITH ISOTOPE DILUTION MASS SPECTROMETRY

11:10 – 12:20  
 Jinying Li<sup>1,2,3</sup>, Guoping Xiao<sup>2,3</sup>, Lei Shi<sup>1,2,3</sup>  
<sup>1</sup>China Resources New Energy Group Co.,Ltd, <sup>2</sup>China Institute of Atomic Energy, Beijing, China; <sup>3</sup>Chinese MS Society, Beijing, China

### PTu-034 When was gold deposited ?

13:30 – 14:40  
 Nobuo Takaoka<sup>1,6</sup>, Nobutaka Shimada<sup>2</sup>, Masako Shima<sup>3</sup>, Tomoki Nakamura<sup>4,7</sup>, Keisuke Nagao<sup>5</sup>, Hitoshi Sagawa<sup>6,8</sup>, Ryuji Okazaki<sup>4</sup>, Kazuhiko Shimada<sup>4</sup>

<sup>1</sup>Kyushu University, Fukuoka, Japan, <sup>2</sup>Kyushu University, Fukuoka, Japan, <sup>3</sup>National Science Museum, Tokyo, Japan, <sup>4</sup>Faculty of Sciences, Kyushu University, Fukuoka, Japan, <sup>5</sup>Faculty of Sciences, University of Tokyo, Tokyo, Japan, <sup>6</sup>Faculty of Sciences, Yamagata University, Yamagata, Japan, <sup>7</sup>Faculty of Sciences, Tohoku University, Sendai, Japan, <sup>8</sup>Human Metabolome, Tsuruoka, Japan

### PTu-035 Surface Desorption Atmospheric Pressure Chemical Ionization (DAPCI) Source based on Graphite needle

11:10 – 12:20  
 Xinglei Zhang, Saijin Xiao, Junqing Yang, Xifang Huang  
 East China Institute of Technology, Nanchang, China

### PTu-036 Rapid 90Sr detection by MALDI-TOF-MS with a new matrix, dipicolinic acid obtained from an eastern Japan-traditional food, Natto.

13:30 – 14:40  
 Masaki Koike, Kaori Chiba-Kamoshida  
 National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

### PTu-038 Spatially Resolved Analysis of Uranium and Plutonium Isotope Ratios in Environmental Samples by Laser Ablation MC-ICP-MS

13:30 – 14:40  
 Siarhei Bulyha<sup>1</sup>, Stefanie Kappel<sup>2</sup>, Thomas Prohaska<sup>2</sup>  
<sup>1</sup>International Atomic Energy Agency, <sup>2</sup>University of Natural Resources and Life Sciences BOKU, Vienna

## Session 16

### New Approaches to Defining the Diversity of Glycans

### PTu-039 MALDI MS analysis of N-glycan structures of a cell adhesion molecule, CADM1, in various cancer cells

11:10 – 12:20  
 Tomoko Maruyama<sup>1</sup>, Mika Sakurai-Yageta<sup>1</sup>, Kaoru Kaneshiro<sup>2</sup>, Sadanori Skiya<sup>2</sup>, Shinichi Iwamoto<sup>2</sup>, Koichi Tanaka<sup>2</sup>, Yoshinori Murakami<sup>1</sup>

<sup>1</sup>The Institute of Medical Science, The University of Tokyo, Tokyo, Japan,  
<sup>2</sup>Shimadzu Corporation, Kyoto, Japan

### PTu-040 Isolation and identification of glycopeptides with isomeric glycans by lectin-column chromatography and negative-ion MALDI-QIT-TOF MSn

13:30 – 14:40  
 Kazuko Hirose, Junko Amano  
 Laboratory of Glycobiology, The Noguchi Institute, Tokyo, Japan

### PTu-041 A workflow for identification of isobaric isoforms of glycans using off-line MALDI-MSn system

11:10 – 12:20  
 Shuichi Nakaya, Yuzo Yamazaki  
 Shimadzu Corporation, Kyoto, Japan

## Tuesday, 18<sup>th</sup> September

- PTu-042** Negative-ion fragmentation of neutral N-glycans derivatized with 3-aminoquinoline and other non-acidic reagents  
 13:30 – 14:40

Takashi Nishikaze, Kaoru Kaneshiro, Shin-Ichirou Kawabata, Koichi Tanaka  
 Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, Japan

### Session 17

#### Non-Covalent Ion-Molecule Interactions

- PTu-043** Atomic metal anions: one-step dehydrogenation and defluororation of linear and cyclic hydrocarbons, alcohols and their fluorinated analogues  
 11:10 – 12:20

Paul M Mayer, Alex Mungham, Jeffery Butson, Jaleh Halvachizadeh, Dhiya Hassan, Sharon Curtis University of Ottawa, Ottawa, Canada

- PTu-044** Energetics of dissociation of polycyclic aromatic hydrocarbons in interstellar environments  
 13:30 – 14:40

Brandi J West<sup>1</sup>, Christine Joblin<sup>2,3</sup>, Valerie Blanchet<sup>3</sup>, Andras Bod<sup>4</sup>, Balint Sztray<sup>5</sup>, Paul M Mayer<sup>1</sup>  
<sup>1</sup>University of Ottawa, Ottawa, Canada, <sup>2</sup>IRAP/CNRS, Toulouse, France, <sup>3</sup>Universite de Toulouse UPS, Toulouse, France, <sup>4</sup>Paul Scherrer Institut, Villigen, Switzerland, <sup>5</sup>University of the Pacific, Stockton, USA

- PTu-045** Gas Phase Acid-Base Chemistry of Cysteine and Serine Homologs  
 11:10 – 12:20

John C Poutsma, Corbin Muettterties, Vincent Yannello, Ashley Janiga College of William and Mary, Williamsburg, VA, USA

- PTu-046** Mass spectrometric analysis of 1,3,5-Trinitroperhydro-1,3,5-triazine (RDX)  
 13:30 – 14:40

Sehwan Park<sup>1</sup>, Soo Gyeong Cho<sup>2</sup>, Eun Mee Goh<sup>2</sup>, Sungman Lee<sup>3</sup>, Sung-Suk Koh<sup>3</sup>, Jeongkwon Kim<sup>1</sup>  
<sup>1</sup>Chungnam National University, Daejeon, South Korea, <sup>2</sup>Agency for Defense Development, Daejeon, South Korea, <sup>3</sup>Sensor Tech Inc., Kyunggi-Do, South Korea

- PTu-047** Formation of hydrated amino acid ions and estimation of their first hydrated shell  
 11:10 – 12:20

Mami Sakai, Kanako Sekimoto, Mitsuo Takayama Yokohama City University, Yokohama, Japan

- PTu-048** Mass Spectrometry Studies of Metal Triflates and Triflimides and Their Interactions with Lewis Bases  
 13:30 – 14:40

Jean-Francois Gal<sup>1</sup>, Ilaria Monfardini<sup>1</sup>, Claudio Iacobucci<sup>1</sup>, Lionel Massi<sup>1</sup>, Sandra Olivero<sup>1</sup>, Elisabet Dunach<sup>1</sup>, Karel Kasemets<sup>2</sup>, Peeter Burk<sup>2</sup>  
<sup>1</sup>University of Nice-Sophia Antipolis, Nice, France, <sup>2</sup>University of Tartu, Tartu, Estonia

- PTu-049** Mass spectrometric approaches to enantioselective complexation system in solution  
 11:10 – 12:20

Motohiro Shizuma<sup>1</sup>, Hirofumi Sato<sup>1</sup>, Takashi Nakakoji<sup>2</sup>, Hideya Kawasaki<sup>2</sup>, Kaori Asano<sup>3</sup>, Tsuyoshi Matsuzaki<sup>3</sup>, Takeyuki Suzuki<sup>3</sup>, Keiji Hirose<sup>4</sup>, Yoshito Tobe<sup>4</sup>, Ryuichi Arakawa<sup>2</sup>, Daisuke Ono<sup>1</sup>

<sup>1</sup>Osaka Municipal Tech. Res. Inst., Osaka, Japan, <sup>2</sup>Kansai University, Osaka, Japan, <sup>3</sup>ISIR, Osaka University, Osaka, Japan, <sup>4</sup>Graduate School of Engineering Science, Osaka University, Osaka, Japan

- PTu-050** Characteristic hydration of saccharides isolated from liquid beams  
 13:30 – 14:40

Namiki Toyama Genesis Research Institute, Inc., Chiba, Japan

- PTu-051** Evaluation of intermolecular association of glycosaminoglycan oligosaccharides using nanoelectrospray ionization mass spectrometry  
 11:10 – 12:20

Yuya Otsuka, Toshikazu Minamisawa Seikagaku corporation, Tokyo, Japan

- PTu-052** Enantioselective binding characteristics of amino acid to chiral copper(II) complex using electrospray ionization mass spectrometry coupling with the deuterium-labeled method  
 13:30 – 14:40

Takashi Nakakoji<sup>1</sup>, Hirofumi Sato<sup>2</sup>, Hiroyuki Miyake<sup>3</sup>, Hideya Kawasaki<sup>1</sup>, Ryuichi Arakawa<sup>1</sup>, Daisuke Ono<sup>2</sup>, Motohiro Shizuma<sup>2</sup>

<sup>1</sup>Kansai University, Osaka, Japan, <sup>2</sup>Osaka Municipal Technical Research Institute, Osaka, Japan, <sup>3</sup>Osaka City University, Osaka, Japan

- PTu-053** MECHANISTIC INVESTIGATION OF ECO-FRIENDLY IODINATION OF AROMATIC DERIVATIVES BY MASS SPECTROMETRY  
 11:10 – 12:20

Diogo Oliveira-Silva, Andre F Rodrigues-Oliveira, Marcelo Serigatti, Cristiano Raminelli Universidade Federal de Sao Paulo - Campus Diadema, Diadema, Brazil

- PTu-054** Comparing the dissociation energies of non-covalent complexes measured with BIRD and RRKM modelling of CID  
 13:30 – 14:40

Justin B Renaud<sup>1</sup>, Lan Liu<sup>2</sup>, John Klassen<sup>2</sup>, Paul M Mayer<sup>1</sup>  
<sup>1</sup>University of Ottawa, <sup>2</sup>University of Alberta

- PTu-055** Molecular recognition in gas phase: a method for quantitative analysis of protein-ligand interactions energy by CID-MS.  
 11:10 – 12:20

Andrey Dyachenko<sup>1</sup>, Sergio Madurga<sup>1,2</sup>, Ernest Giralt<sup>1,2</sup>

<sup>1</sup>Institute for Research in Biomedicine, Barcelona, Spain, <sup>2</sup>Department of Organic Chemistry, Universidad de Barcelona, Barcelona, Spain

- PTu-056** Gas-phase basicity of 2-furaldehyde  
 13:30 – 14:40

Simona Piccolella<sup>1</sup>, Andreina Ricci<sup>1</sup>, Federico Pepi<sup>2</sup>, Alexandros Patsilinakos<sup>2</sup>, Rino Rago<sup>2</sup>, Stefania Garzoli<sup>2</sup>, Pierluigi Giacomello<sup>2</sup>

<sup>1</sup>Second University of Naples, Caserta, Italy, <sup>2</sup>Sapienza' University of Rome, Rome, Italy

## Tuesday, 18<sup>th</sup> September

TUE

- PTu-057** Non-covalent interaction between peptides and its effect on the dissociation process of Bradykinin Molecule  
 11:10 – 12:20

Chuan-Fan Ding, Chen Chen, Xiaodan He  
 Fudan University, Shanghai, China

### Session 18

#### Advances in Resolution and Accuracy of Isotope Ratio Analyses

- PTu-058** A continuous flow system for quantitatively preparation and isotopic measurement of radiogenic argon.  
 13:30 – 14:40

Tatiana Velivetckaia, Aleksandr Ignatev, Sergey Budnitskii  
 Far East Geological Institute FEB Russian Academy of Sciences, Vladivostok, Russia

- PTu-059** High precision analysis stable isotopes of sulfur (32S, 33S, 34S) using UV laser fluorination continuous He flow mass spectrometry  
 11:10 – 12:20

Aleksandr V Ignatev, Tatiana Velivetckaia  
 Far East Geological Institute, FEB RAS, Vladivostok, Russia

- PTu-060** MC-ICPMS: enhanced ion yields for high precision measurement of sub-fg Pu and high mass resolution for S isotope measurements.  
 13:30 – 14:40

Jerome A Johemko<sup>1</sup>, Charles B Douthitt<sup>2</sup>,  
 Johannes Schwieters<sup>3</sup>, Claudia Bouman<sup>3</sup>, Nicholas Lloyd<sup>3</sup>  
<sup>1</sup>Thermo Fisher Scientific, Honolulu, USA, <sup>2</sup>Thermo Fisher Scientific, San Jose, CA, USA, <sup>3</sup>Thermo Fisher Scientific GmbH, Bremen, Germany

- PTu-061** A COMPARATIVE STUDY OF CALCIUM AND STRONTIUM METABOLISM IN THE SHEEP MODEL USING CA-41 AND SR-84 ISOTOPIC TRACERS  
 11:10 – 12:20

Fransiska Dewi<sup>1,2</sup>, Tim Schulze-Koenig<sup>3</sup>, Annette Liesegang<sup>4</sup>,  
 Johanna Irreger<sup>5</sup>, Claudia Weigt<sup>6</sup>, Gisela Kuhn<sup>6</sup>,  
 Hans-Arno Synal<sup>3</sup>, Thomas Prohaska<sup>5</sup>, Thomas Walczyk<sup>1,2,7</sup>  
<sup>1</sup>NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Singapore, <sup>2</sup>Department of Chemistry (Science), National University of Singapore, Singapore, <sup>3</sup>Laboratory of Ion Beam Physics, Swiss Federal Institute of Technology (ETH), Switzerland, <sup>4</sup>Institute of Animal Nutrition, Vetsuisse Faculty, University of Zurich, Germany, <sup>5</sup>Division of Analytical Chemistry, University of Natural Resources and Life Sciences (BOKU), Austria, <sup>6</sup>Institute of Biomechanics, Swiss Federal Institute of Technology (ETH), Switzerland, <sup>7</sup>Department of Biochemistry (Medicine), National University of Singapore, Singapore

- PTu-062** Recent advance in MC-ICP-MS as a tool for the absolute determination of isotopic composition of heavy elements  
 13:30 – 14:40

Masaharu Tanimizu  
 Japan Agency for Marine-Earth Science and Technology

- PTu-063** MEASUREMENT OF IRON TRANSFER FROM DIET TO BRAIN IN THE RAT MODEL  
 11:10 – 12:20

Jiehua Chen, Shahreena Shahnava, Nadia Singh, Wei Yi Ong,  
 Thomas R Walczyk  
 National University of Singapore, Singapore

- PTu-064** Elemental mapping of Eu, Yb, Hf, Pb, Th and U for zircon using high resolution laser ablation-ICP-Mass spectrometry  
 13:30 – 14:40

Kentaro Hattori<sup>1</sup>, Shu-hei Sakata<sup>1</sup>, Hideki Iwano<sup>2</sup>,  
 Takaumi Hirata<sup>1</sup>

<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Kyoto Fission Track Co.Ltd., Kyoto, Japan

- PTu-065** The estimation of the effect of initial 230Th disequilibrium on U-Pb dating of young zircon crystal by LA-ICPMS  
 11:10 – 12:20

Shu-hei Sakata<sup>1</sup>, Hideki Iwano<sup>2</sup>, Kenshi Maki<sup>1</sup>,  
 Takaomi D Yokoyama<sup>1</sup>, Takahumi Hirata<sup>1</sup>

<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Kyoto Fission Track Co. Ltd., Kyoto, Japan

### Session 19

#### Mass Spectrometric Diagnosis

- PTu-066** Developing a human cancer diagnostics system based on the probe electrospray ionization-mass spectrometry and Bayesian statistics  
 13:30 – 14:40

Kentaro Yoshimura<sup>1</sup>, Lee Chuin Chen<sup>2</sup>, Mridul Kanti Mandal<sup>3</sup>,  
 Kunio Tanabe<sup>1,5</sup>, Michio Hara<sup>4</sup>, Hideki Fujii<sup>4</sup>, Masayuki Takeda<sup>6</sup>,  
 Kenzo Hiraoka<sup>3</sup>, Sen Takeda<sup>1</sup>

<sup>1</sup>Department of Anatomy and Cell Biology, Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, <sup>2</sup>Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, <sup>3</sup>Clean Energy Research Center, University of Yamanashi, <sup>4</sup>Department of Surgery, Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, <sup>5</sup>Faculty of Science and Engineering, Waseda University, <sup>6</sup>Department of Urology, Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi

- PTu-067** Ultrasensitive Multiplexed Detection of miRNAs Using Gold Nanoparticles and LDI-TOF MS  
 11:10 – 12:20

Hyunook Kang, Seol-Hye Hong, Woon-Seok Yeo  
 Konkuk University, Seoul, Korea

- PTu-068** Mapping longitudinal proteomic expression levels in brain tissue for an amyloid Alzheimer's disease mouse model using shotgun based mass spectrometry  
 13:30 – 14:40

Ganna Shevchenko<sup>1</sup>, Kim Kultima<sup>2</sup>, Jonas Bergquist<sup>3</sup>,  
 Kina Höglund<sup>4,5</sup>, Lars Andersson<sup>5</sup>, Magnus Wetterhall<sup>6</sup>

<sup>1</sup>Uppsala University, Uppsala, Sweden, <sup>2</sup>Uppsala University, Uppsala, Sweden, <sup>3</sup>Uppsala University, Uppsala, Sweden, <sup>4</sup>AstraZeneca, Södertälje, Sweden, <sup>5</sup>AstraZeneca, Södertälje, Sweden, <sup>6</sup>Uppsala University, Uppsala, Sweden

- PTu-069** Serum metabolome analysis for early detection of colorectal cancer  
 11:10 – 12:20

Masaru Yoshida<sup>1,2,3</sup>, Shin Nishiumi<sup>1</sup>, Yoshihiro Izumi<sup>1</sup>,  
 Atsuki Matsubara<sup>1</sup>, Takeshi Azuma<sup>1</sup>

<sup>1</sup>Division of Gastroenterology, Department of Internal Medicine, Kobe University Graduate School of Medicine, Kobe, Japan, <sup>2</sup>The Integrated Center for Mass Spectrometry, Kobe University Graduate School of Medicine, Kobe, Japan, <sup>3</sup>Division of Metabolomics Research, Kobe University Graduate School of Medicine, Kobe, Japan

## Tuesday, 18<sup>th</sup> September

**PTu-070 Analysis of Drugs and Steroid Hormones in Human Saliva and Serum using Column-switching Ultra-fast LC/MS/MS with On-line Analyte Purification**

13:30 – 14:40  
 Yukiko Hirabayashi<sup>1</sup>, Takashi Shinagawa<sup>2</sup>, Joji Suzuki<sup>2</sup>, Toshio Kaji<sup>2</sup>  
<sup>1</sup>Central Research Laboratory, Hitachi, Ltd., Tokyo, Japan, <sup>2</sup>Hitachi Yokohama Hospital, Hitachi, Ltd., Kanagawa, Japan

**PTu-071 Acylglycine: A Potential Biomarker for the Clinical Diagnosis of Inborn Metabolic Disorders**

11:10 – 12:20  
 Bonnie Fong<sup>1,2</sup>, Sidney Tam<sup>2</sup>, Kelvin Leung<sup>1</sup>  
<sup>1</sup>Department of Chemistry, Hong Kong Baptist University, Hong Kong, <sup>2</sup>Department of pathology and Clinical Biochemistry, Queen Mary Hospital, Hong Kong

**PTu-072 Clinical application of rapid bacterial identification using mass spectrometry**

13:30 – 14:40  
 Kazuyuki Sogawa<sup>1</sup>, Masaharu Watanabe<sup>1</sup>, Fumio Nomura<sup>1,2</sup>  
<sup>1</sup>Chiba University Hospital, Chiba, Japan, <sup>2</sup>Chiba University, Chiba, Japan

**PTu-073 Lectin-capturing and peptide affinity enrichment-based identification of cancer biomarker TIMP1 by high-resolution FT-ICR MS**

11:10 – 12:20  
 Yeong Hee AHN, Kwang Hoe KIM, Park Min SHIN, Eun Sun JI, Jong Shin YOO  
 Korea Basic Science Institute, Cheongwon, Korea

**PTu-074 Relating ESI-MS response with polar-, structural- and primary- characteristics of neuropeptides: Developing a deeper understanding**

13:30 – 14:40  
 Birthe V Nielsen, Daniel A Abaye, Frank Pullen, Minh T Nguyen  
 University of Greenwich, School of Science, Chatham Maritime, Kent, ME4 4TB, UK

**PTu-075 Fabrication of a titanium based MALDI bacterial chip for rapid, sensitive and direct analysis of pathogenic bacteria**

11:10 – 12:20  
 Hui-Fen Wu<sup>1,2,3</sup>, Judy Gopal<sup>1,2</sup>, Nazim Hasan<sup>1</sup>  
<sup>1</sup>Department of Chemistry, National Sun Yat-Sen University, <sup>2</sup>Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, <sup>3</sup>Doctoral Degree Program in Marine Biotechnology, National Sun Yat - Sen University,

**PTu-076 An optimized membrane proteins enrichment strategy for the bottom-up mass spectrometry approach**

13:30 – 14:40  
 Sravani Musunuri, Ganna Shevchenko, Magnus Wetterhall, Jonas Bergquist  
 Uppsala University, Uppsala, Sweden

**PTu-077 alpha-Tocopherol suppresses lipid peroxidation and behavioral impairment in mouse model of Down syndrome**

11:10 – 12:20  
 Mototada Shichiri<sup>1,2</sup>, Noiriko Ishida<sup>1</sup>, Yoshihisa Hagihara<sup>1</sup>, Yasukazu Yoshida<sup>1</sup>, Hiroshi Tamai<sup>2</sup>, Etsuo Niki<sup>1</sup>  
<sup>1</sup>National Institute of Advanced Industrial Science and Technology (AIST), Osaka, Japan, <sup>2</sup>Department of Pediatrics, Osaka Medical College, Osaka, Japan

**PTu-078 PGRN: a novel therapeutic target and biomarker for insulin resistance and obesity identified by differential proteome analysis**

13:30 – 14:40  
 Matsubara Toshiya<sup>1,2</sup>, Minami Kohtaro<sup>2</sup>, Yokoi Norihide<sup>2</sup>, Nishimura Osamu<sup>2</sup>, Seino Susumu<sup>2</sup>  
<sup>1</sup>Shimadzu Co., Kyoto, Japan, <sup>2</sup>Kobe University Graduate School of Medicine, Hyogo, Japan

**PTu-079 Direct molecular analysis by pico-drop sweat trapping from a single gland on a finger**

11:10 – 12:20  
 Harue Hiramoto<sup>1</sup>, Kanako Honda<sup>1</sup>, Naohiro Tsuyama<sup>1</sup>, Hajime Mizuno<sup>1</sup>, Iwao Sakane<sup>2</sup>, Sachiko Date<sup>3</sup>, Tsutomu Masujima<sup>1,3</sup>  
<sup>1</sup>Graduate School of Biomedical Sciences, Hiroshima University, Hiroshima, Japan, <sup>2</sup>ITO EN Ltd., Shizuoka, Japan, <sup>3</sup>Quantitative Biology Center, RIKEN, Japan

**PTu-080 Identifications of amyloidogenic proteins in FFPE tissue sections by MALDI-imaging coupled with on-tissue digestion and immunohistochemical/microscopic examinations**

13:30 – 14:40  
 Toyofumi Nakanishi<sup>1</sup>, Minako Ito<sup>1</sup>, Takashi Nirasawa<sup>2</sup>, Teruo Ueno<sup>1</sup>, Motomu Tsuji<sup>1</sup>, Takayuki Takubo<sup>1</sup>  
<sup>1</sup>Osaka Medical College, Takatsuki, Japan, <sup>2</sup>Bruker Daltonics K.K., Yokohama, Japan

**PTu-081 LC-MS/MS based basal and ACTH-stimulated serum concentrations of adrenal and gonadal steroid hormones and its application on heterozygote CYP21A2 mutations**

11:10 – 12:20  
 Alexandra E Kulle<sup>1</sup>, Juergen Hedderich<sup>2</sup>, Dorothee Roessner<sup>1</sup>, Jessica Schmitz<sup>1</sup>, Lena Niermeyer<sup>1</sup>, Paul-Martin Holterhus<sup>1</sup>, Felix G Riepe<sup>1</sup>  
<sup>1</sup>University Hospital Schleswig-Holstein / Children's Hospital, Kiel, Germany, <sup>2</sup>University Hospital Schleswig-Holstein/Institute of Mediacial Informatics and Statistics, Kiel, Germany

**PTu-082 Discovery of novel urinary biomarker candidates for diagnosis of prostate cancer**

13:30 – 14:40  
 Kenji NAKAYAMA<sup>1</sup>, Takahiro INOUE<sup>2</sup>, Sadanori SEKIYA<sup>3</sup>, Minoru SUZUKI<sup>3</sup>, Hiroki TSUMOTO<sup>1</sup>, Shin-Ichiro KAWABATA<sup>3</sup>, Shinichi IWAMOTO<sup>3</sup>, Kazuharu SHIMIZU<sup>1</sup>, Osamu OGAWA<sup>2</sup>, Gozo TSUJIMOTO<sup>1</sup>, Koichi TANAKA<sup>3</sup>

11:10 – 12:20  
<sup>1</sup>Department of Cancer Omics Research, World-Leading Drug Discovery Research Center, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, JAPAN, <sup>2</sup>Department of Urology, Graduate School of Medicine, Kyoto University, Kyoto, JAPAN, <sup>3</sup>Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, JAPAN

**PTu-083 Mass spectrometric determination of carcinoid syndrome tumor marker 5-HIAA in human serum**

11:10 – 12:20  
 Niina Tohmola<sup>1</sup>, Outi Itkonen<sup>2</sup>, Sakari Joenvaara<sup>1</sup>, Risto Renkonen<sup>1,2</sup>, Esa Hamalainen<sup>2</sup>  
<sup>1</sup>University of Helsinki, Helsinki, Finland, <sup>2</sup>Helsinki University Central Hospital, Helsinki, Finland

## Tuesday, 18<sup>th</sup> September

**PTu-084** Chip-based electrospray ionization tandem mass spectrometry a novel tool for rapid diagnostic of Fabry disease  
 13:30 – 14:40

MIRELA GALUSCA<sup>1</sup>, CORINA FLANGEA<sup>1</sup>, CRISTINA MOSOARCA<sup>1,2</sup>, CLAUDIA COZMA<sup>3</sup>, ALINA D ZAMFIR<sup>1</sup>

<sup>1</sup>Aurel Vlaicu University, Arad, Romania, <sup>2</sup>Physics Department, West University Timisoara, Vasile Parvan Blvd. 4, 300223, Timisoara, Romania,

<sup>3</sup>Laboratory of Analytical Chemistry and Biopolymer Structure Analysis, Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany

**PTu-085** Performance Evaluation of an Analytical LC-MS/MS Method for Accurate Measurement of 25-OH Vitamin-D in Serum  
 11:10 – 12:20

Heather Gamble, Changtong Hao, Sha Joshua Ye, George Scott IONICS Mass Spectrometry, Toronto, Canada

**PTu-086** Phosphoproteomic analysis of an EGFR/HER2 targeted drug-resistant gastric cancer cell line  
 13:30 – 14:40

Yong Yook Lee<sup>1</sup>, Minjueng Kang<sup>1</sup>, Byoung-Kyu Cho<sup>1</sup>, Hwang-Phill Kim<sup>2</sup>, Tae-You Kim<sup>2</sup>, Eugene C Yi<sup>1</sup>

<sup>1</sup>Molecular Medicine and Biopharmaceutical Sciences, Seoul National University, Seoul, Korea, <sup>2</sup>Cancer Research Institute, Seoul National University Hospital, Seoul, Korea

**PTu-087** A Fast Method for Quantitative Determination of Methotrexate in Human Serum by a LC-MS/MS  
 11:10 – 12:20

Sha Joshua Ye, Heather Gamble, George Scott IONICS Mass Spectrometry, Toronto, Canada

**PTu-088** Chip Based MicroLC-MS for Small Molecules Analysis  
 13:30 – 14:40

Remco van Soest<sup>1</sup>, Xiang Zhu<sup>1</sup>, Xiaohong Chen<sup>2</sup>, Nicole Hebert<sup>1</sup>, Hua-Fen Liu<sup>2</sup>  
<sup>1</sup>Eksigent/AB SCIEX, <sup>2</sup>AB SCIEX

**PTu-089** Accurate Mass LC-MS/MS Profiling of Synthetic Cannabinoids  
 11:10 – 12:20

Benjamin J Figard<sup>1</sup>, Christopher L Pennington<sup>2</sup>, Jeff Dahl<sup>3</sup>, Susan Leonard<sup>4</sup>, Jorge R Smith<sup>1</sup>  
<sup>1</sup>Shimadzu Scientific Instruments, South Central Region, Houston, TX, USA, <sup>2</sup>Rice University, Core Mass Spectrometry Facility, Houston, TX, USA, <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD, <sup>4</sup>Shimadzu Scientific Instruments, Marlborough, MA

**PTu-090** A simple GC/MS procedure for vitamin D metabolite analysis  
 13:30 – 14:40

Anna M Przyborowska<sup>1</sup>, Graham D Carter<sup>2</sup>, Julia C Jones<sup>2</sup>, John M Halket<sup>1,2,3</sup>  
<sup>1</sup>King's College London, UK, <sup>2</sup>Imperial College Healthcare NHS Trust, London, UK, <sup>3</sup>Imperial College, London, UK

**PTu-091** Highly sensitive method for arginine vasopressin in human plasma determined by LC-MS/MS  
 11:10 – 12:20

Shin-ichiro Nitta<sup>1</sup>, Yasuko Tsukazaki<sup>1</sup>, Naoto Senda<sup>1,5</sup>, Shigeru Yamada<sup>2</sup>, Kazunobu Yamamoto<sup>2</sup>, Mark M Garner<sup>3</sup>, Hesham Ghobarah<sup>3</sup>, Kunihiro Koriyama<sup>4</sup>, Kinya Kubo<sup>5</sup>  
<sup>1</sup>Mitsubishi Chemical Medience Corporation, Tsukuba, Japan, <sup>2</sup>AB SCIEX, Tokyo, Japan, <sup>3</sup>AB SCIEX, Toronto, Canada, <sup>4</sup>Shimadzu Corporation, Kyoto, Japan, <sup>5</sup>Chromosome Engineering Research Center, Tottori University, Tottori, Japan

## Session 20

### The Ion formation and Dissociation Mechanisms in MALDI

**PTu-092** More and Less Susceptible Amino Acid Residues to In-source Decay of Protein and Peptide in Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry  
 13:30 – 14:40

Mitsuo Takayama, Issei Osaka, Motoshi Sakakura, Ryunosuke Iimuro  
 Yokohama City University, Yokohama, Japan

**PTu-093** New MALDI matrices for negative-mode metabolomics  
 11:10 – 12:20

Stephan R Fagerer, Simone Nielsen, Alfredo J Ibanez, Renato Zenobi  
 ETH Zurich, Zurich, Switzerland

**PTu-094** Surface plasmon-induced cluster ion formation from Au, Ag, Pt, and Cu irradiated by visible laser  
 13:30 – 14:40

Dilshadbek T Usmanov, Lee Chuin Chen, Kenzo Hiraoka  
 University of Yamanashi, Kofu, Japan

**PTu-095** Design and synthesis of new efficient MALDI-MS matrices for low-molecular weight metabolites in negative ionization mode.  
 11:10 – 12:20

Mitsuru Shindo, Terai Yasuaki, Yukihira Daichi, Miura Saisuke, Fujimura Yoshinori, Matsumoto Kenji, Wariishi Hiroyuki  
 Kyushu University, Fukuoka, Japan

**PTu-096** Femtosecond Time-Resolved Mass Spectrometry for Desorption Dynamics of Tetracene Ion from Tetracene-doped Anthracene Crystals  
 13:30 – 14:40

Minagishi Yuuki, Morimoto Daisuke, Matsumoto Jun, Shiromaru Haruo, Hashimoto Kenro, Tatsuya Fujino  
 Tokyo Metropolitan University, Tokyo, Japan

**PTu-097** Matrix-assisted variable wavelength laser desorption ionization of peptides; Influence of the matrix absorption coefficient on expansion cooling  
 11:10 – 12:20

Sung Hee Ahn, Yong Jin Bae, Myung Soo Kim  
 Seoul National University, Seoul, Korea

**PTu-098** Accompanying Compounds induced dehydration of Reserpine in Matrix-assisted Laser Desorption/Ionization Process  
 13:30 – 14:40

Takehiro Watanabe, Tohru Yamagaki  
 Suntory institute for bioorganic research, Osaka, Japan

## Tuesday, 18<sup>th</sup> September

**PTu-100** Highly-Soft-Ionization of Organic Compounds and Polymers by Using Semiconductor Nanoparticels Sample Plate

13:30 – 14:40  
 Tetsu Yonezawa<sup>1</sup>, Hayashi Shinji<sup>2</sup>, Suganuma Takashi<sup>3</sup>,  
 Hideya Kawasaki<sup>3</sup>, Ryuichi Arakawa<sup>3</sup>  
<sup>1</sup>Hokkaido University, Sapporo, Hokkaido, Japan, <sup>2</sup>Kobe University, Kobe, Hyogo, Japan, <sup>3</sup>Kansai University, Suita, Osaka, Japan

**PTu-101** Desorption/Ionization efficiency of 20 common amino acids in SALDI-MS using platinum nanoflowers on silicon substrate

11:10 – 12:20  
 Shuhei Nitta, Hideya Kawasaki, Ryuichi Arakawa  
 Kansai University, Osaka, Japan

**PTu-102** Hydrogen Removing and Compound Properties of Aromatic Carboxylic Acids for Negative-ion Generation in Matrix-assisted Laser Desorption/Ionization Mass Spectrometry

13:30 – 14:40  
 Tohru Yamagaki, Takehiro Watanabe  
 Suntory Institute for Bioorganic Research, Osaka, Japan

**PTu-103** Matrix-assisted Laser Desorption Ionization Mass Spectrometry Using Cation-Substituted Zeolite Surface

11:10 – 12:20  
 Takashi Asano<sup>1</sup>, Junya Suzuki<sup>2</sup>, Tatsuya Fujino<sup>2</sup>  
<sup>1</sup>Metropolitan Police Department, Tokyo, Japan / Hokkaido University, Hokkaido, Japan, <sup>2</sup>Tokyo Metropolitan University, Tokyo, Japan

**PTu-104** Correlation of Ionized Carbohydrate Structure with Peak Intensity of Negative Ion Mass Spectrometry: First Principles Study

13:30 – 14:40  
 Hiromitsu Takaba<sup>1</sup>, Ryuji Miura<sup>1</sup>, Ai Suzuki<sup>1</sup>,  
 Nozomu Hatakeyama<sup>1</sup>, Kazuko Hirose<sup>2</sup>, Takashi Nishikaze<sup>2</sup>,  
 Junko Amano<sup>2</sup>, Akira Miyamoto<sup>1</sup>  
<sup>1</sup>Tohoku University, <sup>2</sup>The Noguchi Institute

**PTu-105** Statistical Investigation of Metabolite Structure to Reveal the Principle for Preferred Ionization in MALDI using 9-Aminoacridine

11:10 – 12:20  
 Daichi Yukihira, Yoshinori Fujimura, Mitsuru Shindo,  
 Daisuke Miura, Hiroyuki Wariishi  
 Kyushu University, Fukuoka, Japan

**PTu-106** Matrix clusters distribution from monomer to clusters with the mass at mega Dalton's region

13:30 – 14:40  
 Su-Hsueh Lai<sup>1,2</sup>, Kuang-Hua Chang<sup>1</sup>, Jung-Lee Lin<sup>1</sup>,  
 Chung-Hsuan Chen<sup>1,2</sup>  
<sup>1</sup>Genomics Research Center, Academia Sinica, Taipei, Taiwan, <sup>2</sup>Department of Chemistry, National Taiwan University, Taiwan

**PTu-107** The initial ion velocity of MALDI-TOFMS matrix DCTB and affect upon the mass accuracy of high molecular weight radical ions.

11:10 – 12:20  
 Mark F Wyatt<sup>1</sup>, Thorsten Jaskolla<sup>2</sup>  
<sup>1</sup>EPSRC Nat. Mass Spec. Service Centre, Swansea University, UK, <sup>2</sup>Institute of Medical Physics and Biophysics, University of Muenster, Germany

## Session 41

### Chemistries of Trapped Ions and their Applications to Biological Mass Spectrometry

**PTu-108** Gas-Phase Fragmentation of Reducing Sugar Modified Small Oligosaccharides

13:30 – 14:40  
 Chiharu Konda<sup>1</sup>, Brad Bendiak<sup>2</sup>, Yu Xia<sup>1</sup>  
<sup>1</sup>Purdue University, West Lafayette, IN, USA, <sup>2</sup>University of Colorado Denver, Aurora, CO, USA

**PTu-109** Radiosensitizers investigated using electrospray ionization mass spectrometry

11:10 – 12:20  
 Linda Feketeova<sup>1</sup>, Niels Bassler<sup>2</sup>, Brita S Sørensen<sup>2</sup>,  
 Michael R Horsman<sup>2</sup>, Jonathan White<sup>1</sup>, Richard A J O'Hair<sup>1</sup>  
<sup>1</sup>School of Chemistry, The University of Melbourne, Parkville, Victoria, Australia, <sup>2</sup>Department of Experimental Clinical Oncology, Aarhus University Hospital, Aarhus C, Denmark

## Session 42

### New Developments in Instruments and Detectors

**PTu-110** Expected possibilities of a new type gas-dynamic interface for preliminary separation and transportation of ions into a mass analyzer

13:30 – 14:40  
 Valeriy V Raznikov, Vladislav V Zelenov  
 The Branch of Institute for Energy Problems of Chemical Physics, Chernogolovka, Russia

**PTu-111** Dramatically Improved Hydrocarbons Analysis with the 5975-SMB GC-MS with Cold EI

11:10 – 12:20  
 Alexander B Fialkov, Aviv Amirav, Alexander Gordin  
 Tel Aviv University, Tel Aviv, Israel

**PTu-112** Suitability of dual solid probe FT-ICR-MS system for gas-phase acidity and basicity measurements of low volatile compounds.

13:30 – 14:40  
 Ivari Kaljurand, Ivo Leito, Ilmar A Koppel  
 University of Tartu, Tartu, Estonia

**PTu-113** Development of mass spectrometer equipped with ECRIS and its application to isotopic analysis of Mo

11:10 – 12:20  
 Tsuyoshi Nagamatsu<sup>1,2</sup>, Masanori Kidera<sup>1</sup>, Masayoshi Toda<sup>3</sup>,  
 Tatsuhiko Tanaka<sup>2</sup>, Kazuya Takahashi<sup>1</sup>  
<sup>1</sup>RIKEN, Wako, Japan, <sup>2</sup>Tokyo University of Science, Shinjuku-ku, Japan, <sup>3</sup>Tokyo University of Marine Science and Technology, Minato-ku, Japan

**PTu-114** Analysis of ion cloud dynamics in different geometry orbitrap mass-analyzers using Particle-in-Cell code based computer simulations

13:30 – 14:40  
 Gleb Vladimirov<sup>1,2</sup>, Eugene N Nikolaev<sup>1,2,3</sup>  
<sup>1</sup>Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia, <sup>2</sup>Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia, <sup>3</sup>Institute of biomedical chemistry, Russian Academy of Medical Sciences, Moscow, Russia

## Tuesday, 18<sup>th</sup> September

- PTu-115 Characteristics of a laser assisted vacuum-type electrospray droplet beam source**  
 11:10 – 12:20

Satoshi Ninomiya, Lee Chuin Chen, Yuji Sakai, Kenzo Hiraoka  
 University of Yamanashi, Kofu, Japan

- PTu-116 New plasma-based ion source mass spectrometer (ECRIS-MS) and its application to rapid detection of volatile compounds**  
 13:30 – 14:40

Tatsuya Urabe<sup>1</sup>, Masanori Kidera<sup>1</sup>, Yasuo Seto<sup>2</sup>, Kazuya Takahashi<sup>1</sup>, Michiko Kitagawa<sup>1</sup>  
<sup>1</sup>RIKEN, <sup>2</sup>National Research Institute of Police Science

- PTu-117 Adaptive Noise reduction in MALDI TOF Mass Spectrometers**  
 11:10 – 12:20

Ian Brookhouse, Andrew R Bowdler, Ian Sherwood  
 Kratos Analytical Ltd., Manchester, England

- PTu-118 Development of an ion transmission enhanced tandem ion guide system for triple quadrupole mass spectrometer**  
 13:30 – 14:40

DAISUKE OKUMURA, MANABU UEDA, TOMOHITO NAKANO  
 Shimadzu Co., Kyoto, Japan

- PTu-119 The A-Wave principle: new way to design ion guides and similar devices**  
 11:10 – 12:20

Alexander S Berdnikov<sup>1</sup>, Nicolay R Gall<sup>2</sup>

<sup>1</sup>Institute for Analytical Instrumentation, St.Petersburg, Russian Federation,  
<sup>2</sup>Ioffe's Physical and Technical Institute RAS, St.Petersburg, Russian Federation

- PTu-120 COUPLING OF AN INERT ION CHROMATOGRAPHIC SYSTEM WITH ICP-Q-MS FOR ROBUST AND ACCURATE ELEMENTAL SPECIATION**  
 13:30 – 14:40

Tomoko Vincent<sup>1</sup>, Daniel Kutscher<sup>1</sup>, Lothar Rottmann<sup>1</sup>,

Julian Wills<sup>1</sup>, Shona McSheehy<sup>1</sup>, Detlef Jenen<sup>2</sup>

<sup>1</sup>Thermo Fisher Scientific, Bremen, Germany, <sup>2</sup>Dionex, Switzerland

- PTu-121 A Two-Dimensional Particle Tracking Velocimetry Investigation for Visualization of Gas Flow inside the Ion Funnel**  
 11:10 – 12:20

Diamantis Kounadis<sup>1</sup>, Dimitris Papanastasiou<sup>1</sup>,  
 Ioannis Orfanopoulos<sup>1</sup>, Alexander Lekkas<sup>1</sup>, Ioannis Nikolos<sup>2</sup>,  
 Emmanuel Raptakis<sup>1</sup>

<sup>1</sup>Fasmatech Science and Technology SA, Athens, Greece, <sup>2</sup>Technical University of Crete, Department of Production Engineering and Management, Chania, Crete, Greece

- PTu-122 Source Cleaning in Maldi Mass Spectrometers by UV Laser Desorption**  
 13:30 – 14:40

John M Allison, Andrew Eaton  
 Kratos Analytical Ltd

- PTu-123 Compensating for Space Charge Effects and Increasing the Mass Accuracy and Dynamic Range of Quadrupole Ion Trap Mass Spectrometers**  
 11:10 – 12:20

Jae Schwartz, Philip M Remes  
 Thermo Fisher Scientific, San Jose USA/CA

- PTu-124 Further expansion of the MCP ion detector output linearity using a current buffering concept.**  
 13:30 – 14:40

ETSUO IIZUKA, MOTOHIRO SUYAMA, TOSHIYUKI UCHIYAMA, YUYA WASHIYAMA, KATSUYUKI ISHIGURO  
 HAMAMATSU PHOTONICS K. K., IWATA, JAPAN

- PTu-125 Sensitivity improvement of MCP-based Ion Detectors for Mass Spectrometry**  
 11:10 – 12:20

Masahiro Hayashi<sup>1</sup>, Yuya Washiyama<sup>1</sup>, Tetsuya Matsushita<sup>1</sup>, Akio Suzuki<sup>1</sup>, Shigetomo Shiki<sup>2</sup>, Masataka Ohkubo<sup>2</sup>

<sup>1</sup>Hamamatsu Photonics K.K., Hamamatsu, Japan, <sup>2</sup>National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

- PTu-126 Round Focusing Magnetic Prisms for Surface Treatment Devices**  
 13:30 – 14:40

Valentina A Mikhalevich, Viacheslav D Sachenko  
 Institute for Analytical Instrumentation of RAS, St.Petersburg, Russia

- PTu-127 From conventional Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) to a universal trace gas analyzer**  
 11:10 – 12:20

Lukas Märk<sup>1</sup>, Alfons Jordan<sup>1</sup>, Achim Edtbauer<sup>1</sup>, Eugen Hartungen<sup>1</sup>, Simone Jürschik<sup>1</sup>, Philipp Sulzer<sup>1</sup>, Tilmann D Märk<sup>1,2</sup>

<sup>1</sup>IONICON Analytik GmbH, Innsbruck, Austria, <sup>2</sup>Institut für Ionenphysik und Angewandte Physik / Leopold Franzens Universität Innsbruck, Innsbruck, Austria

- PTu-128 A Novel Precursor Isolation Method using Digital Ion Trap Mass Spectrometer**  
 13:30 – 14:40

Kei Kodera, Masafumi Jinno, Kiyoshi Watanabe, Makoto Hazama, Masaji Furuta, Sadanori Sekiya, Kaori Kinoshita, Hidenori Takahashi, Kosuke Hosoi, Toshinori Kobayashi, Shinichi Iwamoto, Koichi Tanaka  
 Shimadzu Co., Kyoto, Japan

- PTu-129 A high accuracy FDM field solver for prediction of non-linear resonances in electrodynamic ion traps.**  
 11:10 – 12:20

Matthew C Gill<sup>1</sup>, Alexander Berdnikov<sup>2</sup>, Roger Giles<sup>1</sup>

<sup>1</sup>Shimadzu Research Laboratory (Europe) LTD, Manchester, UK, <sup>2</sup>Institute for Analytical Instrumentation, Rizhskij pr. 26, 190103, St. Petersburg, Russia.

- PTu-130 More than one order of magnitude higher sensitivities with Proton-Transfer-Reaction Time-of-Flight Mass Spectrometry (PTR-TOFMS)**  
 13:30 – 14:40

Eugen Hartungen<sup>2</sup>, Alfons Jordan<sup>2</sup>, Achim Edtbauer<sup>2</sup>, Akio Shimono<sup>1</sup>, Simone Jürschik<sup>2</sup>, Philipp Sulzer<sup>2</sup>, Lukas Märk<sup>2</sup>, Tilmann D Märk<sup>2,3</sup>

<sup>1</sup>Shoreline Science Research Inc., Tokyo, Japan, <sup>2</sup>IONICON Analytik GmbH, Innsbruck, Austria, <sup>3</sup>Institut für Ionenphysik und Angewandte Physik / Universität Innsbruck, Innsbruck, Austria

- PTu-131 A curtain-gas filter that widely protects a mass spectrometer from neutral molecule contaminations**  
 11:10 – 12:20

Hermann Wollnik, Gary Eiceman, Alexander Tarassov, Ryan Blase, Stephen Devila  
 New Mexico State University, Las Cruces, USA

## Tuesday, 18<sup>th</sup> September

### **PTu-132 High Mass Microscope-mode MALDI Imaging Mass Spectrometry**

13:30 – 14:40  
 Yuto Yanagihara<sup>1</sup>, Masahiro Hayashi<sup>1</sup>, Yasuhide Naito<sup>2</sup>  
<sup>1</sup>Hammatsu Photonics K.K., Iwata, Japan, <sup>2</sup>GPI, Hamamatsu, Japan

### **PTu-133 Analysis of neurosteroids by GC-APPI-MS/MS**

11:10 – 12:20  
 Tina J Suominen, Markus Haapala, Anna Takala,  
 Raimo A Ketola, Risto Kostiainen  
 Helsinki University, Helsinki, Finland

### **PTu-134 Potential of direct probe for drug and pharmaceutical**

13:30 – 14:40  
 HARUO HOSODA, NORIYUKI IWASAKI, JOUJI SETA,  
 YOSHIHIKO MORISHITA  
 Bruker Daltonics k.k., Yokohama, Japan

### **PTu-135 Development of high-speed data-streaming system for time-of-flight mass spectrometry**

11:10 – 12:20  
 Ken-ichi Bajo<sup>1</sup>, Osamu Fujioka<sup>2</sup>, Shingo Ebata<sup>1</sup>, Morio Ishihara<sup>3</sup>,  
 Kiichiro Uchino<sup>4</sup>, Hisayoshi Yurimoto<sup>1</sup>  
<sup>1</sup>Hokkaido University, Sapporo, Japan, <sup>2</sup>National Instruments Japan Corporation, Tokyo, Japan, <sup>3</sup>Osaka University, Toyonaka, Japan, <sup>4</sup>Kyushu University, Kasuga, Japan

### **PTu-136 Mass coverage range enhancement of reflectron time-of-flight mass spectrometers by superconducting nano-stripline detectors**

13:30 – 14:40  
 Nobuyuki Zen<sup>1</sup>, Koji Suzuki<sup>1</sup>, Shigetomo Shiki<sup>1</sup>,  
 Masahiro Ukibe<sup>1</sup>, Masaki Koike<sup>1</sup>, Alessandro Casaburi<sup>2</sup>,  
 Mikkel Ejrnaes<sup>2</sup>, Roberto Cristiano<sup>2</sup>, Masataka Ohkubo<sup>1</sup>  
<sup>1</sup>National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, <sup>2</sup>National Research Council, Pozzuoli, Italy

### **PTu-137 An Improvement of MCP Dynamic Range for TOF MS Application**

11:10 – 12:20  
 Yusuke Hayase, Uchiyama Toshiyuki, Ishiguro Katsuyuki  
 Hamamatsu Photonics, Iwata, Japan

## Session 44

### Ambient Ionization

### **PTu-138 Specific analyte ionization using negative atmospheric ions formed in atmospheric pressure corona discharges**

13:30 – 14:40  
 Kanako Sekimoto, Mitsuo Takayama  
 Yokohama City University, Yokohama, Japan

### **PTu-139 Probe Electrospray and Nanoelectrospray Ionization for Direct Biomolecule Analysis and Cancer Diagnostics**

11:10 – 12:20  
 Mridul Kanti Mandal<sup>1</sup>, Lee Chuin Chen<sup>2</sup>, Kentaro Yoshimura<sup>3</sup>,  
 Subhrakanti Saha<sup>1</sup>, Obaidur Rahman<sup>1</sup>, Matiur Rahman<sup>1</sup>,  
 Yasuo Shida<sup>1</sup>, Satoshi Ninomiya<sup>2</sup>, Sen Takeda<sup>3</sup>, Kenzo Hiraoka<sup>1</sup>  
<sup>1</sup>Clean Energy Research Center, University of Yamanashi, Japan,  
<sup>2</sup>Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, Japan, <sup>3</sup>Department of Anatomy and Cell Biology, Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, Japan

### **PTu-140 Development of ultra high sensitive ambient ionization mass spectrometry using Leidenfrost phenomenon-assisted thermal desorption**

13:30 – 14:40  
 Subhrakanti Saha<sup>1</sup>, Lee Chuin Chen<sup>2</sup>, Mridul Kanti Mandal<sup>1</sup>,  
 Kenzo Hiraoka<sup>1</sup>  
<sup>1</sup>Clean Energy Research Center, University of Yamanashi, Japan,  
<sup>2</sup>Interdisciplinary Graduate School of Medicine and Engineering, University of Yamanashi, Japan

### **PTu-141 Scanning Probe Electrospray Ionization for Ambient Mass Spectrometry**

11:10 – 12:20  
 Yoichi Otsuka<sup>1</sup>, Sayuri Shide<sup>2</sup>, Junpei Naito<sup>1</sup>,  
 Masafumi Kyogaku<sup>1</sup>, Hiroyuki Hashimoto<sup>1</sup>, Ryuichi Arakawa<sup>2</sup>  
<sup>1</sup>Frontier Research Center, Canon Inc., Tokyo, Japan, <sup>2</sup>Faculty of Chemistry, Materials and Bioengineering, Kansai University, Osaka, Japan

### **PTu-142 Simultaneous Ionization of Nonpolar and Polar Compounds by Laser Ablation Electrospray Ionization with Heated Gas Jet**

13:30 – 14:40  
 Anu Vaikkinen<sup>1</sup>, Bindesh Shrestha<sup>2</sup>, Akos Vertes<sup>2</sup>,  
 Risto Kostiainen<sup>1</sup>, Tiina J Kauppila<sup>1</sup>  
<sup>1</sup>University of Helsinki, Helsinki, Finland, <sup>2</sup>George Washington University, Washington DC, USA

### **PTu-143 Desorption atmospheric pressure photoionization-mass spectrometry for direct analysis of tetrahydrocannabinol from Cannabis sativa samples**

11:10 – 12:20  
 Tiina J Kauppila<sup>1</sup>, Anu Flink<sup>1</sup>, Ulla-Maija Laakkonen<sup>2</sup>,  
 Laura Aalberg<sup>2</sup>, Raimo A Ketola<sup>1</sup>  
<sup>1</sup>University of Helsinki, Helsinki, Finland, <sup>2</sup>National Bureau of Investigation, Vantaa, Finland

### **PTu-144 Open Spot Ambient Ionization Technology for Near-Instant Determination of Sample Characteristics by using DART-MS**

13:30 – 14:40  
 Musselman D Brian, Joseph LaPointe, Elizabeth Crawford  
 IonSense, Inc.

### **PTu-145 Plasma pencil atmospheric mass spectrometry for the detection and measurement of micronutrients in complex solutions**

11:10 – 12:20  
 Lo Edward, Maria J Stein, David G Castner, Buddy D Ratner  
 University of Washington, Seattle, United States of America

### **PTu-146 Rapid screening and quantitation of pesticides in fruit commodities by Direct Analysis in Real Time (DART) ambient ionization mass spectrometry**

13:30 – 14:40  
 Elizabeth A Crawford, Brian D Musselman  
 IonSense, Inc., Saugus, MA, USA

## Tuesday, 18<sup>th</sup> September

**PTu-147** Study of fragmentaion behaviors for atmospheric negative ion adducts of phenylalanine homologues using atmospheric pressure corona discharge ionization mass spectrometry  
 11:10 – 12:20

Natsuki Matsuda, Nami Sugasawa, Chika Mifune, Kanako Sekimoto, Mitsuo Takayama  
 Yokohama City University, Yokohama, Japan

**PTu-148** Unusual radial cation formation of arginine by atmospheric pressure corona discharge ionization (APCDI)  
 13:30 – 14:40

Atsushi Wada, Kanako Sekimoto, Mitsuo Takayama  
 Yokohama City University, Yokohama, Japan

**PTu-149** Theoretical and experimental studies of ionization of explosive compounds using dielectric barrier discharge ionization  
 11:10 – 12:20

Hirotaka Yabushita<sup>1</sup>, Hirofumi Nagao<sup>1</sup>, Toshinobu Hondo<sup>1</sup>, Michisato Toyoda<sup>2</sup>  
<sup>1</sup>HORIBA STEC, Co., Ltd., Kyoto, Japan, <sup>2</sup>Osaka University, Osaka, Japan

**PTu-150** Quantification of six anti-diabetic drugs in human plasma by indirect spray FT ICR mass spectrometry  
 13:30 – 14:40

Wan Li, T W Dominic Chan  
 The University of Hong Kong, Hong Kong, China

**PTu-151** Physical process hierarchy in ion movement inside a gas dynamic interface for the mass-spectrometer with ambient ionization.  
 11:10 – 12:20

Nicolay R Gall<sup>1</sup>, Alexander S Berdnikov<sup>2</sup>, Lidia N Gall<sup>2</sup>  
<sup>1</sup>Ioffe Physico Technical Inst. of Russian Academt of Sciences, St.Petersburg, Russia,, <sup>2</sup>Institute for Analytical Instrumentation, St.Petersburg, Russia

**PTu-152** Using Thin Layer Chromatography Spray (TLC spray) Ionization Mass Spectrometry to Analyze Drugs in Whole Blood  
 13:30 – 14:40

Yi-Tzu Cho<sup>1</sup>, Chu-Nian Cheng<sup>2</sup>, Hung Su<sup>2</sup>, Jentiae Shiea<sup>\*2</sup>  
<sup>1</sup>Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan,  
<sup>2</sup>National Sun Yat-Sen Univ., Kaohsiung, TAIWAN

**PTu-153** Ambient surface mass spectrometry of polymers and molecules using PADI - Optimising parameters, improving repeatability and damage effects  
 11:10 – 12:20

Tara L Salter, Ian S Gilmore  
 National Physical Laboratory, Teddington, UK

**PTu-154** Thermal Dissociation Atmospheric Chemical Ionization Mass Spectrometry with a Miniature Source for Selective Trace Detection of Dimethoate in Fruit Juices  
 13:30 – 14:40

yongzhong ouyang, Tiqiang zhang, Tenggao Zhu, Huanwen Chen  
 East China Institute of Technology, Nanchang, P.R. China

**PTu-155** Mass analysis of the ions generated by corona discharge ionizers in ambient air  
 11:10 – 12:20

Kenichi Nagato  
 Kochi National College of Technology, Nankoku, Japan

**PTu-156** Rapid Screening of Camphor Wood by Surface Desorption Atmospheric Pressure Chemical Ionization Mass Spectrometry  
 13:30 – 14:40

Jianping Yan, Huanwen Chen  
 Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology, Nanchang, Jiangxi, China

**PTu-157** Hydrocarbons Analysis by Desorption Atmospheric Pressure Chemical Ionization  
 11:10 – 12:20

Fred Paul mark Jjunju Jjunju<sup>1,2</sup>, Badu\_Tawiah K Abraham<sup>2</sup>, Li Anyin<sup>2</sup>, Roqan S Iman<sup>1</sup>, Graham R Cooks<sup>2</sup>

<sup>1</sup>King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division, Thuwal 23955-6900, Saudi Arabia,  
<sup>2</sup>Department of Chemistry Purdue University

**PTu-158** Rapid Detection of Bacterial Lipids, Metabolites and Signalling Compounds by Liquid Extraction Surface Analysis Mass Spectrometry  
 13:30 – 14:40

Martin R Paine<sup>1</sup>, Nicole A Pianegonda<sup>1</sup>, Philip J Barker<sup>2</sup>, Todd W Mitchell<sup>1</sup>, Michael J Manefield<sup>3</sup>, Scott A Rice<sup>3</sup>, Stephen J Blanksby<sup>1</sup>

<sup>1</sup>University of Wollongong, Wollongong, Australia, <sup>2</sup>BlueScope Steel Research, Port Kembla, Australia, <sup>3</sup>University of New South Wales, Sydney, Australia

**PTu-159** A hydrodynamically optimized nanoelectrospray source with 100% transmission  
 11:10 – 12:20

Matthias Pauly<sup>1</sup>, Mario Sroka<sup>2</sup>, Stephan Rauschenbach<sup>1</sup>, Julius Reiss<sup>2</sup>, Gordon Rinke<sup>1</sup>, Alyazan Albargash<sup>1</sup>, Jörn Sesterhenn<sup>2</sup>, Klaus Kern<sup>1</sup>

<sup>1</sup>Max Planck Institute for Solid State Research, Stuttgart, Germany, <sup>2</sup>Technical University Berlin, Berlin, Germany

**PTu-160** Direct analysis of asphaltene by DART FT MS  
 13:30 – 14:40

Hugues PREUD'HOMME<sup>1</sup>, Felipe CARDOSO<sup>2,3</sup>, Bruno GRASSL<sup>4</sup>, Brice BOUSSIÈRE<sup>1</sup>, Hervé CARRIER<sup>2</sup>  
<sup>1</sup>IPREM / LCABIE, University of Pau, Pau, France, <sup>2</sup>LFC-R, UMR 5150, University of Pau, Pau France, <sup>3</sup>Centro de Pesquisas Leopoldo Americo Miquez de Mello, PETROBRAS/CENPES, Rio de Janeiro, Brazil, <sup>4</sup>IPREM / ECP, UMR 5254, University of Pau, France

## Session 45

### Cell Biology / Cellular Pathways

**PTu-161** BRIDGING BETWEEN LIFE SCIENCES AND MATERIAL SCIENCES: MASS SPECTROMETRIC PROTEIN AND METABOLITE ANALYSIS FOR THE PRODUCTION OF BIO-BASED CHEMICALS  
 11:10 – 12:20

Michiel Akeroyd, Rob van der Hoeven, Rene Verwaal, Stefan Turk, Fredoen Valianpour, Marcel Tilborg, Maurien Olsthoorn  
 DSM Biotechnology Center / Delft / The Netherlands

## Tuesday, 18<sup>th</sup> September

### **PTu-162 Large Bio-particle Detection Technologies and Their Applications**

13:30 – 14:40  
Chung Hsuan Chen  
Genomics Research Center/Academia Sinica, Taipei, Taiwan

### **PTu-163 Comparison between Single-cell and traditional MALDI-MS-based workflows for metabolome studies in *Saccharomyces cerevisiae*.**

Alfredo J Ibanez<sup>1</sup>, Stephan R Fagerer<sup>1</sup>, Matthias Heinemann<sup>2</sup>, Renato Zenobi<sup>1</sup>  
<sup>1</sup>ETH Zurich, Zurich, Switzerland, <sup>2</sup>University of Groningen, Groningen, The Netherlands

### **PTu-164 The Cuticular Structure and Lipid Composition of *Arabidopsis thaliana* Organs and Cells Determined by TOF-SIMS**

Gregory L Fisher<sup>1</sup>, Philip C Wong<sup>2</sup>, Christopher Buschhaus<sup>2</sup>, John Hammond<sup>1</sup>, Reinhard Jetter<sup>2</sup>  
<sup>1</sup>Physical Electronics, Minnesota, USA, <sup>2</sup>University of British Columbia, British Columbia, Canada

### **PTu-166 Proteomic Interrogation of MDSC Exosomes by Bottom-up, Middle-out and Top-down strategies**

Catherine Fenselau<sup>1</sup>, Meghan Burke<sup>1</sup>, Waeowalee Chokswangarn<sup>1</sup>, Avantika Dhabaria<sup>1</sup>, Joseph Cannon<sup>1</sup>, Suzanne Ostrand-Rosenberg<sup>2</sup>  
<sup>1</sup>University of Maryland, College Park MD, USA, <sup>2</sup>University of Maryland, Baltimore County, USA

### **PTu-167 Identification of novel cytokinin degradation pathway during adventitious caulogenesis in *Pinus pinea* L. cotyledons with quadrupole-time of flight mass spectrometry**

Ondrej Novak<sup>2</sup>, Candela Cuesta<sup>3</sup>, Karel Dolezal<sup>[1,2]</sup>, Lucie Szucova<sup>2</sup>, Lukas Spichal<sup>2</sup>, Belén Fernández<sup>3</sup>, Ana Rodríguez<sup>3</sup>, Miroslav Strnad<sup>2</sup>  
<sup>1</sup>Institute of Experimental Botany AS CR, Czech Republic, <sup>2</sup>Laboratory of Growth Regulators, Faculty of Science, Palacky University & Institute of Experimental Botany AS CR, Slechtitelu 11, Olomouc, CZ-783 71, Czech Republic, <sup>3</sup>Área de Fisiología Vegetal, Departamento Biología de Organismos y Sistemas, Instituto de Biotecnología de Asturias, Universidad de Oviedo, Oviedo, E-33071, Spain.

### **PTu-168 Activation Kinetics and Dimerization of STAT5 Proteins Followed by Quantitative Mass Spectrometry**

Martin E Boehm, Lorenz Adlung, Marcel Schilling, Ursula Klingmueller, Wolf-Dieter Lehmann  
German Cancer Research Center Heidelberg

### **PTu-169 Lapatinib-resistant gastric cancer cells express cancer stem cell-like cell surface antigens**

Minjueng Kang<sup>1</sup>, Hwang-Phill Kim<sup>2</sup>, Young-dong Yoo<sup>1</sup>, Yong-Tae Kwon<sup>1</sup>, Tae-You Kim<sup>1,2</sup>, Eugene C Yi<sup>1</sup>  
<sup>1</sup>Molecular Medicine and Biopharmaceutical Sciences, Seoul National University, Seoul, Korea, <sup>2</sup>Cancer Research Institute, Seoul National University Hospital, Seoul, Korea

### **PTu-170 Tissue specific profiling of the *Arabidopsis thaliana* auxin metabolome**

13:30 – 14:40  
Ondrej Novak<sup>1,2</sup>, Eva Henykova<sup>1,2</sup>, Ilkka Sairanen<sup>2</sup>, Mariusz Kowalczyk<sup>2</sup>, Tomas Pospisil<sup>3</sup>, Karin Ljung<sup>2</sup>  
<sup>1</sup>Palacky University & Institute of Experimental Botany AS CR, Olomouc, Czech Republic, <sup>2</sup>Umeå Plant Science Centre, Umeå, Sweden, <sup>3</sup>Centre of the Region Hana for Biotechnological and Agricultural Research, Faculty of Science, Olomouc, Czech Republic

### **PTu-171 In Situ Pressure Probe Picoliter Single-Cell Sap Sampling and Mass Spectrometry Metabolite Profiling of Living Plants**

11:10 – 12:20  
Yousef Gholipour<sup>1</sup>, Rosa Erra-Balsells<sup>2</sup>, Hiroshi Nonami<sup>1</sup>  
<sup>1</sup>Ehime University, Matsuyama, Japan, <sup>2</sup>University of Buenos Aires, Argentina

### **PTu-172 In-situ Analysis of Plant Bioactive Molecules by Live Single-cell Mass Spectrometry**

13:30 – 14:40  
Shuichi Matsuda<sup>1</sup>, Sachiko Date<sup>2</sup>, Hajime Mizuno<sup>1</sup>, Naohiro Tsuyama<sup>1</sup>, Takanori Harada<sup>1</sup>, Tsutomu Masujima<sup>1,2</sup>  
<sup>1</sup>Graduate School of Biomedical Sciences, Hiroshima University, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center (QBIC), RIKEN, JAPAN

### **PTu-174 2D-DIGE analysis of the role of S-nitrosoglutathione reductase in lipopolysaccharide-challenged mice**

13:30 – 14:40  
Kentaro Ozawa<sup>1</sup>, Hiroki Tsumoto<sup>1</sup>, Wei Wei<sup>2</sup>, Chi-Hui Tang<sup>2</sup>, Akira T Komatsubara<sup>3</sup>, Hiroto Kawafune<sup>3</sup>, Kazuharu Shimizu<sup>1,4</sup>, Limin Liu<sup>2</sup>, Gozoh Tsujimoto<sup>1,3</sup>  
<sup>1</sup>World-Leading Drug Discovery Research Center, Kyoto University, Kyoto, Japan, <sup>2</sup>Department of Microbiology and Immunology, University of California, San Francisco, USA, <sup>3</sup>Department of Genomic Drug Discovery Science, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan, <sup>4</sup>Department of Nanobio Drug Discovery, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan

### **PTu-175 Proteomic analysis of low temperature resistant system in bacteria**

11:10 – 12:20  
Kadoya Ryosuke, Kasahara Yasuhiro  
Hokkaidou University, Sapporo, Japan

### **PTu-176 IgSF11 is a member of the immunoglobulin superfamily that promotes both neuronal adhesion and cell proliferation**

13:30 – 14:40  
Erika Hayashi<sup>1</sup>, Hiroaki Akutsu<sup>2</sup>, Hiroshi Funakoshi<sup>2</sup>, Yokichi Hayashi<sup>2</sup>  
<sup>1</sup>Hokkaido University, Sapporo, Japan, <sup>2</sup>Asahikawa Medical University, Asahikawa, Japan

### **PTu-177 Live Single-cell Mass Spectrometry for Tracing Metabolic Processes in Organelle**

11:10 – 12:20  
HAJIME MIZUNO<sup>1</sup>, NAOHIRO TSUYAMA<sup>1</sup>, SACHIKO DATE<sup>2</sup>, TAKANORI HARADA<sup>1</sup>, TSUTOMU MASUJIMA<sup>1,2</sup>  
<sup>1</sup>Hiroshima University, Hiroshima, Japan, <sup>2</sup>QBIC, RIKEN, Osaka, Japan

### **PTu-178 Development of Micro-area-specific Extracting Analysis for Molecules in Tissue Section**

13:30 – 14:40  
Sachiko DATE<sup>1</sup>, Tsutomu MASUJIMA<sup>1,2</sup>  
<sup>1</sup>RIKEN QBIC, Osaka, Japan, <sup>2</sup>Hiroshima University, Hiroshima, Japan

Tuesday, 18<sup>th</sup> September

TUE

**PTu-179 In-situ Analysis of Phototropic Molecules in plant by Live Single-cell Mass Spectrometry**

11:10 – 12:20  
TAKASHI FUJII<sup>1</sup>, SACHIKO DATE<sup>2</sup>, HAJIME MIZUNO<sup>1</sup>, NAOHIRO TSUYAMA<sup>1</sup>, TSUTOMU MASUJIMA<sup>1,2</sup>  
<sup>1</sup>Hiroshima University, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center (QBIC), RIKEN, JAPAN

**PTu-180 Analysis of Specific Molecules in Allergic Granule by Live Single-cell Mass Spectrometry**

13:30 – 14:40  
YUKI YAMAMOTO<sup>1</sup>, SACHIKO DATE<sup>2</sup>, HAJIME MIZUNO<sup>1</sup>, NAOHIRO TSUYAMA<sup>1</sup>, TSUTOMU MASUJIMA<sup>1,2</sup>  
<sup>1</sup>Hiroshima University, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center (QBIC), RIKEN, JAPAN

**PTu-181 Time Dependent Changes of Intracellular-Signal-Relating Small Compounds in Allergy Model Cell Line, RBL-2H3**

11:10 – 12:20  
Toshiya Shinasue<sup>1</sup>, Yui Okamura<sup>1</sup>, Hajime Mizuno<sup>1</sup>, Naohiro Tsuyama<sup>1</sup>, Sachiko Date<sup>2</sup>, Tsutomu Masujima<sup>1,2</sup>  
<sup>1</sup>Graduate School of Biomedical Sciences, Hiroshima University, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center, RIKEN, Japan

**PTu-182 Brain proteomics reveals early molecular signature of pathology in pre-symptomatic mouse model of Alzheimer's disease**

13:30 – 14:40  
Hongqian Yang<sup>1</sup>, Jessica L Witnman<sup>2</sup>, Roman A Zubarev<sup>1,3</sup>, Thomas A Bayer<sup>2</sup>

<sup>1</sup>Karolinska Institute, Stockholm, Sweden, <sup>2</sup>University Medicine Göttingen, Göttingen, Germany, <sup>3</sup>Science for Life Laboratory, Stockholm, Sweden

**PTu-184 Realtime molecular analysis of allergenic response in single mast cell by fluorescence probe-assisted Live Single-cell MS**

13:30 – 14:40  
Yosuke Kawai<sup>1</sup>, Naohiro Tsuyama<sup>1</sup>, Hajime Mizuno<sup>1</sup>, Sachiko Date<sup>2</sup>, Tsutomu Masujima<sup>1,2</sup>  
<sup>1</sup>Hiroshima University Graduate School of Biomedical & Health Sciences, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center (QBIC), RIKEN, Osaka, Japan

**PTu-185 A host-pathogen interaction network study of *Shigella flexneri* infection of human cells targeting key metabolic enzymes**

11:10 – 12:20  
Asa Wahlander<sup>1</sup>, Bernd Roschitzki<sup>1</sup>, Paolo Nanni<sup>1</sup>, Claudia Fortes<sup>1</sup>, Christian Trachsel<sup>1</sup>, Nicole Freed<sup>2</sup>, Simon Barkow-Oesterreicher<sup>1</sup>, Christian Panse<sup>1</sup>, Jonas Grossmann<sup>1</sup>, Petra Tienz<sup>2</sup>, Dirk Bumann<sup>2</sup>, Ralph Schlapbach<sup>1</sup>  
<sup>1</sup>Functional Genomics Center Zurich, FGCZ, <sup>2</sup>Infection Biology Biozentrum, University Basel, Basel, Switzerland

**PTu-186 A highly specific and sensitive determination of the sterols in silkworm larva by HPLC/APCI-MS/MS for the investigation to insect steroidogenesis.**

13:30 – 14:40  
Fumihiko Igarashi, Juri Hikiba, Takayoshi Nakaoka, Minoru Suzuki, Hiroshi Kataoka  
Department of Integrated Biosciences, Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan.

**Polymer sciences**

**PTu-187 Evolved gas analysis of a Japanese lacquer film**

11:10 – 12:20  
Noriyasu Niimura  
JEOL, Tokyo, Japan

**PTu-188 Structural characterization of ethylene-vinyl acetate copolymers using high-resolution MALDI-TOFMS with a spiral ion trajectory**

Hiroaki Sato<sup>1</sup>, Hidenobu Aizawa<sup>1</sup>, Sayaka Nakamura<sup>1</sup>, Takafumi Sato<sup>2</sup>

<sup>1</sup>National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, <sup>2</sup>JEOL Ltd., Akishima, Japan

**PTu-189 Determination of Volatile Organic Compounds in Polypropylene Raw Materials by Thermal Desorption-Gas Chromatography/Mass Spectrometry and Head Space-Gas Chromatography-Mass/Spectrometry**

11:10 – 12:20  
Shuqi Sun, Ying Zhang, Song Chen, Yang Song  
SINOPEC Beijing Research Institute of Chemical Industry, Beijing, China

**PTu-190 Characterization of a multi-component liquid crystalline copolyester by high-resolution MALDI-spiral-TOF-MS**

13:30 – 14:40  
Banri Hashimoto, Takanori Sasaki, Hajime Ohtani  
Nagoya Institute of Technology, Aichi, Japan

**PTu-191 Mass-analysis of enzymatic hydrolysis of nylon by argon cluster SIMS**

11:10 – 12:20  
Kensuke Iuchi, Kosuke Moritani, Kozo Mochiji, Keisuke Nagai, Kazuki Iida, Seiji Negoro  
University of Hyogo, Hyogo, Japan

**PTu-192 Characterization of poly(ethylene oxide-propylene oxide) alkyl ether (R-EO-PO) copolymer by LC-ESI-MS**

13:30 – 14:40  
Haruka Yamada<sup>1</sup>, Hirotaka Hisatomi<sup>1</sup>, Mendra Ritonga<sup>2</sup>, Sana Ito<sup>2</sup>, Masaki Morita<sup>2</sup>, Hideya Kawasaki<sup>1</sup>, Ryuichi Arakawa<sup>1</sup>  
<sup>1</sup>Kansai University, Suita, Japan, <sup>2</sup>Niitaka Co., Ltd., Osaka, Japan

**PTu-193 Novel Method for Verification of Trace Amounts of Polymer Contaminants in Photoresist Solution**

11:10 – 12:20  
Min-Soo Suh, Da-Hee Lee, Taehyo Choi, Minjung Kim, Dongju Oh, Jung Dae Park, Pilkwon Jun, Jong Soo Kim  
Samsung Electronics, Hwasung, Korea

**PTu-194 Differential Analysis in sulfenamide-based vulcanizing accelerators for rubber products by High mass Accuracy MS and Multivariate Statistical Technique**

13:30 – 14:40  
Takahiro Goda, Hiroki Nakajima, Satoshi Yamaki, Tsutomu Nishine, Masaru Furuta, Naoki Hamada  
Shimadzu Co., Kyoto, Japan

Tuesday, 18<sup>th</sup> September

- PTu-195** Diagnostics of degradation levels for thermoplastics using pyrolysis-GCxGC-TOFMS  
11:10 – 12:20

Fumie Kabashima, Fumihiko Tsuchiya  
LECO Japan Corporation

**Others**

- PTu-196** Yellow Sand and Seawater Interaction from viewpoint of Silica Speciation  
13:30 – 14:40

Miho Tanaka<sup>1</sup>, Kazuya Takahashi<sup>2</sup>  
<sup>1</sup>Tokyo University of Marine Science and Technology, Tokyo, Japan, <sup>2</sup>RIKEN, Wako, Japan

- PTu-197** High Plasmalogen Content in the Gut of Silkworm (*Bombyx mori*)  
11:10 – 12:20

Takako Aboshi, Ritsuo Nishida, Naoki Mori  
Kyoto University

- PTu-198** Characterization on Oxidation and Hydrolysis of Titanium Ion Using ESI-MS  
13:30 – 14:40

Io Ryumae, Miho Tanaka  
Tokyo University of Marine Science and Technology

- PTu-199** The Development of Multi Elemental Analysis of Ferromanganese Nodule by LA-ICP-MS  
11:10 – 12:20

Junichi Hirata, Miho Tanaka

Tokyo University of Marine Science and Technology, Tokyo, Japan

- PTu-200** Study on Reaction Process of the Complexation of Silicomolybdic and Phosphomolybdic Acids by ESI-MS  
13:30 – 14:40

Mariko Takahashi, Miho Tanaka  
Tokyo University of Marine Science and Technology, Tokyo, Japan

- PTu-201** The Development of Analytical Method for Speciation of Transition Metal Ions in Seawater by CE-ESI-MS  
11:10 – 12:20

Daisuke Nakamoto, Masashi Wakasugi, Miho Tanaka  
Tokyo University of Marine Science and Technology, Tokyo, Japan

- PTu-202** Identification of Silk Proteins Excavated from the Ruin of the Makimuku Site in 3-4 AD Japan by MALDI Mass Spectrometry  
13:30 – 14:40

Kazuki Kawahara<sup>1</sup>, Miho Muguruma<sup>1</sup>, Teruhiko Hashimoto<sup>2</sup>,  
Kaoru Terasawa<sup>2</sup>, Atsuko Miyaji<sup>1</sup>, Takashi Nakazawa<sup>1</sup>  
<sup>1</sup>Nara Women's University, Nara, Japan, <sup>2</sup>Research Center for Makimuku-Gaku, Nara, Japan

Wednesday, 19<sup>th</sup> September

Morning

**Award Lecture**

08:30 – 08:50

Main Hall

**Curt Brunnée Award Lecture**Chair: Catherine E Costello (IMSF Vice-President)  
Boston University School of Medicine, USA**AW1-0830 Curt Brunnée Award Lecture**

08:30 – 08:50

Zheng Ouyang

Purdue University in West Lafayette, USA

**Oral Session**

09:00 – 11:00

Main Hall

**Session 21: Platform Technology for Metabolomics**Chair: Yoshiya Oda  
Eisai Inc, USA

Wed

**AW1-0830 Curt Brunnée Award Lecture**

08:30 – 08:50

Zheng Ouyang

Purdue University in West Lafayette, USA

**S21-0900 [Keynote Lecture] New generation**09:00 – 09:40 **high-field Orbitrap instrumentation in untargeted metabolic profiling**Annie M Evans, Qiang Liu, Brandi Bridgewater,  
Matthew Mitchell, Hongping Dai, Corey DeHaven,  
Sandy Stewart  
Metabolon, Durham, NC, USA**S21-0940 Improving comprehensive analysis for myxobacterial secondary metabolome mining**Thomas Hoffmann<sup>1,2</sup>, Daniel Krug<sup>1,2</sup>, Rolf Mueller<sup>1,2</sup><sup>1</sup>Helmholtz Institute for Pharmaceutical Research Saarland (HIPS),  
Saarbruecken/Germany, <sup>2</sup>Pharmaceutical Biotechnology, Saarland University,  
Saarbruecken/Germany**S21-1000 Understanding alterations of platelets metabolism during storage by using UPLC-Q-TOF-MS strategy.**Giuseppe Paglia<sup>1,2</sup>, Olafur E Sigurjonsson<sup>3</sup>,  
Manuela Magnusdottir<sup>2</sup>, Steinun Thorlacius<sup>2</sup>,Sveinn Gudmundsson<sup>3</sup>, Bernhard O Palsson<sup>2</sup>, Ines Thiele<sup>2</sup>  
<sup>1</sup>University of Iceland, Reykjavik, Iceland, <sup>2</sup>Center for Systems Biology,  
University of Iceland, Reykjavik, Iceland, <sup>3</sup>The Blood Bank, Landspitali-  
University Hospital, Reykjavik, Iceland**S21-1020 Neuroactive Steroids in Plasma Measured by a Novel Mass Spectrometry Platform**Andre Kopoyan, Karin M Green, Kristina M Deligiannidis,  
Scott A Shaffer

University of Massachusetts Medical School, Worcester, MA, USA

**S21-1040 Metabolomics Studies Using a Versatile Microfluidic Platform**Steven A Cohen, Giuseppe Astrarita, Giorgis Isaac,  
Angela Doneanu, Jay Johnson, Jim Murphy  
Waters Corporation, Milford, USA

Wednesday, 19<sup>th</sup> September

Morning

## Oral Session

09:00 – 11:00

Room A

## Session 22: Instrumentation Developments in Mass Spectrometric Imaging

Chair: Anastassios Giannakopoulos  
ThermoFisher Scientific, Germany**S22-0900** [Keynote Lecture] High Resolution in Mass and Space: New Developments and Trends in MALDI Mass Spectrometry Imaging

Bernhard Spengler, Andreas Römpf, Sabine Guenther, Oliver Schulz, Yvonne Schober, Zoltan Takats, Klaus-Peter Hinz, Christian Lotze, Joerg-Ulrich Poetzel, Christian Schinz  
Justus Liebig University, Giessen, Germany

**S22-0940** Development and Applications of New Stigmatic Mass Microscope with High Mass and Spatial Resolving Power using Multi-Turn Time-of-Flight Mass Spectrometer

Jun Aoki, Hisanao Hazama, Kunio Awazu, Michisato Toyoda  
Osaka University, Osaka, Japan

**S22-1000** An Evolution of TOF-SIMS for Biological Samples: From 2D Imaging to 3D FIB-TOF Tomography

John S Hammond, Gregory L Fisher, Scott R Bryan  
Physical Electronics, Chanhassen, Minnesota, USA

**S22-1020** Study of Toxin Distribution in Sprouted Potatoes by Electrospray Laser Desorption Ionization Imaging Mass Spectrometry (ELDI/IMS)

Yichia Huang<sup>1</sup>, Min-Zong Huang<sup>1</sup>, Yi-Tzu Cho<sup>2</sup>, Jentiae Shiea<sup>1</sup>  
<sup>1</sup>National Sun Yat-sen University, Kaohsiung, Taiwan, <sup>2</sup>Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan

**S22-1040** Conventional and stigmatic laser desorption/ionization-imaging mass spectrometry applied to analyses of organic layers in electronic devices

Yuko Tachibana<sup>1</sup>, Yoji Nakajima<sup>1</sup>, Tsuguhide Isemura<sup>1</sup>, Kiyoshi Yamamoto<sup>1</sup>, Takaya Satoh<sup>2</sup>, Jun Aoki<sup>3</sup>, Michisato Toyoda<sup>3</sup>  
<sup>1</sup>Asahi Glass Co., Ltd., Yokohama, Japan, <sup>2</sup>JEOL Ltd., Akishima Tokyo, Japan, <sup>3</sup>Osaka University, Osaka, Japan

## Oral Session

09:00 – 11:00

Room B-1

## Session 23: Gas Phase Fragmentation Mechanisms of Biomolecular Radicals

Chair: Shigeo Hayakawa  
Osaka Prefecture University, Japan**S23-0900** [Keynote Lecture] Gas Phase Chemistry of Biomolecular Radicals - An Overview

Michael Leeming<sup>1,2</sup>, William A Donald<sup>1,2</sup>, Richard A J O'Hair<sup>1</sup>  
<sup>1</sup>The University of Melbourne Victoria 3010 AUSTRALIA, <sup>2</sup>ARC Centre of Excellence for Free Radical Chemistry and Biotechnology

**S23-0940** Mechanism of "Oxygen rearrangement" in mass spectrometry

Nino G Todua, Karl K Irikura, Stephen E Stein, Anzor I Mikaila  
National Institute of Standards and Technology

**S23-1000** The Cn Ions Formed by the Dissociation of an N-terminal Deuterohemin Containing Hexapeptide

Xinhua Guo, Bing Wang, Jiayi Yu  
Jilin University, Changchun, China

**S23-1020** Isomerization of Radical Peptide Ions and Subsequent Radical-Induced Dissociations

Ivan Keung Chu  
Department of Chemistry, The University of Hong Kong, Hong Kong, China

**S23-1040** Cascade Dissociations of Peptide Cation Radicals

Frantisek Turecek  
University of Washington, Seattle, WA, USA

**Wednesday, 19<sup>th</sup> September**

**Morning**

## Oral Session

09:00 – 11:00

Room D

### Session 24: Regulated Bioanalysis

Chair: Shinobu Kudoh

Shimadzu Techno-Research, Inc., Japan

**S24-0900** [Keynote Lecture] Drug regulation and bio-analysis  
09:00 – 09:40

Tatsuo Kurokawa  
Keio University, Tokyo, Japan

**S24-0940** Bioanalytical method validation: Process of preparation and notable points of the draft Japanese guideline  
09:40 – 10:00

Noriko Katori

National Institute of Health Sciences, Tokyo, Japan

**S24-1000** Using of Multistage Mass Spectrometry Techniques in Combinations with Electrophoretic and Chromatographic Separation Techniques for Analysis of Biological Samples  
10:00 – 10:20

Jozef Marak, Andrea Stanova, Monika Kondekova, Monika Radicova, Nikoleta Bihercova, Katarina Krcova  
Comenius University, Bratislava, Slovak Republic

**S24-1020** Quantitative Analysis of Beta casomorphin-7 by SRM using stable isotope labeled peptide as internal standard  
10:20 – 10:40

Xiaomin Song<sup>1</sup>, Thiri Zaw<sup>1</sup>, Ardesir Amirkhani<sup>1</sup>, Andrew Clarke<sup>2</sup>, Mark Molloy<sup>1</sup>  
<sup>1</sup>APAF Macquarie University, Sydney, Australia, <sup>2</sup>A2 Co Ltd, Australia

**S24-1040** Accurate Mass MS/MS an Attractive Option For the Quantification of Biotherapeutics in DMPK Studies  
10:40 – 11:00

Robert S Plumb<sup>1,2</sup>, Christopher Evans<sup>3</sup>, Paul D Rainville<sup>1</sup>, Joanne Mather<sup>1</sup>  
<sup>1</sup>Waters Corporation, <sup>2</sup>Imperial College, London, UK, <sup>3</sup>GlaxoSmithKline, DMPK, PA, USA

## Oral Session

09:00 – 11:00

Room E

### Session 25: New Approaches to Defining the Diversity of Glycans

Chair: Catherine E Costello

Boston University School of Medicine, USA

**S25-0900** [Keynote Lecture] Development and Application of a Rapid and Sensitive Method for Screening Cellular Models of Congenital Disorders of Glycosylation  
09:00 – 09:40

Jane Thomas-Oates<sup>1,2,3</sup>, Salina Abdul Rahman<sup>1,2,3</sup>, Jennifer E Dodd<sup>1,3</sup>, Ed Bergstrom<sup>1,2,3</sup>, David A Ashford<sup>1,2,4</sup>, Jerry Thomas<sup>1,2,4</sup>, Daniel Ungar<sup>1,4</sup>

<sup>1</sup>University of York, York, UK, <sup>2</sup>Centre of Excellence in Mass Spectrometry,

<sup>3</sup>Department of Chemistry, <sup>4</sup>Department of Biology

**S25-0940** Studies of Oligosaccharides and Monosaccharides by LEISD MALDI and 2D-CID-ESI Mass Spectrometry Techniques  
09:40 – 10:00

shuying Liu<sup>1,2</sup>, hongmei Yang<sup>1</sup>, Debin Wan<sup>1</sup>

<sup>1</sup>Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China, <sup>2</sup>Changchun University of Chinese Medicine, 130117, China

**S25-1000** A new approach to the rational synthesis of MALDI matrix. Keeping functional groups and its location but changing the stereochemistry  
10:00 – 10:20

Maria L Salum<sup>2</sup>, Lucia M Itovich<sup>2</sup>, Hiroshi Nonami<sup>1</sup>, Rosa Erra-Balsells<sup>2</sup>

<sup>1</sup>Ehime University, Matsuyama, Japan, <sup>2</sup>University of Buenos Aires, Argentina

**S25-1020** Automated Identification of Intact Glycopeptides from Complex Samples  
10:20 – 10:40

Christopher Becker<sup>1</sup>, Marshall Bern<sup>1</sup>, Yong Kil<sup>1</sup>, Doron Kletter<sup>2</sup>, Mudita Singhal<sup>2</sup>, Julian Saba<sup>3</sup>, David Horn<sup>3</sup>, Sergei Snovida<sup>4</sup>, Rosa Viner<sup>3</sup>

<sup>1</sup>Protein Metrics Inc., <sup>2</sup>Palo Alto Research Center, Palo Alto, CA, USA,

<sup>3</sup>Thermo Fisher Scientific, San Jose, CA, USA, <sup>4</sup>Institute of Biological Chemistry, Academia Sinica, Taipei, TAIWAN

**S25-1040** Ion mobility mass spectrometry of IgG Fc glycopeptides from different subclasses  
10:40 – 11:00

Michiko Tajiri<sup>1</sup>, Yayoi Hongo<sup>2</sup>, Takemichi Nakamura<sup>2</sup>, Kenji Hirose<sup>3</sup>, Yoshinao Wada<sup>1</sup>

<sup>1</sup>Osaka Medical Center and Research Institute for Maternal and Child Health, Izumi, Japan, <sup>2</sup>RIKEN, Wako, Japan, <sup>3</sup>Nihon Waters K.K., Osaka, JAPAN

**Wednesday, 19<sup>th</sup> September**

**Afternoon**

## Oral Session

15:00 – 17:00

Main Hall

### Session 26: Lipidomics : Recent New Techniques and Applications

Chair: Stephen J Blanksby  
University of Wollongong, Australia

- S26-1500** [Keynote Lecture] High-Resolution 'Shotgun' Mass Spectrometry and Chemical Labeling for Comprehensive and Quantitative Lipidome Profiling of Disease  
15:00 – 15:40

Cassie J Fhaner<sup>1</sup>, Hong Ji<sup>2</sup>, Richard J Simpson<sup>2</sup>, Gavin E Reid<sup>1</sup>  
<sup>1</sup>Michigan State University, USA, <sup>2</sup>Latrobe University, Australia

- S26-1540** Tandem MS Methods For Assignment Of Double Bonds And Chain Branching In Fatty Acid Methyl Esters  
15:40 – 16:00

Tom Brenna, Rinat Ran-Ressler, Peter Lawrence  
Cornell University, Ithaca, New York, USA

- S26-1600** The Missing Link between Neurodegeneration and Sphingolipid Metabolism: Integration of Lipidomics and Proteomics  
16:00 – 16:20

Sarita Hebbar, Mayura Nakade, Dominik Schwudke  
National Centre for Biological Sciences, Tata Institute of Fundamental Research, Bangalore, India

- S26-1620** What is a complete lipidome? A snipers approach to shotgun analysis of the human lens.  
16:20 – 16:40

Jane M Deeley, Jessica R Hughes, Shane R Ellis, Jo Ann Seng, Roger J Truscott, Stephen J Blanksby, Todd W Mitchell  
University of Wollongong, Wollongong, Australia

- S26-1640** Toward Total Structural Analysis of Complex Lipids: Electrospray Ionization Multiple-stage Linear ion-trap with High-resolution Mass spectrometric Analysis of Intact Ions  
16:40 – 17:00

Fong-Fu Hsu  
Washington University School of Medicine in St. Louis

## Oral Session

15:00 – 17:00

Room A

### Session 27: Progress in Microbiology

Chair: Catherine Fenselau  
University of Maryland, USA

- S27-1500** [Keynote Lecture] Translating metabolic phenotyping and systems medicine into clinical Practise: Understanding gut microbial-host Interactions in personal and public healthcare problems  
15:00 – 15:40

Jeremy K Nicholson  
Imperial College London

- S27-1540** Distribution and identification of molecular interactions between tomato roots and bacterial biofilms  
15:40 – 16:00

Delphine Debois<sup>1</sup>, Emmanuel Jourdan<sup>2</sup>, Nicolas Smargiasso<sup>1</sup>, Marc Ongena<sup>3</sup>, Philippe Thonart<sup>2</sup>, Edwin De Pauw<sup>1</sup>  
<sup>1</sup>University of Liege, Liege, Belgium, <sup>2</sup>Walloon Centre for Industrial Biology, Liege, Belgium, <sup>3</sup>Gembloux Agro-Bio Tech, Gembloux, Belgium

- S27-1600** Identification of Protein Biomarkers as Diagnostic Targets for Invasive Aspergillosis using Discovery and Targeted Proteomics  
16:00 – 16:20

Chengsi Huang<sup>1,3</sup>, Jason McCarthy<sup>2</sup>, Marta Feldmesser<sup>2</sup>, Vicki H Wysocki<sup>1,3</sup>  
<sup>1</sup>University of Arizona, Tucson, AZ, USA, <sup>2</sup>Albert Einstein College of Medicine, Yeshiva University, Bronx, NY, USA, <sup>3</sup>Ohio State University, Columbus, OH, USA

- S27-1620** Microbial genome mining for novel bioactive natural products with high resolution LC-MS/MS  
16:20 – 16:40

Lijiang Song<sup>1</sup>, JuanPa Gomez-Escribano<sup>2</sup>, Luisa Laureti<sup>3</sup>, Eshwar Mahenthiralingam<sup>4</sup>, Bertrand Agile<sup>3</sup>, Mervyn Bibb<sup>2</sup>, Gregory Challis<sup>1</sup>

<sup>1</sup>University of Warwick, Coventry, UK, <sup>2</sup>John Innes Centre, Norwich, UK,

<sup>3</sup>University of Nancy, Nancy, France, <sup>4</sup>University of Cardiff, Cardiff, UK

- S27-1640** Novel accurate bacterial identification by MALDI-TOFMS based on ribosomal protein coding in S10-spc-alpha Operon at Stain level  
16:40 – 17:00

HIROTO TAMURA<sup>2</sup>, YUDAI HOTTA<sup>2,3</sup>, HIROAKI SATO<sup>4</sup>, KEISUKE SHIMA<sup>1</sup>, AKIFUMI HOSODA<sup>2</sup>, NORIYUKI OJIMA<sup>1</sup>

<sup>1</sup>SHIMADZU Corporation, Analytical & Measuring Instruments Division,

<sup>2</sup>School of Agriculture, Meijo University, <sup>3</sup>Formulation Technology Institute, Kumiai Chemical Industry Co., <sup>4</sup>Research Institute for Environmental Management Technology, National Institute of Advanced Industrial Science and Technology

**Wednesday, 19<sup>th</sup> September**

**Afternoon**

## Oral Session

15:00 – 17:00

Room B-1

### Session 28: IR Spectroscopy of Gas-phase Ions

Chair: Dietmar Kuck  
Bielefeld University, Germany

**S28-1500** [Keynote Lecture] IR Photodissociation Spectroscopy: A new dimension to Tandem Mass Spectrometry

Philippe Maitre  
Paris Sud University / CNRS - Orsay - FRANCE

**S28-1540** Intracavity infrared multiple photon dissociation spectroscopy of transition metal carbene cations: Agostic interactions or not?

Joost M Bakker<sup>1,2</sup>, Vivike Lapoutre<sup>1</sup>, Andrew Sweeney<sup>3</sup>,  
Abhigya Mookherjee<sup>3</sup>, Peter B Armentrout<sup>3</sup>

<sup>1</sup>FOM Institute for Plasma Physics Rijnhuizen, The Netherlands, <sup>2</sup>Radboud University Nijmegen, The Netherlands, <sup>3</sup>University of Utah, Salt Lake City, USA

**S28-1600** Gas-Phase Structure and Chemistry of the Radical Cation of DNA base-pair dGdC

George N khairallah<sup>1</sup>, Linda Feketeova<sup>1</sup>, Bun Chan<sup>2</sup>,  
Vincent Steinmetz<sup>3</sup>, Philippe Maitre<sup>3</sup>, Leo Radom<sup>2</sup>,  
Richard A O'Hair<sup>1</sup>

<sup>1</sup>University of Melbourne, Melbourne, Australia, <sup>2</sup>The University of Sydney, NSW 2006, Australia, <sup>3</sup>Universite Paris Sud, Orsay Cedex, 91405, France

**S28-1620** Infrared spectroscopic studies on isomerization reactions of ionized molecular clusters

Yoshiyuki Matsuda, Naohiko Mikami, Asuka Fujii  
Tohoku University, Sendai, Japan

**S28-1640** IR-MPD investigation of steric constraints on hydrogen bonding in dicarboxylic acid ions

Christine Merkert, Fabian Menges, Yevgeniy Nosenkov,  
Gereon Niedner-Schatteburg  
TU Kaiserslautern, Germany

## Oral Session

15:00 – 17:00

Room D

### Session 29: The Advances in Biological Mass Spectrometry in Drug Discovery and Development: Current State of the Art and Challenges

Chair: Ajai K Chaudhary  
Merck and Company, USA

**S29-1500** [Keynote Lecture] Advances in the Application of Mass Spectrometry to Drug Metabolism and Pharmacokinetics Studies

Ragu Ramanathan<sup>1,2</sup>

<sup>1</sup>Bristol-Myers Squibb, <sup>2</sup>Department of Biotransformation, Princeton, New Jersey 08540, USA

**S29-1540** Development of stable isotope labeling by essential nutrients in cell culture (SILEC) coupled with LC-MS for drug target discovery

Ian A Blair, Nathaniel W Snyder, Zinan Zhou, Andrew Worth, Sankha S Basu  
University of Pennsylvania, Philadelphia, PA 19104, USA

**S29-1600** High-resolution metabolic profiling towards G-protein coupled receptors: rapid and comprehensive screening of histamine H4 receptor ligands

Jeroen Kool<sup>1</sup>, Anders F Rudebeck<sup>1</sup>, Frank Fleurbaaij<sup>1</sup>,  
Saskia Nijmeijer<sup>1</sup>, David Falck<sup>1</sup>, Rogier Smits<sup>2</sup>, Henry F Vischer<sup>1</sup>,  
Rob Leurs<sup>1</sup>, Wilfried M Niessen<sup>1</sup>

<sup>1</sup>VU University, Amsterdam, The Netherlands, <sup>2</sup>Griffin Discoveries B.V., The Netherlands

**S29-1620** THE ROLE OF MASS SPECTROMETRY IN DRUG DISCOVERY AND DEVELOPMENT

ANTHONY TSARBOPoulos  
UNIVERSITY OF PATRAS, PATRAS, GREECE

**S29-1640** Evaluation of fully automated DBS extraction system with LC-MS/MS systems for Sartans and Statins using different DBS card types

Souki Kanda<sup>3</sup>, YASUHIKO BANDO<sup>1,2</sup>, Takemoto Kawamukai<sup>1</sup>,  
Hiroshi Hike<sup>1</sup>, Amane Sakura<sup>3</sup>

<sup>1</sup>AMR, Inc., <sup>2</sup>Biosys Technologies, Inc., Tokyo, Japan, <sup>3</sup>Toray Research Center, Inc., Kanagawa, Japan

Wednesday, 19<sup>th</sup> September

Afternoon

**Oral Session**

15:00 – 17:00

Room E

**Session 30: Data Processing and Informatics for SIMS**

Chair: DaeWon Moon

Center for Nano-Bio Technology, Korea Research Institute of Standards and Science, Korea

**S30-1500 [Keynote Lecture] Image and Spectral Processing for ToF-SIMS Analysis of Biological Materials**  
15:00 – 15:40David G Castner  
University of Washington, Seattle, USA**S30-1540 Multivariate analysis application to ToF-SIMS data of organic layers**  
15:40 – 16:00Yasuko Kajiwara<sup>1,2</sup>, Satoka Aoyagi<sup>2,3</sup>  
<sup>1</sup>MGC Inc., Tokyo, Japan, <sup>2</sup>Tottori University, Tottori, Japan, <sup>3</sup>Shimane University, Shimane, Japan**S30-1600 The Full Spectrum protocol: how to provide quantitative analysis for matrix elements in heterogeneous nanometer scale layers with ToF-SIMS**  
16:00 – 16:20Matthieu Py<sup>1</sup>, Jean-Paul Barnes<sup>2</sup>, Jiro Matsuo<sup>1,3</sup>  
<sup>1</sup>Kyoto University, Uji, Japan, <sup>2</sup>CEA-Leti, MINATEC Campus, Grenoble, France,  
<sup>3</sup>JST-CREST**S30-1620 Evaluation of secondary ions from lysozyme and peptides using G-SIMS and g-ogram**  
16:20 – 16:40Satoka Aoyagi<sup>1</sup>, Ian S Gilmore<sup>2</sup>, Ichiro Mihara<sup>3</sup>  
<sup>1</sup>Shimane University, Matsue, Japan, <sup>2</sup>National Physical Laboratory, UK,  
<sup>3</sup>Kuraray Co., Ltd., Kurashiki, Japan**S30-1640 Ab initio peak identification for SRM/ MRM data**  
16:40 – 17:00Ken Aoshima<sup>1</sup>, Koikegami Shigeru<sup>3</sup>, Fukuda Mitsuru<sup>3</sup>,  
Takahashi Kentaro<sup>1</sup>, Matsuura Kentaro<sup>1</sup>, Watanabe Hideki<sup>1</sup>,  
Sato Yoshiaki<sup>1</sup>, Uehara Taisuke<sup>1</sup>, Kimura Takayuki<sup>1</sup>,  
Nakamura Tatsushi<sup>1</sup>, Parry Howell<sup>2</sup>, Tanaka Satoshi<sup>2</sup>,  
Utsunomiya Shin-ichi<sup>2</sup>, Kajihara Shigeki<sup>2</sup>, Tanaka Koichi<sup>2</sup>,  
Oda Yoshiya<sup>1</sup>  
<sup>1</sup>Eisai Co. Ltd., Tsukuba, Japan, <sup>2</sup>Shimadzu Corp., Kyoto, Japan, <sup>3</sup>Ibio-Tech

## Wednesday, 19<sup>th</sup> September

### Poster Session

Core Time : 11:10 - 12:20 (Odd number),  
13:30 - 14:40 (Even number)

Event Hall

### Session 21

#### Platform Technology for Metabolomics

**PWe-001 Negative ion tandem mass spectrometry of prenylated fungal metabolites and their derivatives**

11:10 – 12:20  
Ramona Heinke, Norbert Arnold, Ludger A Wessjohann,  
Juergen Schmidt  
Leibniz Institute of Plant Biochemistry, Halle, Germany

**PWe-002 Metabolome profiling of human embryonic stem cells by gas chromatography-mass spectrometry**

13:30 – 14:40  
Takashi Suzuki<sup>1</sup>, Masahiro Miyoshi<sup>2</sup>, Katsuhiro Nakagawa<sup>1</sup>,  
Hirofumi Suemori<sup>3</sup>, Shinichiro Chuma<sup>3</sup>, Norio Nakatsuj<sup>3</sup>  
<sup>1</sup>Shimadzu Co., Kyoto, Japan, <sup>2</sup>Shimadzu Analytical and Measuring Center Inc., Kyoto, Japan, <sup>3</sup>Kyoto University, Kyoto, Japan

**PWe-003 Metabolic characterization by mass spectrometry of Cordyceps bassiana mycelium cultivated under various culture medium and light conditions**

11:10 – 12:20  
Sun-Hee Hyun<sup>1</sup>, Seok-Young Lee<sup>1</sup>, So-Hyun Kim<sup>1</sup>, Gi-Ho Sung<sup>2</sup>,  
Seong Hwan Kim<sup>3</sup>, Hyung-Kyo Choi<sup>1</sup>  
<sup>1</sup>College of Pharmacy, Chung-Ang University, Seoul, Korea, <sup>2</sup>Mushroom Research Division, Department of Herbal Crop Research, National Institute of Horticultural & Herbal Science, Suwon, Korea, <sup>3</sup>Department of Microbiology, Dankook University, Cheonan, Korea

**PWe-004 Electrochemical simulation of Phase I and II Drug Metabolism, A Powerful Technique for Metabolite Characterization and Synthesis**

13:30 – 14:40  
Jean-Pierre Chervet<sup>1</sup>, Agnieszka Kraj<sup>1</sup>, Hendrik-Jan Brouwer<sup>1</sup>,  
Nico Reinhoudt<sup>1</sup>, Martin Eysberg<sup>1</sup>, Uwe Karst<sup>2</sup>  
<sup>1</sup>Antec, Zoeterwoude, the Netherlands, <sup>2</sup>Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität, Münster, Germany

**PWe-005 Identification of a new plasma biomarker of Alzheimer Disease using metabolomics technology**

11:10 – 12:20  
YOSHIAKI SATO<sup>1</sup>, Ikumi Suzuki<sup>1</sup>, Tatsuji Nakamura<sup>1</sup>,  
Francois Bernier<sup>1</sup>, Ken Aoshima<sup>1</sup>, Yoshiya Oda<sup>2</sup>  
<sup>1</sup>Eisai Product Creation Systems, Tsukuba, Japan, <sup>2</sup>Eisai Product Creation Systems, Andover, MA 01810

**PWe-006 Metabolic profiling of mouse brain with MALDI-FT-ICR imaging mass spectrometry technique**

13:30 – 14:40  
Kazunori Saito<sup>1</sup>, Daisuke Miura<sup>2</sup>, Fujimura Yoshinori<sup>2</sup>,  
Nirasawa Takashi<sup>1</sup>, Wariishi Hiroyuki<sup>2</sup>  
<sup>1</sup>Bruker Daltonics K.K., <sup>2</sup>Kyushu University

**PWe-007 Ultra Fast Analysis of Amino Acids in Cultured Cell Extracts Using UHPLC/MS/MS**

11:10 – 12:20  
Taku TSUKAMOTO<sup>1</sup>, Yuki SATO<sup>2</sup>, Satoshi YAMAKI<sup>1</sup>

<sup>1</sup>Shimadzu Co., Kyoto, Japan, <sup>2</sup>Shimadzu GLC Ltd., Tokyo, Japan

**PWe-008 Untargeted screening of pesticides metabolites by LC-HRMS: a tool for human exposure evaluation?**

13:30 – 14:40  
Emilien L JAMIN<sup>1,2</sup>, Nathalie BONVALLOT<sup>1,2,3,4</sup>,  
Marie TREMBLAY-FRANCO<sup>1,2</sup>, Jean-Pierre CRAVEDI<sup>1,2</sup>,  
Cecile CHEVRIER<sup>4</sup>, Sylvaine CORDIER<sup>4</sup>, Laurent DEBRAUWER<sup>1,2</sup>  
<sup>1</sup>INRA, UMR1331, Toxalim, Research Centre in Food Toxicology, F-31062 Toulouse, France, <sup>2</sup>Toulouse University, INPT, UPS, UMR1331, F-31062 Toulouse, France, <sup>3</sup>EHESP School of public health, Rennes Sorbonne Paris Cite, France, <sup>4</sup>INSERM UMR 1085 IRSET Institut de recherche en sante, environnement, travail, Rennes, France

**PWe-009 Metabolite profiling of Makgeolli with Different Wild Yeast Strains Saccharomyces cerevisiae 98-5 and Pichia anomala 197-13 During Fermentation**

11:10 – 12:20  
HyeRyun Kim, JeoungMae Son, JaeHo Kim, ByungHak Ahn  
Korea Food Research Institute, Gyeonggi-do, Korea

**PWe-010 Plant metabolite analysis using comprehensive two dimensional gas chromatograph quadrupole mass spectrometer**

13:30 – 14:40  
Shuichi Kawana, Katsuhiro Nakagawa, Yuki Sakamoto,  
Riki Kitano, Haruhiko Miyagawa  
Shimdu Co., Kyoto, Japan

**PWe-011 Differentiation of German and Roman Chamomiles by Comprehensive Chemical Fingerprinting using Ultra Performance Supercritical Fluid Chromatography Coupled**

11:10 – 12:20  
Shinnosuke Horie<sup>1</sup>, Motoji Oshikata<sup>1</sup>, Michael D Jones<sup>2</sup>,  
Bharathi Avula<sup>3</sup>, Kate Yu<sup>2</sup>, Yan-Hong Wang<sup>3</sup>, Mei Wang<sup>3</sup>,  
Dominic Moore<sup>2</sup>, Warren Potts<sup>2</sup>, Ikhlas Khan<sup>3</sup>  
<sup>1</sup>Nihon Waters, Osaka, Japan, <sup>2</sup>Waters Corporation, Milford, MA, <sup>3</sup>University of Mississippi, Oxford, MS

**PWe-012 Synthesis of 13C6- and 13C12-dabsyl chloride to perform amine-targeted clinical profiling**

13:30 – 14:40  
Tetsuo Ishida, Hiroyuki Tanaka, Kihachiro Horiike  
Shiga University of Medical Science, Shiga, Japan

**PWe-013 Use of culture media fingerprinting by LTQ FT Ultra MS to predict human embryonic implantation potential**

11:10 – 12:20  
Eduardo Morgado Schmidt<sup>1,2</sup>, Elaine C Cabral<sup>1</sup>,  
Sylvia Sanches Cortezzi<sup>3</sup>, Marcello Garcia Trevisan<sup>4</sup>,  
Christina Ramires Ferreira<sup>1</sup>, Edson J Borges<sup>5</sup>,  
Marcos Nogueira Eberlin<sup>1</sup>

<sup>1</sup>UNICAMP/ ThoMSon Mass Spectrometry Laboratory, Campinas, Brazil.,

<sup>2</sup>Nova Analitica Importacao e Exportacao LTDA, Sao Paulo, Brazil.,

<sup>3</sup>Sapientiae Institute Educational and Research Center in Assisted Reproduction, Sao Paulo, Brazil., <sup>4</sup>Institute of Exact Sciences, Federal University of Alfenas, Alfenas, Brazil., <sup>5</sup>Fertility Assisted Fertilization Center, Sao Paulo, Brazil.

## Wednesday, 19<sup>th</sup> September

- PWe-014** Ionic liquid-based microextraction for sensitive determination of urinary aromatic amines by liquid chromatography-mass spectrometry  
 13:30 – 14:40

Jingyueh Jeng, Cheng-Yuan Shih  
 Chia nan University of Pharmacy & Science, Tainan, Taiwan

- PWe-015** Adjustment of total cellular metabolite concentration by flow-injection analysis mass spectrometer for metabolomic study  
 11:10 – 12:20

Guan-yuan Chen<sup>1</sup>, Ching-hua Kuo<sup>1,2</sup>  
<sup>1</sup>School of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan, <sup>2</sup>The Metabolomics Core Laboratory, Center of Genomic Medicine, National Taiwan University, Taiwan

- PWe-016** Metabolomics of Curcuma: approaching by studying constituents of wide range polarity using LC-DAD-ECD-MS  
 13:30 – 14:40

Paramitha Messayu, Kuo-Lung Ku  
 National Chiayi University, Chiayi, Taiwan

- PWe-017** Effect of glucose addition against ion suppression by sodium chloride  
 11:10 – 12:20

Megumi Wakimoto<sup>1</sup>, Yui Okamura<sup>1</sup>, Hajime Mizuno<sup>1</sup>, Naohiro Tsuyama<sup>1</sup>, Sachiko Date<sup>2</sup>, Tsutomu Masujima<sup>1,2</sup>  
<sup>1</sup>Graduate School of Biomedical Sciences, Hiroshima University, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center (QBIC), RIKEN, Japan

- PWe-018** Discriminant analysis of Curcuma species grown in different origins using mass spectrometry  
 13:30 – 14:40

Jueun Lee<sup>1,2</sup>, Youngae Jung<sup>1</sup>, Geum Sook Hwang<sup>1,3</sup>  
<sup>1</sup>Korea Basic Science Institute, Seoul, Republic of Korea, <sup>2</sup>Sungkyunkwan Univ. Natural Sciences Campus, Suwon, Republic of Korea, <sup>3</sup>Graduate School of Analytical Science and Technology, Chungnam University, Daejeon, Republic of Korea

- PWe-019** Copper Stress Induced Global Metabolites Profiling of Burdock Roots by 1H NMR, GC-MS and UPLC-QTOF MS Analysis  
 11:10 – 12:20

Youngae Jung<sup>1</sup>, Miyoung Ha<sup>1,2</sup>, Geum-Sook Hwang<sup>1,3</sup>  
<sup>1</sup>Korea Basic Science Institute, Soeul, Korea, <sup>2</sup>Sungkyunkwan University, Suwon, Korea, <sup>3</sup>Graduate School of Analytical Science and Technology, Chungnam National University, Daejoen, Korea

- PWe-020** The impact of high-resolution MS techniques on the discovery of novel natural products from myxobacteria  
 13:30 – 14:40

Yasuhiko Maekawa<sup>1</sup>, Daniel Krug<sup>2,3</sup>, Thomas Hoffmann<sup>2,3</sup>, Aiko Barsch<sup>4</sup>, Gabriela Zurek<sup>4</sup>, Rolf Mueller<sup>2,3</sup>  
<sup>1</sup>Bruker Daltonics K.K., Yokohama, Japan, <sup>2</sup>Helmholtz Institute for Pharmaceutical Research, Saarbrucken, Germany, <sup>3</sup>Saarland University, Saarbrucken, Germany, <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany

- PWe-021** Differential analysis of fermented beverage using fast polarity switching TOFMS acquisition with high mass accuracy and multivariate analysis  
 11:10 – 12:20

Satoshi Yamaki, Manami Kobayashi, Takahiro Goda, Tsutomu Nishine  
 Shimuzu Co., Kyoto, Japan

- PWe-022** Simultaneous Quantitative and Qualitative measurements for Primary Metabolism Investigations using a Quadrupole-Time-of-Flight Mass Spectrometer  
 13:30 – 14:40

Noriyuki Iwasaki<sup>1</sup>, Don Richards<sup>3</sup>, Mark Savage<sup>4</sup>, Angus Nedderman<sup>4</sup>, Carsten Baessmann<sup>2</sup>

<sup>1</sup>Bruker Daltonics K.K., <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany, <sup>3</sup>Bruker UK Ltd, Coventry, UK, <sup>4</sup>Unitabs Bioanalytical Solutions, Sandwich, UK

- PWe-023** Development of accelerate quantification analysis for hydrophilic metabolites using ionpairing chromatography with a high-speed triple quadrupole mass spectrometer  
 11:10 – 12:20

Hashim Zanariah<sup>2</sup>, Yudai Denpo<sup>2</sup>, Tairo Ogura<sup>1</sup>, Ichiro Hirano<sup>1</sup>, Takeshi Bamba<sup>2</sup>, Eiichiro Fukusaki<sup>2</sup>

<sup>1</sup>Shimadzu Co., Kyoto, Japan, <sup>2</sup>Osaka University, Osaka, Japan

- PWe-024** Metabolic changes during aging complementary GC-EI-MS and GC-APCI-TOF-MS analysis of a short-lived mitochondrial knockdown of *Caenorhabditis elegans*  
 13:30 – 14:40

Jouji Seta<sup>1</sup>, Verena Tellstroem<sup>3</sup>, Aiko Barsch<sup>3</sup>, Gabriele Zurek<sup>3</sup>, Carsten Jaeger<sup>2</sup>, Bernd Kammerer<sup>2</sup>

<sup>1</sup>Bruker Daltonics K.K., <sup>2</sup>Center for Biological Systems Analysis (ZBSA), University Freiburg, Germany, <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany

- PWe-025** Development of automated data processing tool for large scale MRM experiment in metabolomics study  
 11:10 – 12:20

Hiroshi Tsugawa<sup>1</sup>, Mitsuhiro Kanazawa<sup>2</sup>, Atsushi Ogiwara<sup>2</sup>, Takeshi Bamba<sup>1</sup>, Eiichiro Fukusaki<sup>1</sup>

<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>Reifycs Inc., Tokyo, Japan

- PWe-027** LC-MS/MS-based plasma metabonomics: finding potential biomarkers for lung cancer  
 11:10 – 12:20

Wei Yang<sup>1</sup>, Yanhua Chen<sup>1</sup>, Cong Xi<sup>1</sup>, Ruiping Zhang<sup>1</sup>, Yongmei Song<sup>2</sup>, Jiuming He<sup>1</sup>, Jinfa Bai<sup>1</sup>, Qimin Zhan<sup>2</sup>, Lvhua Wang<sup>2</sup>, Nan Bi<sup>2</sup>, Zeper Abliz\*<sup>1</sup>

<sup>1</sup>Institute of Materia Medica, Chinese Academy of Medical Sciences and PekingUnionMedicalCollege, Beijing, P. R. China, <sup>2</sup>Cancer Institute and Cancer Hospital, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, P. R. China

- PWe-028** Metabolomics and its application to high resolution phenotype analysis  
 13:30 – 14:40

Eiichiro Fukusaki

Osaka University, Osaka, Japan

- PWe-029** Implementation of a Data Independent MS/MS Acquisition Strategy for Metabolites Identification in a Metabolomics MS-based Workflow  
 11:10 – 12:20

Emmanuel Varesio, Gerard Hopfgartner  
 University of Geneva, Geneva, Switzerland

## Wednesday, 19<sup>th</sup> September

- PWe-030** Alkyl chloroformate - mediated derivatization - extraction platform for parallel GC-MS and LC-MS based metabolomics  
 13:30 – 14:40

Petr Simek, Petr Husek, Helena Zahradnickova, Jana Cimlova, Lucie Rimnacova  
 Biology Centre, Czech Academy of Sciences

- PWe-031** Aberrant Metabolism and Its Response to Treatment in Esophageal Squamous Cell Carcinoma Revealed by Plasma Metabolomics Study  
 11:10 – 12:20

Jing Xu<sup>1</sup>, Yanhua Chen<sup>1</sup>, Ruiping Zhang<sup>1</sup>, Yongmei Song<sup>2</sup>, Nan Bi<sup>2</sup>, Jiuming He<sup>1</sup>, Jinfa Bai<sup>1</sup>, Lvhua Wang<sup>2</sup>, Qimin Zhan<sup>2</sup>, Zeper Abliz<sup>1</sup>

<sup>1</sup>Institute of Materia Medica, Peking Union Medical College, Beijing, China,

<sup>2</sup>Cancer Institute & Cancer Hospital, Peking Union Medical College, Beijing

### Session 22

#### Instrumentation Developments in Mass Spectrometric Imaging

- PWe-032** Imaging mass spectrometry and structural analysis of lipids directly on tissue specimens using a high resolution MALDI-TOF-TOF tandem mass spectrometer  
 13:30 – 14:40

Shuichi Shimma<sup>2</sup>, Ayumi Kubo<sup>3</sup>, Takaya Satoh<sup>3</sup>, Hisanao Hazama<sup>1</sup>, Kunio Awazu<sup>1</sup>, Michisato Toyoda<sup>1</sup>  
<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>National Cancer Center Research Institute, Tokyo, Japan, <sup>3</sup>JEOL Ltd., Tokyo, Japan

- PWe-033** Observation of distributions of Strontium and Cesium stable isotopes in tissues sections of medaka by a new mass imaging system  
 11:10 – 12:20

Shinichiro Ikeda, Jun Aoki, Michisato Toyoda  
 Osaka University, Osaka, Japan

### Session 23

#### Gas Phase Fragmentation Mechanisms of Biomolecular Radicals

- PWe-034** Investigation of fragmentation routes of steroid ethers via MIKES and B2\*E-linked-scan techniques.  
 13:30 – 14:40

Heiko Bannick, Juergen Grotzmeyer  
 Institut of Physical Chemistry University of Kiel, Kiel, Germany

- PWe-035** Marked difference in fragmentation pathway between chemi-excitation and collision-induced excitation of CT-induced decomposition products of dioxetanes in negative-mode MALDI-TOF-MS/MS  
 11:10 – 12:20

Hisako K Ijuin, Mamoru Ohashi, Masatoshi Tanimura, Nobuko Watanabe, Masakatsu Matsumoto  
 Kanagawa University, Hiratsuka, Japan

- PWe-036** Fragmentation of the [M + Na]<sup>+</sup> and [M + Li]<sup>+</sup> Ions of Multiply Benzyloxy-substituted Arenes under ESI/CID conditions  
 13:30 – 14:40

Dietmar Kuck<sup>1</sup>, Sandra Heitkamp<sup>1</sup>, Matthias C Letzel<sup>1</sup>, Ishtiaq Ahmed<sup>2</sup>, Karsten Krohn<sup>2</sup>

<sup>1</sup>Bielefeld University, <sup>2</sup>University of Paderborn

- PWe-037** A functional group substitution effect on the free radical initiated peptide sequencing (FRIPS) method  
 11:10 – 12:20

Han Bin Oh<sup>1</sup>, Jihye Lee<sup>1</sup>, Hyeyeon Park<sup>1</sup>, Kun Cho<sup>1,2</sup>, Bongjin Moon<sup>1</sup>

<sup>1</sup>Sogang University, Seoul, Korea, <sup>2</sup>Korea Basic Science Institute, Ochang, Korea

### Session 24

#### Regulated Bioanalysis

- PWe-038** Evaluation of peptide fractionation strategies used in proteome analysis  
 13:30 – 14:40

Chih-Wei Chiu, Chun-Lun Chang, Sung-Fang Chen\*  
 National Taiwan Normal University, Taipei, Taiwan

- PWe-039** Simultaneous analysis of 8-oxo-7, 8-dihydroguanine and 8-oxo-7, 8-dihydro-2'-deoxyguanosine in plasma by liquid chromatography-tandem mass spectrometry with automated solid-phase extraction  
 11:10 – 12:20

Yi-Hung Tsai, Mu-Rong Chao

Department of Occupational Safety and Health, Chung Shan Medical University, Taichung 402, Taiwan

- PWe-041** Quantitative analysis of nine N-nitrosamines in human urine by isotope-dilution liquid chromatography-tandem mass spectrometry with on-line solid-phase extraction  
 11:10 – 12:20

Ming-Yen Hsieh, Chiung-Wen Hu

Department of Public Health, Chung Shan Medical University, Taichung, Taiwan

- PWe-042** Ultra-Performance Liquid Chromatography/Mass Spectrometric Method for the determination of venlafaxine and its metabolite in plasma: Application to pharmacokinetic study  
 13:30 – 14:40

Sunil Kumar Dubey<sup>1</sup>, Hemanth Jangala<sup>1</sup>, R N Saha<sup>1</sup>, S Pasha<sup>2</sup>

<sup>1</sup>Birla Institute Of Technology & Science, Pilani, India, <sup>2</sup>Institute of Genomics and Integrative Biology, Mall Road, Delhi, India

- PWe-043** Quantitative evaluation of synthase and hemisynthase activity of glucosamine-6P synthase by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry  
 11:10 – 12:20

Vincent Guerineau, David Touboul, Florence Wieczorek, Marie-Ange Badet-Denisot, Bernard Badet, Alain Brunelle, Philippe Durand

ICSN CNRS, Gif sur Yvette, France

Wed

Wednesday, 19<sup>th</sup> September

- PWe-044 Optimization of ESI method for the LC-MS analysis of phosphorylated peptide**  
13:30 – 14:40

Issey Osaka, Mitsuo Takayama  
Yokohama City University

- PWe-045 Amino acid analysis by LC/MS with LC columns designed for hydrophilic compounds**  
11:10 – 12:20

Hiroko Arai<sup>1</sup>, Tsuneaki Kaneko<sup>1</sup>, Taketoshi Kanda<sup>1</sup>, Yanli Guo<sup>2</sup>,  
Osamu Shiota<sup>2</sup>  
<sup>1</sup>Shiseido, <sup>2</sup>Shiseido China

- PWe-046 Accelerate Method Development using Fast Screening of Mobile Phases Additives and Solvents for Optimum Sensitivity in LC-MS**  
13:30 – 14:40

Mikael LEVI, Stephane MOREAU  
Shimadzu France, Noisiel, France

- PWe-047 Effective Strategies for Phospholipid Removal using Supported Liquid Extraction (SLE) with LC-MS/MS Analysis**  
11:10 – 12:20

Gavin J Jones, Lee Williams, Rhys Jones, Maiko Kaneko,  
Steve Jordan  
Biotage, Cardiff, UK

- PWe-048 Simultaneous determination seven hydroxyacids by capillary electrophoresis and liquid chromatography mass spectrometry**  
13:30 – 14:40

Yen-Ling Chen, Pei-Yu Liu  
Kaohsiung Medical University, Kaohsiung , Taiwan

- PWe-049 Fast determination of phosphopeptides by nanoLC-MS/MS in biological samples**  
11:10 – 12:20

Rong-Chun Chen, Chi-Yu Lu  
Department of Biochemistry, College of Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan

- PWe-050 Derivatization of lipoic acid for analysis by capillary liquid chromatography and mass spectrometry**  
13:30 – 14:40

Chia-Ju Tsai, Chia-Hsien Feng  
Department of Fragrance and Cosmetic Science, College of Pharmacy,  
Kaohsiung Medical University, Kaohsiung, Taiwan

- PWe-051 Highly-Selective Reaction Monitoring (H-SRM) with Automated Mass and Resolution Calibration in Testing of Anabolic Steroids in Equine Plasma and Urine**  
11:10 – 12:20

Harald Oser<sup>1</sup>, Hans Schweingruber<sup>1</sup>, Mary L Blackburn<sup>1</sup>,  
Shane E Tichy<sup>1</sup>, Cornelius E Uboh<sup>2</sup>  
<sup>1</sup>Thermo Scientific, San Jose, CA USA, <sup>2</sup>Pennsylvania Equine Toxicology and Research Laboratory

- PWe-052 Selective enrichment of histidine-tagged proteins and peptides on MALDI plate**  
13:30 – 14:40

shin-yi Huang, Yu-Chie Chen  
Department of Applied Chemistry, National Chiao Tung University, Taiwan

- PWe-053 Determination of Fluconazole and 5-Fluoro Cytosine in human plasma and cerebrospinal fluid using protein precipitation and LC-MS/MS**  
11:10 – 12:20

Carmen A de Kock, Peter J Smith, Jennifer Norman,  
Lubbe Wiesner  
University of Cape Town, Cape Town, South Africa

## Session 25

### Glycoanalytical Technology for Systems Glycobiology and Functional Glycomics

- PWe-054 Studies on the selective binding of divalent metals to cyclodextrins by ESI mass spectrometry**  
13:30 – 14:40

Xiaodan He, chuanfan Ding  
Fudan University, Shanghai, China

- PWe-055 Dual Lectin-based Enrichment Method of N-linked Glycopeptides Using Asymmetrical Flow Field-Flow Fractionation and Applications to Human Blood Serum**  
11:10 – 12:20

Jinyong Kim<sup>1</sup>, Duk Jin Kang<sup>2</sup>, Myeong Hee Moon<sup>1</sup>  
<sup>1</sup>Yonsei University, Seoul, Korea, <sup>2</sup>Korea Research Institute of Standards and Science, Daejeon, South Korea

- PWe-056 A nanoprobe-based strategy combined with HILIC enrichment for targeted glycoprotein profiling**  
13:30 – 14:40

Kai-Yi Wang<sup>1,2</sup>, Ying-Wei Lu<sup>3</sup>, Chun-Cheng Lin<sup>3</sup>, Yu-Ju Chen<sup>1,2,4</sup>  
<sup>1</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan, <sup>2</sup>Nano Science and Technology Program, Taiwan International Graduate Program, Institute of Physics, Academia Sinica, Taipei, Taiwan, <sup>3</sup>Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, <sup>4</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan

- PWe-057 Alteration of glycan profile during early stage of mesenchymal stem cells differentiation**  
11:10 – 12:20

Noritaka Hashii, Ryosuke Kurabayashi, Nana Kawasaki  
National Institute of Health Sciences, Tokyo, Japan

- PWe-058 Data-dependent acquisition system for N-linked glycopeptides using MALDI-DIT-TOF MS**  
13:30 – 14:40

Masaki Murase, Hidenori Takahashi, Yoshihiro Yamada,  
Sadanori Sekiya, Shigeki Kajihara, Shinichi Iwamoto,  
Koichi Tanaka  
Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corp, Kyoto, Japan

- PWe-059 SRM analysis of chondroitin sulfate terminal regions**  
11:10 – 12:20

Harumi Osago<sup>1</sup>, Tomoko Shibata<sup>2</sup>, Suguru Kuwata<sup>3</sup>,  
Michihaya Kono<sup>3</sup>, Nobumasa Hara<sup>1</sup>, Kazuo Yamada<sup>1</sup>,  
Yuji Uchio<sup>3</sup>, Mikako Tsuchiya<sup>1</sup>

<sup>1</sup>Dept. of Biochem., Faculty of Med., Shimane Univ., Shimane, Japan, <sup>2</sup>Cent. for Integ. Res. in Sci., Shimane Univ., Shimane, Japan, <sup>3</sup>Dept. of Orthopaedic Surgery, Faculty of Med., Shimane Univ., Shimane, Japan

## Wednesday, 19<sup>th</sup> September

**PWe-060 Novel Bioinformatics Tool: Interpretation of Glycan Mass Spectra with Metal Adducts and Multiple Adduct Combinations**

13:30 – 14:40 Julian Saba<sup>2</sup>, Kentaro Takahara<sup>1</sup>, Ningombam Meitei<sup>3</sup>, Arun Apte<sup>3</sup>

<sup>1</sup>Thermo Fisher Scientific, Yokohama, Japan, <sup>2</sup>Thermo Fisher Scientific, San Jose, CA, <sup>3</sup>PREMIER Biosoft, Palo Alto, CA

**PWe-061 Determination of Extensive Glycosylation on Glycoproteins and Glycolipids in High-density Lipoprotein using Mass Spectrometry**

11:10 – 12:20 Jincui Huang, Hyeyoung Lee, Nancy Rivera, Angela M Zivkovic, Jennifer Smilowitz, Bruce J German, Carlito B Lebrilla  
University of California, Davis

### Session 26

#### Lipidomics : Recent New Techniques and Applications

**PWe-062 Quantitative analyses of phosphatidylcholine hydroperoxides in oxidized lipoproteins by LC/MS**

13:30 – 14:40 Shu-Ping Hui<sup>1</sup>, Toshihiro Sakurai<sup>1,2</sup>, Seiji Takeda<sup>1</sup>, Shigeki Jin<sup>1</sup>, Hirotoshi Fuda<sup>1</sup>, Takao Kurosawa<sup>3</sup>, Hitoshi Chiba<sup>1</sup>

<sup>1</sup>Hokkaido University, Sapporo, Japan, <sup>2</sup>Research Fellow of the Japan Society for the Promotion of Science, Japan, <sup>3</sup>Faculty of Pharmaceutical Sciences, Health Sciences University of Hokkaido, Ishikari-Tobetsu, Hokkaido, Japan

**PWe-064 In situ analysis of soybean and nuts by Probe Electrospray Ionization mass spectrometry. Sequential ionization of carbohydrates and lipids**

13:30 – 14:40 Gabriela Petroselli<sup>1</sup>, Mridul K Mandal<sup>2</sup>, Lee C Chen<sup>2</sup>, Kenzo Hiraoka<sup>2</sup>, Hiroshi Nonami<sup>3</sup>, Rosa Erra-Balsells<sup>1</sup>

<sup>1</sup>University of Buenos Aires, <sup>2</sup>Yamanashi University, <sup>3</sup>Ehime University

**PWe-065 Comprehensive Lipid Profiling with Multiplexed Precursor Ion Scanning using the New AB SCIEX QTRAP® 4500 LC/MS/MS System**

11:10 – 12:20 Tomoko Nembai, Toshiyuki Yamazaki, Noriko Fueki, Kaoru Karasawa  
K.K.ABSCIEX

**PWe-066 Comprehensive fatty acid profiling using a single lipidomic approach**

13:30 – 14:40 futoshi sato<sup>1</sup>, Giorgis Isaac<sup>2</sup>, Amrita Cheema<sup>3</sup>, Kieran J Neeson<sup>2</sup>, Jeff Goshawk<sup>2</sup>, Jayne Kirk<sup>2</sup>, Andrew Baker<sup>2</sup>, Alan Millar<sup>2</sup>, Albert J Fornace Jr<sup>3</sup>, Jim Langridge<sup>2</sup>, Giuseppe Astarita<sup>2</sup>

<sup>1</sup>Nihon Waters K.K., Tokyo, Japan, <sup>2</sup>Waters Corporation, Milford, US,

<sup>3</sup>Georgetown University, Washington D.C., US

**PWe-067 MALDI-TOF MS analysis of phosphatidic acid using phosphate capture molecule, Phos-tag**

11:10 – 12:20 Mai Urikura<sup>1</sup>, Yoshino Kondo<sup>1</sup>, Jun-ichi Morishige<sup>1</sup>, Tamotsu Tanaka<sup>2</sup>, Kiyoshi Satouchi<sup>1</sup>

<sup>1</sup>Fukuyama University, Fukuyama, Japan, <sup>2</sup>University of Tokushima Graduate School, Tokushima, Japan

**PWe-068 Novel Non-targeted Lipidomic Quantitation using HILIC-HPLC/MS**

13:30 – 14:40 Eva Cifkova, Miroslav Lisa, Michal Holcapek  
University of Pardubice, Pardubice, Czech Republic

**PWe-069 Shotgun analysis of lipid extract from mouse brain by using comprehensive LC/MS**

11:10 – 12:20 Jisun Yoo, Eun Jung Bae, Taeseong Park, Young Hwan Kim  
Korea Basic Science Institute, Ochang, Korea

**PWe-070 Top-Down Analysis of Lipoproteins by On-Line Field-Flow Fractionation and ESI-MS-MS**

13:30 – 14:40 Ki Hun Kim, Ju Yong Lee, Myeong Hee Moon  
Yonsei University, Seoul, Korea

**PWe-071 Potential Biomarkers of Coronary Artery Disease by Flow Field-Flow Fractionation and Nanoflow LC-ESI-MS-MS**

11:10 – 12:20 Seul Kee Byeon, Ju Yong Lee, Myeong Hee Moon  
Yonsei University, Seoul, Korea

**PWe-072 Profiling of the Oxidized Phospholipids in Human Lipoprotein by Nanoflow LC-ESI-MS-MS**

13:30 – 14:40 Ju Yong Lee, Myeong Hee Moon  
Yonsei University, Seoul, South Korea

**PWe-073 Discovery of lipid markers by LC-ESI/MS for early detection of low dose radiation exposure**

11:10 – 12:20 Nai-Chun Huang, Jui-Ping Li, Chia-Hwa Chen, Chung-Shi Yang, Jen-Kun Chen  
National Health Research Institutes, Zhunan, Taiwan

**PWe-074 Characterization of mosquito cuticular lipids for age, species, and sex discrimination by MALDI-IT-TOF-MS**

13:30 – 14:40 Kevin A Schug<sup>1</sup>, Sheheli Islam<sup>1</sup>, Jaroslaw Krzywinski<sup>2</sup>, Seoung Bum Kim<sup>3</sup>

<sup>1</sup>The University of Texas at Arlington, Arlington TX USA, <sup>2</sup>Liverpool School of Tropical Medicine, Liverpool UK, <sup>3</sup>Korea University, Seoul, Korea

**PWe-075 Liquid extraction surface analysis for local profile of lipid molecular species on mammalian tissue slices**

11:10 – 12:20 Ryo Taguchi<sup>1</sup>, Akinori Mizuno<sup>1</sup>, Yoshiki Mizuno<sup>1</sup>, Miho Goto<sup>1</sup>, Kazutaka Ikeda<sup>2</sup>

<sup>1</sup>Chubu University, Kasugai, Aichi, Japan, <sup>2</sup>Institue for Advanced Biosciences, Keio University, Yamagata, Japan

**PWe-076 Comprehensive Standardized Methods of Lipid Profiling**

13:30 – 14:40 Toshiyuki Yamazaki, Noriko Fueki, Nembai Tomoko, Karasawa Kaoru  
AB SCIEX, Tokyo, Japan

## Wednesday, 19<sup>th</sup> September

**PWe-077** The utility of acetonitrile-related adducts formed in APCI sources for localization of double bonds in lipids  
 11:10 – 12:20

Josef Cvacka<sup>1</sup>, Vladimir Vrkoslav<sup>1</sup>, Eva Hakova<sup>2</sup>, Petra Horka<sup>1,2</sup>  
<sup>1</sup>Institute of Organic Chemistry and Biochemistry AS CR, v.v.i., Prague, Czech Republic, <sup>2</sup>Charles University in Prague, Prague, Czech Republic

**PWe-078** New mass spectrometric methods for structural characterization of hydrocarbons  
 13:30 – 14:40

Vladimir Vrkoslav, Josef Cvacka  
 Institute of Organic Chemistry and Biochemistry AS CR, v.v.i., Prague, Czech Republic

**PWe-079** Comparison of triacylglycerols in commercial DHA supplements utilizing MALDI-TOF-TOF tandem MS with spiral ion trajectory  
 11:10 – 12:20

Ayumi Kubo, Yoshiyuki Itoh, Masahiro Hashimoto, Jun Tamura  
 JEOL Ltd., Tokyo, Japan

**PWe-080** Analysis of oxidized lipid derived volatiles by Gas Chromatography/Mass Spectrometry  
 13:30 – 14:40

Shoji KAKUTA<sup>1</sup>, Yasuhiro BANDO<sup>2</sup>, Eiichiro FUKUSAKI<sup>1</sup>,  
 Takeshi BAMBA<sup>1</sup>  
<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>AMR Inc., Tokyo, Japan

**PWe-081** Structural analysis of triacylglycerols using desorption electrospray ionization mass spectrometry with precursor ion scanning and neutral loss scanning  
 11:10 – 12:20

Mayuko Morita<sup>1,2</sup>, Toshie Takahashi<sup>3</sup>, Ryo Taguchi<sup>2,4</sup>  
<sup>1</sup>Kyoto Prefectural University of Medicine, Kyoto, Japan, <sup>2</sup>Department of Metabolome, Graduate School of Medicine, The University of Tokyo, Tokyo, Japan, <sup>3</sup>Department of Biochemistry and Molecular Biology, Graduate School of Medicine, The University of Tokyo, Tokyo, Japan, <sup>4</sup>Department of Biomedical Sciences, College of Life and Health Sciences, Chubu University, Kasugai, Japan

**PWe-082** Multidimensional lipidomics for untargeted and targeted analyses  
 13:30 – 14:40

Giuseppe Astarita<sup>2</sup>, Marc V Gorenstein<sup>2</sup>, Andrew Baker<sup>2</sup>,  
 Mark A Ritchie<sup>1</sup>, John P Shockcor<sup>2</sup>  
<sup>1</sup>Waters Pacific, Singapore, <sup>2</sup>Waters, Milford, MA, USA

**PWe-083** Development of comprehensive identification and quantification of polyunsaturated fatty acids and eicosanoids in human plasma using LC-MS/MS  
 11:10 – 12:20

Fumiuki Nakagawa<sup>1</sup>, Katsutaro Morino<sup>2</sup>, Atsushi Ishikado<sup>2</sup>,  
 Chiho Ikeda<sup>1</sup>, Yoko Hoshiya<sup>1</sup>, Hiroshi Maekawa<sup>2</sup>  
<sup>1</sup>JCL Bioassay Corporation, Osaka, Japan, <sup>2</sup>Shiga University of Medical Science, Shiga, Japan

**PWe-084** Chiral HPLC/MS Analysis of Triacylglycerol Enantiomers and Regiosomers  
 13:30 – 14:40

Miroslav Lisa, Michal Holcapek  
 University of Pardubice, Pardubice, Czech Republic

**PWe-085** Structural analysis of oxidized triacylglycerols by using MALDI-SpiralTOF-TOF tandem mass spectrometer with high precursor ion selectivity and high-energy CID  
 11:10 – 12:20

Akihiko Kusai<sup>2</sup>, Ayumi Kubo<sup>1</sup>, Yoshiyuki Itoh<sup>1</sup>,  
 Masahiro Hashimoto<sup>1</sup>, Yoshihisa Ueda<sup>1</sup>

<sup>1</sup>JEOL Ltd., Tokyo, Japan, <sup>2</sup>JEOL (Europe) SAS, CROISSY-SUR-SEINE, France

**PWe-086** Development of a high-throughput lipid profiling method by using a quadrupole orbitrap mass spectrometer and an automated lipid identification software  
 13:30 – 14:40

Takayuki Yamada<sup>1</sup>, Takato Uchikata<sup>1</sup>, Shigeru Sakamoto<sup>2</sup>,  
 Yasuto Yokoi<sup>3</sup>, Eiichiro Fukusaki<sup>1</sup>, Takeshi Bamba<sup>1</sup>

<sup>1</sup>Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Suita, JAPAN, <sup>2</sup>Thermo Fisher Scientific, Yokohama, JAPAN, <sup>3</sup>Mitsui Knowledge Industry, Tokyo, JAPAN

**PWe-087** Simultaneous profiling of polar lipids by supercritical fluid chromatography/tandem mass spectrometry with methylation  
 11:10 – 12:20

Jaewon Lee<sup>1</sup>, Shin Nishiumi<sup>2</sup>, Masaru Yoshida<sup>2</sup>,  
 Eiichiro Fukusaki<sup>1</sup>, Takeshi Bamba<sup>1</sup>

<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>Kobe University, Kobe, Japan

**PWe-088** A screen using DART-MS to identify novel components of a pheromone synthesis pathway in *Drosophila melanogaster*  
 13:30 – 14:40

Yin Ning Chiang<sup>1</sup>, Joanne Y Yew<sup>1,2</sup>

<sup>1</sup>National University of Singapore, Singapore, Singapore, <sup>2</sup>Temasek Life Sciences Laboratory, Singapore, Singapore

**PWe-089** Inter-strain comparative lipidomics of microalgae using an online multi-dimensional HILIC-RP-UPLC-QToF-MS  
 11:10 – 12:20

Jeremy Dietrich Netto<sup>1</sup>, Sophie Fon Sing<sup>2,3</sup>, William Ditcham<sup>4</sup>,  
 Michael Borowitzka<sup>2</sup>, Mark Ritchie<sup>1</sup>

<sup>1</sup>Waters Pacific Private Limited, Singapore, <sup>2</sup>School of Biological Sciences and Biotechnology, Murdoch University, Australia, <sup>3</sup>Muradel Proprietary Limited, Australia, <sup>4</sup>Separation Science and Metabolomics Laboratory, Murdoch University, Australia

**PWe-090** Lipid identification through MS and MS/MS analyses combined with new database search software  
 13:30 – 14:40

Rainer Paape, Aiko Barsch, Jens Fuchser, Andrea Schneider,  
 Ulrike Anders, Sebastian Goetz, Detlev Suckau  
 Bruker Daltonik GmbH, Bremen, Germany

**PWe-091** Lipidomic profiling of mammalian brain and biofluids by RP-LC/MS: Global approaches and structural analysis using LTQ-Orbitrap.  
 11:10 – 12:20

Benoit COLSCH, Samia BOUDAH, Christophe JUNOT  
 CEA, Gif-sur-Yvette, France

## Wednesday, 19<sup>th</sup> September

**PWe-092 Development of ultra-high sensitive detection method of sphingosine-1-phosphate and its related sphingoids by LC/MS/MS**

13:30 – 14:40  
 Daisuke Saigusa, Tomohiro Takahashi, Shiori Ootaku,  
 Daisuke Jinno, Asuka Inoue, Michiyo Okutani, Takaaki Abe,  
 Naoto Suzuki, Junken Aoki, Yoshihisa Tomioka  
 Tohoku University, Miyagi, Japan

**PWe-093 Mass spectrometry based assessment chimeric mouse liver metabolite profiles following oral dosing of troglitazone**

11:10 – 12:20  
 Alan J Barnes<sup>1</sup>, Neil J Loftus<sup>1</sup>, David R Baker<sup>1</sup>, Ian Wilson<sup>2</sup>,  
 Yoshio Morikawa<sup>3</sup>

<sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom, <sup>2</sup>Astra Zeneca,  
 Alderley Park, UK, <sup>3</sup>PhoenixBio Co. Ltd, Higashi-Hiroshima, Japan

**PWe-094 High-throughput lipid profiling system for dried plasma spots by using online-supercritical fluid extraction-supercritical fluid chromatography/mass spectrometry**

13:30 – 14:40  
 Takato Uchikata, Atsuki Matsubara, Eiichiro Fukusaki,  
 Takeshi Bamba  
 Osaka University, Osaka, Japan

**PWe-095 Systems based LC-MS metabolite profiling of mice treated with ethanol enriched liquid diets**

11:10 – 12:20  
 Ashton Simon<sup>1</sup>, Neil J Loftus<sup>1</sup>, Alan J Barnes<sup>1</sup>,  
 Filippou Michopoulos<sup>2</sup>, Ian Wilson<sup>2</sup>, Ji Cheng<sup>3</sup>  
<sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom, <sup>2</sup>Astra Zeneca,  
 Alderley Park, UK, <sup>3</sup>University of Southern California, Los Angeles, USA

**PWe-096 Identification of Insect Species by Direct UV-Laser Desorption/ Ionization Mass Spectrometry of Cuticular Lipids and Pheromones**

13:30 – 14:40  
 Jacqueline Chin<sup>1,2</sup>, Qi Ling Koh<sup>3</sup>, Joanne Yew<sup>1,2</sup>  
<sup>1</sup>Temasek Life Sciences Laboratory, Singapore, <sup>2</sup>National University of Singapore, Singapore, <sup>3</sup>Nanyang Technological University, Singapore

**PWe-097 Systems-Based Approaches to Elucidating Gender-Specific Mechanisms in the Etiology of Atherosclerosis**

11:10 – 12:20  
 F L D'Alessandro<sup>1</sup>, Dmitry Grapov<sup>2</sup>, Peddinti Gopalacharyulu<sup>3</sup>,  
 T L Pedersen<sup>2</sup>, A Razuvayev<sup>1</sup>, S Arvidson<sup>1</sup>, H Hedin<sup>1</sup>, K Lund<sup>1</sup>,  
 T Gustavsson<sup>1</sup>, K Caidahl<sup>1</sup>, Jesper Z Haeggstrom<sup>1</sup>,  
 R Laaksonen<sup>4</sup>, M Janis<sup>4</sup>, T Hyotylainen<sup>3</sup>, M Oresic<sup>3</sup>,  
 J W Newman<sup>2</sup>, Craig E Wheelock<sup>1</sup>

<sup>1</sup>Karolinska Institute, <sup>2</sup>United States Department of Agriculture ARS Western Human Nutrition Research Center, Davis, CA, USA, <sup>3</sup>VTT Technical Research Centre of Finland, Espoo, Finland, <sup>4</sup>Zora Biosciences, Oy, Espoo, Finland

**PWe-098 Molecular lipidomic workflow solution identifies a single lipid marker for the diagnosis of statin myalgia**

13:30 – 14:40  
 Kim Ekoos<sup>1</sup>, Dimple Kauhanen<sup>1</sup>, Tuulia Sylvänen<sup>1</sup>,  
 Kirill Tarasov<sup>1</sup>, Reini Hurme<sup>1</sup>, Giuliana Mombelli<sup>2</sup>,  
 Cesare R Sirtori<sup>3</sup>, Michael Phillips<sup>4</sup>, Marie-Pierre Dube<sup>4</sup>,  
 Nathalie Laplante<sup>4</sup>, Jean-Claude Tardif<sup>4</sup>, Reijo Laaksonen<sup>1</sup>  
<sup>1</sup>Zora Biosciences, Espoo, Finland, <sup>2</sup>Niguarda Hospital, Milan, Italy,  
<sup>3</sup>University of Milan, Milan, Italy, <sup>4</sup>Montreal Heart Institute, Montreal, Canada

**PWe-099 Development of comprehensive glycerophospholipid profiling methods using liquid chromatography / high-speed triple quadrupole mass spectrometry**

11:10 – 12:20  
 Suzumi M Tokuoka<sup>1</sup>, Yoshihiro Kita<sup>1</sup>, Masaki Yamada<sup>1,2</sup>,  
 Takao Shimizu<sup>1</sup>

<sup>1</sup>The University of Tokyo, Tokyo, Japan, <sup>2</sup>Shimadzu Corporation, Kyoto, Japan

**PWe-100 Development of a comprehensive detection method for quantifying eicosanoids using high-speed liquid chromatography / mass spectrometry**

Masaki Yamada<sup>1,2</sup>, Yoshihiro Kita<sup>1</sup>, Suzumi Tokuoka<sup>1</sup>,  
 Takao Shimizu<sup>1</sup>

<sup>1</sup>The University of Tokyo, Tokyo, Japan, <sup>2</sup>Shimadzu Co., Kyoto, Japan

**PWe-101 Formation and collision-induced dissociation (CID) of unsaturated fatty acid-alkali metal anionic complexes: A new approach for determining double bond position**

Michael C Thomas, Thomas Gallagher, Geoffrey W Nette  
 Independent Marine Biochemical Research, Dunwich, Australia

**PWe-102 Phosphoinositides analysis by liquid chromatography and mass spectrometry**

13:30 – 14:40  
 Federico Torta, Pradeep Narayanaswamy, Michael P Sheetz,  
 Markus R Wenk  
 National University of Singapore, Singapore, Singapore

## Session 27

### Progress in Microbiology

**PWe-103 Secondary metabolite profile of Fusarium oxysporum by LCMS using QTOF,different sources, ion modes and metal solution post-column addition**

11:10 – 12:20  
 Adriana M Cirigliano<sup>1</sup>, Brenda V Bertinetto<sup>1</sup>, Maria A Rodriguez<sup>2</sup>,  
 Alicia M Godeas<sup>2</sup>, Gabriela M Cabrera<sup>1</sup>

<sup>1</sup>Depto Quimica Organica y UMYMFOR-CONICET Buenos Aires University,  
 Buenos Aires, Argentina, <sup>2</sup>Depto Biodiversidad y biología experimental  
 Buenos Aires University, Buenos Aires, Argentina

**PWe-104 Pyruvate Phosphate Dikinase Phosphorylation Increases Lipid Production in Rhodopseudomonas palustris: a Phosphoproteomic Analysis**

13:30 – 14:40  
 Chia-Wei Hu<sup>2</sup>, Miao-Hsia Lin<sup>1,3</sup>, Tsun-Hsuan Yi<sup>2</sup>,  
 Hsuan-Cheng Huang<sup>4</sup>, Wei-Chi Ku<sup>1</sup>, Chia-Feng Tsai<sup>5</sup>,  
 Yu-Ju Chen<sup>5</sup>, Naoyuki Sugiyama<sup>6</sup>, Yasushi Ishihama<sup>1,6</sup>,  
 Hsueh-Fen Juan<sup>2,7</sup>, Shih-Hsiung Wu<sup>2</sup>

<sup>1</sup>Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan, <sup>2</sup>Institute of Molecular and Cellular Biology, National Taiwan University, Taipei, Taiwan, <sup>3</sup>Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan, <sup>4</sup>Institute of Biomedical Informatics and Center for Systems and Synthetic Biology, National Yang-Ming University, Taipei, Taiwan,

<sup>5</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan, <sup>6</sup>Institute for Advanced Biosciences, Keio University, Daihoji, Tsuruoka, Japan,

<sup>7</sup>Department of Life Sciences, National Taiwan University, Taipei, Taiwan

## Wednesday, 19<sup>th</sup> September

**PWe-105 Rapid and Simple Characterization of Mycolic Acids in the Suborder Corynebacterineae Using MALDI Spiral-TOFMS**

11:10 – 12:20  
 Kanae Teramoto<sup>1</sup>, Takafumi Sato<sup>1</sup>, Shinichi Mukosaka<sup>1</sup>, Tomohiko Tamura<sup>2</sup>, Moriyuki Hamada<sup>2</sup>, Ken-ichiro Suzuki<sup>2</sup>

<sup>1</sup>JEOL Ltd., Tokyo, Japan, <sup>2</sup>NITE Biological Resource Center, Kisarazu, Japan

**PWe-106 Evaluation of Proteomic Profile with Principal Component Analysis in Group A Streptococci**

13:30 – 14:40  
 Akira Okamoto<sup>1</sup>, Taguchi Yoshihiro<sup>2</sup>

<sup>1</sup>Aichi University of Education, Aichi, Japan, <sup>2</sup>Chuo University, Tokyo, Japan

**PWe-107 Glycopeptidolipids with novel peptide composition from *Mycobacterium avium-intracellulare* complex**

11:10 – 12:20  
 Naoya Ichimura, Takeshi Kasama  
 Tokyo Medical and Dental University, Tokyo, Japan

**PWe-108 Identification of Medically Important *Candida* Species by LC-Selective Tandem Mass Spectrometry**

13:30 – 14:40  
 Po-Chih Chang<sup>1</sup>, Muralidhar Reddy<sup>1</sup>, Chien-Liang Chen<sup>1</sup>, Tsung C Chang<sup>2</sup>, Hsien-Chang Chang<sup>3</sup>, Yen-Peng Ho<sup>1</sup>

<sup>1</sup>Department of Chemistry, National Dong Hwa University, Hualien, Taiwan,

<sup>2</sup>Department of Medical Laboratory Science and Biotechnology, National Cheng-Kung University, Taiwan, <sup>3</sup>Department of Biomedical Engineering, National Cheng-Kung University, Taiwan

**PWe-109 Metabolome of Aspergillus: Towards the Early Diagnosis of Invasive Aspergillosis**

11:10 – 12:20  
 Havlicek Vladimir<sup>1</sup>, Strohalm Martin<sup>1</sup>, Kavan Daniel<sup>1</sup>, Lemr Karel<sup>1</sup>, Schug Kevin<sup>2</sup>, Sulc Miroslav<sup>1</sup>

<sup>1</sup>Institute of Microbiology, Prague, Czech Republic, <sup>2</sup>University of Texas at Arlington, TX, USA

**PWe-110 Design Of Specific methodology For The Identification Of Beta-Lactamase Producing Enterobacteriaceae Using MALDI Mass Spectrometry**

13:30 – 14:40  
 Emmanuel Q wey<sup>1</sup>, Matthew Openshaw<sup>2</sup>, Philippa Hart<sup>2</sup>, Omar Belgacem<sup>2</sup>, Pranav Somaiya<sup>3</sup>, Shervanthi Homer-Vanniasinkam<sup>3</sup>, Indran Balakrishnan<sup>1</sup>

<sup>1</sup>Royal Free Hospital Foundation Trust London United Kingdom, <sup>2</sup>Shimadzu, Manchester, United Kingdom, <sup>3</sup>NPIMR-UCL, London, United Kingdom

**PWe-111 Differentiation of Single Attachment versus Double Attachment of Phycoerythrobilin Chromophores to Phycobiliproteins of *Fremyella diplosiphon* Cyanobacteria using MALDI Mass Spectrometry**

11:10 – 12:20  
 M Nazim Boutaghous<sup>2</sup>, Christina M Kronfel<sup>2</sup>, Leanora S Hernandez<sup>2</sup>, Avijit Biswas<sup>2</sup>, Wendy M Schluchter<sup>2</sup>, Richard B Cole<sup>1,2</sup>

<sup>1</sup>Université Pierre et Marie Curie (Paris 6), Paris, France, <sup>2</sup>University of New Orleans, New Orleans, LA, USA

**PWe-112 The study and characterization of growth factors produced by murine herpes virus using multistage MS techniques**

13:30 – 14:40  
 Andrea Stanova, Jozef Marak, Miroslava Supolikova, Livia Cikova, Frantisek Golais, Pavol Kois

Comenius University, Bratislava, Slovak Republic

**PWe-113 MALDI Mass Spectrometry and MALDI-MS/MS Investigation into Chemically Induced Peptides of Beta-Lactamase Producing Enterobacteriaceae**

11:10 – 12:20  
 Emmanuel Q Wey<sup>2</sup>, Philippa J Hart<sup>1</sup>, Matthew Openshaw<sup>1</sup>, Omar Belgacem<sup>1</sup>, Pranav Somaiya<sup>3</sup>,

Shervanthi Homer-Vanniasinkam<sup>3</sup>, Indran Balakrishnan<sup>2</sup>

<sup>1</sup>Shimadzu, UK, <sup>2</sup>Royal Free Hospital NHS Foundation Trust, London , UK,

<sup>3</sup>NPIMR-UCL, London, UK

**PWe-114 Exploring the Patellamide Biosynthetic Pathway**

13:30 – 14:40  
 Shirran L Sally<sup>1</sup>, Fuszard Matthew<sup>1</sup>, Koehne Jesko<sup>1</sup>, Bent Andrew<sup>1</sup>, Houssen Wael<sup>2</sup>, Jaspars Marcel<sup>2</sup>, Botting H Catherine<sup>1</sup>, Naismith H James<sup>1</sup>

<sup>1</sup>University of St Andrews, <sup>2</sup>University of Aberdeen

**PWe-115 Liquid chromatography-electrospray ionization mass spectrometry for metabolism studies of mogroside V by Ganoderma lucidum mycelium**

11:10 – 12:20  
 Chun-Hui Chiu, Ting-Jang Lu  
 National Taiwan University, Taipei, Taiwan

**PWe-116 Identification of Bacteria and Fungi by Rapid Evaporative Ionization Mass Spectrometry**

13:30 – 14:40  
 Ákos Szekeres<sup>1</sup>, Imola Körtvélyessyén Györi<sup>2</sup>, Júlia Balogh<sup>2</sup>, Tamás Szaniszló<sup>3</sup>, Katalin Dr Kristóf<sup>3</sup>, Judit M Dr Molnár<sup>3</sup>, Zoltán Dr Takáts<sup>4</sup>

<sup>1</sup>Masprox Ltd., Budapest, Hungary, <sup>2</sup>Medimass Ltd., Budapest, Hungary,

<sup>3</sup>Semmelweis University, Budapest, Hungary, <sup>4</sup>Imperial College London, London, UK

**PWe-117 Lysosomal storage diseases diagnostics in dry blood spots by fluorimetry and multiple reaction monitoring mass spectrometry**

11:10 – 12:20  
 Claudia Cozma<sup>1</sup>, Marius-Ionut Iurascu<sup>1</sup>, Laura Ion<sup>1</sup>, Stefan Maeser<sup>2</sup>, Michael Przybylski<sup>1</sup>

<sup>1</sup>University of Konstanz, Germany, <sup>2</sup>Centogen GmbH, Germany

## Session 28

### IR Spectroscopy of Gas-phase Ions

**PWe-118 UV action spectroscopy of peptides and proteins via photodissociation of iodine labelled tyrosine residues.**

13:30 – 14:40  
 Benjamin B Kirk<sup>1</sup>, Adam T Trevitt<sup>1</sup>, Haibo B Yu<sup>1</sup>, Yuanqi Tao<sup>2</sup>, Benjamin N Moore<sup>2</sup>, Ryan R Julian<sup>2</sup>, Stephen J Blanksby<sup>1</sup>

<sup>1</sup>University of Wollongong, Wollongong, Australia, <sup>2</sup>University of California, Riverside, USA

## Wednesday, 19<sup>th</sup> September

### Session 29

#### The Advances in Biological Mass Spectrometry in Drug Discovery and Development: Current State of the Art and Challenges

- PWe-120** Influence of end-capping reagent of LC column on sensitive determination using LC/MS  
13:30 – 14:40

Chiaki Aoyama, Yuko Yui, Kensuke Okusa, Kosuke Osaka, Takao Tamura, Masakazu Takahashi  
GL Sciences Inc., Iruma, Japan

- PWe-121** Simultaneous, Fast Analysis of Melamine and Analogues in Pharmaceutical Components Using Q Exactive - Benchtop Orbitrap LC-MS/MS  
11:10 – 12:20

Kate J Comstock, Hongxia (Jessica) Wang, Tim Stratton, Yingying Huang  
ThermoFisher Scientific

- PWe-122** Measurement and Optimization of Organic Chemical Reaction Yields by GC-MS with Supersonic Molecular Beams  
13:30 – 14:40

Aviv Amirav, Alexander Gordin, Youlia Hagoory, Shlomo Rozen, Bogdan Belgorodsky, Boaz Seemann, Hanit Marom, Michael Gozin, Alexander B Fialkov  
Tel Aviv University

- PWe-123** The Utility of a Novel High Resolution Quadrupole Time-of-Flight Mass Spectrometer for Improved Characterization of Antibodies and Immuno-Conjugates  
11:10 – 12:20

Asish Chakraborty<sup>1</sup>, St John Skilton<sup>1</sup>, Steve Pringle<sup>2</sup>, Nick Tomczyk<sup>2</sup>, Weibin Chen<sup>1</sup>  
<sup>1</sup>Waters, Milford, USA, <sup>2</sup>Water MS Technologies, Manchester UK

- PWe-124** Method Development for Quality Control of Traditional Chinese Herbal Medicine- Guizhi Tang by HPLC and Electrospray Ion Trap Mass Spectrometry  
13:30 – 14:40

Ming-Yu Chao, Ying-Yu Kuo, Jui-Ching Chen, Che-Yi Lin, Yuan-Ling Ku, Leah Lo  
Medical and Pharmaceutical Industry Technology and Development Center, Taipei, Taiwan (R.O.C.)

- PWe-125** High-throughput sequence determination of screened 90 micron single beads on which a cyclic octapeptide is immobilized  
11:10 – 12:20

Kiyoshi NOKIHARA<sup>1</sup>, Takafumi OHYAMA<sup>1</sup>, Noriko ONO<sup>1</sup>, Takeshi KASAMA<sup>2</sup>  
<sup>1</sup>HiPep Laboratories, Kyoto, Japan, <sup>2</sup>Tokyo Medical and Dental University, Tokyo, Japan

- PWe-127** MsXelerator: A Software Platform for (Reactive) Drug Metabolite Detection and Identification using High-Resolution Mass Spectrometry and Post-Acquisition Data Mining  
11:10 – 12:20

Marco Ruijken  
MsMetrix, Maarssen, the Netherlands

- PWe-128** Non-targeted identification of novel Buspirone metabolites using a Spectral Similarity score derived from common fragment ion and neutral loss species  
13:30 – 14:40

Kirsten Hobby, Alan Barnes, Neil Loftus  
Shimadzu MSO, Manchester, UK

- PWe-129** Analysis of interaction between TNF-alpha and anti-TNF-alpha agents by hydrogen deuterium exchange/mass spectrometry  
11:10 – 12:20

Shiori Nakazawa<sup>1,2</sup>, Noritaka Hashii<sup>2</sup>, Nana Kawasaki<sup>1,2</sup>  
<sup>1</sup>Hokkaido University, Sapporo, Japan, <sup>2</sup>National Institute of Health Sciences, Tokyo, Japan

- PWe-130** Validation and application of UHPLC-ESI-MS/MS method for the quantification of probe-drugs and metabolites of CYP3A4 and UGT1A1 in pharmacokinetics study  
13:30 – 14:40

Daryl Kim Hor Hee, Zhangyan Yao, Lawrence Soon-U Lee  
National University of Singapore, Singapore

- PWe-131** MALDI High Resolution Mass Spectrometry in the Identification of Atorvastatin and Its Oxidative Metabolites  
11:10 – 12:20

Robert Jirasko<sup>1</sup>, Veronika Jedlickova<sup>1</sup>, Tomas Mikysek<sup>1</sup>, Michal Holcapek<sup>1</sup>, Ales Svatos<sup>2</sup>, Martin Kunes<sup>3</sup>, Milan Nobilis<sup>3</sup>  
<sup>1</sup>Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentska 573, 53210 Pardubice, Czech Republic, <sup>2</sup>Max Planck Inst. Chem. Ecol., Res. Grp. Mass Spectrometry, D-07745 Jena, Germany, <sup>3</sup>Faculty of Pharmacy, Charles University, Heyrovskeho 1203, CZ-50005 Hradec Kralove, Czech Republic

- PWe-132** Metabolic Stability Screening Workflow using a Second Generation High Resolution Accurate Mass Benchtop Instrument  
13:30 – 14:40

Shigeru Sakamoto<sup>1</sup>, Sun Hai-Ling<sup>3</sup>, Soohoo Daniel<sup>3</sup>, Comstock Kate<sup>2</sup>, Stratton Tim<sup>2</sup>

<sup>1</sup>ThermoFisher Scientific, Yokohama, Japan, <sup>2</sup>ThermoFisher Scientific, San Jose, CA, USA, <sup>3</sup>Gilead Sciences, Foster City, CA, USA

## Wednesday, 19<sup>th</sup> September

**PWe-133** Development of High Performance Liquid Chromatography Tandem Mass Spectrometry Method for Analysis of Bacopaside-I in Rat Urine and Feces Samples  
 11:10 – 12:20

Sontaya Sookying<sup>2</sup>, Kornkanok Ingkaninan<sup>\*2</sup>, Dumrongsak Pekthong<sup>3</sup>, Sarawut Oo-puthinan<sup>3</sup>, Jie Xing<sup>1</sup>, Zhaoqi Zhan<sup>1</sup>

<sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, CINTECH IV, Singapore, <sup>2</sup>Department of Pharmaceutical Chemistry and Pharmacognosy, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand, <sup>3</sup>Department of Pharmacy Practice, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand

**PWe-134** Novel Mass Spectrometry Based Method for Quantitation of Antibody Drug Conjugates  
 13:30 – 14:40

Kim Alving<sup>1</sup>, James Stefano<sup>1</sup>, Richard Gregory<sup>2</sup>, Diego Gianolio<sup>2</sup>, William Brondyke<sup>1</sup>, Pradeep Dhall<sup>1</sup>, Aharon Cohen<sup>1</sup>, Bing Wang<sup>1</sup>  
<sup>1</sup>Genzyme - A Sanofi company, <sup>2</sup>Sanofi Oncology

**PWe-135** Method for the direct injection and on-line sample clean-up of whole methanolic extracts from dried blood spots  
 11:10 – 12:20

Reiko Iizuka<sup>1</sup>, Motoji Oshikata<sup>1</sup>, Paul Rainville<sup>2</sup>, Jennifer Simeone<sup>2</sup>, Thomas Wheat<sup>2</sup>, Robert Plumb<sup>2</sup>  
<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>Waters, Milford, MA

**PWe-136** Metabolite analysis using a novel relationship and database driven software platform approach for screening and understanding metabolism  
 13:30 – 14:40

Etsuko Suzuki<sup>1</sup>, Motoji Oshikata<sup>1</sup>, Mark Wrona<sup>2</sup>, David Deans<sup>3</sup>, Jeff Goshawk<sup>3</sup>, Debadeep Bhattacharya<sup>2</sup>, Joanne Mather<sup>2</sup>, Robert Plumb<sup>2</sup>  
<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>Waters Corporation, Milford, MA, <sup>3</sup>Waters, Manchester, UK

**PWe-137** HILIC-UHPLC-MS/MS determination of entecavir in rat plasma, urine and plasma ultrafiltrate using various sample preparation techniques  
 11:10 – 12:20

Lucie Novakova<sup>1</sup>, Hana Vlckova<sup>1</sup>, Tomas Gottvald<sup>1</sup>, Jaroslav Janak<sup>1</sup>, Frantisek Trejtnar<sup>2</sup>, Jana Mandikova<sup>2</sup>, Petr Solich<sup>1</sup>

<sup>1</sup>Charles University in Prague, Faculty of Pharmacy in Hradec Kralove, Department of analytical chemistry, <sup>2</sup>Department of Pharmacology and Toxicology, Faculty of Pharmacy, Charles University in Prague, Heyrovskeho 1203, 500 05 Hradec Kralove, Czech Republic

**PWe-138** Determining The Pharmacokinetics And Metabolic Fate Of A Novel Anti-Cancer Compound Using LC/MS/MS With Comprehensive Data Collection  
 13:30 – 14:40

Shunya Sasaki<sup>1</sup>, Motoji Oshikata<sup>1</sup>, Joanne Mather<sup>2</sup>, Robert Plumb<sup>3</sup>, Ian Wilson<sup>4</sup>  
<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>Waters Corporation, Milford, MA, <sup>3</sup>Imperial College, London, UK, <sup>4</sup>AstraZeneca, Macclesfield, UK

**PWe-139** Development of a Highly Sensitive Methodology for Quantitative Determination of Fexofenadine in Microdose Studies by Multiple Injection Method Using UHPLC-MS/MS  
 11:10 – 12:20

Yukari Tanaka<sup>1,2</sup>, Yutaka Yoshikawa<sup>2</sup>, Hiroyuki Yasui<sup>2</sup>

<sup>1</sup>SHIONOGI & CO., LTD., Osaka, Japan, <sup>2</sup>Kyoto Pharmaceutical University, Kyoto, Japan

**PWe-140** Mass spectrometric analysis of ginsenosides in Panax ginseng root and callus using pseudo two-dimensional liquid chromatogram  
 13:30 – 14:40

Yumiko Ueno<sup>1</sup>, Issey Osaka<sup>2</sup>, Hirotaka Hisatomi<sup>1</sup>, Shu Taira<sup>3</sup>, Hideya Kawasaki<sup>1</sup>, Ryuichi Arakawa<sup>1</sup>

<sup>1</sup>Kansai University,Suita,Japan, <sup>2</sup>Yokohama City University, Yokohama, Japan, <sup>3</sup>Japan Advanced Institute of Science and Technology, Nomi, Japan

**PWe-141** Metabolic site elucidation of glucuronide metabolites using ion mobility and molecular modeling  
 11:10 – 12:20

Motoji Oshikata<sup>1</sup>, Masayo Yabu<sup>1</sup>, Yutaka Takahashi<sup>2,3</sup>, Mitsuo Takayama<sup>3</sup>

<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>MS Solution, Tokyo, Japan, <sup>3</sup>Graduate School of Nanobioscience, Yokohama City University, Yokohama, Japan

**PWe-142** Mimicking of the phase I metabolism of drugs by photocatalytic reactions  
 13:30 – 14:40

Miina Ruokolainen, Tiina Sikanen, Petri Kylli, Risto Kostainen, Tapio Kotiaho  
 University of Helsinki, Helsinki, Finland

**PWe-143** Streamlining the Metabolite Identification Workflow Using High Resolution QTOF Data and Mass-MetaSite.  
 11:10 – 12:20

Lester C Taylor<sup>1</sup>, Ismael Zamora<sup>2</sup>, Gabriele Cruciani<sup>2</sup>

<sup>1</sup>Agilent Technologies, <sup>2</sup>Molecular Discovery Ltd

**PWe-144** The development of multistatin method for determination of statins, their metabolites and interconversion products in human serum  
 13:30 – 14:40

Hana Vlckova, Karolina Skraskova, Pavel Svoboda,

Helena Tomsikova, Petr Solich, Lucie Novakova

Charles University in Prague, Faculty of Pharmacy, Hradec Kralove, Czech Republic

**PWe-145** Electrochemical generation of oxidative and reductive metabolites of selected drugs and their UHPLC/MS/MS characterization  
 11:10 – 12:20

Michal Holcapek<sup>1</sup>, Robert Jirasko<sup>1</sup>, Veronika Jedlickova<sup>1</sup>, Tomas Mikysek<sup>1</sup>, Milan Nobilis<sup>2</sup>, Lenka Skalova<sup>2</sup>

<sup>1</sup>University of Pardubice, Czech Republic, <sup>2</sup>Faculty of Pharmacy, Charles University, Hradec Kralove, Czech Republic

**PWe-146** In-depth pharmaco-phosphoproteomics using meter-long monolithic columns to evaluate molecular-targeting drugs  
 13:30 – 14:40

Masaki Wakabayashi<sup>1</sup>, Ayaka Sato<sup>1</sup>, Mio Iwasaki<sup>1</sup>,

Naoyuki Sugiyama<sup>2</sup>, Yasushi Ishihama<sup>1</sup>

<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Keio University, Tsuruoka, Japan

## Wednesday, 19<sup>th</sup> September

- PWe-147** A Semi-Automated Method for Sequencing Oligonucleotides using ISD and Pseudo-MS3 on a MALDI-Ion Trap-TOF Mass Spectrometer  
 11:10 – 12:20

Matthew E Openshaw<sup>1</sup>, Omar Belgacem<sup>1</sup>, Marco Smith<sup>2</sup>  
<sup>1</sup>Shimadzu, Manchester, UK, <sup>2</sup>GlaxoSmithKline, Stevenage, UK

- PWe-148** Caco-2 PERMEABILITY STUDIES AND DETERMINATION BY LC/MSMS OF MEMANTINE  
 13:30 – 14:40

Banu Erdem<sup>1</sup>, Seval Korkmaz<sup>2</sup>, Murat Onul<sup>3</sup>, Engin Bayram<sup>3</sup>  
<sup>1</sup>Marmara University Faculty of Engineering Department of Bioengineering,  
<sup>2</sup>Abdi Ibrahim Pharmaceuticals Inc., Istanbul, Turkey, <sup>3</sup>Ant Teknik Cih. Ltd. Sti., Istanbul, Turkey

- PWe-149** Development of mass spectrometric method for pharmacokinetic study of Herceptin  
 11:10 – 12:20

Jin Nyoung Choi<sup>1</sup>, Jeong Won Kang<sup>1</sup>, Do Young Choi<sup>1</sup>,  
 Gyu-Tae Park<sup>2</sup>, Soyong Jang<sup>2</sup>, Kwang Pyo Kim<sup>1</sup>  
<sup>1</sup>Konkuk University, Seoul, Korea, <sup>2</sup>CKD Research Institute, Yongin, Korea

- PWe-150** Caco-2 PERMEABILITY STUDIES AND DETERMINATION BY LC/MSMS OF THIOCTIC ACID  
 13:30 – 14:40

Murat Onul<sup>1</sup>, Seval Korkmaz<sup>2</sup>, Banu Erdem<sup>3</sup>  
<sup>1</sup>Ant Teknik, Istanbul, Turkey, <sup>2</sup>Abdi Ibrahim Pharmaceuticals Inc., Istanbul, Turkey, <sup>3</sup>Marmara University Faculty of Engineering, Department of Bioengineering, Istanbul, Turkey

- PWe-151** Chemical modomics: Alternative analytical platform for efficient biomarker discovery  
 11:10 – 12:20

Tomoyuki Oe  
 Tohoku University, Sendai, Japan

- PWe-152** Metal Modified Nanoparticle as a Probe for Quantitative Analysis of Clodronate Drug by MALDI-MS in Human Plasma  
 13:30 – 14:40

Wei Hsu<sup>1</sup>, Yi-Chi Ho<sup>1</sup>, Mei-Chun Tseng<sup>1</sup>, An-Kai Su<sup>1</sup>, Ping-Yu Lin<sup>1</sup>, Huan-Ting Wu<sup>2</sup>, Chun-Cheng Lin<sup>2</sup>, Ming-Ren Fuh<sup>3</sup>, Yu-Ju Chen<sup>1</sup>  
<sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan, <sup>2</sup>Department of Chemistry, Tsing Hua University, Hsinchu, Taiwan, <sup>3</sup>Department of Chemistry, Soochow University, Taipei, Taiwan

- PWe-153** Caco-2 PERMEABILITY STUDIES AND DETERMINATION BY LC/MSMS OF TRIMEBUTINE  
 11:10 – 12:20

Murat Yayla<sup>1</sup>, Seval Korkmaz<sup>2</sup>, Banu Erdem<sup>3</sup>, Murat ONUL<sup>4</sup>  
<sup>1</sup>Ant Teknik, Ankara, Turkey, <sup>2</sup>Abdi Ibrahim Pharmaceutical Inc., Turkey, <sup>3</sup>Marmara University Faculty of Engineering, Department of Bioengineering, Istanbul, Turkey, <sup>4</sup>Ant Teknik, Istanbul, Turkey

- PWe-154** Caco-2 PERMEABILITY STUDIES AS A NEW ALTERNATIVE MODEL TO BIOEQUIVALENCE AND BIOWAIVER TESTS  
 13:30 – 14:40

Seval Korkmaz  
 Abdi Ibrahim Pharmaceuticals, Istanbul, TURKEY

- PWe-156** Selectivity test: Potential Interfering substances evaluation during LDTD-MS/MS quantification  
 13:30 – 14:40

Alex Birsan, Serge Auger, Annick Dion-Fortier, Pierre Picard  
 Phytronix Technologies, Quebec, Canada

- PWe-157** Intact Monoclonal Antibody Characterization Using A Bench-Top Orbitrap Mass Spectrometer  
 11:10 – 12:20

Zhiqi Hao<sup>1</sup>, Yi Zhang<sup>1</sup>, Dave Horn<sup>1</sup>, Shiaw-Lin Wu<sup>2</sup>,  
 Patrick K Bennett<sup>1</sup>, Andreas F Huhmer<sup>1</sup>

<sup>1</sup>Thermo Fisher Scientific, <sup>2</sup>Barnett Institute, Northeastern University, Boston, MA

- PWe-158** Novel approaches in the imitation of oxidative drug metabolism by electrochemistry-mass spectrometry  
 13:30 – 14:40

Hjalmar P Permentier<sup>1</sup>, Eslam Nouri-Nigjeh<sup>1,2</sup>, Andries P Bruins<sup>1</sup>, Rainer Bischoff<sup>1</sup>

<sup>1</sup>University of Groningen, Groningen, The Netherlands, <sup>2</sup>New York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, USA

- PWe-159** Analysis of lipid composition in stimulated human cancer cells by LC-MS/MS following treatment with protolichesterinic acid isolated from Cetraria islandica  
 11:10 – 12:20

Finnur F Eiriksson<sup>1,2</sup>, Baldur B Sigurdsson<sup>2</sup>, Sesselja S Omarsdottir<sup>1</sup>, Helga M Ogmundsdottir<sup>1</sup>, Margret Thorsteinsdottir<sup>1,2</sup>

<sup>1</sup>University of Iceland, Reykjavik, Iceland, <sup>2</sup>ArcticMass, Reykjavik, Iceland

- PWe-160** UHPLC-MS-MS with Precursor Ion Scanning, Neutral Loss Scanning and Polarity Switching for the Detection of Glutathione Conjugates of Reactive Metabolites  
 13:30 – 14:40

Richard B van Breemen, Ke Huang  
 University of Illinois College of Pharmacy, Chicago, IL USA

## Session 30

### Data Processing and Informatics for SIMS

- PWe-161** Comparison of titanate nanosheets by G-SIMS and g-ogram  
 11:10 – 12:20

Ichiro Mihara<sup>1</sup>, Satoko Aoyagi<sup>2</sup>, Keizo Nakagawa<sup>3</sup>

<sup>1</sup>Kuraray CO., LTD, Tokyo, Japan, <sup>2</sup>Shimane University, Shimane, Japan, <sup>3</sup>The University of Tokushima, Tokushima, Japan

- PWe-162** Adaptive Thresholding for Three-Dimensional Wavelet Denoising of TOF-SIMS Images : Toward Digital Staining of Pathological Specimens  
 13:30 – 14:40

Koichi Tanji, Manabu Komatsu, Hiroyuki Hashimoto  
 Canon Inc. Tokyo, Japan

## Wednesday, 19<sup>th</sup> September

### Session 43

#### Novel Proteomics Methodologies

- PWe-163** Elucidating the aberrant PK Profiles of Monoclonal Antibody by Proteomics Approaches  
 11:10 – 12:20

Wai Siang Law<sup>1</sup>, A P Warren<sup>1</sup>, P Lloyd<sup>1</sup>, J Sims<sup>1</sup>, J Balthasar<sup>2</sup>, Carsten Krantz<sup>1</sup>

<sup>1</sup>Novartis Pharma AG, Basel, Switzerland, <sup>2</sup>Department of Pharmaceutical Sciences School of Pharmacy and Pharmaceutical Sciences University at Buffalo, The State University of New York, Buffalo, New York 14260

- PWe-165** Mass spectrometry-based non-invasive proteomic analysis of human skin keratins for discovery of biomarkers of oxidative skin damage  
 11:10 – 12:20

Seon Hwa Lee, Kohei Miyamoto, Takaaki Goto, Tomoyuki Oe Tohoku University, Sendai, Japan

- PWe-166** RELATIVE QUANTITATION OF TMT-LABELED PROTEOMES FOCUS ON QUANTITATIVE PRECISION AND ACCURACY  
 13:30 – 14:40

Rosa I Viner<sup>1</sup>, Michaela Scigelova<sup>2</sup>, Martin Zeller<sup>2</sup>, Madalina Oppermann<sup>2</sup>, Thomas Moehring<sup>2</sup>, Vlad Zabrouskov<sup>1</sup>  
<sup>1</sup>Thermo Fisher Scientific, San Jose, USA, <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany

- PWe-167** Mobility Assisted Data Independent Label-Free LC-MS Analysis of Citrobacter rodentium Infected Mouse Colon  
 11:10 – 12:20

Maki Terasaki<sup>1</sup>, Chris Hughes<sup>2</sup>, Johannes P Vissers<sup>2</sup>, James Collins<sup>3</sup>, Gad Frankel<sup>3</sup>

<sup>1</sup>Nihon Waters K. K., Tokyo, Japan, <sup>2</sup>Waters, Manchester , UK, <sup>3</sup>Imperial College, London, UK

- PWe-168** A method for isolation of endogenous disulfide-containing peptides from a biological sample.  
 13:30 – 14:40

Caroline D Pereira<sup>1</sup>, Naoto Minamino<sup>2</sup>, Toshifumi Takao<sup>1</sup>  
<sup>1</sup>Institute for Protein Research, Osaka University, Osaka, Japan, <sup>2</sup>National Cardiovascular Center, Osaka, Japan

- PWe-169** A Targeted Quantitative Phosphoproteomic Approach using iTRAQ-Labelled Synthetic Peptides as Internal Standards  
 11:10 – 12:20

Andre C Mueller, Leonhard Heinz, Kumaran Kandasamy, Manuela Bruckner, Christoph L Baumann, Giulio Superti-Furga, Keiryn L Bennett

CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences/Vienna/Austria

- PWe-170** The study of aging processes using in vitro glycation experiments applied to low density lipoproteins using MALDI Mass Spectrometry  
 13:30 – 14:40

Omar Belgacem<sup>1</sup>, Matthew Openshaw<sup>1</sup>, Grazyna Sobald<sup>2</sup>, Katharina Pock<sup>3</sup>, Gerald Stuebiger<sup>4</sup>  
<sup>1</sup>Shimadzu, Manchester, UK, <sup>2</sup>Dept. of Nuclear Medicine, Medical University Vienna, Austria, <sup>3</sup>Octapharma Pharmazeutika Produktionsges.m.b.H, Vienna, Austria, <sup>4</sup>Center of Biomolecular Medicine and Pharmacology, Medical University Vienna, Austria

- PWe-171** Phosphoprotein analysis using a combination of an online monolithic trypsin-immobilized enzyme reactor and TiO<sub>2</sub> enrichment column with tandem mass spectrometry  
 11:10 – 12:20

Kun Cho<sup>1</sup>, Hyo Jin Hwang<sup>2</sup>, Jisun Yoo<sup>1</sup>, Jin Young Kim<sup>1</sup>, Young Hwan Kim<sup>1</sup>, Han Bin Oh<sup>2</sup>

<sup>1</sup>Korea Basic Science Institute, Ochang, South Korea, <sup>2</sup>Department of Chemistry, Sogang University, Seoul, South Korea

- PWe-172** Label-Free Phosphopeptide Quantitation and Occupancy Determination from a Single Protein Using LC-MALDI  
 13:30 – 14:40

Oliver Drews, Anja Resemann, Waltraud Evers, Eckhard Belau, Asperger Arndt, Detlev Suckau  
 Bruker Daltonik GmbH, Bremen, Germany

- PWe-173** Ion-Trap Quantitative Proteomics of Glycoproteome from Pancreatic Cancer Patients based on the Label-Free and iTRAQ Approaches  
 11:10 – 12:20

Anna Drabik<sup>1</sup>, Piotr Suder<sup>1</sup>, Marek Sierzega<sup>2</sup>, Radoslaw Pach<sup>2</sup>, Jan Kulig<sup>2</sup>, Anna Bodzon-Kulakowska<sup>1</sup>, Jerzy Silberring<sup>1,3</sup>

<sup>1</sup>AGH University of Science and Technology, Krakow, Poland, <sup>2</sup>Jagiellonian University Medical College, Krakow, Poland, <sup>3</sup>Polish Academy of Sciences, Gliwice, Poland

- PWe-174** Screening of Oxidative Stress induced LDL-modifications using (LC-)MALDI-MS/(MS) based Lipoproteomics  
 13:30 – 14:40

Gerald Stübiger<sup>1</sup>, Ulrike Resch<sup>1</sup>, Michael Wuczkowski<sup>2</sup>, Helmut Sinzinger<sup>1</sup>, Omar Belgacem<sup>3</sup>

<sup>1</sup>Medical University Vienna, Vienna, Austria, <sup>2</sup>Technoclone GmbH, Vienna, Austria, <sup>3</sup>Shimadzu, Manchester, UK

- PWe-176** In-depth human proteome analysis by one-shot LC-MS/MS with meter-scale monolithic silica capillary columns  
 13:30 – 14:40

Mio Iwasaki<sup>1</sup>, Masaki Wakabayashi<sup>1</sup>, Naoyuki Sugiyama<sup>2</sup>, Nobuo Tanaka<sup>3</sup>, Yasushi Ishihama<sup>1</sup>

<sup>1</sup>Kyoto University, <sup>2</sup>Keio University, Yamagata, Japan, <sup>3</sup>GL Sciences, Tokyo, Japan

- PWe-177** Automated Quality Control of Biopharmaceutical N-/C-Terminal Sequences by Routine Top-Down Mass Spectrometry  
 11:10 – 12:20

Rainer Paape<sup>2</sup>, Anja Resemann<sup>2</sup>, Lars Vorwerg<sup>2</sup>, Jens Hoehndorf<sup>2</sup>, Detlev Suckau<sup>2</sup>, Hank Wang<sup>1</sup>

<sup>1</sup>Bruker Daltonics Inc., Beijing, China, <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany

- PWe-178** Evaluation of targeted proteomic approaches on a Q-TOF system  
 13:30 – 14:40

Carsten Funke, Stephanie Kasper, Wolfgang Jabs, Carsten Baessmann  
 Bruker Daltonik GmbH

- PWe-179** Electron Transfer Dissociation differentiates the isobaric deamidation products Aspartate and IsoAspartate.  
 11:10 – 12:20

Andrea Kiehne<sup>1</sup>, Ralf Hartmer<sup>1</sup>, Laxmi Adhikary<sup>2</sup>, Anand Khedkar<sup>2</sup>, Harish Iyer<sup>2</sup>, Raju Mukherjee<sup>2</sup>

<sup>1</sup>Bruker Daltonik GmbH, <sup>2</sup>Biocon

## Wednesday, 19<sup>th</sup> September

- PWe-180** Identification and quantification of concentration-dependent biomarkers in MCF-7/BOS cells exposed to 17beta-estradiol by 2-D DIGE and label-free proteomics  
 13:30 – 14:40

Mike Collodoro, Pascale Lemaire, Gauthier Eppe, Virginie Bertrand, Rowan Dobson, Gabriel Mazzucchelli, Joelle Widart, Edwin De Pauw, Marie-Claire A Gillet  
 Liege University, Liege, Belgium

- PWe-181** Quantitative phosphoproteome analysis of apoptotic human cell cultures using SILAC combined with complementary ESI-MS techniques  
 11:10 – 12:20

Yumiko Matsuyama<sup>1</sup>, Benjamin Mueller<sup>2</sup>, Wolfgang Jabs<sup>3</sup>, Carsten Baesemann<sup>3</sup>, Stephanie Kaspar<sup>3</sup>, Karsten Niehaus<sup>4</sup>, Thomas Noll<sup>2</sup>, Raimund Hoffrogge<sup>2</sup>  
<sup>1</sup>Bruker Daltonics K.K., Yokohama, Japan, <sup>2</sup>Institute of Cell Culture Technology, Faculty of Technology, Bielefeld University, Germany, <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany, <sup>4</sup>Proteome and Metabolome Research, Faculty of Biology, Bielefeld University, Germany

- PWe-182** Validating a novel Parkinson's Disease SRM-based assay using automated sample preparation  
 13:30 – 14:40

Christine A Jelinek<sup>1</sup>, Liana Rosenthal<sup>1</sup>, Yan Jia<sup>1</sup>, Kevin W Meyer<sup>2</sup>, Ted Dawson<sup>1</sup>, Robert J Cotter<sup>1</sup>  
<sup>1</sup>Johns Hopkins School of Medicine, Baltimore, United States of America, <sup>2</sup>Perfinity Biosciences, West Lafayette, United States of America

- PWe-183** In vitro phosphorylation to manipulate the abundance profiles in proteomic samples  
 11:10 – 12:20

Shunsuke Takagi<sup>1</sup>, Haruna Immura<sup>1</sup>, Masaki Wakabayashi<sup>1</sup>, Naoyuki Sugiyama<sup>2</sup>, Yasushi Ishihama<sup>1</sup>  
<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Keio University, Yamagata, Japan

- PWe-184** Identification of kinase substrates by siRNA-induced kinase knock-down coupled with quantitative phosphoproteomics  
 13:30 – 14:40

Ayaka Sato<sup>1</sup>, Sayaka Iwano<sup>1</sup>, Wei-Chi Ku<sup>1</sup>, Masaki Wakabayashi<sup>1</sup>, Naoyuki Sugiyama<sup>2</sup>, Fumiko Toyoshima<sup>1</sup>, Yasushi Ishihama<sup>1</sup>  
<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Keio University, Yamagata, Japan

- PWe-185** Comprehensive Targeted Quantitative Proteomics - Assessing Quantitation Quality of Highly Multiplexed Assays  
 11:10 – 12:20

Christie L Hunter, Sean L Seymour  
 AB SCIEX, Foster City, CA, United States

- PWe-186** Global profiling and quantification of histones, histone PTM's and histone-modifying enzymes in mesenchymal stem cells using a multiplexed SRM assay  
 13:30 – 14:40

Mei Ying Han<sup>1</sup>, Bryan Krastins<sup>2</sup>, Alejandra Garces<sup>2</sup>, Victoria V Lunyak<sup>3</sup>, Benjamin Blackwell<sup>3</sup>, David Sarracino<sup>2</sup>, Amol Prakash<sup>2</sup>, Shadab Ahmad<sup>2</sup>, Maryann S Vogelsang<sup>2</sup>, Mary F Lopez<sup>2</sup>  
<sup>1</sup>Thermo Fisher Scientific, Yokohama, Japan, <sup>2</sup>BRIMS, Thermo Fisher Scientific, Cambridge, MA, <sup>3</sup>Buck Institute for Research on Aging, Novato, CA

- PWe-187** Polyhedral approach to comprehensive quantitative analysis for membrane proteomics  
 11:10 – 12:20

Kazuaki Takaishi, Seiji Takashima, Akira Kikuchi  
 Osaka University, Osaka, Japan

- PWe-188** Separation of polypeptides by isoelectric point focusing in electrospray-friendly solution using multiple-junction capillary fractionator  
 13:30 – 14:40

Konstantin Chingin<sup>1</sup>, Juan Astorga-Wells<sup>1,2</sup>, Mohammad Pirmoradian Najafabadi<sup>1,2</sup>, Thorleif Lavold<sup>2</sup>, Roman A Zubarev<sup>1,3</sup>

<sup>1</sup>Karolinska Institutet, Stockholm, Sweden, <sup>2</sup>Biomotif AB, Stockholm, Sweden, <sup>3</sup>Science for Life Laboratory, Stockholm, Sweden

- PWe-189** Comprehensive variability analysis of nutrients absorption mechanism in small intestine by quantitative proteomics  
 11:10 – 12:20

Takashi Nishiyama, Shushi Nagamori, Kazuaki Takaishi, Yoshikatsu Kanai  
 Osaka University Graduate School of Medicine, Suita, Japan

## Others

- PWe-190** Laser Spectroscopic Investigations of 1,3-Dichloro-2-fluorobenzene by REMPI and MATI Spectroscopy  
 13:30 – 14:40

Sascha Krüger, Juergen Grottemeyer  
 Kiel University, Kiel, Germany

- PWe-191** Selective Extraction and Absolute Quantification of Glutathione using Nanoengineered Micro Gold Shells and LDI-TOF MS  
 11:10 – 12:20

Jeongwook Lee, Woon-Seok Yeo  
 Konkuk University, Korea

- PWe-192** Coulomb-Interaction-Induced Effects on Xe Isotopic Ion FT-ICR Mass Spectra: A Many-Particle Simulation Using GRAPE  
 13:30 – 14:40

Makoto Fujiwara, Naohisa Hoppo, Koichi Tanaka  
 Hiroshima City University, Hiroshima, Japan

- PWe-193** Analysis of flavonoids by Graphene-Based SALDI-TOF MS  
 11:10 – 12:20

Min-Wei Chien<sup>1</sup>, Ching-Yuan Su<sup>2</sup>, Lain-Jong Li<sup>3</sup>, Chien-Chen Lai<sup>1</sup>  
<sup>1</sup>Institute of Molecular Biology, National Chung Hsing University, Taiwan, <sup>2</sup>Department of Electronic Engineering, Chang Gung University, Taiwan, <sup>3</sup>Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

- PWe-194** Quantification of eight catechins and caffeine in black, white and green tea samples using UHPLC coupled to tandem mass spectrometry  
 13:30 – 14:40

Karolina Skraskova, Michaela Mudrova, Hana Vlckova, Lucie Novakova  
 Charles University in Prague, Faculty of Pharmacy in Hradec Kralove, Hradec Kralove, Czech Republic

Wednesday, 19<sup>th</sup> September

- PWe-195** Low-energy ion scattering (LEIS) study of Cs-sputtering effects on III-V semiconductor hetero-structures during SIMS analysis  
11:10 – 12:20

Helena Tellez<sup>1</sup>, David M McPhail<sup>1</sup>, Jose M Vadillo<sup>2</sup>  
<sup>1</sup>Imperial College, London, UK, <sup>2</sup>University of Malaga, Malaga, Spain

- PWe-196** Quality control of multilayered/nanoheterostructured solar cells by secondary ion mass spectrometry and ion beam etching techniques  
13:30 – 14:40

Jose M Vadillo<sup>1</sup>, Diana J Padilla<sup>1</sup>, Helena Tellez<sup>2</sup>, John W Druce<sup>2</sup>, David S McPhail<sup>2</sup>, Jose J Laserna<sup>1</sup>  
<sup>1</sup>University of Málaga, <sup>2</sup>Imperial College

- PWe-197** Ultra high pressure comprehensive two-dimensional liquid chromatography combined with hybrid mass spectrometry for the elucidation of carotenoids in chilired peppers  
11:10 – 12:20

Marcus Mreyen<sup>1</sup>, Francesco Cacciola<sup>2,3</sup>, Paola Donato<sup>3,4</sup>, Daniele Giuffrida<sup>5</sup>, Germana Torre<sup>3</sup>, Paola Dugo<sup>3,4</sup>, Luigi Mondello<sup>3,4</sup>  
<sup>1</sup>Shimadzu Europa GmbH, Duisburg, Germany, <sup>2</sup>Chromaleont S.r.l., Messina, Italy, <sup>3</sup>Dipartimento Farmaco-chimico, Messina, Italy, <sup>4</sup>Centro Integrato di Ricerca (C.I.R.), Roma, Italy, <sup>5</sup>Dipartimento di Scienze degli Alimenti e dell'Ambi, Messina, Italy

- PWe-198** Identification of Organic Contaminants on Silicon Surface by Mass Spectrometry  
13:30 – 14:40

Yoon Mi Lee, Sang Yoon Shin, Jung Dae Park, Pil Kwon Jun, Jong Soo Kim  
Semiconductor Business, Samsung Electronics / Gyeonggi-Do, Korea

- PWe-199** Comprehensive Targeted Compound Identification Using Pseudo-Precursor Ion Scan and Neutral Loss Scan for Degradation Analysis of Electrolytes  
11:10 – 12:20

Kaoru Karasawa, Toshiyuki Yamazaki, Sumie Ando  
ABSCIEX

- PWe-200** Analysis of degradation products in electrolyte for rechargeable lithium-ion battery through high mass accuracy MSn and multivariate statistical technique  
13:30 – 14:40

Hiroki Nakajima, Yamaki Satoshi, Nishine Tsutomu, Furuta Masaru  
Shimadzu Co., Kyoto, Japan

- PWe-201** GC/MS Determination of N-Nitrosamines in Rubber Teats  
11:10 – 12:20

Peng Gao, Jun Fan, Li X Deng, Hong T Huang  
SHIMADZU(CHINA)CO.,LTD,ShangHai,China

- PWe-202** Analysis of black tea by GC-MS and high-resolution UPLC-MS  
13:30 – 14:40

Christian Grün, Boudewijin Hollebrands, Julien Boelhouwer  
Unilever R&D, Vlaardingen, The Netherlands

Thursday, 20<sup>th</sup> September

Morning

## Plenary Lecture

08:00 – 08:45

Main Hall

## Plenary Lecture 4: Hisayoshi Yurimoto

Chair: Robert J. Cotter

Johns Hopkins University School of Medicine, USA

## PL4-0800 Science of asteroid sample return mission "HAYABUSA"

08:00 – 08:45

Hisayoshi Yurimoto

Hokkaido University, Sapporo, Japan

## Oral Session

09:00 – 11:00

Main Hall

## Session 31: Native Mass Spectrometry and Structural Biology

Chair: Satoko Akashi

Yokohama City University, Japan

## S31-0900 [Keynote Lecture] Integrating Native Mass Spectrometry and Top-Down MS for Defining Protein Interactions Important in Biology and Medicine

Joseph A Loo

University of California-Los Angeles, USA

## S31-0940 Ion mobility-mass spectrometry for the study of conformational space and topology of proteins and protein-DNA complexes

Frank Sobott

Antwerp University, Antwerp/Belgium

## S31-1000 Structure of a Beta-Crystallin Heterodimer by Ion Mobility and Radical Probe Mass Spectrometry

Kevin Downard<sup>1</sup>, Yuichi Kokabu<sup>2</sup>, Mitsunori Ikeguchi<sup>2</sup>,  
Satoko Akashi<sup>2</sup><sup>1</sup>University of Sydney, <sup>2</sup>Yokohama City University

## S31-1020 Application of Backbone Amide Hydrogen/Deuterium Exchange-Mass Spectrometry (HDX-MS) to Characterize Protein-Ligand Interactions and Protein-Protein Interactions

Yoshitomo Hamuro

ExSAR, Monmouth Junction, NJ, USA

## S31-1040 An integrated workflow for structural mass spectrometry: combining X-linking technology with ionmobility for the structural characterisation of macromolecular assemblies

Florian Stengel<sup>1</sup>, Argyris Politis<sup>2</sup>, Zoe Hall<sup>2</sup>, Eri Sakata<sup>3</sup>,  
Helena Hernandez<sup>2</sup>, Alexander Leitner<sup>1</sup>, Thomas Walzthoeni<sup>1</sup>,  
Carol V Robinson<sup>2</sup>, Ruedi Aebersold<sup>1,4</sup><sup>1</sup>Department of Biology, Institute of Molecular Systems Biology, ETH Zurich,<sup>2</sup>Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield Road, Oxford, UK, <sup>3</sup>Laboratory of Protein Metabolism, Tokyo Metropolitan Institute of Medical Science, Setagaya-ku, Tokyo, 156-8506, Japan, <sup>4</sup>Faculty of Science, University of Zurich, Switzerland

**Thursday, 20<sup>th</sup> September**

**Morning**

## Oral Session

09:00 – 11:00

Room A

### Session 32: Formation and Dissociation of Peptide Radical Ions

Chair: Dominic T.W. Chan

The Chinese University of Hong Kong, Hong Kong SAR

#### S32-0900 [Keynote Lecture] Formation and Dissociation of Peptide Radical Ions

09:00 – 09:40 Roman A Zubarev  
Karolinska Institutet, Stockholm, Sweden

#### S32-0940 Ab initio MO Study on the Fragmentation Mechanisms of Protonated Phosphopeptides in “On-Resonance” and “Off-Resonance” Pulsed Gas Introduction Collision-Induced Dissociations

Takae Takeuchi<sup>1,2</sup>, Ayaka Takahashi<sup>1</sup>, Erika Sugawara<sup>1</sup>, Tomoko Kimura<sup>1</sup>, Yuka Kuroasaki<sup>1</sup>, Shigeki Kajihara<sup>3</sup>, Hiroko Morinaga<sup>4</sup>, Shinichi Iwamoto<sup>3</sup>, Koichi Tanaka<sup>3</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, Nara Women's University, Nara, Japan, <sup>2</sup>National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka, Japan, <sup>3</sup>Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, Japan,

<sup>4</sup>Technical Research Laboratory, Shimadzu Corporation, Kyoto, Japan

#### S32-1000 Electron transfer dissociation of protonated disulfide linked peptides and analogs without S-S bond

10:00 – 10:20 Shigeo Hayakawa<sup>1</sup>, Shinya Matsumoto<sup>1</sup>, Michisato Toyoda<sup>2</sup>, Yasushi Shigeri<sup>3</sup>, Michiko Tajiri<sup>4</sup>, Yoshinao Wada<sup>4</sup>

<sup>1</sup>Osaka Prefecture University, Sakai, Japan, <sup>2</sup>Osaka University, Toyonaka, Japan, <sup>3</sup>AIST, Ikeda, Japan, <sup>4</sup>Osaka MCHRI, Izumi, Japan

#### S32-1020 Ionization energy of gas phase proteins and its dependence on charge state and structure

Alexandre Giuliani<sup>1</sup>, Alexksandar R Milosavljevic<sup>2</sup>, Konrad Hinsen<sup>1</sup>, Francis Canon<sup>1</sup>, Laurent Nahon<sup>1</sup>, Matthieu Regrefgiers<sup>1</sup>

<sup>1</sup>Synchrotron SOLEIL, Gif-sur-Yvette, France / INRA, CEPIA, Nantes, France, <sup>2</sup>University of Belgrade, Institute of Physics, Belgrade, Serbia

#### S32-1040 Direct ECD and CID sequencing intra disulfide C-terminal loops of non-tryptic natural peptides

10:40 – 11:00 Tatiana Y Samgina, Yegor A Vorontsov, Konstantin V Karandashev, Albert T Lebedev  
M.V.Lomonosov Moscow State University

## Oral Session

09:00 – 11:00

Room B-1

### Session 33: JMS Award Symposium

Chair: Richard M Caprioli

Vanderbilt University, Nashville, TN, USA / Editor-in-Chief, Journal of Mass Spectrometry

#### S33-0900 JMS Award -Overview and Award Ceremony-

Richard M Caprioli<sup>1, 2</sup>

<sup>1</sup>Vanderbilt University, Nashville, TN, USA, <sup>2</sup>Editor-in-Chief, Journal of Mass Spectrometry

#### S33-0920 Integral Membrane Proteins by High-mass MALDI-MS: Direct Access to the Stoichiometry of their Complexes and to Posttranslational Modifications

FAN CHEN<sup>1</sup>, Sabina Gerber<sup>2</sup>, Katrin Heuser<sup>2</sup>, Volodymyr Kokhov<sup>2</sup>, Christian Lizak<sup>2</sup>, Kaspar Locher<sup>2</sup>, Renato Zenobi<sup>1</sup>

<sup>1</sup>Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland,

<sup>2</sup>Institute of Molecular Biology and Biophysics, ETH Zurich, Switzerland

#### S33-0940 Great Insights from a Small System: Structure and reactivity of [VPO<sub>4</sub>]<sup>+</sup> in comparison with [V<sub>2</sub>O<sub>4</sub>]<sup>+</sup>.

10:40 – 10:00 Nicolas Dietl, Maria Schlangen, Helmut Schwarz  
Technical University Berlin, Berlin, Germany

#### S33-1000 Charge-State Dependent Compaction and Dissociation of Protein Complexes: Insights from Ion Mobility and Molecular Dynamics

Zoe Hall<sup>1</sup>, Argyris Politis<sup>1</sup>, Matthew F Bush<sup>1,2</sup>, Lorna J Smith<sup>1</sup>, Carol V Robinson<sup>1</sup>

<sup>1</sup>University of Oxford, Oxford, UK, <sup>2</sup>University of Washington, Seattle, USA

#### S33-1020 Odd products from even-electron ions: Exploiting charge-remote bond homolysis to compare bond dissociation energies

10:20 – 10:40 David L Marshall<sup>1</sup>, Martin Paine<sup>1</sup>, Philip J Barker<sup>2</sup>, Stephen J Blanksby<sup>1</sup>

<sup>1</sup>University of Wollongong, Wollongong, Australia, <sup>2</sup>BlueScope Steel Research, Port Kembla, Australia

Thursday, 20<sup>th</sup> September

Morning

**Oral Session**

09:00 – 11:00

Room D

**Session 34: MS Informatics for Identification and Characterization**

Chair: Shigeki Kajihara

Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Co., Japan

- S34-0900** [Keynote Lecture] The value of different types of information in MS based identification  
09:00 – 09:40

David Fenyö

New York University, New York, NY, USA

- S34-0940** Improving endogenous peptide sequence characterization using electron-capture dissociation and collision-induced dissociation.  
09:40 – 10:00

Eisuke Hayakawa<sup>1</sup>, Gerben Menschaert<sup>2</sup>, Walter Luyten<sup>1</sup>, Geert Baggerman<sup>3</sup>, Liliane Schoofs<sup>1</sup><sup>1</sup>K.U. Leuven, Leuven, Belgium., <sup>2</sup>Ghent University, Ghent, Belgium, <sup>3</sup>VITO, Mol, Belgium

- S34-1000** LipidXplorer software supports high-throughput shotgun lipidomics at any mass spectrometer platform and acquisition mode  
10:00 – 10:20

Ronny Herzog<sup>1</sup>, Dominik Schwudke<sup>2</sup>, Kai Schuhmann<sup>1</sup>, Julio Sampaio<sup>1</sup>, Andrej Shevchenko<sup>1</sup><sup>1</sup>Max Planck Institute of Cell Biology and Genetics, Dresden, Germany, <sup>2</sup>National Centre for Biological Science, Bangalore, India

- S34-1020** MassBank: Public Mass Spectral Database  
10:20 – 10:40

Takaaki Nishioka, Yoshito Nihei, Yuya Ojima, Tasuku Ikeda  
Nara Institute of Science and Technology, Nara, Japan

- S34-1040** MSPTM-DB: a known PTM database for high-speed and accurate search available on the “ProteoAnalysis” web site  
10:40 – 11:00

Akiyasu C Yoshizawa<sup>1</sup>, Tsuyoshi Tabata<sup>2</sup>, Takayuki Kimura<sup>2</sup>, Ken Aoshima<sup>2</sup>, Yoshiya Oda<sup>2</sup>, Shigeki Kajihara<sup>1</sup>, Koichi Tanaka<sup>1</sup>  
<sup>1</sup>Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>Eisai Product Creation Systems, Eisai Corporation, Ltd., Tsukuba, Japan**Oral Session**

09:00 – 11:00

Room E

**Session 35: Environment I**Chair: Peter Haglund  
Umeå University, Sweden

- S35-0900** [Keynote Lecture] Chiral Chemicals as Tracers of Sources and Fate Processes in a World of Changing Climate  
09:00 – 09:40

Terry F Bidleman<sup>1,2,3</sup>, Liisa M Jantunen<sup>2</sup>, Perihan B Kurt-Karakus<sup>4</sup>, Fiona Wong<sup>5</sup><sup>1</sup>Chemistry Department, Umeå University, Umeå, Sweden, <sup>2</sup>Centre for Atmospheric Research Experiments, Environment Canada, Egbert, ON, Canada, <sup>3</sup>Department of Chemistry, University of Toronto, Toronto, ON, Canada, <sup>4</sup>Department of Environmental Engineering, Bahcesehir University, Istanbul, Turkey, <sup>5</sup>Department of Applied Environmental Science (ITM), Stockholm University, Stockholm, Sweden

- S35-0940** POLLUTION OF MOSCOW AIR: GC/MS STUDY OF SNOW SAMPLES  
09:40 – 10:00

Olga V Polyakova<sup>1</sup>, Viatcheslav V Artaev<sup>2</sup>, Dmitry M Mazur<sup>1</sup>, Albert T Lebedev<sup>1</sup><sup>1</sup>M.V.Lomonosov Moscow State University, <sup>2</sup>LECO Corporation, 3000 Lakeview Avenue, St. Joseph, MI, USA

- S35-1000** AQUEOUS-PHASE REACTIONS OF ATMOSPHERICALLY RELEVANT VOLATILE ORGANIC COMPOUNDS THROUGH TANDEM MASS SPECTROMETRY: AN INTRIGUING STORY OF AEROSOL FORMATION  
10:00 – 10:20

Rafal Szmigielski, Krzysztof Jan Rudzinski, Inna Kuznietsova  
Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland

- S35-1020** HRAM Screening and Quantitative Analysis of Pesticides in Environmental & Food Matrices using a bench top LCMS Orbitrap system  
10:20 – 10:40

Dipankar Ghosh, Charles Yang, Leo Wang, Jonathan Beck  
Thermo Fisher Scientific

- S35-1040** Development and validation of methodology using liquid chromatography-tandem mass spectrometry (LC-MS/MS) for monitoring for use of anabolic steroids in animals  
10:40 – 11:00

Simon J Hird, George Stubbings  
The Food and Environment Research Agency

**Thursday, 20<sup>th</sup> September**

**Afternoon**

## Oral Session

15:00 – 17:00

Main Hall

### Session 36: Advances in Ion Mobility Mass Spectrometry

Chair: Joseph A Loo  
University of California-Los Angeles, USA

**S36-1500** [Keynote Lecture] Peptide and protein aggregation: Mechanisms, inhibition and disease  
15:00 – 15:40

Michael T Bowers  
University of California at Santa Barbara, Santa Barbara CA USA

**S36-1540** Behavior of intrinsically disordered regions within a protein complex of Swi5-Sfr1 characterized by IM-MS and SAXS  
15:40 – 16:00

Kazumi Saikusa<sup>1</sup>, Naoyuki Kuwabara<sup>2</sup>, Yuichi Kokabu<sup>1</sup>,  
Yu Inoue<sup>1</sup>, Mamoru Sato<sup>1</sup>, Hiroshi Iwasaki<sup>3</sup>, Toshiyuki Shimizu<sup>2</sup>,  
Mitsunori Ikeguchi<sup>1</sup>, Satoko Akashi<sup>1</sup>

<sup>1</sup>Yokohama City University, Yokohama, Japan, <sup>2</sup>University of Tokyo, Tokyo, Japan, <sup>3</sup>Tokyo Institute of Technology, Yokohama, Japan

**S36-1600** Probing Protein Quaternary Structures by Surface Induced Dissociation and Ion Mobility - Mass Spectrometry  
16:00 – 16:20

Mowei Zhou<sup>1,2</sup>, Shai Dagan<sup>1</sup>, Vicki H Wysocki<sup>1,2</sup>  
<sup>1</sup>University of Arizona, Tucson, United States, <sup>2</sup>Ohio State University, Columbus, Ohio, United States

**S36-1620** Energy-resolved ion mobility tandem mass spectrometry: A new approach for probing fragmentation pathways involving ion isomerization  
16:20 – 16:40

Yayoi Hongo<sup>1</sup>, Takemichi Nakamura<sup>1</sup>, Takae Takeuchi<sup>2</sup>,  
Shunya Takahashi<sup>1</sup>, Hiroyuki Koshino<sup>1</sup>  
<sup>1</sup>RIKEN, Wako, Japan, <sup>2</sup>Nara Women's University

**S36-1640** Understanding protein-DNA Interactions and Tumorigenic Mutations in IDPs: IM-MS rises to the challenge  
16:40 – 17:00

Ewa Jurneczko<sup>1</sup>, Faye Cruickshank<sup>1</sup>, Penka Nikolova<sup>2</sup>,  
Ian Campuzano<sup>3</sup>, Michael Morris<sup>3</sup>, Perdita E Barran<sup>1</sup>  
<sup>1</sup>The University of Edinburgh, <sup>2</sup>King's College London, London, UK, <sup>3</sup>Waters Corporation, Manchester, UK

## Oral Session

15:00 – 17:00

Room A

### Session 37: Challenges in High Resolution and High Accuracy Mass Measurement Mass Spectrometry

Chair: Evgeny N. Nikolaev  
The Institute for energy problems of chemical physics Russian Academy of Sciences, Russia

**S37-1500** [Keynote Lecture] Mass Resolution and Mass Accuracy: How Much is Enough?  
15:00 – 15:40

Alan G Marshall, Greg T Blakney, Nathan K Kaiser, Yuan Mao, Amy M McKenna, Ryan P Rodgers, Brian M Ruddy, Christopher L Hendrickson  
Florida State University, Tallahassee, Florida, U.S.A.

**S37-1540** Enhanced Fourier transform and filter diagonalization method mass spectrometry for top-down analysis of antibodies and petroleomics  
15:40 – 16:00

Yury O Tsybin, Ünige A Laskay, Luca Fornelli, Konstantin O Zhurov, Anton N Kozhinov  
Ecole Polytechnique Federale de Lausanne, Switzerland

**S37-1600** Characterization and Selective Classification of Petroleum Crude Oils using High Resolution Time-of-Flight Mass Spectrometry  
16:00 – 16:20

Clecio Klitzke<sup>2</sup>, Marcos Eberlin<sup>2</sup>, Kevin Siek<sup>1</sup>, Jeffrey S Patrick<sup>1</sup>, Joe Binkley<sup>1</sup>, Yuri Corillo<sup>2</sup>  
<sup>1</sup>LECO Corporation, <sup>2</sup>UNICAMP, Thermo Mass Spectrometry Laboratory, Campinas, São Paulo Brasil

**S37-1620** Detailed structure analysis of fluorinated polymer by means of pyrolysis comprehensive two-dimensional gas chromatography / high-resolution time-of-flight mass spectrometry  
16:20 – 16:40

Yoji Nakajima, Yuko Arinami, Tsuguhide Isemura, Kiyoshi Yamamoto  
Asahi Glass Co., Kanagawa, Japan

**S37-1640** Dynamically harmonized FTICR cell with specially shaped electrodes for compensation of inhomogeneity of the magnetic field.  
16:40 – 17:00

Yury Kostyukevich<sup>1</sup>, Gleb Vladimirov<sup>1</sup>, Eugene Nikolaev<sup>1,2,3</sup>  
<sup>1</sup>Institute for Energy problems of chemical physics, Russia, <sup>2</sup>Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia,  
<sup>3</sup>Institute of Biomedical Chemistry of Russian Academy of Medical Sciences, Moscow, Russia

**Thursday, 20<sup>th</sup> September**

**Afternoon**

## Oral Session

15:00 – 17:00

Room B-1

### Session 38: Mass Spectrometry for Metabolic Diseases

Chair: Makoto Yoshino  
Kurume University, Japan  
Seiji Yamaguchi  
Shimane University, Japan

#### S38-1500 LC/MS/MS analysis of protein-bound uremic toxins in hemodialysis patients

15:00 – 15:20 Toshimitsu Niwa<sup>1</sup>, Yoshiharu Itoh<sup>2</sup>, Atsuko Ezawa<sup>2</sup>, Kaori Kikuchi<sup>2</sup>, Yoshinari Tsuruta<sup>3</sup>

<sup>1</sup>Nagoya University, Nagoya, Japan, <sup>2</sup>Biomedical Research Laboratories, Kureha Corporation, Tokyo, Japan, <sup>3</sup>Meijo Clinic, Aichi, Japan

#### S38-1520 Early indicator of hepatic fibrosis in patients with chronic hepatitis C: discovery, assay optimization and clinical validation

15:20 – 15:40 Fumio Nomura<sup>1</sup>, Kazuyuki Sogawa<sup>1</sup>, Kenta Noda<sup>1</sup>, Toshihide Miura<sup>1</sup>, Yoshio Kodera<sup>2</sup>, Osamu Yokosuka<sup>1</sup>  
<sup>1</sup>Chiba University, Chiba, Japan, <sup>2</sup>Kitasato University, Kanagawa, Japan

#### S38-1540 Liquid chromatography-mass spectrometry based analysis of the cerebrospinal fluid metabolome for the study of inborn errors of metabolism

15:40 – 16:00 Maria del Mar Amadore<sup>2</sup>, Foudil Lamari<sup>2,5</sup>, Benoit Colsch<sup>1</sup>, Fanny Mochel<sup>2,3</sup>, Francois Seguin<sup>4</sup>, Frederic Sedel<sup>2</sup>, Christophe Junot<sup>1</sup>

<sup>1</sup>CEA, Gif-sur-Yvette, France, <sup>2</sup>Pitie-Salpetriere Hospital, AP-HP & University Pierre and Marie Curie, Paris, France, <sup>3</sup>INSERM UMR S975, Paris, France,

<sup>4</sup>INSERM U1082, Paris, France, <sup>5</sup>Department of Metabolic Biochemistry- Pitie-Salpetriere Hospital, Paris, France

#### S38-1600 Highly sensitive and specific clinical diagnostics of lysosomal storage diseases using multiple reaction monitoring mass spectrometry, fluorimetry, and affinity-proteomics

16:00 – 16:20 Michael Przybylski<sup>1</sup>, Claudia Cozma<sup>1</sup>, Marius I Iurascu<sup>1</sup>, Laura Ion<sup>1</sup>, Adolf Muehl<sup>2</sup>, Alina Petre<sup>1,3</sup>, Michael L Gross<sup>3</sup>, Stefan Maeser<sup>2</sup>

<sup>1</sup>University of Konstanz, Konstanz, Germany, <sup>2</sup>Centogene GmbH, Freiburg & Rostock, Germany, <sup>3</sup>Washington University St. Louis, St. Louis, MO, USA

#### S38-1620 Mass spectrometry in newborn screening of fatty acid oxidation disorders - diagnostic approach using lymphocytes

16:20 – 16:40 Yosuke Shigematsu<sup>1</sup>, Ikue Hata<sup>1</sup>, Go Tajima<sup>2</sup>  
<sup>1</sup>University of Fukui, Fukui, Japan, <sup>2</sup>Hiroshima University Graduate School of Biomedical Sciences, Hiroshima, Japan

#### S38-1640 Application of in-vitro probe acylcarnitine assay using tandem mass spectrometry for the evaluation of mitochondrial fatty acid oxidation

Jamiyan Purevsuren, Hironori Kobayashi, Yuki Hasegawa, Kenji Yamada, Tomoo Takahashi, Seiji Yamaguchi  
Shimane University School of Medicine, Shimane, Japan

## Oral Session

15:00 – 17:00

Room D

### Session 39: MS Informatics for Quantitation

Chair: David Fenyö  
New York University, USA

#### S39-1500 [Keynote Lecture] Detection of differential expression of splice variants

15:00 – 15:40 in the MaxQuant framework for quantitative proteomics

Jürgen Cox<sup>1,2</sup>, Nagarjuna Nagaraj<sup>1,2</sup>, Cornelia Schoenbauer<sup>1,2</sup>, Frank Schnorrer<sup>1,2</sup>, Matthias Mann<sup>1,2</sup>

<sup>1</sup>Max Planck Institute for Biochemistry, Martinsried, Germany, <sup>2</sup>Max Planck Institute for Biochemistry

#### S39-1540 Peptide Yields Depend on Digestion Conditions

15:40 – 16:00 Stein E Stephen, Yuxue Liang, Eric Yan  
National Institute of Standards and technology, Gaithersburg, MD, USA

#### S39-1600 Quantitative Proteomics of Embryonic Stem Cells Differentiation to Cardiomyocytes

16:00 – 16:20 Ekaterina Mostovenko, André M Deelder, Christine L Mummary, Robert Passier, Magnus Palmlad Leiden University Medical Center, Leiden, Netherlands

#### S39-1620 Estimation of relative protein abundance and statistical analysis of proteomic data from multiple iTRAQ experiments, to assess micronutrient deficiencies.

16:20 – 16:40 Ingo Ruczinski, Keith P West, Robert N Cole, Kerry Schulze, Shelley Herbrich, Parul Christian, Jim D Yager, John D Groopman  
Johns Hopkins University, Baltimore MD, USA

#### S39-1640 Accurate mass quantitation of in vivo plasma samples using high resolution QToF and MSE data analysis across a global network

16:40 – 17:00 McDonald Stephen<sup>1</sup>, Mark Wrona<sup>1</sup>, Julie Laterre<sup>2</sup>, Nigel Ewing<sup>3</sup>, Eric Lanlois<sup>2</sup>, Joanne Mather<sup>1</sup>, Debadeep Bhattacharya<sup>1</sup>, Robert S Plumb<sup>1</sup>

<sup>1</sup>Waters Corporation, Milford, USA, <sup>2</sup>Vertex, Laval, Canada, <sup>3</sup>Vertex, Cambridge, USA

Thursday, 20<sup>th</sup> September

Afternoon

## Oral Session

15:00 – 17:00

Room E

## Session 40: Environment II

Chair: Takeshi Nakano  
Osaka University, Japan**S40-1500** [Keynote Lecture] Powerful GC-ToF-MS Techniques for Quantification of Legacy Pollutants and Screening and Identification of Emerging Pollutants

15:00 – 15:40 Peter S Haglund, Conny Danielsson, Mikael Harju, Patricia Moreira-Bastos, Ulrika Olofsson Umeå University, Umeå, Sweden

**S40-1540** Dioxin Food Crises and New POPs: Challenges in Analyses15:40 – 16:00 Jef Focant  
University of Liege, Liege, Belgium**S40-1600** New Perspectives in the Mass Spectroscopy Determination of Dioxin-like Substances in Environmental and Food Samples16:00 – 16:20 Angel Garcia-Bermejo<sup>2</sup>, Manuela Abalos<sup>1</sup>, Lisa Mattioli<sup>1</sup>, Maria Jose Gonzalez<sup>2</sup>, Belen Gomara<sup>2</sup>, Esteban Abad<sup>1</sup>  
<sup>1</sup>Lab. of Dioxins, IDAEA-CSIC, <sup>2</sup>Department of Instrumental Analysis and Environmental Chemistry, IQOG-CSIC**S40-1620** GC-MS studies on POPs in Brazilian Ecosystems16:20 – 16:40 Joao Paulo M Torres<sup>1</sup>, Jose Lailson-Brito<sup>2</sup>, Paulo R Dorneles<sup>1</sup>, Rodrigo O Meire<sup>1</sup>, Larissa S Cunha<sup>1</sup>, Daniele Botaro<sup>1</sup>, Giselle C Saldanha<sup>3</sup>, Claudio E Azevedo e Silva<sup>1</sup>, Dayse Aline M Rocha<sup>1</sup>, Olaf Malm<sup>1</sup>, Karl W Schramm<sup>4</sup>, Begona Jimenez<sup>5</sup><sup>1</sup>Universidade Federal do Rio de Janeiro, Brazil, <sup>2</sup>Universidade do Estado do Rio de Janeiro - MAQUA, Brazil, <sup>3</sup>Instituto Federal de Educacao Tecnologica - Rondonia, Brazil, <sup>4</sup>Helmholtz Centrum, Munich, Germany, <sup>5</sup>Instituto de Quimica Organica General - CSIC, Spain**S40-1640** Structural Analysis of Cyclodextrin Inclusion Complexes Formed in Nonpolar Solvents16:40 – 17:00 Toshiyuki Kida, Haruyasu Asahara, Takuya Iwamoto, Mitsuru Akashi  
Osaka University, Suita, Japan

## Award Lecture

17:10 – 18:10

Main Hall

## Thomson Medal Award Lecture

Chair: Marcos N. Eberlin (IMSF President)  
University of Campinas, Brazil**AW2-1710** Thomson Medal Award Lecture

17:10 – 18:10

Ruedi Aebersold

ETH, Switzerland

Alexander Makarov

ThermoFisher Scientific, Germany

František Tureček

University of Washington, USA

Thursday, 20<sup>th</sup> September

## Poster Session

Core Time : 11:10 - 12:20 (Odd number),  
13:30 - 14:40 (Even number)

Event Hall

## Session 31

## Native Mass Spectrometry and Structural Biology

**PTh-001 Development, Evaluation and Comparison of Calibration Standards for MALDI-MS in the > 100 kDa m/z Range**

11:10 – 12:20 Simon Weidmann<sup>1</sup>, Konstantin Barylyuk<sup>1</sup>, Stefanie Maedler<sup>1,2</sup>, Renato Zenobi<sup>1</sup>

<sup>1</sup>ETH Zurich, Zurich, Switzerland, <sup>2</sup>Current address: York University, Toronto, Canada

**PTh-002 Relative electrospray response factor in homodimer-monomer equilibrium system of DNA oligonucleotides**

13:30 – 14:40 Konstantin Barylyuk<sup>1</sup>, Xueshu Xie<sup>2</sup>, Renato Zenobi<sup>1</sup>  
<sup>1</sup>ETH Zurich, Zurich, Switzerland, <sup>2</sup>Karolinska Institutet, Stockholm, Sweden

**PTh-003 Protein Flexibility is Key to Cisplatin Cross-linking in Calmodulin**

11:10 – 12:20 Huilin Li, Stephen A Wells, J E Jimenez-Roldan, Rudolf A Römer, Yao Zhao, Peter J Sadler, Peter B O'Connor  
University of Warwick, Coventry, UK

**PTh-004 High resolution hydrogen/deuterium exchange mass spectrometry maps contact surfaces of VEGF and a novel recombinant monoclonal antibody fragment (CIGB-166A)**

13:30 – 14:40 Marta Vilaseca<sup>1</sup>, Marina Gay<sup>1</sup>, Andrey Dyachenko<sup>2</sup>, Claudio Diema<sup>1</sup>, Mar Vilanova<sup>1</sup>, Michael Goldflam<sup>2</sup>, Humberto Lamdan<sup>3</sup>, Ernest Giralt<sup>2</sup>, Gabriel Padron<sup>3</sup>  
<sup>1</sup>Mass Spectrometry Core Facility, Institute for Research in Biomedicine, IRBBBarcelona, Barcelona, Spain, <sup>2</sup>Institute for Research in Biomedicine, IRBBBarcelona, Barcelona, Spain, <sup>3</sup>Centro Ingenieria Genetica y Biotecnologia, CIGB, La Habana, Cuba

**PTh-005 Following amyloid fibril formation by ion mobility spectrometry mass spectrometry: are all pathways the same?**

11:10 – 12:20 Charlotte A Scarff, Lydia Young, Aneika C Leney, Lucy A Woods, Sheena E Radford, Alison E Ashcroft  
University of Leeds, Leeds, United Kingdom.

**PTh-006 Structural Characterisation of Protein Complexes by Chemical Cross-linking and Ion Mobility-Mass Spectrometry**

13:30 – 14:40 Antonio Calabrese, Danielle Williams, Yanqin Liu, Tara L Pukala  
University of Adelaide, Adelaide, Australia

**PTh-007 The effect of gas molecules for the structural dynamics of GAPDH revealed by mass spectrometry coupled with H/D exchange**

11:10 – 12:20 Tatsuya Yamamoto, Yasuaki Kabe, Makoto Suematsu  
Japan Science and Technology Agency / Keio University, Tokyo, Japan

**PTh-008 A systematic survey of protein kinase specificity by in vitro phosphoproteomic approaches**

13:30 – 14:40 Haruna Imamura<sup>1</sup>, Naoyuki Sugiyama<sup>2</sup>, Masaki Wakabayashi<sup>1</sup>, Yasushi Ishihama<sup>1</sup>

<sup>1</sup>Kyoto University, Kyoto, Japan, <sup>2</sup>Keio University, Tsuruoka, Japan

**PTh-009 Cellobiose dehydrogenase represents a real challenge for hydrogen/deuterium exchange mass spectrometry**

11:10 – 12:20 Petr Man<sup>1,2</sup>, Alan Kadek<sup>1,2</sup>, Roland Ludwig<sup>3</sup>, Petr Novak<sup>1,2</sup>, Petr Halada<sup>1</sup>

<sup>1</sup>Institute of Microbiology v.v.i., Prague, Czech Republic, <sup>2</sup>Faculty of Science, Charles University in Prague, Czech Republic, <sup>3</sup>University of Natural Resources and Applied Life Sciences, Vienna, Austria

**PTh-010 Improved analysis of biopharmaceutical samples using an MS-only Orbitrap mass spectrometer**

13:30 – 14:40 Maciej P Bromirscki, Jan-Peter Hauschild, Eduard Denisov, Eugen Damoc, Alexander Makarov  
Thermo Fisher Scientific, Bremen, Germany

**PTh-011 Topology of cytochrome P450 2B4 and cytochrome b5 interaction and membrane orientation by photoactivatable nanoprobe/chemical cross-linking and mass spectrometry**

11:10 – 12:20 Tomas Jecmen<sup>1,2</sup>, Monika Koberova<sup>2</sup>, Bozena Kubickova<sup>2</sup>, Petr Novak<sup>1,2</sup>, Petr Hodek<sup>2</sup>, Jiri Hudecek<sup>2</sup>, Miroslav Sulc<sup>1,2</sup>

<sup>1</sup>Institute of Microbiology, Prague, Czech Republic, <sup>2</sup>Charles University, Prague, Czech Republic

**PTh-012 Structural Examination of hexadecameric and octameric G-quadruplexes, exchange-studies and H/D-exchange on Supramolecular Architectures**

13:30 – 14:40 Dominik Sattler<sup>1</sup>, José M Rivera<sup>2</sup>, Christoph A Schalley<sup>1</sup>

<sup>1</sup>Freie Universität Berlin, Berlin, Germany, <sup>2</sup>University of Puerto Rico, Rio Piedras, San Juan, Puerto Rico

**PTh-013 Identification of on-pathway intermediates of beta-2 microglobulin fibril formation**

11:10 – 12:20 Lucy A Woods, Claire J Sarell, Sheena E Radford, Alison A Ashcroft  
University of Leeds, Leeds, UK

**PTh-014 Mapping the interaction between Hsp90 and TOM by chemical cross-linking coupled to mass spectrometry**

13:30 – 14:40 Fabio C Gozzo, Alana R Figueiredo, Carlos I Ramos, Leticia M Zanphorlin, Lisandra M Gava  
University of Campinas, Campinas, Brazil

## Thursday, 20<sup>th</sup> September

**PTh-015** **Chemical Cross-linking Coupled to Mass Spectrometry Applied to the Characterization of the Interaction Domains in FimX-PilZ Complex**

11:10 – 12:20 Mariana Fioramonte<sup>1</sup>, Cristiane R Guzzo<sup>2</sup>, Shaker C Farah<sup>2</sup>,

Fabio C Gozzo<sup>1</sup>

<sup>1</sup>University of Campinas, <sup>2</sup>University of São Paulo

**PTh-016** **Inter-molecular interactions of SMC proteins studied by MS under non-denaturing condition and HDX-MS**

13:30 – 14:40 Susumu Uchiyama<sup>1</sup>, Masanori Noda<sup>1</sup>, Rie Takino<sup>1</sup>, Yuya Miyahara<sup>1</sup>, Kazuki Kawahara<sup>2</sup>, Yuki Hosokawa<sup>1</sup>, Daisuke Motoooka<sup>1</sup>, Shota Nakamura<sup>1</sup>, Tadayasu Ohkubo<sup>1</sup>, Kiichi Fukui<sup>1</sup>

<sup>1</sup>Osaka University, <sup>2</sup>Nara Women's University

### Session 34

#### MS Informatics for Identification and Characterization

**PTh-017** **StavroX - a software for analyzing crosslinked products in protein interaction studies.**

11:10 – 12:20 Michael Götze, Jens Pettelkau, Sabine Schaks, Konstanze Bosse, Christian Ihling, Fabian Krauth, Romy Fritzsche, Uwe Kühn, Andrea Sinz

Martin-Luther-University,Halle,Germany

**PTh-018** **Electrospray mass spectrometry for detailed mechanistic studies of an aldolreaction catalyzed with L-proline**

13:30 – 14:40 Mohammed Wasim Alachraf, Wolfgang Schrader

Max Planck Institut for Coal research

**PTh-019** **LC/MS and surface ionization techniques in classification of red wine**

11:10 – 12:20 Petr Bednar<sup>1</sup>, Barbora Papouskova<sup>1</sup>, Lucie Hartmanova<sup>1</sup>, Karel Hron<sup>2</sup>, Jan Stavek<sup>3</sup>, Josef Balik<sup>3</sup>, Renata Myjavcova<sup>1</sup>, Petr Bartak<sup>1</sup>, Eva Tomankova<sup>3</sup>, Karel Lemr<sup>1</sup>

<sup>1</sup>Regional Centre of Advanced Technologies and Materials, Department of Analytical Chemistry, Faculty of Science, Palacky University, Olomouc, Czech Republic, <sup>2</sup>Department of Mathematical Analysis and Applications of Mathematics, Faculty of Science, Palacky University, <sup>3</sup>Department of Post-Harvest Technology of Horticultural Products, Faculty of Horticulture in Lednice, Mendel University in Brno

**PTh-020** **Higher-Order Structural Characterization of an IgG2 Monoclonal Antibody by Disulfide Mapping and Hydrogen Deuterium Exchange Mass Spectrometry**

13:30 – 14:40 Taiji Kawase<sup>1</sup>, Kenji Hirose<sup>1</sup>, Joomi Ahn<sup>2</sup>, Stephane Houel<sup>2</sup>, Asish Chakraborty<sup>2</sup>, Ying Qing Yu<sup>2</sup>, Justin B Sperry<sup>3</sup>

<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>Waters Corporation, Milford, MA, <sup>3</sup>Analytical R&D, Biotherapeutics Pharm. Sci., Pfizer Inc., Chesterfield, MO

**PTh-021** **Compound search technique for overlapping peaks of LC/MS with a unique algorithm for simultaneous multicomponent identification**

11:10 – 12:20 Yuka Noritake<sup>1</sup>, Haruo Shimada<sup>1</sup>, Yoshimasa Nakatani<sup>1</sup>, Rakan Matsui<sup>1</sup>, Kazumasa Kinoshita<sup>2</sup>, Satoru Kamikubo<sup>2</sup>, Yasuo Shida<sup>3</sup>

<sup>1</sup>Shiseido Research Center, Yokohama, Japan, <sup>2</sup>Bio Chromato, Inc., Fujisawa, Japan, <sup>3</sup>Clean Energy Research Center, University of Yamanashi, Koufu, Japan

**PTh-022** **To determine the activity of Essential Oil from Blumea eriantha from Indian origin by HSGC and GCMS.**

13:30 – 14:40 Jitendra G Kelkar<sup>1</sup>, Deepa Kulkarni<sup>1</sup>, Ajit Datar<sup>1</sup>, Dheeraj Handique<sup>1</sup>, Aarti Karkhanis<sup>1</sup>, Prajakta Pednekar<sup>2</sup>

<sup>1</sup>Shimadzu Analytical (India) Pvt Ltd, Mumbai, India, <sup>2</sup>(2)Guru Nanak Institute of Research and Development, G. N. Khalsa College, Matunga, Maharashtra, India

**PTh-023** **Screening of antioxidants present in unripe Manilkara zapota fruit of Indian origin by using LCMS/MS.**

11:10 – 12:20 Shailendra A Rane<sup>1</sup>, Deepa Bhandarkar<sup>1</sup>, Rashi Kochhar<sup>1</sup>, Shruti Raju<sup>1</sup>, Bhairavi Saraf<sup>1</sup>, Ajit Datar<sup>1</sup>, Jeetendra Kelkar<sup>1</sup>, Bhagyashree Jadhav<sup>2</sup>

<sup>1</sup>Shimadzu Analytical (India) Pvt Ltd, Mumbai, India, <sup>2</sup>(2)Bioanalytical Department, Ramnarain Ruia College, Matunga, Maharashtra, India.

**PTh-024** **Rapid development of functional extensions for mass spectrometry using freeware Mass++**

13:30 – 14:40 Howell E Parry<sup>1</sup>, Satoshi Tanaka<sup>1</sup>, Tsuyoshi Tabata<sup>2</sup>, Ken Aoshima<sup>2</sup>, Yoshiya Oda<sup>2</sup>, Shinichi Utsunomiya<sup>1</sup>, Shigeki Kajihara<sup>1</sup>, Koichi Tanaka<sup>1</sup>

<sup>1</sup>Shimadzu Corporation, <sup>2</sup>Eisai Co., Ltd.

**PTh-025** **UHPLC-MS/MS, an Alternative Solution to Conventional Biosensor Approach for Quorum Sensing Signalling Molecules Detection in Complex Environmental Samples**

11:10 – 12:20 Chuan Hao (Grant) Tan<sup>2,4</sup>, Kai Shyang Koh<sup>4</sup>, Scott A Rice<sup>2,4,5</sup>, Yan Zhou<sup>2,3</sup>, Staffan Kjelleberg<sup>4,5</sup>, Wun Jern Ng<sup>\*2,3</sup>, Peiting Zeng<sup>1</sup>, Zhaoqi Zhan<sup>1</sup>

<sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore, <sup>2</sup>Advanced Environmental Biotechnology Centre, Singapore, Singapore, <sup>3</sup>Nanyang Environment and Water Research Institute, Singapore, Singapore, <sup>4</sup>Singapore Centre on Environmental Life Sciences Engineering, Nanyang Technological University, Singapore, Singapore, <sup>5</sup>The Centre for Marine Bio-Innovation, The University of New South Wales, Sydney, Australia

**PTh-027** **Strategy for key odor component discovery using GC×GC-TOFMS**

11:10 – 12:20 Fumihiko Tsuchiya, Fumie Kabashima, Wataru Uchikawa, Michiko Kanai

LECO Japan, Tokyo, Japan

**PTh-028** **Coordination Polymer Formation Observed by Cold-Spray Ionization Mass Spectrometry**

13:30 – 14:40 Kazuaki Ohara, Kentaro Yamaguchi

Tokushima Bunri University, Sanuki, Japan

## Thursday, 20<sup>th</sup> September

**PTh-029 Mass Spectral Libraries for Analysis of Complex Plant Metabolomics Datasets - Algorithms**

11:10 – 12:20 Wm Gary Mallard<sup>1</sup>, Steve Stein<sup>1</sup>, Yuri Mirokhin<sup>1</sup>,

Nirina Rabe Andriamaharavo<sup>1</sup>, John Halket<sup>2</sup>

<sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD USA,

<sup>2</sup>Kings College, London, UK

**PTh-030 Structure estimation of triacylglycerol by comparing calculated peak pattern with high energy CID spectrum using MALDI-TOF-TOF tandem MS**

13:30 – 14:40 Takaya Satoh, Kubo Ayumi, Hizume Takehiro, Sato Takayoshi, Ueda Yoshihisa  
JEOL Ltd.

**PTh-031 Identification of antioxidants in Fructus aurantii and its quality evaluation3 using a new on-line combination of analytical techniques**

11:10 – 12:20 ZONGTAO LIN<sup>2</sup>, JING DONG<sup>1</sup>, HONG WANG<sup>2</sup>, YING XU<sup>2</sup>, YUKI HASHI<sup>3</sup>, SHIZHONG CHEN<sup>2</sup>

<sup>1</sup>Shimadzu(China), Beijing, China, <sup>2</sup>School of Pharmaceutical Sciences, Peking University, Beijing, China, <sup>3</sup>Shimadzu (China) Co., Ltd., Shanghai Office,ShangHai, China

**PTh-032 Use specific proteins of Taiwan tea as biomarkers for the certification of origin**

13:30 – 14:40 Han-Ju Chien, Chien-Chen Lai  
Institute of molecular biology/National Chung Hsing University, Taichung, Taiwan

**PTh-033 JobRequest - an easy-to-use software platform for proteomic analysis - and ProteoAnalysis, its application for protein identification.**

11:10 – 12:20 Tsuyoshi Tabata<sup>1</sup>, Akiyasu C Yoshizawa<sup>2</sup>, Takayuki Kimura<sup>1</sup>, Tatsushi Nakamura<sup>1</sup>, Ken Aoshima<sup>1</sup>, Yoshiya Oda<sup>1</sup>, Shigeki Kajihara<sup>2</sup>, Koichi Tanaka<sup>2</sup>

<sup>1</sup>Eisai Product Creation Systems / Eisai Co., Ltd., <sup>2</sup>Koichi Tanaka Laboratory of Advanced Science and Technology, Shimadzu Corporation

**PTh-034 Fragmentation analysis of glucuronide metabolites using hybrid ion-trap/orbitrap mass spectrometer with electrospray ionization**

13:30 – 14:40 Kazuyoshi Nozaki<sup>1</sup>, Mitsuo Takayama<sup>2</sup>  
<sup>1</sup>Astellas Pharma Inc, Tsukuba, Japan, <sup>2</sup>Yokohama City University, Yokohama, Japan

**PTh-035 Proteomic analysis of salt-responsive ubiquitin-related proteins in rice root.**

11:10 – 12:20 Yen-Fu Chen<sup>1</sup>, Chang-Sheng Wang<sup>2</sup>, Chien-Chen Lai<sup>1</sup>  
<sup>1</sup>Institute of Molecular Biology College of Life Science, National Chung Hsing University, Taichung, Taiwan, <sup>2</sup>Department of Agronomy, National Chung Hsing University, Taichung, Taiwan

**PTh-036 Application of high speed LC-MSMS technology towards unambiguous characterization of degraded products of Lenalidomide, an anticancer molecule**

13:30 – 14:40 Janani Thyagarajan, Raman Palavannathan, Saravanan Subramanyam, Govindarajan Chandramohan, Mohan Kasi, Manohar VENKAT

Indian Institute of Chromatography & Mass Spectrometry

**PTh-037 Metabolite ID analysis using UNIFI, a novel database driven software platform approach for screening and understanding metabolism**

11:10 – 12:20 Milar Alan<sup>1</sup>, Mark Wrona<sup>1</sup>, Stephen McDonald<sup>1</sup>, Robert Plumb<sup>2</sup>, Joanne Mather<sup>1</sup>

<sup>1</sup>Waters Corporation, <sup>2</sup>Imperial College, London, UK

**PTh-038 Metabolite Identification Workflow Software**

13:30 – 14:40 Graham A McGibbon<sup>1</sup>, Vitaly Lashin<sup>2</sup>, Alexey Aminov<sup>2</sup>, Dmitry Mitushev<sup>2</sup>, Hans de Bie<sup>1</sup>

<sup>1</sup>Advanced Chemistry Development (ACD/Labs), Toronto, Canada, <sup>2</sup>ACD Ltd., Moscow, Russia

**PTh-039 Integration of spectral library in standard data processing pipeline for shotgun proteomics data**

11:10 – 12:20 Junko Kimata<sup>1</sup>, Kai Fritzemeier<sup>2</sup>, Torsten Ueckert<sup>2</sup>, Bernard Delanghe<sup>2</sup>

<sup>1</sup>Thermo Fisher Scientific K.K., Yokohama, Japan, <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

**PTh-040 Application of MALDI-TOF Mass Spectrometry Characterization in the Development of Nano-porous Metallophthalocyanin Sensor Electrodes**

13:30 – 14:40 Siau Gek Ang, Chuan Ming Yap, Guo Qin Xu  
National University of Singapore

**PTh-041 Highly accurate chemical formula prediction tool utilizing high-resolution mass spectra, MS/MS fragmentation, heuristic rules, and isotope pattern matching**

11:10 – 12:20 Tomas Pluskal<sup>1</sup>, Taisuke Uehara<sup>2</sup>, Mitsuhiro Yanagida<sup>1</sup>

<sup>1</sup>Okinawa Institute of Science and Technology, Onna, Japan, <sup>2</sup>Eisai Co. Ltd., Tsukuba, Japan

### Session 35

#### Environment I

**PTh-042 SBSE probe desorption GC-IT-MS analysis of degradation products of esfenvalerate obtained by chemical oxidation process**

13:30 – 14:40 Renata Colombo, Marcos Roberto V Lanza, Janete H Yariwake  
University of Sao Paulo/IQSC, Sao Carlos, Brazil

## Thursday, 20<sup>th</sup> September

**PTh-043 Adosorption property of PCB 209 congeners by gamma-cyclodextrin polymer**

11:10 – 12:20  
Yasunori Fukuda<sup>1</sup>, Kazuhiro Miyawaki<sup>1</sup>, Eiichi Kato<sup>1</sup>, Toshiyuki Kida<sup>2</sup>, Takeshi Nakano<sup>2</sup>, Mitsuru Akashi<sup>2</sup>

<sup>1</sup>NEOS Co.,Ltd., Konan, Japan, <sup>2</sup>Osaka University, Suita/Japan

**PTh-044 Charge exchange ionization in reversed-phase liquid chromatography-atmospheric pressure photoionization mass spectrometry of hormones**

13:30 – 14:40  
David Matejicek  
Mendel University in Brno, Brno, Czech Republic

**PTh-045 Identification of Biodegradation Products of High-Molecular-Weight Perfluorinated Compounds Using Two-Dimensional Liquid Chromatography/High-Resolution Mass Spectrometry**

11:10 – 12:20  
Atsushi Yamamoto<sup>1,2</sup>, Hirotaka Hisatomi<sup>1</sup>, Daisuke Ono<sup>3</sup>, Shuusuke Takemine<sup>4</sup>, Mikiya Kitagawa<sup>5</sup>, Hideya Kawasaki<sup>1</sup>, Ryuichi Arakawa<sup>1</sup>  
<sup>1</sup>Kansai University, Suita, Japan, <sup>2</sup>Osaka City Inst. Pub. Health Environ. Sci., Osaka, Japan, <sup>3</sup>Osaka Municipal Tech. Res. Inst., Osaka, Japan, <sup>4</sup>Hyogo Pref. Inst. Environ. Sci., Hyogo, Japan, <sup>5</sup>Nippon Dionex K.K., Osaka, Japan

**PTh-046 Current status of organophosphorus compounds contaminants in Maizuru Bay, Japan**

13:30 – 14:40  
Emi Yatsuzuka<sup>1</sup>, Hiroya Harino<sup>1</sup>, Chiaki Yamao<sup>1</sup>, Masaaki Ueno<sup>2</sup>, Madoka Ohji<sup>3</sup>  
<sup>1</sup>Kobe College, <sup>2</sup>Kyoto University, <sup>3</sup>Tokyo University of Agriculture and Technology

**PTh-047 Tandem SPE clean up/extraction: strategy to minimize matrix effects on LC-MS determination of endocrine disrupters and pharmaceuticals in sewage samples**

11:10 – 12:20  
Robson J Afonso<sup>1</sup>, Fernanda B Queiroz<sup>2</sup>, Julio C Silva<sup>3</sup>, Rafaela P Gomes<sup>1,2</sup>, Mauricio X Coutrim<sup>1,2</sup>, Sergio F Aquino<sup>1</sup>  
<sup>1</sup>Federal University of Ouro Preto/Minas Gerais/Brazil, <sup>2</sup>Molecular Characterization/Mass Spectrometry Laboratory, <sup>3</sup>Federal University of Minas Gerais/Minas Gerais/Brazil

**PTh-048 Simultaneous analysis of anionic, amphoteric and non-ionic surfactants using ultra-high speed LC-MS/MS**

13:30 – 14:40  
Keiko Matsumoto, Jun Watanabe, Junko Iida  
Shimadzu Corporation., Kyoto, Japan

**PTh-049 Limitations of a commercially available plasma air purifier**

11:10 – 12:20  
Stefan Schmid<sup>1</sup>, Andreas Gerecke<sup>2</sup>, Herbert Haechler<sup>3</sup>, Hubert Hilbi<sup>4</sup>, Simon Weidmann<sup>1</sup>, Renato Zenobi<sup>1</sup>  
<sup>1</sup>ETH Zurich, Zurich, Switzerland, <sup>2</sup>Swiss Federal Laboratories for Material Science and Technology, Dubendorf, Switzerland, <sup>3</sup>University of Zurich, Zurich, Switzerland, <sup>4</sup>Ludwig-Maximilians-Universitaet, Munich, Germany

**PTh-050 Multi-component quantitative analysis of pharmaceuticals and personal care products in the environment by LC-MS/MS with fast polarity switching**

13:30 – 14:40  
Natsuyo Asano, Kiyomi Arakawa, Shinjiro Fujita, Manabu Ueda, Kazuo Mukaibatake, Ichiro Hirano  
Shimadzu Co., Kyoto, Japan

**PTh-051 Screening and library search of Environmental pollutants in Japanese environmental water using LC-MS/MS**

11:10 – 12:20  
Ushio Takeda<sup>1</sup>, Kozue Asakura<sup>1</sup>, Yuji Kakazu<sup>1</sup>, Andre Schreiber<sup>2</sup>  
<sup>1</sup>AB SCIEX, Tokyo, Japan, <sup>2</sup>AB SCIEX, Concord, Canada

**PTh-052 OPTIMIZATION OF SOLID PHASE EXTRACTION FOR PERFLUORINATED COMPOUNDS ANALYSIS IN WATER SAMPLE**

13:30 – 14:40  
Chinagarn Kunacheva, Tanaka Shuhei, Fujii Shigeo, Suzuki Yuji, Chularueangaksorn Pattarawan  
Kyoto University, Kyoto, Japan

**PTh-053 Analytical method and homolog distribution of OH-PCBs in ambient Air**

11:10 – 12:20  
Yuki Haga<sup>1</sup>, Motoharu Suzuki<sup>2</sup>, Masahiro Tsurukawa<sup>1</sup>, Yoshiya Yamoto<sup>3</sup>, Chisato Matsumura<sup>1</sup>, Takeshi Nakano<sup>4</sup>  
<sup>1</sup>Hyogo Pref. Inst. of Env. Sci., Kobe, Japan, <sup>2</sup>Kobe University, Kobe, Japan, <sup>3</sup>Kansai University, Osaka, Japan, <sup>4</sup>Osaka University, Osaka, Japan

**PTh-054 Application of combined UPLC-TOF-MS and combustion ion chromatography for electrolytic degradation mechanism of PFOS in water**

13:30 – 14:40  
Shogo Taniguchi<sup>1</sup>, Ayumi Hashiguchi<sup>2</sup>, Rabindra R Giri<sup>1</sup>, Hiroaki Ozaki<sup>1</sup>

<sup>1</sup>Osaka Sangyo University, Osaka, Japan, <sup>2</sup>Kyoto University, Kyoto, Japan

**PTh-055 2,3,7,8-tetrachlorodibenzo-p-dioxin congener in breast milk among 3 hot spots in Vietnam**

11:10 – 12:20  
Manh D Ho<sup>1</sup>, Teruhiko Kido<sup>1</sup>, Rie Okamoto<sup>1</sup>, Tai T Pham<sup>2</sup>, Muneko Nishijo<sup>2</sup>, Hideaki Nakagawa<sup>2</sup>, Shoko Maruzeni<sup>2</sup>, Hung N Nguyen<sup>3</sup>, Nhu D Dang<sup>3</sup>

<sup>1</sup>Kanazawa University, Kanazawa, Japan, <sup>2</sup>Kanazawa Medical University, Japan, <sup>3</sup>Ha Noi Medical University, Vietnam

**PTh-056 Profiling waters from natural sources and areas of oil sands activity using Fourier transform ion cyclotron resonance mass spectrometry**

13:30 – 14:40  
Mark P Barrow<sup>1</sup>, John V Headley<sup>2</sup>, Kerry M Peru<sup>2</sup>, Brian Fahlman<sup>2</sup>, Richard Frank<sup>3</sup>, L Mark Hewitt<sup>3</sup>

<sup>1</sup>University of Warwick, Coventry, United Kingdom, <sup>2</sup>Environment Canada, Saskatoon, Canada, <sup>3</sup>Environment Canada, Burlington, Canada

**PTh-057 Analysis of biomarkers of the pesticide imazalil using LC/MS/MS.**

11:10 – 12:20  
Moosa Faniband, Bo A Jönsson, Christian H Lindh  
Occupational and Environmental Medicine, Lund University, Sweden

## Thursday, 20<sup>th</sup> September

**PTh-058** **Mass spectrometric investigation of mechanisms for methane formation from epicuticular wax under aerobiosis and UV**

13:30 – 14:40 helge Egsgaard<sup>1</sup>, Dan Bruhn<sup>2,3</sup>, Teis Mikkelsen<sup>2</sup>, Morten M Rolsted<sup>3</sup>, Per Ambus<sup>2</sup>

<sup>1</sup>Department of Chemical and Biochemical Engineering, <sup>2</sup>Department of Chem. and Biochem. Engineering, Technical University of Denmark, Denmark,

<sup>3</sup>Department of Biology, University of Copenhagen, Denmark

**PTh-059** **Application of HPLC/MS in determination of heroin metabolites in saliva and urine samples**

11:10 – 12:20 Marijana Curcic<sup>2</sup>, Vesna Milovanovic<sup>3</sup>, Biljana Ceric<sup>4</sup>, Marina Pijanovic<sup>5</sup>, Vesna Kilibarda<sup>4</sup>, Slavica Vucinic<sup>4</sup>, Nobutake Sato<sup>1</sup>, Takeshi Nakano<sup>6</sup>, Biljana Antonijevi<sup>2</sup>

<sup>1</sup>Nihon Waters, Tokyo, Japan, <sup>2</sup>University of Belgrade, Belgrade, Serbia,

<sup>3</sup>Serbian Chemicals Agency, Belgrade, Serbia, <sup>4</sup>Poison Control Center, Belgrade, Serbia, <sup>5</sup>Medilab Polyclinic, Cacak, Serbia, <sup>6</sup>Osaka University, Osaka, Japan

**PTh-060** **Analysis method of polybrominated diphenyl ether using GC-MS and GC-MS/MS coupled with automated identification and quantification system with a database**

13:30 – 14:40 Katsuhiro Nakagawa, Tomoaki Kondo, Kouki Tanaka, Yuki Sakamoto, Shuichi Kawana, Haruhiko Miyagawa Shimadzu Co., Kyoto, Japan

**PTh-061** **LC-HRMS investigation of the human in vitro metabolism of brominated flame retardants using APPI and ESI.**

11:10 – 12:20 CHARLOTTE MARTEAU<sup>1</sup>, SYLVIE CHEVOLLEAU<sup>1</sup>, ISABELLE JOUANIN<sup>1</sup>, ELISABETH PERDU<sup>1</sup>, GEORGES DE SOUSA<sup>2</sup>, ROGER RAHMANI<sup>2</sup>, DANIEL ZALKO<sup>1</sup>, LAURENT DEBRAUWER<sup>1</sup>

<sup>1</sup>INRA, UMR 1331, Toxalim/AXIOM/Metatoul, Toulouse, FRANCE, <sup>2</sup>INRA, UMR 1331, Toxalim, Sophia Antipolis, FRANCE

**PTh-062** **Information of the behavior of the persistent organic pollutants in the sea around Japan**

13:30 – 14:40 Masahiro Tsurukawa<sup>1</sup>, Motoharu Suzuki<sup>2</sup>, Yuki Haga<sup>1</sup>, Chisato Matsumura<sup>1</sup>, Takeshi Nakano<sup>3</sup>, Masayuki Kunugi<sup>4</sup>  
<sup>1</sup>HYOGO Prefectural Institute of Environmental Sciences, Kobe, Japan, <sup>2</sup>Kobe University, Kobe, Japan, <sup>3</sup>Osaka University, Osaka, Japan, <sup>4</sup>Tokyo University of Science, Chiba, Japan

**PTh-063** **LC/ESI(-)-MS/MS analyses of the biotransformation products of dibenz-p-dioxin by *Sphingobium* sp. strain KK2**

11:10 – 12:20 Allyn H Maeda, Emi Aoki, Robert A Kanaly  
Yokohama City University, Yokohama, Japan

**PTh-064** **Analysis of Sea-Dumped Chemical Warfare Agents from Sediment Samples Taken at in Baltic Sea**

13:30 – 14:40 Ullastiina Hakala, Martin Söderström, Olli Kostiainen, Jenni Taipalus, Paula Vanninen  
VERIFIN/Department of Chemistry/University of Helsinki, Finland

**PTh-065** **Online SPE LC-MSMS for screening and quantifying anti-cancer drugs and metabolites in hospital's wastewaters and rivers**

11:10 – 12:20 Mikael Levi<sup>2</sup>, Claude Villard<sup>3</sup>, Therese Schembri<sup>3</sup>, Anja Gruening<sup>1</sup>, Stephane Moreau<sup>2</sup>, Pierre Boissery<sup>4</sup>, Daniel Lafitte<sup>2</sup>

<sup>1</sup>Shimadzu Europa GmbH, Duisburg, Germany, <sup>2</sup>Shimadzu France SAS, Marne la Vallee, France, <sup>3</sup>Aix Marseille Universite, Marseille , France, <sup>4</sup>Agence de l'Eau Rhone Mediterranee & Corse, Marseille, France

**PTh-066** **Identification of chlorinated aromatics as impurity of chlorinated paraffins by GC-HRMS or GC-HR-Tof-MS**

13:30 – 14:40 Takumi Takasuga<sup>1</sup>, Takeshi Nakano<sup>2</sup>, Yasuyuki Shibata<sup>3</sup>

<sup>1</sup>Shimadzu Techno-Research Inc., Kyoto, Japan, <sup>2</sup>Osaka University, Osaka, Japan, <sup>3</sup>National Institute for Environmental Studies, Tsukuba, Japan

**PTh-068** **Determination of absolute configuration of PCB atropisomer and analysis of enantiomeric excess in the human sample**

13:30 – 14:40 Takeshi Nakano<sup>1</sup>, Chisato Matsumura<sup>2</sup>, Masahiro Tsurukawa<sup>2</sup>, Toshihiro Okuno<sup>2</sup>, Mitsunobu Toda<sup>1</sup>, Tadashi Mori<sup>1</sup>, Yoshihisa Inoue<sup>1</sup>

<sup>1</sup>Osaka University, Suita, Japan, <sup>2</sup>Hyogo prefectural Institute of Environmental Sciences

**PTh-069** **Analysis of natural organic dyestuffs extracted from textiles.**

11:10 – 12:20 Ivan Viden, David Kohout, Jiri Kosina, Josef Chudoba  
Institute of Chemical Technology, Prague, Czech Republic

**PTh-070** **Atmospheric pressure ionisation and ion mobility novel techniques for the analysis of the POPs on the Stockholm convention including dioxins**

13:30 – 14:40 Bert van Bavel<sup>1</sup>, Jody Dunstan<sup>2</sup>, Peter Hancock<sup>2</sup>, Rhys Jones<sup>2</sup>, Ingrid Ericson<sup>1</sup>, Jessika Hagberg<sup>1</sup>

<sup>1</sup>MTM Research Center, Örebro University, Sweden, <sup>2</sup>Waters Corporation, Manchester, Great Britian

**PTh-071** **Mixed-mode Liquid Chromatography/Tandem Mass Spectrometry Analysis of Glyphosate and Its Application in Exposure Study**

11:10 – 12:20 Chunyan Hao<sup>1</sup>, Christopher B Edge<sup>2</sup>, David Morse<sup>1</sup>, Dean G Thompson<sup>3</sup>, Jeff E Houlahan<sup>2</sup>

<sup>1</sup>Ontario Ministry of the Environment, <sup>2</sup>Biology Department, University of New Brunswick, <sup>3</sup>Great Lakes Forestry Center, Canadian Forest Service

**PTh-072** **Desorption atmospheric pressure photoionization-mass spectrometry for the determination of chemical composition of atmospheric aerosols**

13:30 – 14:40 Evgeny Parshintsev<sup>1</sup>, Ingrid Lamazere<sup>1,2</sup>, Jose Ruiz-Jimenez<sup>1</sup>, Tiina Kauppila<sup>1</sup>, Kari Hartonen<sup>1</sup>, Tapio Kotiaho<sup>1</sup>, Marja-Liisa Riekola<sup>1</sup>

<sup>1</sup>University of Helsinki, Helsinki, Finland, <sup>2</sup>IUT Paul Sabatier, Castres, France

**Thursday, 20<sup>th</sup> September**

## Session 36

### Advances in Ion Mobility Mass Spectrometry

- PTh-073** Evaluating multiplex fragmentation and ion mobility separations to improve the quality of rapid LCMS peptide mapping analyses for biotherapeutic proteins.  
 11:10 – 12:20

KATSUTOSHI NAGASE<sup>1</sup>, KENJI HIROSE<sup>1</sup>, Scott Berger<sup>2</sup>,  
 Henry Shion<sup>2</sup>, St John Skilton<sup>2</sup>, Weibin Chen<sup>2</sup>  
<sup>1</sup>Waters, Tokyo, Japan, <sup>2</sup>Waters Corporation, Milford, MA

- PTh-074** Conformational and functional analysis for quality control of protein drugs using ion mobility mass spectrometry  
 13:30 – 14:40

Haruhiko Kamada<sup>1,2</sup>, Masaki Inoue<sup>1</sup>, Yasuhiro Abe<sup>1</sup>,  
 Kazuya Nagano<sup>1</sup>, Kenji Hirose<sup>3</sup>, Yasuo Tsutsumi<sup>1,2</sup>,  
 Shin-ichi Tsunoda<sup>1,2</sup>  
<sup>1</sup>NIBIO, Osaka, Japan, <sup>2</sup>Osaka University, Osaka, Japan, <sup>3</sup>Nihon Waters KK, Tokyo, Japan

- PTh-075** Effects of hydrophobic oligopeptides on the aggregation process of Parkinson's disease target protein alpha-Synuclein  
 11:10 – 12:20

Kathrin Lindner<sup>1</sup>, Christiaan Karreman<sup>1</sup>, Hanne Gerdin<sup>1</sup>,  
 Marcel Leist<sup>1</sup>, Michael Gross<sup>2</sup>, David Clemmer<sup>3</sup>,  
 Michael Przybylski<sup>1</sup>  
<sup>1</sup>University of Konstanz, Konstanz, Germany/Baden-Württemberg,

<sup>2</sup>Washington University St. Louis, St. Louis, USA/MO, <sup>3</sup>Indiana University, Bloomington, USA/IN

- PTh-076** Analysis of different conformers of carbonic anhydrase2 using ion mobility coupled with electrospray ionization  
 13:30 – 14:40

KENJI HIROSE<sup>1</sup>, TAIJI KAWASE<sup>1</sup>, YOSHIAKI NABUCHI<sup>2</sup>,  
 MITSUO TAKAYAMA<sup>2</sup>  
<sup>1</sup>Nihon Waters K.K., Osaka, Japan, <sup>2</sup>Yokohama City University, Kanagawa, Japan

- PTh-077** The Accuracy and Reproducibility of Calibration in Trapped Ion Mobility Spectrometry  
 11:10 – 12:20

Victor Fursey, Mark Ridgeway, Desmond Kaplan, Melvin A Park  
 Bruker Daltonics, Billerica, MA, USA

- PTh-078** Enhancement of Nanowire Formation by Mixing Multiple Modified Amyloid Peptides: Mechanism and Application  
 13:30 – 14:40

Hiroki Sakai<sup>1</sup>, Ken Watanabe<sup>1</sup>, Christian Bleiholder<sup>2</sup>,  
 Thomas Wyttenbach<sup>2</sup>, Michael T Bowers<sup>2</sup>, Kazuyasu Sakaguchi<sup>1</sup>  
<sup>1</sup>Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan, <sup>2</sup>Department of Chemistry and Biochemistry, University of California, Santa Barbara, California, USA

- PTh-079** Internal energy of ions in travelling wave ion mobility spectrometry: dependence on instrument parameters and ion properties  
 11:10 – 12:20

Denis Morsa, Valerie Gabelica, Edwin A De Pauw  
 Mass Spectrometry Laboratory, University of Liege

- PTh-080** An ion mobility mass spectrometer with an axial sector TOF analyzer  
 13:30 – 14:40

Alexey A Sysoev, Alexander A Sysoev, Sergey S Poteshev,  
 Denis M Chernyshev  
 National Research Nuclear University MEPhI, Moscow, Russia

- PTh-081** Energy-resolved ion-mobility tandem mass spectrometry: a new tool for probing gas-phase isomerization and fragmentation of small molecules  
 11:10 – 12:20

Yayoi Hongo<sup>1</sup>, Takemichi Nakamura<sup>1</sup>, Takae Takeuchi<sup>2</sup>  
<sup>1</sup>RIKEN, Wako, Japan, <sup>2</sup>Nara Women's University, Nara, Japan

- PTh-082** Separation of Peptide Sequence Isomers by Capillary Electrophoresis Coupled with Ion Mobility Mass Spectrometer  
 13:30 – 14:40

Yury E Glazyrin<sup>1,2</sup>, Gleb G Mironov<sup>2</sup>, Robert N Ben<sup>2</sup>,  
 Maxim V Berezovski<sup>2</sup>  
<sup>1</sup>Krasnoyarsk State Medical University, Krasnoyarsk, Russia, <sup>2</sup>University of Ottawa, Ottawa, Canada

## Session 37

### Challenges in High Resolution and High Accuracy Mass Measurement Mass Spectrometry

- PTh-083** Challenges in high resolution and accuracy mass measurement for drug discovery and development using FT ICR and Orbitrap mass spectrometers  
 11:10 – 12:20

Zenzaburo Tozuka  
 Osaka University

- PTh-085** Silicon speciation in petroleum products using a multi-technical approach by Mass Spectrometry for a better understanding of catalyst poisoning  
 11:10 – 12:20

Fabien Chainet<sup>2</sup>, Jeremie Ponthus<sup>1,2</sup>,  
 Charles-Philippe Lienemann<sup>2</sup>, Marion Courtiade<sup>2</sup>,  
 Olivier Francois X Donard<sup>3</sup>  
<sup>1</sup>IFP Energies Nouvelles, <sup>2</sup>IFP Energies Nouvelles, Solaize, France, <sup>3</sup>LCBIE-IPREM, UMR 5254, CNRS UPPA, Pau, France

- PTh-086** Development and validation of high resolution liquid chromatography-time of flight method of Bacopaside-I and metabolites for pharmacokinetic study  
 13:30 – 14:40

Sontaya Sookying<sup>2</sup>, Kornkanok Ingkaninan<sup>\*2</sup>,  
 Dumrongsak Pekthong<sup>3</sup>, Sarawut Oo-puthinan<sup>3</sup>, JIE XING<sup>1</sup>,  
 Zhaoqi Zhan<sup>1</sup>

<sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, Singapore, <sup>2</sup>Department of Pharmaceutical Chemistry and Pharmacognosy, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand, <sup>3</sup>Department of Pharmacy Practice, Faculty of Pharmaceutical Sciences, Naresuan University, Phitsanulok 65000, Thailand

- PTh-087** Characterization of Humic and Fulvic acid fractions separated by size exclusion chromatography and application of 15T FT-ICR MS  
 11:10 – 12:20

Min-Hui Son, Yoon-Seok Chang  
 POSTECH, Pohang, Korea

Thursday, 20<sup>th</sup> September**PTh-088** Dependence of Field Evaporation in Three-Dimensional Atom Probe on the Crystallographic Orientation

13:30 – 14:40  
Mahito Shimizu, Masato Morita, Yuya Hanaoka,  
Masanori Owari  
The University of Tokyo, Tokyo, Japan

**PTh-089** Theoretical Verification of a Strategy for Determining Elemental Composition Based on Ultrahigh-resolution Mass Spectrometric Data

11:10 – 12:20  
Tatsuhiko Nagao<sup>1</sup>, Daichi Yukihira<sup>1</sup>, Yoshinori Fujimura<sup>1</sup>,  
Kazunori Saito<sup>2</sup>, Daisuke Miura<sup>1</sup>, Hiroyuki Wariishi<sup>1</sup>  
<sup>1</sup>Kyushu University, Fukuoka, Japan, <sup>2</sup>Bruker Daltonics K.K., Yokohama, Japan

**PTh-090** Analysis of Wedelia trilobata flower extract using Liquid Chromatography-Orbitrap Mass Spectrometry

13:30 – 14:40  
Jhih-Yang Huang<sup>1</sup>, Ean-Tun Alex Liaw<sup>1</sup>, Chien-Kuo Han<sup>2</sup>,  
Ming-Feng Chen<sup>3</sup>, Jean Chih-Chun Huang<sup>1</sup>  
<sup>1</sup>National Pingtung University of Science & Technology, Pingtung, Taiwan,  
<sup>2</sup>Asia University, Taichung, Taiwan, <sup>3</sup>National Cheng Kung University, Tainan, Taiwan

**PTh-091** Relevance of Gas and Pressure for Thermalization of Cluster Ions in the Hexapole Ion Trap of a FT-ICR Mass Spectrometer

11:10 – 12:20  
Jürgen H Gross, Doris Lang, Iris Mitsch  
Heidelberg University, Heidelberg, Germany

**Session 38**  
Mass Spectrometry for Metabolic Diseases**PTh-092** A quantitative analytical method for determining the levels of glucose-dependent insulinotropic polypeptides GIP1-42 and GIP3-42 in human plasma using LC-MS/MS/MS

13:30 – 14:40  
Atsushi Miyachi<sup>1</sup>, Nana Morimoto<sup>1</sup>, Yuichiro Yamada<sup>2</sup>,  
Ken-ichi Harada<sup>3</sup>  
<sup>1</sup>SANWA KAGAKU KENKYUSHO CO.,Mie,Japan, <sup>2</sup>Akita University School of Medicine, Akita, Japan, <sup>3</sup>Meijo University, Nagoya, Japan

**PTh-093** Metabolomic Analysis of Autism Spectrum Disorders Using Saliva

11:10 – 12:20  
KEIJI GAMOH, KAZUTAKA SUGAI  
Kochi University, Kochi, Japan

**PTh-094** Affinity - Mass Spectrometry: A Proteome Signature for Intra-Uterine Growth Restriction Reveals Pathological Protein Glycosylation Alterations in Umbilical Cord Blood

13:30 – 14:40  
Manja Wölter<sup>1</sup>, Claudia Röwer<sup>1</sup>, Cornelia Koy<sup>1</sup>, Ulrich Pecks<sup>2</sup>,  
Michael O Glocker<sup>1</sup>  
<sup>1</sup>Proteome Center Rostock, <sup>2</sup>Womens Clinic, University of Aachen

**PTh-095** Automated Analysis of 25-hydroxyvitamin D2 and D3 with APCI-MS/MS Coupled with ZIVAK ONH-200BD Sample Preparation System

11:10 – 12:20  
MURAT CELIK, HASAN OZGEN  
ZIVAK TECHNOLOGIES, KOCAELI, TURKEY

**PTh-096** A LC/MS/MS Method Enables Simultaneous Detection of Diagnostic Biomarkers of Alkaptonuria, Ornithine Carbamoyltransferase Deficiency and Neuroblastoma Disease

13:30 – 14:40  
Chien-Chen Lai<sup>1</sup>, Wei-Yi Hsu<sup>2</sup>, Fuu-Jen Tsai<sup>2</sup>  
<sup>1</sup>National Chung Hsing University, Taichung, Taiwan, <sup>2</sup>Department of Medical Research, China Medical University Hospital, Taichung, Taiwan

**PTh-097** Development of a high sensitive quantitation method for serum C-peptide by isotope-dilution mass spectrometry

11:10 – 12:20  
Tomoya Kinumi, Mari Goto, Akiko Takatsu  
National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

**PTh-098** Label-Free Screening for Epigenetic Drug Discovery Using Mass Spectrometry to Monitor Protein and Nucleic Acid Modification Events

13:30 – 14:40  
Jennifer Rossi, Peter Rye, Lauren Frick, Hisashi Iwase, Masahiro Maeda, William LaMarr  
Agilent Technologies

**PTh-099** Comprehensive analysis of human proteome in hippocampus tissue from Alzheimer disease patient.

11:10 – 12:20  
hyekyeong Min<sup>1</sup>, Hyung Joo Lee<sup>2</sup>, Se-Young Kim<sup>1</sup>, Gun Wook Park<sup>1</sup>, In Jung Ji<sup>1</sup>, Kyung-Hoon Kwon<sup>1</sup>, Jong Shin Yoo<sup>1</sup>, Young Mok Park<sup>1</sup>, Jin Young Kim<sup>1</sup>  
<sup>1</sup>Korea Basic Science Institute,Ochang-eup,Cheongwon-gun,Chungbuk,Korea,  
<sup>2</sup>Yonsei Proteome Research Center, Yonsei University, Seoul, Korea

**PTh-100** Rapid and sensitive determination of the intermediates of advanced glycation end products in human nail by UPLC-ESI-TOF-MS

13:30 – 14:40  
Jun Zhe MIN<sup>1</sup>, Makoto Yamamoto<sup>1</sup>, Tatsuya Higashi<sup>2</sup>, Kenichiro Todoroki<sup>1</sup>, Koichi Inoue<sup>1</sup>, Toshimasa Toyo'oka<sup>1</sup>  
<sup>1</sup>School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, Japan,  
<sup>2</sup>Faculty of Pharmaceutical Sciences, Tokyo University of Science, Japan

**PTh-101** Determination of flavonoids in infected plants using LC-MS/MS

11:10 – 12:20  
Jong Sung Jin<sup>1</sup>, Hae Gyeong Kim<sup>1</sup>, Mee Sung Lee<sup>1</sup>, Mi Jin Kim<sup>1</sup>, Sung Chul Shin<sup>2</sup>  
<sup>1</sup>Korea Basic Science Institute, Busan, Korea, <sup>2</sup>Gyeongsang National University, Jinju, Korea

## Thursday, 20<sup>th</sup> September

- PTh-102** Development of methods to identify previously unknown secondary metabolites from myxobacteria based on a comprehensive metabolic profiling workflow  
 13:30 – 14:40

Thomas Hoffmann<sup>2,3</sup>, Daniel Krug<sup>2,3</sup>, Clive Seymour<sup>1</sup>,

Gabriela Zurek<sup>4</sup>, Aiko Barsch<sup>4</sup>, Rolf Mueller<sup>2,3</sup>

<sup>1</sup>Bruker BioSciences Pty. Ltd., Preston, Australia, <sup>2</sup>Pharmaceutical Biotechnology, Saarland University, Saarbruecken, Germany, <sup>3</sup>Helmholtz-Institute for Pharmaceutical Research Saarland (HIPS), Saarbruecken, Germany, <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany

- PTh-103** Use of proton-affinitive derivatization in HPLC-positive-ESI-MS analysis of biologically important carboxylic acids  
 11:10 – 12:20

Hajime Kato, Shin Mitsuzuka, Kowa Yamashita, Mitsuteru Numazawa

Tohoku Pharmaceutical University, Sendai, Japan

- PTh-104** Comprehensive CID with accurate mass measurement for analyte identification in metabolomics and natural products: HPLC-TOF-MS analysis with database searching  
 13:30 – 14:40

Joe Binkley, Binkley Joe, Kevin Siek, Li Zhang

LECO Corporation

- PTh-105** Acylcarnitine analysis by ESI-MS/MS with smaller amount of sample and rapid analytical time  
 11:10 – 12:20

Hironori Kobayashi<sup>1</sup>, Yuichi Mushimoto<sup>1</sup>, Yuki Hasegawa<sup>1</sup>, Kenji Yamada<sup>1</sup>, Jamiyan Purevsuren<sup>1</sup>, Tomoo Takahashi<sup>1</sup>, Toshikazu Minohata<sup>2</sup>, Junko Iida<sup>2</sup>, Yamaguchi Seiji<sup>1</sup>

<sup>1</sup>Shimane University, Izumo, Japan, <sup>2</sup>Shimadzu Corporation, Kyoto, Japan

- PTh-106** Simultaneous determination of acylcarnitines and amino acids for inborn error of metabolism using UPLC/MS/MS  
 13:30 – 14:40

Haruka Oda<sup>1</sup>, Yasuhiro Maeda<sup>1</sup>, Tetsuya Ito<sup>1</sup>, Yuji Hotta<sup>1</sup>, Yoko Nakajima<sup>1</sup>, Sayaka Kato<sup>1</sup>, Shinji Saito<sup>1</sup>, Naruji Sugiyama<sup>2</sup>, Kazunori Kimura<sup>1</sup>

<sup>1</sup>Nagoya City University, Nagoya, Japan, <sup>2</sup>Aichi-Gakuin University, Nagoya, Japan

## Session 39

### MS Informatics for Quantitation

- PTh-107** An Attempt to Quantitative Analysis for Clinical Proteomics by Nano LC-nano-ESI-SRM-MS Using Stable Isotope-labeled Iodoacetanilide as well as N-Ethylmaleimide  
 11:10 – 12:20

Sadamu Kurono<sup>1,2</sup>, Yuka Kaneko<sup>1,2</sup>, Shuji Matsuura<sup>1</sup>, Satomi Niwayama<sup>3</sup>

<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>Wako Pure Chemical Industries, Ltd., Osaka, Japan, <sup>3</sup>Texas Tech University, Lubbock, TX

- PTh-108** Multivariate analysis software to support large scale MRM study  
 13:30 – 14:40

Atsushi Ogiwara<sup>1</sup>, Hisae Anyoji<sup>1</sup>, Jun Watanabe<sup>2</sup>, Junko Iida<sup>2</sup>, Mitsuhiro Kanazawa<sup>1</sup>

<sup>1</sup>Reifycs, Inc., Tokyo, Japan, <sup>2</sup>Shimadzu Corporation, Kyoto, Japan

- PTh-109** High Pressure Acid Dissolution of alpha-alumina for trace elements determination by ICP-MS  
 11:10 – 12:20

Jung Ki Suh, Chang Soo Kim

Korea Research Institute for Standards and Science, 267 Gajeong Ro, Yuseong Gu, Daejeon 305-340, Rep. of Korea

## Session 40

### Environment II

- PTh-110** High-Speed Survey Method for Photo-degradation Products of Pharmaceuticals Using UV-LED Lighting Device and DART-TOF Mass Spectrometer  
 13:30 – 14:40

Toshio Tashima<sup>1</sup>, Kaori Asano<sup>2</sup>, Takeyuki Suzuki<sup>2</sup>, Tsuyoshi Matsuzaki<sup>2</sup>, Takeshi Nakano<sup>3</sup>

<sup>1</sup>GeneStem Co. Ltd., Osaka, Japan, <sup>2</sup>The Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan, <sup>3</sup>Research Center for Environmental Preservation, Osaka University, Osaka, Japan

- PTh-111** Hydrophilic-interaction liquid chromatography (HILIC)-tandem mass spectrometry for quantification of oseltamivir and zanamivir in surface water and sediment samples  
 11:10 – 12:20

Ryohei Takanami, Hiroaki Ozaki, Rabindra Raj Giri, Shogo Taniguchi, Shintaro Hayashi  
 Osaka Sangyo University, Osaka, Japan

- PTh-112** Determination of chlorinated/brominated polycyclic aromatic hydrocarbons (Cl/BrPAHs) in flue gas and ash from waste incinerator  
 13:30 – 14:40

Liang Tang<sup>1</sup>, Yuichi Miyake<sup>1</sup>, Yuichi Horii<sup>2</sup>, Kiyoshi Nojiri<sup>2</sup>, Nobutoshi Ohtsuka<sup>2</sup>, Takashi Amagai<sup>1</sup>

<sup>1</sup>University of Shizuoka, Shizuoka, Japan, <sup>2</sup>Center for Environmental Science in Saitama, Kazo, Japan

- PTh-113** SELECTIVE EXTRACTION OF ORGANOHALOGENS FROM GCxGC-HRToFMS DATA FOR GLOBAL ANALYSIS OF ENVIRONMENTAL AND BIOLOGICAL SAMPLES  
 11:10 – 12:20

Shunji Hashimoto, Yasuyuki Zushi, Akihiro Fushimi, Yoshikatsu Takazawa, Kiyoshi Tanabe, Yasuyuki Shibata  
 National Institute for Environmental Studies, Tsukuba, Japan

- PTh-114** Electrospray mass spectrometric observation of the interaction between environmental pollutants and biologic compounds  
 13:30 – 14:40

Hiroshi Moriwaki, Takahiro Nakagawa  
 Shinshu University

- PTh-115** Characterization of organic pollutants in River Water by GC/MS ion profiles  
 11:10 – 12:20

Zaharie Moldovan<sup>1</sup>, Olivian Marincas<sup>1</sup>, Veronica Avram<sup>1</sup>, Florina Tusa<sup>1</sup>, Alfredo C Alder<sup>2</sup>

<sup>1</sup>National Institute for Research and Development of Isotopic and Molecular Technology, Cluj-Napoca, Romania, <sup>2</sup>Swiss Federal Institute of Aquatic Science and Technology, EAWAG, Environmental Chemistry Department, Dübendorf, Switzerland

## Thursday, 20<sup>th</sup> September

**PTh-116 A Sensitive measurement of sucralose and acesulfame in inland and offshore waters around Japan by LC/MS and LC/MS/MS.**

13:30 – 14:40  
 Shigeru Suzuki<sup>1</sup>, Atsuko Hasegawa<sup>2</sup>, Rina Higuchi<sup>1</sup>,  
 Takahiro Yamaguchi<sup>1</sup>, Hisato Nishikawa<sup>1</sup>, Takuhei Miyaki<sup>1</sup>,  
 Chiaki Oshima<sup>1</sup>, Ryosuke Otsubo<sup>1</sup>

<sup>1</sup>Chubu University, Aichi, Japan, <sup>2</sup>Kanagawa Environmental Research Center, Kanagawa Japan

**PTh-117 Real-time ambient air monitoring using selected ion flow tube-mass spectrometry (SIFT-MS)**

11:10 – 12:20  
 Vaughan S Langford<sup>1</sup>, Murray J McEwan<sup>1,2</sup>

<sup>1</sup>Syft Technologies Limited, Christchurch, New Zealand, <sup>2</sup>University of Canterbury, Christchurch, New Zealand

**PTh-118 Development of UPLC-MS/MS method with large volume injection for simultaneous determination of regulated pesticides in drinking water.**

13:30 – 14:40  
 Jun Yonekubo, Nobutake Sato  
 Nihon Waters K.K., Japan

**PTh-119 Development of Automated Identification and Quantification System with a Database**

11:10 – 12:20  
 Kiwao Kadokami<sup>1</sup>, Terumi Miyazaki<sup>5</sup>, Chiaki Karaki<sup>1</sup>,  
 Daisuke Jinya<sup>2</sup>, Tomomi Iwamura<sup>2</sup>, Kaori Ohkubo<sup>4</sup>,  
 Takashi Miyawaki<sup>3</sup>, Yoko Nakazono<sup>4</sup>, Kouji Takahashi<sup>3</sup>  
<sup>1</sup>The University of Kitakyushu, Kitakyushu, Japan, <sup>2</sup>Kitakyushu City Institute of Environmental Sciences, <sup>3</sup>Fukuoka Institute of Health and Environmental Sciences, <sup>4</sup>Saga Prefectural Institute of Public Health and Pharmaceutical Research, <sup>5</sup>Nippon Steel Kankyo Engineering

**PTh-120 Metal speciations in environmental and clinical applications**

13:30 – 14:40  
 Yeuk-Ki Tsui, Kelvin Sze-Yin Leung  
 Hong Kong Baptist University, Hong Kong

**PTh-121 Occurrence of 92 pharmaceuticals in river water in agricultural or urban areas**

11:10 – 12:20  
 Koya Komori, Mizuhiko Minamiyama, Yutaka Suzuki  
 Public Works Research Institute, Tsukuba, Japan

**PTh-122 Application of tandem mass spectrometry for the structure confirmation of a wide range of peptides synthesized by cyanobacteria *Woronichinia naegeliana***

13:30 – 14:40  
 Beata Bober<sup>1,2</sup>, Zbigniew Lechowski<sup>2</sup>, Jan Bialczyk<sup>2</sup>,  
 Piotr Suder<sup>3</sup>, Ken-ichi Harada<sup>1</sup>  
<sup>1</sup>Meijo University, Nagoya, Japan, <sup>2</sup>Jagiellonian University, Krakow, Poland,  
<sup>3</sup>University of Science and Technology, Krakow, Poland

**PTh-123 A search for active ingredients in cigarette smoke that modify significant biomolecules**

11:10 – 12:20  
 Shizuyo Horiyama<sup>1</sup>, Chie Honda<sup>1</sup>, Kiyoko Suwa<sup>1</sup>,  
 Kiyoharu Nishide<sup>1</sup>, Yuta Takahashi<sup>1</sup>, Kazuki Nakamura<sup>1</sup>,  
 Masaru Kunitomo<sup>1</sup>, Hirofumi Sato<sup>2</sup>, Motohiro Shizuma<sup>2</sup>,  
 Mitsuo Takayama<sup>3</sup>

<sup>1</sup>Mukogawa Women's University, Nishinomiya, Japan, <sup>2</sup>Osaka Municipal Technical Research Institute, Osaka, Japan, <sup>3</sup>International Graduate School of Arts and Sciences, Yokohama, Japan

**PTh-124 Development of smoke diagnostic assays: When the smoke clears, will it end up in the wine bottle?**

13:30 – 14:40  
 Yoji Hayasaka, Gayle Baldock, Mango Parker, Kevin Pardon, Cory Black, Markus Herderich  
 The Australian Wine Research Institute

**PTh-125 Ions Observed in DART-MS Analysis of Pharmaceuticals Containing Various Functional Groups on Normal and Reverse Phase TLC Plates**

11:10 – 12:20  
 Kaori Asano<sup>1</sup>, Toshio Tashima<sup>2</sup>, Takeyuki Suzuki<sup>1</sup>,  
 Tsuyoshi Matsuzaki<sup>1</sup>, Takeshi Nakano<sup>3</sup>  
<sup>1</sup>The Institute of Scientific and Industrial Research, Osaka University, <sup>2</sup>GeneStem Co., Ltd, <sup>3</sup>Research Center for Environmental Preservation, Osaka University

**PTh-126 Concentration profiles of PCB congeners in Steller sea lion, Hokkaido, Japan**

13:30 – 14:40  
 Keiko Kubo<sup>1</sup>, Katsuyuki Yamaguchi<sup>2</sup>, Wakana Yamada<sup>3</sup>,  
 Tsuyoshi Ishinazaka<sup>4</sup>, Masaki Mitsuhashi<sup>6</sup>, Kaoru Hattori<sup>5</sup>,  
 Shunitz Tanaka<sup>1</sup>

<sup>1</sup>Hokkaido University, Sapporo, Japan, <sup>2</sup>Hokkaido Research Organization, Sapporo, Japan, <sup>3</sup>Hokkaido University, Hakodate, Japan, <sup>4</sup>Shiretoko Nature Foundation, Rausu, Japan, <sup>5</sup>Fisheries Research Agency, Kushiro, Japan, <sup>6</sup>Hokkaido Research Organization, Kushiro, Japan

**PTh-127 Investigation of metabolites formed during activated sludge treatment of clarithromycin**

11:10 – 12:20  
 Masakazu Morita<sup>1</sup>, Koya Komori<sup>2</sup>, Mizuhiko Minamiyama<sup>2</sup>  
<sup>1</sup>NS Environmental Science Consultant Co., Tokyo, Japan, <sup>2</sup>Public Works Research Institute, Ibaraki, Japan

**PTh-128 A NEW CHEMOMETRIC APPROACH FOR THE QUANTITATION OF STEROIDAL COMPOUNDS IN WASTEWATER BY GCxGC-TOFMS**

13:30 – 14:40  
 Matias Kopperi, Jose Ruiz-Jimenez, Kari Hartonen, Marja-Liisa Riekola  
 University of Helsinki, Finland

**PTh-129 High-Resolution Tandem Mass Spectrometry Analysis of the Interactions of Oligonucleotides with Selected River Basin Specific Pollutants**

11:10 – 12:20  
 Janna Anichina, Andre Schreiber, Ron Bonner, Takeo Sakuma AB SCIEX, Concord, Canada

## Thursday, 20<sup>th</sup> September

### PTh-130 Formation of Hydroxy Polychlorinated Biphenyl

13:30 – 14:40  
Shiho Fukuzawa<sup>1</sup>, Takeshi Morita<sup>1</sup>, Masahiro Shimase<sup>1</sup>, Akinobu Kunitake<sup>1</sup>, Takanori Sakiyama<sup>2</sup>, Tameo Okumura<sup>3</sup>

<sup>1</sup>Nippon Steel Kankyo Engineering Co., Ltd., Chiba, Japan, <sup>2</sup>Osaka City Institute of Public Health and Environmental Sciences, Osaka, Japan, <sup>3</sup>Environmental Pollution Control Center, Osaka Prefectural, Government, retirement

### PTh-131 High Resolution LC-MS for Screening and Quantitative Analysis of Antibiotics in Drinking Water using an Orbitrap and Online Sample Preparation

11:10 – 12:20  
Jonathan R Beck, Dipankar Ghosh, Charles T Yang  
Thermo Fisher Scientific, San Jose, USA

### PTh-132 Rapid screening and confirmation of emerging contaminants in UK river waters by UHPLC-IT-TOF

13:30 – 14:40  
David R Baker<sup>1</sup>, John Bagnall<sup>2</sup>, Alan J Barnes<sup>1</sup>, Barbara Kasprzyk-Hordern<sup>2</sup>, Neil J Loftus<sup>1</sup>  
<sup>1</sup>Shimadzu Co., Manchester, UK, <sup>2</sup>University of Bath, Bath, UK

### PTh-133 Degradation of Pentachlorobenzene by Fungi Screened from Nature

11:10 – 12:20  
Ajeng A Sari<sup>1</sup>, Sanro Tachibana<sup>2</sup>, Kazutaka Itoh<sup>2</sup>  
<sup>1</sup>The United Graduate School of Agriculture Sciences, Ehime University, Matsuyama, Japan, <sup>2</sup>Department of Applied Bioscience, Faculty of Agriculture, Ehime University

### PTh-134 Analysis of thermal products of chlorpyrifos using LC/FTMS

13:30 – 14:40  
Yoshinari Yamoto<sup>1</sup>, Takanori Sakiyama<sup>2</sup>, Hideya Kawasaki<sup>1</sup>, Ryuichi Arakawa<sup>1</sup>, Takeshi Nakano<sup>3</sup>  
<sup>1</sup>Kansai University, Osaka, Japan, <sup>2</sup>Osaka City Institute of Public Health and Env. Sciences, Osaka, Japan, <sup>3</sup>Osaka University, Osaka, Japan

### PTh-135 Behavior of Hexabromocyclododecane (HBCD) stereoisomers in water, sediment, and biological samples.

11:10 – 12:20  
Hitomi Hasegawa<sup>1,2</sup>, Masatoshi Watanabe<sup>1</sup>, Shigeru Suzuki<sup>2</sup>  
<sup>1</sup>Nagoya City Env.Sci.Res.Inst., Nagoya, Japan, <sup>2</sup>Chubu University, Kasugai, Japan

### PTh-136 LC/MS/MS determination of hair-dye ingredients in products, water and urine: estimation of human exposure and environmental release.

13:30 – 14:40  
Mari Takazawa, Shigeru Suzuki  
CHUBU University,Aichi,Japan

### PTh-137 Qualitative analysis of waste leachate by using exact mass of LC/Q-ToFMS/MS

11:10 – 12:20  
Akira Murakami<sup>1</sup>, Shigeru Suzuki<sup>1</sup>, Masahiko Takino<sup>2</sup>  
<sup>1</sup>CHUBU University,Aichi,Japan, <sup>2</sup>Agilent Technologies,Tokyo,Japan

### PTh-138 Investigation of Perfluorinated compounds in Osaka-bay over past three years

13:30 – 14:40  
Shusuke Takemine<sup>1,2</sup>, Chisato Matsumura<sup>1</sup>, Katsuya Yamamoto<sup>1</sup>, Masahiro Tsurukawa<sup>1,2</sup>, Takeshi Nakano<sup>2</sup>, Akira Kondo<sup>2</sup>  
<sup>1</sup>Hyogo Prefectural Institute of Environmental Sciences, Kobe, Japan, <sup>2</sup>Graduate School of Engineering Osaka University, Osaka, Japan

### PTh-139 Computational Chemistry Study on Negative Ion Chemical Ionization Mechanism of Peroxyacetyl Nitrate

11:10 – 12:20  
Yasuyuki ITANO<sup>1</sup>, Mamoru SAKAI<sup>1</sup>, Yasuhiro SADANAGA<sup>2</sup>, Hiroshi BANDOW<sup>2</sup>

<sup>1</sup>Osaka City Institute of Public Health and Environmental Sciences, Osaka, Japan, <sup>2</sup>Osaka Prefecture University, Sakai, Japan

### PTh-140 Analysis of inadvertent PCBs contained in consumer goods

13:30 – 14:40  
Masanobu Yokota<sup>1</sup>, Akiko Sawada<sup>1</sup>, Yoshikuni Deguchi<sup>1</sup>, Takeshi Nakano<sup>2</sup>

<sup>1</sup>Kaneka Techno Research Corporation, Hyogo, Japan, <sup>2</sup>Osaka University, Osaka, Japan

### PTh-141 Method development for simultaneous analysis of hydroxylated polychlorinated biphenyl by GC-ECNI/MS in biota sample

11:10 – 12:20  
Eguchi Akifumi<sup>1</sup>, Nomiyama Kei<sup>1</sup>, Katsuhiro Nakagawa<sup>2</sup>, Tanaka Kouki<sup>2</sup>, Miyagawa Haruhiko<sup>2</sup>, Tanabe Shunsuke<sup>1</sup>  
<sup>1</sup>Center for Marine Environmental Studies (CMES), Ehime University, Matsuyama, Japan, <sup>2</sup>Shimadzu Corporation, Japan

### PTh-142 Suspended solid as a disturbance of PFOS analysis in case of wastewater

13:30 – 14:40  
Hitomi Oka<sup>1</sup>, Akiko Sawada<sup>1</sup>, Yoshikuni Deguchi<sup>1</sup>, Takeshi Nakano<sup>2</sup>

<sup>1</sup>Kaneka Techno Research Corporation, Hyogo, Japan, <sup>2</sup>Osaka University, Osaka, Japan

### PTh-143 Analysis of Metabolites emitted by Soil-Derived Fungi using Ion Mobility Spectrometry based on GC/MS Data Analysis

11:10 – 12:20  
Shoko Ichii<sup>1</sup>, Tomoko Kimura<sup>2</sup>, Haruna Tanaka<sup>1</sup>, Sachio Kaneko<sup>3</sup>, Yoko Kiuchi<sup>3</sup>, Takahito Suzuki<sup>4</sup>, Toshiki Sugai<sup>5</sup>, Takae Takeuchi<sup>1,6</sup>

<sup>1</sup>Department of Chemistry, Graduate School of Humanities and Sciences, Nara Women's University, Nara, Japan, <sup>2</sup>Department of Chemistry, Faculty of Science, Nara Women's University, Nara, Japan, <sup>3</sup>Department of Biological Science, Graduate School of Humanities and Sciences, Nara Women's University, Nara, Japan, <sup>4</sup>Department of Biological Science, Faculty of Science, Nara Women's University, Nara, Japan, <sup>5</sup>Department of Chemistry, Faculty of Science, Toho University, Funabashi, Chiba, Japan, <sup>6</sup>National Institute of Advanced Industrial Science and Technology (AIST), Osaka Japan

### PTh-144 Measurement of brominated flame retardants in the environment near factories by LC/MS/MS.

13:30 – 14:40  
Itaru Oue, Shigeru Suzuki  
CHUBU University,Aichi,Japan

### PTh-145 Determination of sulfonamides and tetracyclines in livestock wastewater using hybrid ion trap - time of flight mass spectrometer

11:10 – 12:20  
Youngmin Hong<sup>1</sup>, Hyunook Kim<sup>2</sup>

<sup>1</sup>Dong-il Shimadzu Corp., Seoul, Korea, <sup>2</sup>Department of Energy & Environmental System Engineering, The University of Seoul, Seoul, Korea

## Thursday, 20<sup>th</sup> September

**PTh-146** Dechlorane Plus, a highly chlorinated flame retardant in Japanese environment samples.  
13:30 – 14:40

Takanori Sakiyama<sup>1</sup>, Takeshi Nakano<sup>2</sup>

<sup>1</sup>Osaka City Institute of Public Health and Environmental Sciences, Osaka, Japan, <sup>2</sup>Osaka University, Osaka, Japan

**PTh-147** Multi-residue method for rapid screening of veterinary drugs in muscle matrices by UHPLC-MS/MS  
11:10 – 12:20

Youngmin Hong<sup>1</sup>, Sujeong Park<sup>2</sup>, Insun Lee<sup>1</sup>, Minhye Lee<sup>1</sup>

<sup>1</sup>Dong-il Shimadzu Corp., Seoul, Korea, <sup>2</sup>Animal, Plant and Fisheries Quarantine and Inspection Agency, Seoul, Korea

**PTh-148** Development of LC-MS/MS method to monitor pharmaceuticals in environmental wastewater  
13:30 – 14:40

Youngmin Hong, Insun Lee, Minhye Lee

Dongil Shimadzu, Seoul, Korea

**PTh-149** Analysis of Ultraviolet Absorbers in Urine Samples by Functionalized Nanomaterial-assisted Electrospray Mass Spectrometry  
11:10 – 12:20

Tzung-Jie Yang, Maw-Rong Lee

National Chung Hsing university, Taichung, Taiwan

**PTh-150** Determination of diuretics in urine using immobilized-multiwalled carbon nanotubes hollow fiber liquid-phase microextraction combined with liquid chromatography-mass spectrometry  
13:30 – 14:40

Tse-Tsung Ho, Maw-Rong Lee

National Chung Hsing university, Taichung, Taiwan

**PTh-151** In-line preconcentration capillary electrophoresis-electrospray ionization-mass spectrometry for the analysis of haloacetic acids in tap water  
11:10 – 12:20

Sih-Hua Hung, Guor-Rong Her

National Taiwan University, Taipei, Taiwan(R.O.C)

**PTh-152** Effects of silver on Chlamydomonas reinhardtii; insights from proteome analysis and physiological endpoints  
13:30 – 14:40

Marc J Suter, Smitha Pillai, Holger Nestler, Rene Schoenenberger, Renata Behra, Kristin Schirmer Eawag, Dubendorf, Switzerland

**PTh-154** on-site analysis of gases emitted from soils using MULTUM-S II  
13:30 – 14:40

Takahiro Anan<sup>1</sup>, Shuichi Shimma<sup>2</sup>, Yo Toma<sup>3</sup>, Yasuyuki Hashidoko<sup>4</sup>, Ryusuke Hatano<sup>4</sup>, Morio Ishihara<sup>1</sup>, Jun Aoki<sup>1</sup>, Michisato Toyoda<sup>1</sup>

<sup>1</sup>Osaka University,Osaka,Japan, <sup>2</sup>National Cancer Center Research Institute, Tokyo, Japan, <sup>3</sup>Ehime University, Ehime, Japan, <sup>4</sup>Hokkaido University, Hokkaido, Japan

**PTh-155** Level of Dechlorane Plus in ambient air and development of monitoring method  
11:10 – 12:20

Koichiro MATSUMOTO<sup>1</sup>, Yuko ODASHIMA<sup>1</sup>, Yuji KASHIMA<sup>1</sup>, Takanori SAKIYAMA<sup>2</sup>, Takeshi NAKANO<sup>3</sup>

<sup>1</sup>Japan Environmental Sanitation Center, Kanagawa, Japan, <sup>2</sup>Osaka City Institute of Public Health and Environmental Sciences, Osaka, Japan,

<sup>3</sup>Graduate School of Engineering, Osaka University, Osaka, Japan

**PTh-156** Determination of hydroxylated polycyclic aromatic hydrocarbons in mariner's urine by high performance liquid chromatography-tandem mass spectrometry  
13:30 – 14:40

Tetsuya Hirai<sup>1,2</sup>, Hiroaki Kinoshita<sup>1</sup>, Hideo Okamura<sup>2</sup>, Yoshiji Yano<sup>2</sup>, Takeshi Nakano<sup>2</sup>

<sup>1</sup>Otsuka Pharmaceutical Co., Tokushima, Japan, <sup>2</sup>Graduate School of Maritime Sciences Kobe University, Kobe, Japan

**PTh-157** Thermal solid phase extraction for GC-MS analysis of complex samples  
11:10 – 12:20

Vivi Kofoed-Soerensen, Asger W Noergaard, Peder Wolkoff, Per Axel Clausen

National Research Centre for the Working Environment (NRCWE)

**PTh-158** Organic coatings of engineered nanomaterials characterized by mass spectrometry  
13:30 – 14:40

Per Axel Clausen, Renie Birkedal, Vivi Kofoed-Sorensen, Asger W Norgaard, Keld A Jensen

National Research Centre for the Working Environment, Denmark (pac@nrcwe.dk)

**PTh-159** Simultaneous determination of cationic and anionic compounds using a high-speed polarity switching ESI and an online-SPE LC-MS/MS  
11:10 – 12:20

Shoji F Nakayama<sup>1</sup>, Yayoi Suzuki<sup>1</sup>, Tairo Ogura<sup>2</sup>, Ichiro Hirano<sup>2</sup>, Mitsuha Yoshikane<sup>3</sup>

<sup>1</sup>National Institute for Environmental Studies, Tsukuba, Japan, <sup>2</sup>Shimadzu Corporation, Kyoto, Japan, <sup>3</sup>The University of Tokyo, Kashiwanoha, Japan

**PTh-160** The analysis of olefine and aromatic hydrocarbon in hydrocarbon mixture using Multi-Dimensional GC/GCMS system  
13:30 – 14:40

LiBin Liu, GuiXiang Yang, TaoHong Huang, Lei Cao  
Shimadzu Co.,Beijing, China

**PTh-161** A Novel Sensing Material for Iron(III) Ions based on Poly (gamma-Glutamic acid)-grafted-3,4-dihydro-3'-ethylhydroxyl-6-methyl-1,3,2H-benzoxazine  
11:10 – 12:20

Nuorn Choothong<sup>1</sup>, Attaphon Kaewvilai<sup>1</sup>, Apirat Laobuthee<sup>1,2</sup>, Amornrat Lertworasirikul<sup>1,2</sup>

<sup>1</sup>Kasetsart University, Bangkok, Thailand, <sup>2</sup>Center of Advanced Studies in Industrial Technology, Faculty of Engineering, Kasetsart University

## Thursday, 20<sup>th</sup> September

**PTh-162 Analysis of perfluorinated compounds in sediment samples from wastewater canal of Pancevo industrial area, Serbia**

13:30 – 14:40  
 Vladimir P Beskoski<sup>1</sup>, Shuusuke Takemine<sup>2</sup>, Takeshi Nakano<sup>3</sup>, Latinka Slavkovic-Beskoski<sup>4</sup>, Gordana Gojic-Cvijovic<sup>1</sup>, Mila Ilic<sup>1</sup>, Srdjan Miletic<sup>1</sup>, Miroslav M Vrvić<sup>1,5</sup>

<sup>1</sup>Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia, <sup>2</sup>Hyogo Prefectural Institute of Environmental Science, Kobe, Japan,

<sup>3</sup>Center for Advanced Science and Innovation, Osaka University, Japan,

<sup>4</sup>Institute of Nuclear Sciences, <sup>5</sup>Faculty of Chemistry, University of Belgrade, Serbia

**PTh-163 Study of On-site sampling method for Dioxin in water with high concentrations of suspended solids.**

11:10 – 12:20  
 Takeshi Enomoto<sup>1</sup>, Miho Okimoto<sup>1</sup>, Chuanpit Boonyoy<sup>2</sup>, Areerat Jaksakul<sup>2</sup>, Ruchaya Boonyatumanond<sup>2</sup>, Genta Takahashi<sup>5</sup>, Kenji Tawara<sup>5</sup>, Tohru Matsumura<sup>3</sup>, Takeshi Nakano<sup>4</sup>

<sup>1</sup>JEOL Ltd., Tokyo, Japan, <sup>2</sup>ERTC, Pathumthani, Thailand, <sup>3</sup>IDEA Consultant Inc., Shizuoka, Japan, <sup>4</sup>Osaka University, Osaka, Japan, <sup>5</sup>Hyogo Environmental Advancement Association, Kobe, Japan

**PTh-164 Multi-residue analysis of pesticides in animal and fishery products, and their processed foods by dual-column GC-MS/MS**

13:30 – 14:40  
 Eiji Ueno, Haruka Ohno, Minae Watanabe, Harumi Oshima, Eiichi Mikami  
 Aichi Prefectural Institute of Public Health, Nagoya, Japan

**PTh-165 Simultaneous analysis of cationic, anionic and neutral surfactants from different matrices using LCMS/MS.**

11:10 – 12:20  
 Rashi Kochhar<sup>1</sup>, Shruti Raju<sup>1</sup>, Deepthi Bhandarkar<sup>1</sup>, Bhairavi Saraf<sup>1</sup>, Shailendra Rane<sup>1</sup>, Jitendra Kelkar<sup>1</sup>, Ajit Datar<sup>1</sup>, Zhaoqi Zhan<sup>2</sup>

<sup>1</sup>Shimadzu Analytical (India) Pvt.Ltd., Mumbai, India, <sup>2</sup>Shimadzu Asia Pacific Pte.Ltd.

## Food safety

**PTh-166 Detection of Melamine in Human Renal Uric Acid Stone by Matrix-Assisted Laser Desorption / Ionization Time-Of-Flight Mass Spectrometry (MALDI-TOF MS)**

13:30 – 14:40  
 Chia-Fang Wu<sup>1</sup>, Chia-Chu Liu<sup>2,3,4,5</sup>, Jentae Shiea<sup>6</sup>, Yi-Tzu Cho<sup>7</sup>, Yii-Her Chou<sup>2,3</sup>, Bai-Hsiun Chen<sup>8</sup>, Chao-Yi Chien<sup>1</sup>, Shu-Pin Huang<sup>2,3</sup>, Wen-Jeng Wu<sup>2,3,9</sup>, Jung-Tsung Shen<sup>9</sup>, Mei-Yu Chang<sup>9</sup>, Chun-Hsiung Huang<sup>2,3</sup>, Ai-Wen Chang<sup>2</sup>, Ming-Tsang Wu<sup>\*1,4,10,11</sup>

<sup>1</sup>Department of Public Health, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>2</sup>Department of Urology, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>3</sup>Department of Urology, Faculty of Medicine, College of Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>4</sup>Graduate Institute of Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>5</sup>Pingtung Hospital, Department of Health, Executive Yuan, Pingtung, Taiwan, <sup>6</sup>Department of Chemistry, National Sun Yat-Sen University, Kaohsiung, Taiwan, <sup>7</sup>Department of Cosmetic Applications and Management, Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan, <sup>8</sup>Department of Laboratory Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan, <sup>9</sup>Department of Urology, Kaohsiung Municipal Hsiao-Kang Hospital, Kaohsiung, Taiwan, <sup>10</sup>Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan, <sup>11</sup>Center of Environmental and Occupational Medicine, Kaohsiung Municipal Hsiao-Kang Hospital, Kaohsiung, Taiwan

**PTh-167 Urinary oxidative metabolites of di(2-ethylhexyl)phthalate can predict the daily intake of phthalate-tainted foods in Taiwanese children**

11:10 – 12:20  
 I-Chen Wu<sup>1</sup>, Chia-Fang Wu<sup>2</sup>, Jentae Shiea<sup>3</sup>, Bai-Hsiun Chen<sup>4</sup>, Jiunn-Ren Wu<sup>5</sup>, Ming-Tsang Wu<sup>\*2,6,7</sup>

<sup>1</sup>Division of Gastroenterology, Department of Internal Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan, <sup>2</sup>Department of Public Health, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>3</sup>Department of Chemistry, National Sun Yat-Sen University, Kaohsiung, Taiwan, <sup>4</sup>Department of Laboratory Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>5</sup>Department of Pediatrics, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan, <sup>6</sup>Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan, <sup>7</sup>Center of Environmental and Occupational Medicine, Kaohsiung Municipal Hsiao-Kang Hospital, Kaohsiung, Taiwan

**PTh-168 LC-MS analysis of neonicotinoid insecticides in the crops using a novel selective solid-phase extractant having dipole type functional group**

13:30 – 14:40  
 Toshio Miwa<sup>1</sup>, Isao Saito<sup>1</sup>, Atsushi Yamamoto<sup>1</sup>, Yoshinori Inoue<sup>2</sup>, Mitsuru Saito<sup>2</sup>

<sup>1</sup>Chubu University, Aichi, Japan, <sup>2</sup>Nippon Filcon Co., Tokyo, Japan

**PTh-169 Studies on Residual Characteristics of Growth Regulator 6-BA in Bean Sprout**

11:10 – 12:20  
 Wan-Hee Seo, Young-Mo Jeong, Soon-Kil Cho, Bong-Suk Oh  
 Jeonnam Provincial Office, National Agricultural Products Quality Management Service, MIAFF, Korea

**PTh-170 Improvement of Determination Method for Pesticide Residues in Bean Sprout**

13:30 – 14:40  
 Soon-Kil Cho, Wan-Hee Seo, Young-Mo Jeong, Ji-Mi Cho  
 Jeonnam Provincial Office, National Agricultural Products Quality Management Service, MIAFF, Korea

**PTh-171 Screening of five mycotoxins by using immunoaffinity column and HPLC-orbitrapMS in processed foods**

11:10 – 12:20  
 Dong Sik Jeong, Seung Lim Baek, Dae Hyun Kim, Jong Ho Lee, Cheong-Tae Kim  
 NONGSHIM Co., LTD., Seoul, South Korea

**PTh-172 Simultaneous determination of melamine and its analogues in various processed foods using LTQ-orbitrap HRMS**

13:30 – 14:40  
 JONG HO LEE, DONGSIK JEONG, DAE HYUN KIM, CHEONG-TAE KIM  
 NONGSHIM Co., Ltd., Seoul, Korea

**PTh-174 Determination of DNA adducts originating from methyleugenol using isotope-dilution UPLC-ESI-MS/MS**

13:30 – 14:40  
 Wolfram Engst<sup>1</sup>, Kristin Herrmann<sup>1</sup>, Fabian Schumacher<sup>1</sup>, Simone Florian<sup>1</sup>, Klaus E Appel<sup>2</sup>, Hansruedi Glatt<sup>1</sup>

<sup>1</sup>German Institute of Human Nutrition Potsdam-Rehbrücke, Nuthetal, Germany, <sup>2</sup>Federal Institute for Risk Assessment, Berlin, Germany

Thursday, 20<sup>th</sup> September**PTh-175** Exploring the application of a universal method for pesticide screening in foods using a high data acquisition speed MS/MS

11:10 – 12:20 Hirano Ichiro<sup>1</sup>, Yuka Fujito<sup>2</sup>, Kiyomi Arakawa<sup>1</sup>, Yusuke Inohana<sup>1</sup>  
<sup>1</sup>Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>Shimadzu Analytical and Measuring Center Inc., Kyoto, Japan

**PTh-176** Multi-class pesticide analysis in challenging vegetable matrices using fast 5 msec MRM with 15 msec polarity switching

13:30 – 14:40 Yuka Fujito<sup>1</sup>, Yusuke Inohana<sup>2</sup>, Kiyomi Arakawa<sup>2</sup>, Hirano Ichiro<sup>2</sup>  
<sup>1</sup>Shimadzu Analytica & Measuring Center, Inc., Kyoto, Japan, <sup>2</sup>Shimadzu Co., Kyoto, Japan

**PTh-177** High Throuput Quantitative Analysis of Multi-mycotoxin in Beer-based Drinks using UHPLC-MS/MS

11:10 – 12:20 Masayoshi Tamura<sup>1</sup>, Keiko Matsumoto<sup>2</sup>, Jun Watanabe<sup>2</sup>,  
Junko Iida<sup>2</sup>, Yasushi Nagatomi<sup>1</sup>, Naoki Mochizuki<sup>1</sup>  
<sup>1</sup>Asahi Group Holdings, LTD., Ibaraki, Japan, <sup>2</sup>Shimadzu Co., Kyoto, Japan

**PTh-178** Molecular Imprinted Polymer@Magnetic Nanoparticles Combined with Liquid Chromatography Mass Spectrometry for Determination of Glycoalkaloids in Potato

Cheng-Hsin Yeh, Maw-Rong Lee  
National Chung Hsing University, Taichung, Taiwan

**PTh-179** Determination of cyromazine and melamine in chicken eggs by using QuEChERS coupled with liquid chromatography tandem mass spectrometry

11:10 – 12:20 Pei-Cheng Wang, Ren-Jye Lee, Chi-Chung Chou, Maw-Rong Lee  
National Chung Hsing University, Taichung, Taiwan

**PTh-180** DIFFERENTIATION OF FARMED FISH AND WILD SEAFISH USING ISOTOPIC SIGNATURES

13:30 – 14:40 Lian Jie Bay<sup>1</sup>, Jaime Wong<sup>1</sup>, Daniel Fliegel<sup>2</sup>,  
Sheot Harn Joanne Chan<sup>3</sup>, Thomas R Walczyk<sup>1</sup>  
<sup>1</sup>National University of Singapore, Singapore, <sup>2</sup>National Institute of Nutrition and Seafood Research, Bergen, Norway, <sup>3</sup>Health Sciences Authority, Singapore

**PTh-181** Evaluation of a new ion source to improve the limit of quantitation for chloramphenicol on a UHR-TOF

11:10 – 12:20 Karin Wendt, Thomas Zey, Amalia Apalategui,  
Carsten Baessmann, Peter Brechlin  
Bruker Daltonik GmbH, Bremen, Germany

**PTh-182** MASS SPECTROMETRY IDENTIFICATION AND CHARACTERIZATION OF GIBBERELLINES IN FRUITS

13:30 – 14:40 ENCARNACION MOYANO, GABINO BOLIVAR-SUBIRATS,  
HECTOR GALLART-AYALA, MARIA TERESA GALCERAN  
Barcelona University, Barcelona, Spain

**PTh-183** EVALUATION OF ATMOSPHERIC PRESSURE IONIZATION SOURCES FOR MASS SPECTROMETRIC ANALYSIS OF PHENICOL DRUGS

11:10 – 12:20 ELIDA ALECHAGA, ENCARNACION MOYANO,  
MARIA TERESA GALCERAN  
Barcelona University, Barcelona, Spain

**PTh-184** High-throughput simultaneous analysis of pesticide residues in food by supercritical fluid chromatography/tandem mass spectrometry

13:30 – 14:40 Megumi Ishibashi<sup>1</sup>, Ando Takashi<sup>2</sup>, Sakai Miho<sup>2</sup>,  
Matsubara Atsuki<sup>1</sup>, Uchikata Takato<sup>1</sup>, Fukusaki Eiichiro<sup>1</sup>,  
Bamba Takeshi<sup>1</sup>  
<sup>1</sup>Osaka University, Osaka, Japan, <sup>2</sup>Miyazaki Agricultural Research Institute, Miyazaki, Japan

**PTh-185** Chromatographic Separation of Chrysene and Triphenylene in Smoked Fish

11:10 – 12:20 Mirja L Hokkanen, Marika N Jestoi, Kimmo E Peltonen  
Finnish Food Safety Authority Evira, Helsinki, Finland

**PTh-186** Assessing the impact of a novel ion source design in food safety applications using MS/MS detection

13:30 – 14:40 Neil J Loftus<sup>1</sup>, Simon Hird<sup>2</sup>, David Baker<sup>1</sup>, Alan Barnes<sup>1</sup>  
<sup>1</sup>Shimadzu, Manchester, UK, <sup>2</sup>FERA, York, UK

**PTh-187** Development and applications of a pesticide multiresidue analysis turn-key system utilizing UHPLC-Orbitrap MS and post data processing

James Chang<sup>2</sup>, Jon Wong<sup>3</sup>, Kai Zhang<sup>3</sup>, Serei Thach<sup>4</sup>,  
Paul Yang<sup>4</sup>, Charles Yang<sup>2</sup>, Kristi Akervik<sup>2</sup>, Maciej Bromirski<sup>2</sup>,  
Yoko Yamagishi<sup>1</sup>, Dipankar Ghosh<sup>2</sup>  
<sup>1</sup>Thermo Fisher Scientific K.K., Yokohama, Japan, <sup>2</sup>ThermoFisher Scientific, San Jose, CA, <sup>3</sup>Food and Drug Administration, Center for Food Safety and Applied Nutrition, MD, <sup>4</sup>Ontario Ministry of the Environment, Ontario, Canada

**PTh-188** Multi-residue method for the confirmation of six avermectin residues in food products of animal origin by liquid-chromatogrphy tandem mass spectrometry

13:30 – 14:40 Myeong-Ae Kim, Jeong Woo Kang, Myung-Sin Lim,  
Young Hoon Bong, Chae-Mi Lim, Seoung-Wan Son  
Animal, Plant and Fisheries Quarantine and Inspection Agency, Anyang, Korea

**PTh-189** Multi-residue analysis of 59 pesticides in raw bovine milk using GC-MS/MS and UPLC-MS/MS

11:10 – 12:20 JinYoung Shin, Dong-Gyu Kim, Kyung Yuk Ko, MeeKyung Kim,  
Chae-Mi Lim, Seong-Wan Son  
Animal, Plant and Fisheries Quarantine and Inspection Agency, Anyang, Korea

## Thursday, 20<sup>th</sup> September

### Others

- PTh-190 Untargeted Plasma Metabolomics using <sup>13</sup>C-Glucose: Glycated-Metabolites as Novel Biomarkers for Aging and Diabetes**  
 13:30 – 14:40

Daiki Setoyama, Yoshinori Fujimura, Hiroyuki Wariishi,  
 Daisuke Miura  
 Kyushu University, Fukuoka, Japan

- PTh-191 The examination of high-throughput, high-sensitive and more-ecological measurement by micro flow UHPLC/MS/MS system**  
 11:10 – 12:20

Seiji Horie<sup>1</sup>, Kazuhide Inoue<sup>1</sup>, Masazumi Yasumoto<sup>1</sup>,  
 Kayoko Hagiwara<sup>2</sup>, Shigeru Yamada<sup>2</sup>, Yasutoshi Kawase<sup>1</sup>  
<sup>1</sup>TAKARA BIO INC., Shiga, Japan, <sup>2</sup>K.K. AB SCIEX, Tokyo, Japan

- PTh-192 Screening analysis for drugs of abuse by LC-MS/MS enables fast polarity switching MRM triggered product ion scanning on the fly**  
 13:30 – 14:40

Toshikazu Minohata<sup>1</sup>, Ichiro Hirano<sup>1</sup>, Junko Iida<sup>1</sup>, Keiko Kudo<sup>2</sup>,  
 Noriaki Ikeda<sup>2</sup>, Kei Zaitsu<sup>3</sup>, Noriaki Shima<sup>3</sup>, Munehiro Katagi<sup>3</sup>,  
 Hitoshi Tsuchihashi<sup>4</sup>, Koichi Suzuki<sup>4</sup>

<sup>1</sup>Shimadzu Co., Kyoto, Japan, <sup>2</sup>Kyushu University, Fukuoka, Japan, <sup>3</sup>Osaka  
 Prefectural Police, Osaka, Japan, <sup>4</sup>Osaka Medical Collage, Takatsuki, Japan

- PTh-193 HPLC method scouting system using ultra high performance liquid chromatography coupled to single quadrupole mass spectrometer**  
 11:10 – 12:20

Yusuke Inohana, Taku Tsukamoto, Hidetoshi Terada,  
 Kiyomi Arakawa, Ichiro Hirano  
 Shimadzu Co., Kyoto, Japan

- PTh-194 Detection of Emerging Legal Highs and Common Drugs of Abuse in Drug Seizures by Fast LC-MS/MS Method**  
 13:30 – 14:40

Kheng Aik Lim<sup>1</sup>, Yuan Yuan Cheryl Yeo<sup>1</sup>, Peiting Zeng<sup>2</sup>, Lijie Yu<sup>1</sup>,  
 Mei Ching Ong<sup>1</sup>, Tiong Whei Angeline Yap<sup>1</sup>

<sup>1</sup>Health Sciences Authority, Singapore, <sup>2</sup>Shimadzu (Asia Pacific) Pte Ltd,  
 Singapore

- PTh-195 Untargeted detection of novel abused substances using high-resolution time-of-flight mass spectrometry with comprehensive collision-induced dissociation**  
 11:10 – 12:20

Michiko Kanai<sup>1</sup>, Kevin Siek<sup>2</sup>, Joe Binkley<sup>2</sup>, Jeffrey S Patrick<sup>2</sup>,  
 David Alonso<sup>2</sup>

<sup>1</sup>LECO Japan Corporation, Tokyo, Japan, <sup>2</sup>LECO Corporation, MI, USA

- PTh-196 Identification of triazolam, etizolam and their metabolites by liquidchromatography tandem mass spectrometry**  
 13:30 – 14:40

Mayumi Matsui<sup>1</sup>, Toshikazu Minohata<sup>1</sup>, Noriko Shoji<sup>2</sup>,  
 Naohiro Kuriyama<sup>2</sup>, Chie Yokoyama<sup>2</sup>, Keiko Matsumoto<sup>1</sup>,  
 Jun Watanabe<sup>1</sup>, Junko Iida<sup>1</sup>

<sup>1</sup>Shimadzu Corporation, Kyoto, Japan, <sup>2</sup>YMC Co., LTD., Komatsu, JAPAN

- PTh-197 Determination of Prohibited Components in Hair Dyes by Solid Phase Extraction Coupled with Liquid Chromatography-Tandem Mass Spectrometry**  
 11:10 – 12:20

Chung-Yu Chen, Tsai-Jung Lin, Maw-Rong Lee  
 National Chung Hsing University, Taichung, Taiwan

- PTh-198 Doubly-Etched Microfabricated Gas Chromatography Columns for High Resolution Mass Spectrometry**  
 13:30 – 14:40

Sanggoo Kim, Sung Min Lim, Sejong Yong  
 Korea Basic Science Institute

- PTh-199 Coupling of Capillary Electrophoresis with Solvent Assisted Inlet Ionization-Mass Spectrometry Using a Poly(dimethylsiloxane)-based Sheath Liquid Interface**  
 11:10 – 12:20

Che-Wei Wang, Guor-Rong Her  
 National Taiwan University, Taipei, Taiwan

- PTh-200 The Development of a Sheathless CE/ESI-MS interface Based on Thin Conducting Liquid Film**  
 13:30 – 14:40

Ju-Li Huang, Ren-Yu Hsu, Guor-Rong Her  
 National Taiwan University, Taipei, Taiwan

- PTh-201 Proteome analysis with molecular simulation can reveal the TTR amyloidogenesis**  
 11:10 – 12:20

Kenji Miura<sup>1</sup>, Naoya Hatano<sup>1</sup>, Mika Ohta<sup>1</sup>, Hirotaka Sato<sup>2</sup>,  
 Aki Sugano<sup>1</sup>, Eiichi Maeda<sup>1</sup>, Yoshiyuki Sakaki<sup>3</sup>,  
 Ken-ichi Yamamura<sup>4</sup>, Yutaka Takaoka<sup>1</sup>

<sup>1</sup>Kobe University Graduate School of Medicine, Kobe, Japan, <sup>2</sup>Iwate Medical University School of Dentistry, Iwate, Japan, <sup>3</sup>Toyohashi University of Technology, Aichi, Japan, <sup>4</sup>Kumamoto University, Kumamoto, Japan

Friday, 21<sup>st</sup> September

Morning

## Plenary Lecture

08:00 – 08:45

Main Hall

## Plenary Lecture 5: Richard M Caprioli

Chair: Dominic M Desiderio

University of Tennessee Health Science Center, USA

**PL5-0800** Molecular Imaging of Tissues by Mass Spectrometry: Looking Beyond the Microscope

08:00 – 08:45

Richard M Caprioli

Vanderbilt University, Nashville, TN, USA

## Oral Session

09:00 – 11:00

Main Hall

**Session 41: Chemistries of Trapped Ions and their Applications to Bio- logical Mass Spectrometry**

Chair: Gavin E Reid

Michigan State University, USA

**S41-0900** [Keynote Lecture] Bioconjugation in the Gas Phase: New Chemistry for Tandem Mass Spectrometry

09:00 – 09:40

Scott A McLuckey

Purdue University

**S41-0940** Trap that Fat: Structure elucidation of ionized lipids by selective ion-molecule reactions and radical directed dissociationHuong T Pham<sup>1</sup>, Alan T Maccarone<sup>1</sup>, Tony Ly<sup>2</sup>, Adam J Trevitt<sup>1</sup>, Larry J Campbell<sup>3</sup>, Todd W Mitchell<sup>1</sup>, Stephen J Blanksby<sup>1</sup><sup>1</sup>University of Wollongong, Wollongong, Australia, <sup>2</sup>University of Dundee, UK,<sup>3</sup>AB Sciex, Concord, Canada**S41-1000** Harvesting High-Level Structural (Stereo- and Anomeric-) Information from Oligosaccharides with Single Sugar Resolution - A Tandem Mass Spectrometric Approach

10:00 – 10:20

Chiharu Konda<sup>1</sup>, Frank A Londry<sup>2</sup>, Brad Bendiak<sup>3</sup>, Yu Xia<sup>1</sup><sup>1</sup>Purdue University, West Lafayette, IN, USA, <sup>2</sup>AB Sciex, Concord, Ontario,<sup>3</sup>University of Colorado Denver, Aurora, CO , USA**S41-1020** Measurement of the Peptide Ion Temperature by Using N-Acylated Dipeptide Tags as Internal Standards

10:20 – 10:40

Seung Koo Shin, Jongcheol Seo, Min-Soo Suh, Hye-Joo Yoon

Pohang University of Schence and Technology, Pohang, Korea

**S41-1040** Gas phase reactions of trapped bioorganic ions

10:40 – 11:00

Gianluca GIORG

University of Siena

**Friday, 21<sup>st</sup> September**

**Morning**

## Oral Session

09:00 – 11:00

Room A

### Session 42: New Developments in Instruments and Detectors

Chair: **Takaya Sato**  
JEOL, Japan

- S42-0900** [Keynote Lecture] From supercomputer modeling to highest mass resolution in FT ICR  
09:00 – 09:40

Evgeny N Nikolaev<sup>1,2</sup>

<sup>1</sup>The Institute for energy problems of chemical physics Russian Academy of Sciences, <sup>2</sup>The Institute of biochemical physics Russian Academy of Sciences

- S42-0940** A New magnetic TOF Detector with 1.5 ns Pulse Width and Very High Dynamic Range  
09:40 – 10:00

Dick Stresau, Yair Benari, Kevin Hunter  
ETP Electron Multipliers, Melrose Park (Sydney), Australia

- S42-1000** Novel Compact Double Focusing Mass-Analyzer for Biochemical and Elemental Analysis.  
10:00 – 10:20

Viacheslav D Sachenko, L N Gall, R N Gall  
Institute for analytical Instrumentation of RAS

- S42-1020** Penning traps and ICR MS in physics research: From highly-charged atomic ions to metal-clusters to short-lived atomic nuclei  
10:20 – 10:40

Lutz Schweikhard  
University of Greifswald, Greifswald, Germany

- S42-1040** A multi-reflection time of flight mass spectrograph for short-lived nuclei and heavy molecules  
10:40 – 11:00

Peter Schury<sup>1</sup>, Michiharu Wada<sup>2</sup>, Yuuta Ito<sup>1,2</sup>, Sarah Naimi<sup>2</sup>, Hermann Wollnik<sup>3</sup>, Tetsu Sonoda<sup>2</sup>, Sousuke Nakamura<sup>1,2</sup>  
<sup>1</sup>Tsukuba University, Ibaraki, Japan, <sup>2</sup>RIKEN, Wako, Japan, <sup>3</sup>Geissen University, Geissen, Germany

## Oral Session

09:00 – 11:00

Room B-1

### Session 43: Novel Proteomics Methodologies

Chair: **Yasushi Ishihama**  
Kyoto University, Japan

- S43-0900** [Keynote Lecture] Shifting Proteomics from a Hypothesis Generating Workflow to a Hypothesis Testing Workflow  
09:00 – 09:40

Michael J MacCoss<sup>1</sup>, Jarrett Egertson<sup>1</sup>, Michael Bereman<sup>1</sup>,

Richard Johnson<sup>1</sup>, Christine C Wu<sup>2</sup>, Brendan MacLean<sup>1</sup>

<sup>1</sup>University of Washington, <sup>2</sup>University of Pittsburgh

- S43-0940** Profiling of Human Kinome Using In Vitro Kinase Assay in Combination with Quantitative Phosphoproteomics  
09:40 – 10:00

Naoyuki Sugiyama<sup>1</sup>, Masaki Gouda<sup>2</sup>, Haruna Imamura<sup>3</sup>,  
Masaru Tomita<sup>1</sup>, Yasushi Ishihama<sup>1,3</sup>

<sup>1</sup>Institute for Advanced Biosciences, Keio University, Tsuruoka, Japan, <sup>2</sup>Carna Biosciences, Inc., Kobe, Japan, <sup>3</sup>Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan

- S43-1000** In-depth analysis of human proteome by High Resolution Isoelectric Focusing (HirIEF)-LC-MS/MS  
10:00 – 10:20

Kie Kasuga, Rui M Branca, Henrik J Johansson, Janne Lehtiö  
Karolinska Institutet / Science for Life Laboratory, Stockholm, Sweden

- S43-1020** Enrichment of plasma membrane proteins using cationic nanoparticle pellicles  
10:20 – 10:40

Waeowalee Choksaengkarn<sup>1</sup>, Sung-Kyoung Kim<sup>1</sup>,  
Joe Cannon<sup>1</sup>, Nathan Edwards<sup>2</sup>, Sang Bok Lee<sup>1,3</sup>,  
Catherine Fenselau<sup>1</sup>

<sup>1</sup>Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742, United States, <sup>2</sup>Department of Biochemistry and Molecular & Cellular Biology, Georgetown University Medical Center, Washington, D. C. 20074, United States, <sup>3</sup>Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea

- S43-1040** Informatics-Assisted Label-free EDC-MRM Quantitation for Targeted Signaling Pathway Analysis  
10:40 – 11:00

Yi-Ting Wang<sup>2,3</sup>, Chia-Feng Tsai<sup>1,4</sup>, Pei-Yi Lin<sup>1</sup>, Hsin-Yi Wu<sup>1</sup>,  
Szu-Hua Pan<sup>5</sup>, Sung-Liang Yu<sup>5</sup>, Pan-Chyr Yang<sup>3,7</sup>, Yu-Ju Chen<sup>1,2,4</sup>

<sup>1</sup>Institute of Chemistry, Academia sinica, Taiwan, <sup>2</sup>Chemical Biology and Molecular Biophysics Program, Taiwan International Graduate Program, Institute of Chemistry, Academia Sinica, Taipei, Taiwan, <sup>3</sup>Institute of Biochemical Sciences, National Taiwan University, Taipei, Taiwan,

<sup>4</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan,

<sup>5</sup>Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan, <sup>6</sup>Institute of Biomedical Science, Academia Sinica, Taipei, Taiwan, <sup>7</sup>College of Medicine, National Taiwan University, Taipei, Taiwan

**Friday, 21<sup>st</sup> September**

**Morning**

## Oral Session

09:00 – 11:00

Room D

### Session 44: Ambient Ionization

Chair: Jentae Shiea

National Sun Yat-Sen University, Taiwan

**S44-0900 [Keynote Lecture] Ambient desorption/ionization mass spectrometry for minimal samples**

09:00 – 09:40 Kenzo Hiraoka<sup>1</sup>, Mridul K Mandal<sup>1</sup>, Lee C Chen<sup>1</sup>, Hideki Fujii<sup>2</sup>, Kentaro Yoshimura<sup>2</sup>, Sen Takeda<sup>2</sup>

<sup>1</sup>University of Yamanashi, Kofu, Japan, <sup>2</sup>University of Yamanashi, Chuo, Japan

**S44-0940 Advances in Ambient Ionization and Imaging using DART and Microplasma Ion Sources**

09:40 – 10:00 Facundo M Fernandez<sup>1</sup>, Joel Keelor<sup>1</sup>, Rachel Bennett<sup>1</sup>, Prabha Dwivedi<sup>1</sup>, Joshua Symonds<sup>2</sup>, Reuben Gann<sup>1</sup>, Thomas Orlando<sup>1,2</sup>

<sup>1</sup>Georgia Institute of Technology/School of Chemistry and Biochemistry, Atlanta, GA, USA, <sup>2</sup>Georgia Institute of Technology, School of Physics

**S44-1000 Monitoring intra- and inter-day human breath metabolic signatures supports the existence of individual phenotypes**

10:00 – 10:20 Pablo M-L Sinues<sup>1</sup>, Lukas Meier<sup>1</sup>, Christian Berchtold<sup>1</sup>, Noriane Sievi<sup>2</sup>, Giovanni Camen<sup>2</sup>, Malcolm Kohler<sup>2</sup>, Renato Zenobi<sup>1</sup>

<sup>1</sup>ETH, Zurich, Switzerland, <sup>2</sup>University Hospital Zurich, Zurich, Switzerland

**S44-1020 Alternative Desorption/Ionization Processes of Low-Temperature Plasma Probe Ambient Mass Spectrometry**

10:20 – 10:40 Joshua S Wiley, Jobin Cyriac, Jacob T Shelley, R Graham Cooks  
Purdue University, West Lafayette, IN, USA

**S44-1040 Analysis of Polar Components in Heavy Oils by Gas Chromatography Electrospray Ionization Mass Spectrometry (GC-ESI/MS) and Multivariate Analysis**

10:40 – 11:00 Chu-Nian Cheng<sup>1</sup>, Yi-Tzu Cho<sup>2</sup>, Hung Su<sup>1</sup>, Jentae Shiea<sup>1</sup>  
<sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan, <sup>2</sup>Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan

## Oral Session

09:00 – 11:00

Room E

### Session 45: Cell Biology / Cellular Pathways

Chair: Renato Zenobi

ETH Zurich, Switzerland

**S45-0900 [Keynote Lecture] Future of Cell Analyses and Mass Spectrometry**

09:00 – 09:40 Tsutomu Masujima

Hiroshima University, Hiroshima, Japan/RIKEN QBiC, Suita, Japan

**S45-0940 Telling the Biological Story - Post Processing of -Omics Data**

09:40 – 10:00 Michael Kohl<sup>1</sup>, Hagen Meckel<sup>1</sup>, Maike Ahrens<sup>1</sup>,

Helmut E Meyer<sup>1</sup>, Martin Hofmann-Apitius<sup>2</sup>, Martin Eisenacher<sup>1</sup>

<sup>1</sup>Medizinisches Proteom-Center, Ruhr University, Bochum, Germany,

<sup>2</sup>Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Sankt Augustin, Germany

**S45-1000 Realtime Molecular Analysis of Single Cell State by Fluorescence-assisted Live Single-cell Mass Spectrometry**

10:00 – 10:20 Naohiro Tsuyama<sup>1</sup>, Hajime Mizuno<sup>1</sup>, Takanori Harada<sup>1</sup>,

Sachiko Date<sup>2</sup>, Tsutomu Masujima<sup>1,2</sup>

<sup>1</sup>Hiroshima University Graduate School of Biomedical & Health Sciences, Hiroshima, Japan, <sup>2</sup>Quantitative Biology Center (QBiC), RIKEN, Osaka, Japan

**S45-1020 Multi-omics Approach to study the effect of rapamycin treatment on a human cell line**

10:20 – 10:40 Sudha Rajagopalan, Siji Joseph, Guha Nilanjan, Syed S Lateef, Yugandhar Reddy

Agilent Technologies India Pvt.Ltd

**S45-1040 Screening and identification of sulfur mustard metabolites from in vitro samples using different LC-MS experiments for new biomarker development**

10:40 – 11:00 Mia Halme<sup>1</sup>, Maija Pesonen<sup>2</sup>, Marja Hagström<sup>3</sup>,  
Markku Pasanen<sup>2</sup>, Paula Vanninen<sup>1</sup>

<sup>1</sup>VERIFIN, Department of Chemistry, University of Helsinki, Finland, <sup>2</sup>School of Pharmacy, Faculty of Health Sciences, University of Eastern Finland, Finland,

<sup>3</sup>Center of Drug Research, Faculty of Pharmacy, University of Helsinki, Finland

Friday, 21<sup>st</sup> September

Morning

**Plenary Lecture**

11:45 – 12:30

Main Hall

**Plenary Lecture 6: R Graham Cooks**Chair: Yoshinao Wada  
Osaka MCHRI, Japan**PL6-1145** Through a Glass Darkly: Glimpses into  
11:45 – 12:30 the Future of Mass SpectrometryR Graham Cooks  
Purdue University, West Lafayette, IN/USA

## Workshop

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**Monday, 17<sup>th</sup> September, 17:15-19:15**

**Workshop 1 (Room B-1):**

**Mass Spectrometry of Polymers and Industrial Materials**

Organizer: Hiroaki Sato

Scope of Session: Mass spectrometry is commonly used as a technique for the characterization of polymeric industrial materials. This session will discuss the recent progress in the structural characterization of polymers (especially for degraded materials) by advanced mass spectrometry such as high-resolution techniques and ion separation techniques.

Keywords: Structural characterization, High-resolution TOF, Ion mobility, Polymer degradation

**Workshop 2 (Room D):**

**Hydrogen/Deuterium Exchange Mass Spectrometry**

Organizers: Yoshitomo Hamuro, Rachel A Garlish

Scope of Session: Hydrogen/deuterium exchange mass spectrometry (HDX-MS) is an increasingly popular protein characterization method. This session covers both the application and new method development of HDX-MS. The application of HDX-MS includes higher order structure analysis, protein-ligand interaction, and protein-protein interaction, particularly epitope mapping. Method development includes opportunities for higher resolution analysis using ETD fragmentation, data generation automation, and data extracting software.

Keywords: Hydrogen/deuterium exchange, Higher order structure, Protein-ligand interaction, Protein-protein interaction, Epitope mapping, ETD fragmentation, Automation, Software

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**Tuesday, 18<sup>th</sup> September, 17:15-19:15**

**Workshop 3 (Room B-1):**

**Careers in Mass Spectrometry**

Organizer: Anthony W T Bristow

Chair: John Langley

Scope of Session: The session is designed to outline a variety of career paths that begin and stay within mass spectrometry and also expand beyond a starting point in mass spectrometry. Several international speakers will briefly describe their career paths (for example: academia, industry, instrument manufacturer). These short presentations will outline the choices made during career development, any challenges encountered and the opportunities available in the different career pathways. In addition, there will be a presentation that describes the current job market for people with a background in mass spectrometry and more broadly in analytical science. The workshop will be very interactive, and we actively encourage attendees to question the speakers about their careers and the choices made.

**Workshop 4 (Room D):****Mass++ and MassBank: Tools for Data Processing and Database on PC**

Organizers: Satoshi Tanaka, Takaaki Nishioka

Scope of Session: Mass++ (mass plus plus) is freeware for viewing and manipulating various types of mass spectrometric data. Mass++ 2.1.0, which was released recently, is easy to use as search engines such as Mascot and MassBank. MassBank is a public repository for sharing mass spectra of small molecules among research community. A bottleneck in metabolomics is to submit a large amount of mass spectra from LC-MS as the queries to database searches manually. Mass++ and MassBank projects have collaboratively developed a tool that relieves the users from the repeated manual works. Two projects will give tutorials of their tools.

Key words: Freeware, Proteomics, Metabolomics, Multi-vendor, Chemical identification

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**Wednesday, 19<sup>th</sup> September, 17:15-19:15****Workshop 5 (Room B-1):****Path to Next-generation IMS: New Concepts, Advanced Instrumentation, and Leveraging the Ion-molecule Chemistry**

Organizers: Toshiki Sugai, Alexandre A Shvartsburg

Scope of Session: Ion mobility separations coupled to mass spectrometry have become a mainstream analytical tool, and both conventional IMS and FAIMS are available in commercial systems now applied in various areas. This workshop will look beyond established products and methods into qualitatively new approaches that would take IMS to the next level. Topics of presentations and discussion will include multi-stage platforms of much greater specificity and peak capacity, use of ion-molecule chemistry to expand the separation space and modify resolution of specific targets, and various integrative measurements incorporating the IMS dimension.

**Workshop 6 (Room D):****Mass Spectrometry for Food Safety**

Organizer: Jentae Shiea

Scope of Session: Recent food incidents have drawn the public's awareness of how food supply is regulated and inspected to be deemed safe for consumption. The common food harmful substances include foodborne microorganisms, mycotoxins, chemical residues, pesticides, melamine, plasticizers, and chemical contaminants from food packaging and processing. Only trace amount of these harmful substances is sufficient to cause harmful health effects. Thus, mass spectrometry plays a critical role as an excellent analytical tool to identify food contaminants accurately and efficiently. This workshop explores the recent advances and application of mass spectrometry to food safety, and challenges in food sample preparation.

Keywords: Food safety, Mass spectrometry, Foodborne microorganisms, Mycotoxins, Chemical residues, Pesticides, Food packaging and processing

## The 3<sup>rd</sup> Asian-Oceanic Mass Spectrometry Conference (AOMSC-3)

Australian and New Zealand Society for Mass Spectrometry (ANZSMS)  
 Chinese Mass Spectrometry Society (CMSS)  
 Hong Kong Society of Mass Spectrometry (HKSMS)  
 Indian Society for Mass Spectrometry (ISMAS)  
 Korean Society for Mass Spectrometry (KSMS)  
 Mass Spectrometry Society of Japan (MSSJ)  
 Singapore Society for Mass Spectrometry (SSMS)  
 Taiwan Society for Mass Spectrometry (TSMS)

### Day 1 (Monday, 17<sup>th</sup> September) 17:15-19:15 (Room A)

#### **“OMICs and Biological Mass Spectrometry”**

Chair: Yu-Ju Chen (TSMS) / Tohru Yamagaki (MSSJ)

1	Top-down analysis of lipoproteins by on-line field-flow fractionation and ESI-MS-MS	Ki Hun Kim; Ju Yong Lee; <b>Myeong Hee Moon</b>	Korea
2	Serum metabolome analysis for early detection of colorectal cancer	Masaru Yoshida; Shin Nishiumi; Yoshihiro Izumi; Atsuki Matsubara; Takeshi Azuma	Japan
3	Identification of insect species by direct UV-laser desorption/ ionization mass spectrometry of cuticular lipids and pheromones	Jacqueline Chin; Qi Ling Koh; Joanne Yew	Singapore
4	Acylglycine: a potential biomarker for the clinical diagnosis of inborn metabolic disorders	Bonnie Fong; Sidney Tam; Kelvin Leung	Hong Kong
5	Caco-2 permeability studies as a new alternative model to bioequivalence and bioequivalent tests	Seval Korkmaz	Turkey
6	Clinical application of rapid bacterial identification using mass spectrometry	Kazuyuki Sogawa; Masaharu Watanabe; Fumio Nomura	Japan

### Day 2 (Tuesday, 18<sup>th</sup> September) 17:15-19:15 (Room A)

#### **“New Technologies”**

Chair: Myeong Hee Moon (KSMS) / Kanako Sekimoto (MSSJ)

1	Radiosensitizers investigated using electrospray ionization mass spectrometry	Linda Feketeova; Niels Bassler; Brita S Sørensen; Michael R Horsman; Jonathan White; Richard A J O'Hair	Australia
2	Combining quantum mechanical and MS analysis to understanding the source of H <sup>+</sup> during APPI of PAH dissolved in toluene	Arif Ahmed; Chell Ho Choi; Kim Sungwan	Korea
3	Application of high speed LC-MSMS technology towards unambiguous characterization of degraded products of Lenalidomide, an anticancer molecule	Janani Thyagarajan; Raman Palavannathan; Saravanan Subramanyam; Govindarajan Chandramohan; Mohan Kasi; Manohar Venkat	India
4	Sensitive ionization of non-volatile analytes using multiply charged primary ions in desorption electrospray ionization mass spectrometry	Zhiqiang Zhu; Qiliang Gong; Yafei Zhou; Ning Xu; Haiwei Gu; Huanwen Chen; Tenggao Zhu	China
5	Hydrocarbons analysis by desorption atmospheric pressure chemical ionization	Fred Paul mark Jjunju Jjunju; Badu_Tawiah K Abraham; Li Anyin; Roqan S Iman; Graham R Cooks	Saudi Arabia
6	Miniaturized peptide sample pretreatment platform for indirect spray analysis	Hoi Sze Yeung; Tak-Wah Dominic Chan	Hong Kong
7	Large bio-particle detection technologies and their applications	Chung Hsuan Chen	Taiwan

## Pre-Conference Programme

### Mass Spectrometry Summer School 2012

The Kansai-area colloquium in Mass Spectrometry Society of Japan (MSSJ) will take place a mass spectrometry summer school for students and young scientists as a joint workshop of the 19<sup>th</sup> IMSC. The purpose of the workshop is to make research colleagues among young scientists in several countries. This summer school will be mainly composed of group discussion and free discussion. The venue place, Koyasan (Mount Koya), is the center of Shingon Buddhism, an important Buddhist sect which was introduced to Japan in 805 by Kobo Daishi. In the 1200-years history and UNESCO World Cultural Heritage Sites, participants will enjoy scientific discussion with touching Japanese culture. Through this opportunity, the collaboration in the young generation in mass spectrometry will be closely united.

The details of the summer school are as follows:

Date: 13<sup>th</sup> – 14<sup>th</sup> September

Venue: Ekoin temple (497 Koyasan, Koya-cho, Ito-gun, Wakayama, Japan)

Number of participants: 60

Finally, this summer school is financially supported by MSSJ, 19<sup>th</sup> IMSC and Kato Biomedical Memorial Foundation. The organizer would like to thank for these supports.

### Short Course

#### Fundamentals of Mass Spectrometry

Instructor: O David Sparkman, Pacific Mass Spectrometry Facility, Chemistry Department, College of the Pacific, University of the Pacific, Stockton, CA USA  
Jürgen Gross, Org.-Chem. Inst. der Universität, Heidelberg, Germany

Schedule: Saturday, 15<sup>th</sup> September, 10:00 – 17:00

Sunday, 16<sup>th</sup> September, 10:00 – 15:00

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 LIFDI), electrospray ionization (ESI), and matrix-assisted laser desorption/ionization (MALDI) will be included.

**Fragmentation Methods, Their Fundamentals and Application in Proteomics**

Instructor: Professor Roman A Zubarev, Karolinska Institutet, Stockholm, Sweden

Schedule: Saturday, 15<sup>th</sup> September, 10:00 – 17:00

Fragmentation of biomolecules in tandem mass spectrometry is the basis for structure identification of polypeptides, which is a cornerstone of proteomics. The excitation methods for fragmentation fall into three categories: slow or rapid heating, electronic excitation, and radical initiation. What happens to a peptide when it is excited by one of the three methods? What makes the bond break and the molecule fall apart? Why do negative ions fragment differently than positive ions? How fast does bond rupture happen and how much energy is required? The answer to these questions will be given during the course. Collisional dissociation in an ion trap or by infrared irradiation (slow heating), collisions in a qTOF or Orbitrap instrument (rapid heating), ultraviolet dissociation (electronic excitation), electron capture/transfer dissociation and electron ionization dissociation (radical initiation) will be discussed. On a practical note, real-life examples of peptide fragmentation will be considered, MS/MS spectra explained, and de novo sequencing illustrated. Analysis of peptide modifications will also be considered in detail.

**Introduction to Imaging Mass Spectrometry**

Instructor: Mitsutoshi Setou, Hamamatsu University School of Medicine, Hamamatsu, Shizuoka, Japan

Schedule: Saturday, 15<sup>th</sup> September, 10:00 – 17:00

Matrix-assisted laser desorption/ionization (MALDI)-imaging mass spectrometry (IMS) is emerging as a powerful tool for investigating the distribution of molecules, such as proteins and metabolites, within biological systems through the direct analysis of thin tissue sections. Unique among imaging methods, MALDI-IMS can determine the distribution of hundreds of unknown compounds in a single measurement and identify the molecules on tissue sections. Recently, Mass Microscopes were introduced to the research community, enabling us to detect conventional molecules in tissue structures by optical microscopes with an objective lens, as well as volatile ones using an atmospheric ion source chamber. Altogether, this offers the opportunity to visualize molecular distributions with more high-spatial resolution by the minimum laser diameter (< 10 μm) and identify them from their individual fragmentation patterns. Moreover, our group together with the Japanese foundation for cancer research have developed an analyzing software for IMS datasets. Using this software, we can easily extract meaningful signals based on common and/or specific expressions from enormous IMS datasets. This course covers the fundamental principal and techniques of MALDI-IMS, assuming no previous experience in IMS or basic mass spectrometry. The following topics are covered: introduction to principles and applications of IMS technology, such as making tissue sections, applying matrices onto tissue sections, acquiring IMS datasets from tissue sections, creating ion images from the IMS dataset, and statistical analyses of data.

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**Open Lecture for General Public (in Japanese)**

The Conference co-chair Koichi Tanaka will deliver a lecture to high school & university students and young researchers on science, technology and study. (pre-registration required)

Schedule: Saturday, 15<sup>th</sup> September, 14:00 – 16:00

Venue: Main Hall, ICC Kyoto

## Users' Day

AB SCIEX	Room A	Saturday, 15 <sup>th</sup> September	10:00-17:00
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- 10:00 Registration  
10:30-12:10 Seminar sessions  
12:30-16:00 "Kyoto experience with AB SCIEX"  
Leave the venue for Kyoto downtown by bus for Lunch & Attraction

Shimadzu	Room A	Sunday, 16 <sup>th</sup> September	10:00-15:00
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- 10:30 Biological Profiling: Complementary Qualitative and Quantitative Analysis using IT-TOF and QQQ Mass Spectrometry  
Kevin Schug, Department of Chemistry & Biochemistry, University of Texas at Arlington, U.S.A  
11:25 Top-down Proteomics using MALDI ISD and MS<sup>n</sup>  
Daniel Lafitte, University Aix-Marseille, France  
12:10 GC×GC-qMS with chemical ionization for highly specific, sensitive, and quantitative steroids  
J Thomas Brenna, Professor, Cornell University, U.S.A  
12:40 Serum Metabolome Analysis for Early Detection of Colorectal Cancer  
Masaru Yoshida, Chief, Division of Metabolomics Research, Kobe University Graduate School of Medicine, Japan

The registration will open from 9:00AM and the Users' Day starts from 10:00AM. Some other presentations are planned.

The presentations will last until 13:15 and then we will host a lunch event featuring buffet style food and drinks from

13:30 in the Gold Room, Grand Prince Hotel Kyoto, close to the congress location. We also encourage you to enjoy Japanese traditional attractions with us!

## Company Luncheon Seminars

### AB SCIEX

**Monday, 17<sup>th</sup> September 12:20-13:30 Room A**

Moderator: Mark Cafazzo (AB SCIEX)

**Advancing technologies and workflow solutions for successful lipidomics research and identification and quantitation of lipid species**

Prof. Stephen Blanksby (University of Wollongong, Wollongong, Australia)

Fadi Abdi (AB SCIEX)

This luncheon seminar will focus on the use of innovative mass spec technologies and workflow solutions for lipidomics research and qualitative and quantitative studies of lipid species.

**Tuesday, 18<sup>th</sup> September 12:20-13:30 Room A**

Moderator: Johnny Cardenas (AB SCIEX)

**Transformative MS-Technologies and Workflows for Biotherapeutics**

Gary Impey (AB SCIEX)

Byung-Hee Shin (AB SCIEX, Korea)

This luncheon seminar will focus on the use of innovative mass spectrometry technologies and workflow solutions for biotherapeutics applications and bioanalytical quantitation analysis.

**Wednesday, 19<sup>th</sup> September 12:20-13:30 Room A**

Moderator: Fabienne Le Floch (AB SCIEX)

**New technologies and workflows to enhance General Unknown Screening applications for food, environmental, or toxicological testing**

Lauryn Bailey (AB SCIEX)

Janna Anichina (AB SCIEX)

This luncheon seminar will present innovative mass spectrometry technologies and software enhancing general unknown screening workflows for use in food safety testing, environmental analysis and forensic toxicology applications.

**Thursday, 20<sup>th</sup> September 12:20-13:30 Room A**

Moderator: Mark Cafazzo (AB SCIEX)

**Pushing the limits of global quantitative strategies for Proteomics**

Prof. Rudolf Aebersold (ETH Zurich, Zurich, Switzerland)

Sean L. Seymour (AB SCIEX)

This luncheon seminar will focus on the use of innovative mass spectrometry technologies and workflow solutions for proteomics and biomarker research including MS/MS/ALL with SWATH™ Acquisition strategy.

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**Advion****Tuesday, 18<sup>th</sup> September 12:20-13:30 Room E**

Moderator: Daniel Eikel, Ph.D.

**Chip-based Nanoelectrospray Seminar**

Dr. Ryo Taguchi, Dr. Zoltan Takats, Dr. Kim Ekroos, Dr. Daniel Eikel

IMSC Meeting attendees are invited to attend Advion's Luncheon to be held on 18 September. Leading scientists present their work with Advion's chip-based nanoelectrospray ion source technology. In addition, a new chip-based nanoelectrospray ion source will be introduced at the meeting.

Moderated by Advion's Product Manager, Daniel Eikel, Ph.D., the meeting includes brief presentations that highlight the key aspects of work being conducted in lipids analysis, metabolomics, liquid extraction analysis, and proteomics.

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**Agilent Technologies****Monday, 17<sup>th</sup> September 12:20-13:30 Room E**

Moderator: Maryann Shen, Ph.D.

**(1) Novel Approaches for Phosphoprotein Analysis using ICP-QQQ**

Amir Liba Ph.D. (Agilent Technologies)

**(2) High Sensitivity Protein Identification from a pathway perspective**

Keith Waddell (Agilent Technologies)

This workshop will focus on new technology that can be brought to bear in the field of proteomics.

The new ICP-triple quadrupole mass spectrometer from Agilent allows low level analysis of phosphopeptides to help identify where in chromatograms the phospho groups are. The technology involving the filtering of oxygen adducts on the phosphorus element through the Q3 region has enabled low level detection in the same sensitivity range that would normally be expected on a LC/MS set up for phosphopeptide analysis. This offers possibilities for absolute quantitation and avoidance of the use of radioactive <sup>32</sup>P.

The new ion funnel based Q-TOF LC/MS/MS system allows a deeper level of protein identification. Combined with new HPLC-Chip based technology and improved data dependent software this technology has now been used to enable linkage of protein ID to protein, metabolite and gene pathway analysis. The combination of transcriptomics, metabolomics and proteomics allows true integrated biology.

**Wednesday, 19<sup>th</sup> September 12:20-13:30 Room E**

Moderator: Maryann Shen, Ph.D.

**1) Recent Advances of Plant Metabolomics Based on Mass Spectrometry**

Kazuki Saito, Ph.D. (Riken Plant Science Center)

Metabolomics plays a major role in plant functional genomics and biotechnology. We have established an excellent analytical platform of plant metabolome based on the combination of multiple mass spectrometers. This presentation will describe the recent development of cutting-edge metabolomics technology and successful application in plant functional genomics and crop biotechnology.

## 2) Advances in Instrumentation and Software: Data Directed Multi-Omics Mining of Biological Pathways

Theodore Sana, Ph.D. (Agilent Technologies)

The field of Metabolomics requires rigorous statistical analysis and confident identification of metabolites. This session will also explore the use of transcriptomics, proteomics and metabolomics to elucidate an integrated biology approach to determine biological changes in disease systems. Pathway analysis software has enabled a viewing of the changes in metabolites from a pathway perspective rather than from just a metabolite perspective. This integrated approach allows linkage on a Multiomic level and allows better confirmation and understanding of biological change.

## 3) Metabolic Profiling of Yeast Sterols Using the Agilent 7200 Series GC/Q-TOF System

Terry Sheehan, Ph.D. (Agilent Technologies)

Targeted analysis of the relative levels of ergosterol biosynthesis pathway intermediates was combined with an untargeted approach, empowered by accurate mass high resolution GC/Q-TOF technology, to obtain the most comprehensive results. EI spectral information was complemented with MS/MS accurate mass product ion spectral data to confirm the identity of the compounds accumulated in yeast as a result of drug treatment.

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### Bruker

#### Wednesday, 19<sup>th</sup> September 12:20-13:30 Main Hall

Moderator: Clive Seymour

##### 1. Innovations in Mass Spectrometry

Dr. Arnd Ingendoh (Bruker Daltonik Germany)

##### 2. MALDI Imaging Mass Spectrometry: Practical Considerations

Prof. Richard Caprioli (Vanderbilt University School of Medicine, Nashville TN)

##### 3. Exact and fast: QTOF Technology for Qualitative and Quantitative Analysis

Dr. Peter Brechlin (Bruker Daltonik Germany)

Currently, a wide range of novel mass spec approaches for clinical, pharmaceutical analysis, proteomics as well as for applied markets like food safety, forensics and environment is developing. This is truly driven by recent innovations in instrumentation, methods and technology. The seminar will provide an overview of the current status of mass spectrometry for those new approaches.

#### Thursday, 20<sup>th</sup> September 12:20-13:30 Room E

Moderator: Rohan Thakur

##### Game Changing Technologies in MRM Analysis

Removing bottlenecks from sample to reports in MRM analysis

Jonathan McNally (Bruker Daltonics)

An introduction to a triple quadrupole designed for a singular purpose - to reliably quantify thousands of real samples in the fastest 'Sample-to-Report' time possible. Delivering exceptional precision, accuracy, linearity, and a wide dynamic range for your multiple reaction monitoring (MRM) assays. Innovations in software and ionization technology make it a 'game changer' for routine high-sensitivity, quantitative analysis.

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**JEOL****Monday, 17<sup>th</sup> September 12:20-13:30 Room D**

Moderator: Yoshihisa Ueda

**1. Direct Analysis in Real Time (DART®): new applications and future prospects**

Robert B Cody, Jr.

New applications and future prospects of the Direct Analysis in Real Time (DART®) technology will be presented by Dr. Robert B. Cody, one of the inventors of the technology.

**2. Analyses of lipids using SpiralTOF™ MALDI-TOF-TOF tandem MS: structural analyses and highly selective imaging**

Jun Tamura

Analyses of simple and complex lipids using SpiralTOF™ MALDI-TOF-TOF tandem MS will be presented. Structural analyses of lipids, including regio-specific analysis of triacylglycerols, utilizing high precursor ion selectivity and high-energy collision induced dissociation capability of the SpiralTOF™ and highly selective imaging of lipids on biological specimens utilizing high mass resolving power and high mass accuracy of the SpiralTOF™ will be discussed.

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**IonSense/AMR****Thursday, 20<sup>th</sup> September 12:20-13:30 Room D**

Moderator: Yasuhiko Bando (AMR, Inc.)

**1. DART-MS Strategies for Rapid Screening and Quantitation of Pesticides**

Elizabeth Crawford (IonSense, Inc.)

Pesticides and fungicides can be detected rapidly by using DART-MS. The capability for screening and quantitation of residues in order to efficiently monitor produce products before reaching the consumer market is the topic of this presentation. The Direct Analysis in Real Time (DART) ambient ionization technique offers the ability to rapidly screen the surface of produce for pesticides by a direct swabbing method and permits direct analysis of fruit juices in seconds. With automated sample introduction rapid screening and quantitative measurements can be completed using DART ionization coupled to high resolution accurate mass and triple quadrupole mass spectrometers.

**2. OpenSpot® Mass Spectrometry tools for Real-Time Quality Assessment using DART ionization sources**

Brian Musselman (IonSense, Inc.)

The rapid sampling of DART-MS permits monitoring of reaction products in seconds per sample using only a few microliters of sample. A rapid desorption system that allows for both detection of the acids by negative ion detection of the deprotonated molecule. The utility of this method for quality control experiments will be discussed using determination of fatty acids from edible oil. In these experiments the mesh is attached to a variable-current power supply that can deliver sufficient current to heat the sample at a rate > 20X faster than the conventional DART cartridge heater.

As monitoring of the production of fatty acids is completed in seconds per sample the method shows promise as a tool for detection of low and moderate levels of contaminants, monitoring the progress of biofuel production, detection of adulterants and non-specific threats.

### 3. Advantages of Using DART Ionization with Different Types of Mass Specs

Teruhisa Shiota (AMR, Inc.)

Various examples of DART-MS analysis will be presented to illustrate the advantages of using the Direct Analysis in Real Time ionization method with different types of mass spectrometers such as single/triple quadrupole and Orbitrap. The new DART ID CUBE features more powerful heating mechanism to allow analyses of metal organic complexes and pigments that were difficult to analyze with the conventional DART ionization sources.

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#### Shimadzu

**Monday, 17<sup>th</sup> September 12:20-13:30 Main Hall**

Moderator: Iwamoto Shinichi (Shimadzu)

#### “Let's Fish Mass”

Koichi Tanaka (Shimadzu)

Daniel J Capon (Blood Systems Research Institute San Francisco, U.S.A)

**Tuesday, 18<sup>th</sup> September 12:20-12:30 Room D**

Moderator: Neil Loftus (Shimadzu)

#### “Challenges in (un)-supervised LC-MS/MS-based metabolomics.”

Gérard Hopfgartner (School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, Geneva, Switzerland)

Qualitative and quantitative analysis of endogenous and exogenous compounds in biological fluids such as plasma or urine is mainly performed using high performance liquid chromatography with mass spectrometric detection. While high resolution mass spectrometry is gaining of interest for unsupervised analysis and compound identification triple quadrupoles still play an important role for sensitive and accurate quantitation of targeted analytes simultaneously in the positive and negative mode. Due to the large polarity range of the metabolites multiple separation strategies need to be considered including reversed phase, HILIC or ANP chromatography, generally in the ultra-high pressure mode. As the analytes of interest are covering a large dynamic range of at least 5-6 orders of magnitude direct injection of urine or the supernatant after plasma protein precipitation are of limited interest. Pooling extracts from different sample preparation (protein precipitation and liquid liquid extraction) procedures starting with different sample volume is one approach which equalizes the analytes of interest and allows them to be analyzed in a single run. In that case column-switching is used as an injector for the LC separation. Finally, as most of the compounds are endogenous construction of calibration curves in the matrix investigated for quantification is challenging requiring the use of surrogate matrices or surrogate analytes.

**Wednesday, 19<sup>th</sup> September 12:20-13:30 Room D**

Moderator: Jeff Dahl (Shimadzu Scientific Instruments Inc.)

**"Ultra Fast and Sensitive: Shimadzu UHPLC-Triple Quadrupole Mass Spectrometers "**

Richard van Breemen (University of Illinois, UIC/NIH Botanical Center for Dietary Supplements Research, U.S.A)

UHPLC-MS-MS applications of the new Shimadzu LCMS-8040 and LCMS-8080 triple quadrupole mass spectrometers will be discussed with an emphasis on the quantitative analysis of natural products in clinical specimens and botanical dietary supplements. The Nexera UHPLC system was used as an ideal complement for the ultra fast LCMS-8040 and the ultra sensitive LCMS-8080. Examples include the quantitative analysis of carotenoids, retinol and retinyl esters in human liver biopsies and serum, hepatotoxic pyrrolizidine alkaloids in borage oil dietary supplements, anthocyanidins in freeze-dried grapes, and enzyme assays for the inhibition of cytochrome P450 enzymes by hops and prenylated flavonoids from hops. UHPLC combined with fast and sensitive tandem mass spectrometry facilitated separations that were up to 12-fold faster and more sensitive than previous methods.

**Thursday, 20<sup>th</sup> September 12:20-13:30 Main Hall**

Moderator: Yoshinao Wada (Osaka MCH)

**" Induction of Pluripotency of Defined Factors"**

Shinya Yamanaka (Center for iPS Cell Research and Application, Kyoto University, Japan)

Induced pluripotent stem (iPS) cells were originally generated from mouse and human fibroblasts by retroviral introduction of Oct3/4, Sox2, c-Myc, and Klf4. iPS cells are similar to embryonic stem (ES) cells in morphology, proliferation, gene expression, and most importantly, pluripotency. Compared to ES cells, iPS cells have less ethical controversy and can be generated from various genetically identified individuals including disease patients or those having specific human leukocyte antigen (HLA) types. Patient-specific iPS cells provide unprecedented opportunities in disease research, drug screening, and toxicology. A bank of iPS cells constructed from HLA-homozygous donors would provide significant resources for stem cell therapy. However, recent reports of tumor formation following transplantation, and the large diversity between iPS cell clones highlight potential problems. Furthermore, the mechanism of reprogramming remains unclear.

In addition to fibroblasts, iPS cells can be generated from various somatic cells, such as hepatic cells, gastric epithelial cells, neural cells, dental pulp cells, peripheral blood cells, and cord blood cells. As alternatives to retroviral transduction, iPS cells can be generated by lentiviruses, adenoviruses, plasmids, transposons, recombinant proteins, or synthesized mRNA. Recently, we reported an integration-free induction method using episomal vectors. This method can induce human iPS cells efficiently and reproducibly. Regarding iPS cell induction factors, we discovered that L-Myc and the transcription factor Glis1, which is strongly expressed in the unfertilized egg, can establish iPS cells with a high efficiency and quality, replacing the oncogene c-Myc. Other reports suggest that chemicals can further enhance induction efficiency.

Each induction experiment can result in up to 100 or more independent iPS cell clones. These iPS cell clones may vary qualitatively, considering responses to in vitro directed differentiation protocols and their propensity to produce tumors. In fact, we have previously shown that the origins of mouse iPS cells have profound effects on tumorigenicity. It is therefore essential to

determine the best origins, the best induction protocols, and the best methods to evaluate iPS cell clones and subclones for future clinical applications. From this point of view, the need for genetic and epigenetic analyses, such as DNA methylation, histone modification, and genomic imprinting becomes more significant. It is also important to note that iPS cell within a clone can be heterogeneous, despite their common derivation from a single progenitor cell. This is likely because the process requires multiple cell division and cannot be completed by the four exogenous factors alone. Additional endogenous factors are required to achieve full reprogramming. Better understanding of the reprogramming mechanism will facilitate more uniform and complete reprogramming during iPS cell generation.

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**Thermo Fisher Scientific**

**Tuesday, 18<sup>th</sup> September 12:20-13:30 Main Hall**

**NEW Mass Spectrometry Technologies from Thermo Fisher Scientific**

August Specht Ph.D. (Thermo Fisher Scientific SanJose USA)

New LC-MS, GC-MS, ICP-MS and IOMS instruments from Thermo Fisher Scientific deliver exciting new capabilities to solve critical analytical challenges . Technology breakthroughs enable systems that deliver higher performance – faster - and with sample prep and software to support key application workflows. Learn about the new TSQ 8000 GC/MS,a robust instrument that delivers unstoppable prouctivity for MS/MS simplicity. The new Exactive Plus LC/MS is a next generation orbitrap system for routine screening and quantitation. The iCAP Q ICP-MS offers leading sensitivity, increased productivity and simplified operation with the smallest footprint in the industry. Come learn about these important new systems and see many test cases demonstrating their impressive performance in key applications.

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**Waters**

**Wedensday, 19<sup>th</sup> September 12:20-13:30 Room B-1**

Moderator: Kenji Hirose (Waters)

**Characterisation of Large Molecules by Advanced Mass Spectrometry**

Dr St John Skilton (Waters)

Abstract: As the market for Biotherapeutics accelerates and as Biosimilars are increasingly developed, the analytical market has boomed because of the power and detail available from mass spectrometry. Waters has developed a number of unique tools for this market and they have been further refined, augmented and enhanced in response to immediate need. For an organisation like Waters, these tools are now moving towards being incorporated into system solutions that are regulated – the first time that an analytical instrument vendor has taken on this challenge.

In this seminar we will examine the progress that has been made so far in designing and implementing advanced tools, the work in moving these tools into a routine framework, where non-specialists are able to access relevant technology with ease. In addition, the future pathway will be explored with a view to extending this to ever larger molecules and ever greater complexity.

**Tuesday, 18<sup>th</sup> September 12:20-13:30 Room B-1**

Moderator: Futoshi Sato (Waters)

**Advances in Mass Spectrometry for Protein Biomarker Discovery**

Dr. Jim Langridge (Waters)

Abstract: Advances in liquid chromatography and mass spectrometry are driving the ability to rapidly and accurately characterise complex systems samples. This workshop will focus upon these advances and the associated informatics to integrate proteomics with other 'omics data streams.

**Wednesday, 19<sup>th</sup> September 12:20-13:30 Room B-1**

Moderator: Motoji Oshikata (Waters)

**Advances in Drug Metabolism and Bioanalysis**

Dr. Robert Plumb (Waters)

Abstract: The Drug Metabolism and Pharmacokinetics has seen new scientific challenges and important regulatory changes over recent years. These changes and challenges require new innovative thinking and solutions to meet the business and scientific needs. Join the Waters DMPK team in this session to discuss recent advancements in metabolite identification, bioanalysis and the analysis of therapeutic proteins. The session will be interactive with technology updates from the Waters staff, industry perspectives from leading scientist and open forum discussions.

**Thursday, 20<sup>th</sup> September 12:20-13:30 Room B-1**

Moderator: Futoshi Sato (Waters)

**Novel Tools for the Analysis of Complex Mixtures Using an “Omics-Based” Approach**

Dr. John Shockcor (Waters)

Abstract: During this presentation, gene expression and its involvement in lipid metabolism and energy homeostasis will be discussed. Learn how to characterize the metabolic effects of Peroxisome Proliferator Activated Receptor (PPAR)-pan drug on white adipose tissue (WAT) using a mass spectrometry based lipidomic approach. Find out if the observed effects of drug administration resulted in up-regulated fatty acid oxidation or increased fatty acid sequestration and elongation.

## Company Information

### Exhibitors

#### AB SCIEX Pte. Ltd.

Booth B

500 Old Connecticut Path, Framingham, MA 01701, USA.

Phone 508-383-7700

[www.absciex.com](http://www.absciex.com)

AB SCIEX helps to improve the world we live in by enabling scientists and laboratory analysts to push the limits in their field and address the complex analytical challenges they face. The company's global leadership and world-class service and support in the mass spectrometry industry have made it a trusted partner to thousands of the scientists and lab analysts worldwide who are focused on basic research, drug discovery and development, food and environmental testing, forensics and clinical research. With over 25 years of proven innovation, AB SCIEX excels by listening to and understanding the ever-evolving needs of its customers to develop reliable, sensitive and intuitive solutions that continue to redefine what is achievable in routine and complex analysis. For more information, please go to [www.absciex.com](http://www.absciex.com). Follow AB SCIEX on Twitter @ABSCIEX and on Facebook.

#### Advion, Inc.

Booth 5

10 Brown Road, Ithaca, NY 14850 USA

Yoshiharu Naito ([info.advj@advion.com](mailto:info.advj@advion.com))

Amy Lummus ([alummus@advion.com](mailto:alummus@advion.com))

Advion develops, manufactures and globally supports mass spectrometers, chip-based ion sources, microfluidic flow chemistry systems and consumables for life science and related industries. We seek to enhance analysis performance and workflows. Using our deep scientific and engineering knowledge of mass spectrometry and microfluidics, we leverage our passionate employees' commitment to create quality, flexible and fit-for-purpose solutions. More about Advion, Inc. can be found on their website, [www.advion.com](http://www.advion.com).

#### Agilent Technologies, Inc.

Booth A

5301 Stevens Creek Blvd Santa Clara, CA 95051 USA

1-800-227-9770

[www.agilent.com/chem/contact](http://www.agilent.com/chem/contact)

Agilent Technologies is the world-wide leader in mass spectrometry, with proven, reliable GC/MS, LC/MS, CE/MS, and ICP-MS instruments and solutions for diverse application areas including pharmaceutical, food safety, environmental, forensic, metabolomic, proteomic analysis and clinical research. Agilent mass spectrometers work seamlessly with our industry-leading GC, LC, SPE and CE separation technologies. This comprehensive portfolio of innovative instruments uses MassHunter software which provides a single, consistent user interface that dramatically accelerate data acquisition, processing and reporting. With our sample preparation supplies, separation columns, Agilent provides complete solutions which are backed by Agilent's legendary world-wide service and support organization that ensures 24/7 reliability, maximum uptime and productivity.

**Antec**

Booth 37

**Industrieweg 12, 2382NV, Zoeterwoude the Netherlands****info@myAntec.com****TEL +31-71-5813333****FAX +31-71-5813334**

Antec is a worldwide supplier of Electrochemistry (EC) and (U)HPLC hardware used upfront MS, for the on-line coupling of EC with LC/MS. The award winning ROXY™ EC and ROXY™ EC/LC Systems are on display. They are known for their superior performance and unique features, e.g., versatility - they fit with any MS!

In many cases, Electrochemistry complements MS and allows for faster and superior MS analysis with substantial cost savings. Typical examples are in the mimicking and prediction of drug/xenobiotic metabolism, Protein chemistry, i.e., reduction of disulfide bonds, oxidative stability of nutrients and healthcare products, etc.

Special drivers are available and will be introduced such as XCalibur (Thermo) to allow easy instrument control and operation. Other products such as the new chip based electrochemical flow cells and new electrodes for optimal disulfide bond reduction in proteomics will be shown.

**APRIORI CORPORATION**

Booth 31

**1-7, KANDA-SUDACHO, CHIYODA-KU, TOKYO 101-0041, JAPAN****KOICHIRO NAKADA****info@apriori.co.jp****TEL: 03-5296-5521****www.apriori.co.jp**

Syft Technologies' Voice200® is based on the technology of Selected ion flow tube mass spectrometry (SIFT-MS) and it provides capability to detect and quantifies volatile organic compounds (VOCs) and certain inorganic compounds down to part-per-trillion concentrations in real-time usually with no sample preparation. The instrument is user-friendly and can be operated by non-technical personnel.

These characteristics mean that SIFT-MS can easily be applied to the variety of R&D and manufacturing field such as Ambient air monitoring and other environmental and occupational safety, Medical and breath research, Food and flavour research, Monitoring hydrocarbons in oil and gas exploration and drilling operations, and Detection of residual fumigants and other toxic industrial compounds in shipping and air-freight containers, etc.

If you need to detect or quantify VOCs rapidly and accurately, SIFT-MS Voice200® has a solution for you.

**Biologica Co.**

Booth 39

**Ohsu 4-10-40 Naka-ku, Nagoya 460-0011****sales@biologica.co.jp****www.biologica.co.jp**

Biologica exhibits the products as distributor of Antec and New objective that are ROXY, EC potentiostat for online EC/MS, and electrospray tips and Nano-column for LC/MS respectively.

**Biotage JAPAN, Ltd.**

Booth 4

1-14-4, Kameido, Koto-ku, Tokyo, Japan 136-0071

Japan\_info@biotage.com

Sample preparation doesn't have to be difficult or time consuming. Biotage offers instrumentation and consumables for many industries, including pharmaceutical, environmental, forensic, clinical and food testing. Through our application chemists and many application notes, we are here to help you establish the most cost-effective and appropriate sample preparation prior to LC/MS, GC/MS or other analytical method. We will present a poster with title of "Effective Strategies for Phospholipid Removal using Supported Liquid Extraction (SLE) with LC-MS/MS" on 19th September. Stop by booth #4 and poster #PWe-047 at IMSC 2012 to speak to one of our Technical Representatives!

**Bruker**

Booth E

Bruker Daltonics K.K. Japan Office

3/9, Moriya-cho Kanagawa-ku Yokohama-city, KANAGAWA 221-0022 Japan

Yasuhiko Maekawa

045-440-0471

info@bruker-daltonics.jp

<http://www.bdal.com>

While you've always known us as the leader in MALDI TOF and TOF/TOF technology, today Bruker Daltonics is about so much more. From pioneering ultra-high resolution mass spectrometry with the maXis series of LC-MS/MS qTOFs, to developing the most compact GC-MS/MS on the market, Bruker is your partner for system solutions and workflows to enhance your productivity and provide the answers to your analytical challenges.

**CTC Analytics AG**

Booth 2,3

[www.palsystem.com](http://www.palsystem.com)

info@ctc.ch

CTC Analytics AG, a privately owned Swiss and ISO 9001/13485 registered company, is a leader in front-end automation for gas and liquid chromatography. Over the course of the last 25 years we have invested in the continuous development of a flexible, highly reliable, advanced laboratory sample handling platform, primarily designed for use by researchers and scientists in the pharmaceutical, life science, chemical, environmental and food & flavor industries. The PAL products are distributed through OEM channels as well as through a selected net of independent CTC distributors around the world.

CTC Analytics shows at IMSC 2012 its brand new Sample Prep Automation system - the PAL RTC. This unique PAL System features a Robotic Tool Changer and completely new Software, the Cycle Composer 3. The PAL RTC is the new platform for efficiently automating complex sample preparation steps.

Wherever increased precise and accurate sample loading/throughput, fast cycles, modular architecture in combination with flexibility, near zero carryover and exceptional reproducibility is required the PAL product family is the right choice.

**Fujitsu Limited / Advanced Chemistry Development, Inc.**

Booth 36,43

**Fujitsu:**

9-3, Nakase 1-chome, Mihamaku, Chiba City, Ciba 261-8588, Japan

ACD/Labs Team

Computational Science and Engineering Solution Div.

Technical Computing Solutions Unit

tcsu-acd@ml.css.fujitsu.com

TEL:(043)299-3680 FAX:(043)299-3011

Advanced Chemistry Development, Inc(ACD/Labs):

8 King Street East, Suite 107,Toronto, Ontario, Canada M5C 1B5

info@acdlabs.com

Phone: Toll free (USA &amp; Canada): 1-800-304-3988

Voice: 1 (416) 368-3435

Fax: 1 (416) 368-5596

Advanced Chemistry Development, Inc., (ACD/Labs) is a chemistry software company that develops and commercializes enterprise and desktop solutions to support R&D efforts, and preserve and re-use legacy chemical and analytical knowledge. We also provide integration with existing informatics systems and undertake custom projects including enterprise-level automation. ACD/Labs develops desktop and enterprise software solutions for chemical, biochemical, and pharmaceutical R&D. Our expertise lies in vendor-neutral spectroscopic and chromatographic data processing and prediction, physicochemical and ADMET property prediction, analytical knowledge management, interactive reporting, and integrating analytical data with chemical structures to help protect and leverage valuable research knowledge.

**GL Sciences Inc.**

Booth 49

22-1 Nishishinjuku 6-chone,Shinjuku-ku,Tokyo,163-1130 Japan

world@gls.co.jp

GL Sciences is a Japanese chromatograph maker who deals with consumables and equipments from sample preparation to analysis. As HPLC columns, InertSustain series(C18, C8, Phenyl, NH2) have been developed and manufactured from Silica Gel which was controlled. InertSustain are very inertness, longer durability and high sensitivity. For GC analysis, Gas Leak Detector LD239 is an high sensitivity, convenience, and incredible downsizing to use. Let's try to use.

**Hakuto Co., Ltd.**

Booth 14

1-13, Shinjuku 1-Chome, Shinjuku-Ku, Tokyo 160-8910, Japan  
SECOND SALES DEPT. ELECTRONIC EQUIPMENT DIV.  
Tel +81-3-3225-8939(Direct), Fax +81-3-3225-9011

Hakuto Co., Ltd. has started handling of Alcatel Lucent's Vacuum (adixen) products in addition to Pfeiffer Vacuum products as an exclusive distributor in Japan since July, 2011.

Pfeiffer Vacuum has produced and developed advanced vacuum pumps, measurements and analysis equipments since they founded in 1890. Pfeiffer Vacuum invented turbopump at first in the world more than 50 years ago. Thank to continue to innovate their technology, Pfeiffer Vacuum becomes as leading company in this field to provide optimized vacuum environment for a wide variety of customers in all of the world.

Jan. 2010 Pfeiffer Vacuum Technology AG acquired Trinos Vacuum System.

Dec. 2010 Pfeiffer Vacuum Technology AG acquired Alcatel Lucent's Vacuum Technology Unit (adixen).

From standard turbopumps to pumps especially suited for mass spectrometry and electron microscopy, we deliver perfect vacuum solutions that will allow your analytical instrument to exceed expectations.

**HAMAMATSU PHOTONICS K.K.**

Booth 45

314-5 Shimokanzo, Iwata-City, Shizuoka Pref., 438-0193, Japan  
E-mail: salespro@etd.hpk.co.jp  
TEL: 0539-62-5248, FAX: 0539-62-2205  
Web site: <http://www.hamamatsu.com/>

Hamamatsu Photonics, as a technological group of light, is pursuing the limit of light, carving out unexplored fields one after another, and taking an active part in a wide range of fields.

We manufacture and sell MCP (micro channel plate) assemblies for TOF-MS.

**Hitachi, Ltd., Central Research Laboratory**

Booth 7

1-280, Higashi-koigakubo, Kokubunji-shi, Tokyo, 185-8601, Japan  
<https://www8.hitachi.co.jp/inquiry/hqrd/rd/en/form.jsp>

Hitachi Central Research Laboratory (HCRL), nestled among the natural flora of the Musashino area, was established in 1942 by the founder of Hitachi, Ltd., Mr. Namihei ODAIRA, with the mission of "Confronting today's developmental challenges as well as pursuing research for 10 to 20 years in the future." HCRL has fostered three core technologies: Measurement Technology, beginning with the electron microscope in 1942; Electronics, beginning with the transistor in 1952; and Computing, beginning with general purpose computers in 1956. These three core technologies have been fused together and further developed, contributing to Hitachi's large-scale businesses in energy generation, semiconductor devices, computers and communications. Today, we continue to strive to create new technologies in the fields of information and communication, electronics, life sciences and measurement technology.

**HORIBA, Ltd.**

Booth 10, 11

**2 Miyanohigashi, Kisshoin, Minami-ku Kyoto 601-8510 Japan****<http://www.horiba.com> info.hstec@jp.horiba.com**

The HORIBA Group of worldwide companies provides an extensive array of instruments and systems for applications ranging from automotive R&D, process and environmental monitoring, in-vitro medical diagnostics, semiconductor manufacturing and metrology, to a broad range of scientific R&D and QC measurements. Proven quality and trustworthy performance have established widespread confidence in the HORIBA Brand.

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Realize your optimal manufacturing process and improve your Overall Equipment Efficiency with world-class analysis, monitoring, and control technology from HORIBA - the company you can trust to adapt to your needs and always be there to provide expertise and support today, tomorrow, and into the future.

HORIBA-STEC “MICROPOLE System” is one of the world’s most compact and lightest\* residual gas analyzers with the capability to detect trace gas in a low vacuum. We explored the possibility of using this system under various conditions and designed a mass detector with 9 quadrupoles. (\*From HORIBA STEC 2011 research)

**Hudson Surface Tech**

Booth 15,16

**2 Executive Dr, Suite 580, Fort Lee, NJ, USA****Don Lee****[www.maldiplate.com](http://www.maldiplate.com)**

Hudson Surface Technology is the leading source for single-use third party sample plates for MALDI-MS for ABSciex, Bruker, Shimadzu and JEOL instruments.  $\mu$ Focus MALDI targets provide precisely defined hydrophilic islands on a hydrophobic surface so that your dried drop sample spots are focused onto repeatable, defined spots. HST offers these in standard formats for ABSciex, Bruker, Shimadzu and JEOL instruments, and also include ITO slide glass for MALDI imaging. For instruments, HST offers protein sample prep system which is Rapid Enzyme Digestion System (REDS) and  $\mu$ Matrix Spotter as well.

**INFOCOM CORPORATION**

Booth 27

**Sumitomo Fudosan Harajuku Building, 2-34-17, Jingumae, Shibuya-ku, Tokyo 150-0001, Japan****<http://infocom-science.jp/> info-science@infocom.co.jp**

Innovative software solutions for data analysis of mass spectroscopy are exhibited.

PEAKS is a complete software package for proteomics mass spectrometry data analysis. It effectively performs peptide and protein identification, PTM and mutation characterization, as well as results validation, visualization and reporting.

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MetaCore is an integrated knowledge database and software suite for pathway analysis of experimental data, genomics, proteomics and metabolomics. It's manually curated database contains human protein-protein, protein-DNA and protein compound interactions, metabolic

and signaling pathways, supported by proprietary ontologies and controlled vocabulary. AnalyzerPro is vendor-independent data-mining/deconvolution software for mass spectrometry. Its proprietary algorithms provide accurate components which existing software is unable to determine without additional information.

### IONICON Analytik GmbH

Booth 9

Eduard-Bodem-Gasse 3 6020 Innsbruck Austria

Phone +43 512 214 800

Email: [info@ionicon.com](mailto:info@ionicon.com)

Web: <http://www.ionicon.com>

IONICON is the world's leading PTR-MS company, producing ultra-sensitive mass spectrometers for real-time trace gas analysis featuring unique Proton-Transfer-Reaction Mass Spectrometry as well as related technologies such as Switchable Reagent Ions (SRI), where besides H<sub>3</sub>O<sup>+</sup> also NO<sup>+</sup>, O<sub>2</sub><sup>+</sup>, Kr<sup>+</sup> and Xe<sup>+</sup> are available as reagent ions to be used in IONICON's universal trace gas analyzers (patent pending). The IONICON product portfolio includes ultra-sensitive quadrupole and high-resolution time of flight based systems, capable of reaching a market-leading detection limit < 1 pptv with an excellent linear dynamic range of more than 6 orders of magnitude and mass resolution up to 8000 m/Δm. Application areas include VOC monitoring and quantification in environmental and biological research, atmospheric chemistry, emissions, exhaust and industrial process monitoring, food, flavor & fragrance science, breath analysis and illicit substances detection. In Japan IONICON PTR-MS instruments are available exclusively through Shoreline Science Research, Inc. (<http://www.shorelinesci.jp>).

### IONICS Mass Spectrometry

Booth 38

32 Nixon Road, Bolton, Ontario, Canada, L7E 1W2

Erik Hansen (905-857-5665 ext. 242, [erikh@ionics.ca](mailto:erikh@ionics.ca))

Founded in 2001, IONICS develops and manufactures triple quad mass spectrometers with industry leading sensitivity, robustness and throughput. Our recently launched second generation 3Q Series 100 and 3Q Series 200 offer the end user a broad range of capabilities that benefit from IONICS advances in source design, ion path and signal detection. IONICS instruments are available with a multi-option dual source which enables ESI/ESI, ESI/APCI and APCI/APCI configurations. Data acquisition, processing and reporting is facilitated with our MolAna Software. IONICS offers a full range of service and support options including method development support and is committed to enabling our users to achieve the highest quality results day-after-day. Continually innovating, IONICS has a commitment to producing the most sensitive and robust triple quads, which are capable of pushing the limits of detection to new levels.

**IonSense, Inc. / AMR, Inc.**

Booth 48

999 Broadway, Suite 404, Saugus, MA 01906

Phone 781 231 1739 [www.ionsense.com](http://www.ionsense.com)

AMR, Inc.

Phone +81-3-5731-2281 [www.amr-inc.co.jp/](http://www.amr-inc.co.jp/)

DART is a novel open air ionization methodology that enables ionization of compounds from gas, liquids, and solid at atmospheric pressure. IonSense develops DART® (Direct Analysis in Real Time) technology for mass spectrometry. The company completes product development, manufacturing, as well as sales and marketing activities associated with the interface of DART®SVP and OpenSpot® Sample Card enable ID-CUBE® sources to commercial mass spectrometers from Agilent, Thermo, AB-SCIEX, Bruker, JEOL, Waters and most recently Shimadzu API-series instruments.

**JCL Bioassay Corporation**

Booth 50

1-4-2, Shinsenri-higashimachi, Toyonaka-shi, Osaka 560-0082, Japan

Head Office +81-6-4863-5020

Yokohama Office +81-45-478-0747

Email [info@jclbio.com](mailto:info@jclbio.com)

<http://www.jclbio.com/>

JCL Bioassay Corporation is a leading Contract Research Organization (CRO) for bioanalysis in Japan. Our researchers have a wealth of knowledge in bioanalysis as well as acquired skills since the establishment of our company. By using state-of-the-art analytical instruments, our researchers have been able to produce a top-notch level work in ultramicro analysis. This has led to the continuous growth of our company as a leader in the bioanalytical field in Japan.

Our corporate group made its way into the world's largest U.S. market in 2010.

We will adapt our world's top-ranked technologies to the U.S. market, and streamline our operations to improve price competitiveness. With the collaboration of both domestic and overseas laboratories, we aim to be the top bioanalytical CRO in the world.

**JEOL Ltd.**

Booth C

1-2, Musashino 3-chome, Akishima,Tokyo,196-8558,JAPAN

<http://www.jeol.com>, phone:+81-42-543-1111

JEOL has been challenging to the state-of-the-art technology including Spiral TOF (MALDI-TOF), DART-MS, GC-TOF, Double-focusing magnetic sector MS, GC-QMS.

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**LECO Corporation**

Booth 41

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marcom@leco.co.jp

<http://www.leco.co.jp>

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**LMS Co., Ltd.**

Booth 42

3-6-7 Hongo, Bunkyo-Ku, Tokyo, 113-0033 Japan

SI division Mr. Yoichi Kadooka

<http://www.prosolia.com/>

Prosolia, Inc. is a scientific instrument company developing and marketing novel sample introduction technologies for mass spectrometry. Our portfolio scientific analytical tool are part of workflows that reduce complexity and accelerate results. Desorption Electrospray Ionization (DESI) is our flagship product. DESI enables rapid spot sampling and chemical imaging of surfaces under ambient conditions using mass spectrometry. Prosolia's current products retro-fit onto instruments produced by the major instrument companies including AB SCIEX, Thermo Scientific, Waters, Agilent, Bruker and LECO Corp.

**Matrix Science K.K.**

Booth 29

KN-Bldg 3F, 6-10-12 Sotokanda, Chiyoda, Tokyo 1010021 Japan.

TEL:+ 81-3-5807-7895

FAX:+81-3-5807-7896

<http://www.matrixscience.com> Info-jp@matrixscience.com

Mascot Server is a powerful search engine which uses mass spectrometry data to identify proteins from primary sequence databases. We will exhibit new version V2.4, and presenting a new feature, "Database Manager", "Report Builder" and more.

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**MS NOISE**

Booth 6

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Contact : Pieter DEKOCKER

Email : [contact@msnoise.com](mailto:contact@msnoise.com)

Website : [www.msnoise.com](http://www.msnoise.com) or [www.ionbench.com](http://www.ionbench.com)

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Booth 44

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Reiji Kobayashi([reiji\\_kobayashi@ap.pall.com](mailto:reiji_kobayashi@ap.pall.com))

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- LCMS certified – Be confident about your LCMS (Liquid Chromatography/Mass Spectrometry) results. The Acrodisc MS syringe filter is the first LCMS-certified filter with extremely low levels of extractables to minimize interference in LCMS chromatograms.
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## PEAK SCIENTIFIC JAPAN KK

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## PHOTONIS USA

Booth 25, 26

660 Main Street, Sturbridge, MA USA 01566

Mr. Bruce Laprade ([b.laprade@usa.photonis.com](mailto:b.laprade@usa.photonis.com))

Ms. Valerie Grib ([v.grib@usa.photonis.com](mailto:v.grib@usa.photonis.com))

Mr. John Harper ([j.harper@usa.photonis.com](mailto:j.harper@usa.photonis.com))

Phone: +1 508 347 4000

Fax: +1 508 347 3849

<http://www.photonis.com/en/ism/88-mass-spectrometry.html>

PHOTONIS USA is the world's leader in the design and manufacture of mass spectrometer, residual gas and ion mobility detectors and sensors. We hold a number of patents on our products which ensures that PHOTONIS detectors bring quality analysis.

PHOTONIS manufactures a wide range of custom and standard products for most major mass spectrometers, including:

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PHOTONIS introduces a new Ion Mobility Analyzer which can be used as a stand-alone product or coupled with a mass spectrometer. It features a high resolving power for simple and quick analysis.

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Booth 28

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The leader in high throughput solution in mass spectrometry presents the LDTD-96 and LDTD-384 ion sources. These platforms are the unique way to achieve up to 1400 samples analysis per hours. This shotgun approach introduces the sample into the mass spectrometer by fast Laser Diode Thermal Desorption (LDTD) process combined to an atmospheric pressure chemical reactions (LDTD-APCI). No matter what your application field is, the LDTD technology is an unmatchable alternative to increase your throughput.

**Polymer Factory Sweden AB**

Booth 46

**Teknikringen 48****114 28 Stockholm, Sweden****Andreas Nyström, CEO****andreas.nystrom@polymerfactory.com****Jonas Bengtsson, Project Manager****jonas.bengtsson@polymerfactory.com**

Polymer Factory is a provider of advanced dendritic and polymeric materials, such as dendrimers and dendrons, and a contract research company. We are committed to deliver cutting edge know-how and groundbreaking materials to accelerate our customer's success in material and life science. Our products are used to support research and development projects in a broad array of applications, ranging from pharmaceuticals to semiconductor materials.

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To learn more about Polymer Factory or SpheriCal®, head to our webpage at [www.PolymerFactory.com](http://www.PolymerFactory.com).

**Shimadzu Corporation**

Booth F

**1 Nishinokyo Kuwabara-cho,Nakagyo-ku,Kyoto 604-8511,Japan****imsc2012@group.shimadzu.co.jp**

Shimadzu Corporation is approving IMSC2012 (The 19th International Mass Spectrometry Conference) as a platinum sponsor.

We present newly-developed Ultra Fast Technologies and three new triple quadrupole mass spectrometers: LCMS-8040 which incorporates newly ion optics and collision cell technology to provide higher MRM sensitivity, LCMS-8080 which developed to realize high sensitivity less than a low femtogram even if in a complicated matrix represented by plasma, and GCMS-TQ8030 which is the first domestically product at IMSC2012. Moreover we provide various plans, such as user's day and a luncheon seminar. We all are looking forward to your participation of IMSC2012.

**SYSTEM INSTRUMENTS CO., LTD**

Booth 8

**776-2 Komiya, Hachioji, Tokyo 192-0031, Japan****TEL: 81-42-648-0533 FAX: 81-42-646-8228****Email: sice@sic-tky.com****<http://www.sic-tky.com/>**

System Instruments Co., Ltd is a manufacturer of analytical instruments. We have the biggest share of the market of Nitrogen Gas Generator for LCMS in Japan .System instruments insist on offering our customers the products of best quality and fast maintenance services.

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Booth 17-24

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The Thermo Scientific brand represents Thermo Fisher Scientific's broad range of laboratory solutions for the life sciences industries. Our product offerings include chromatography and mass spectrometry products as well as guaranteed support to meet your analysis needs.

**ULVAC-PHI, Inc.**

Booth 1

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ULVAC-PHI, Inc., started as a joint venture of Physical Electronics (PHI) and ULVAC, Japan. We are now the world's leading manufacture of advanced surface analysis apparatus aiming to the number one product of SIMS, XPS, and AES. Surface characterization technique is an essential technology in materials research and development, not only for basic research for new materials, green energy and biotechnology, but also the manufacturing sector. At IMSC exhibition, we mainly exhibit the latest time-of-flight secondary ion mass spectrometry (TOF-SIMS) PHI TRIFT V nanoTOF, and its brand-new application using gas cluster ion beam (GCIB). It includes biological tissue imaging, polymer materials characterizations, and organic thin film device.

**VRS**

Booth 30

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VRS are the leading Recruitment Consultancy specialising in jobs within Analytical Chemistry, predominantly Mass Spectrometry & Chromatography (HPLC, GC, LC-MS, GC-MS, ICP-MS, MALDI, etc).

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**Waters Corporation**

Booth D

Worldwide and Americas Headquarters

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<http://www.waters.com/imsc>

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Booth 40

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Our company provides columns and bulk packings for HPLC, UHPLC, SFC, LC, SEC, and flash chromatography for the analysis and purification of small and large molecules. Innovative products include the YMC Triart family of hybrid particles with C18, C8, phenyl, and Diol-HILIC phases, YMC BioPro ion exchange materials for analysis and purification of biomolecules, YMC DispoPackAT flash cartridges, and distribution of various stationary phases built on particles from 1.9 to 150 um. In addition to columns and bulk packings, our company also provides flowreactor systems for chemical synthesis, hydrogenation, and photoreaction, and their related products such as syringe pumps, hydrogen generator, and protein crystallization system.

**Zivak Technologies**

Booth 47

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Hüseyin Avni ÇAVDAR  
Phone Number: +90 212 210 5435  
avni.cavdar @zivak.com  
Elif Esin TANIŞ  
Phone Number: +90 212 210 5435  
elif.tanis @zivak.com  
<http://www.zivak.com>

Zivak Technologies was founded in 2005 at the TÜBITAK Marmara Research Centre Technological Free Zone, MARMARA TEKNOKENT A.Ş. It's principal aim was to develop and produce analysis kits for the parameters that are needed to be analyzed in food industry, health sector, and in environmental issues.

In 2006, the firm has added to its range of activities the acquisition of the LC/MS/MS platforms that the kits run on, and has implemented changes in their design to obtain a greater degree of analytical precision and ease of use in order to increase the service quality and customer satisfaction.

## Publications' Exhibitors

### AAAS/Science

Table H

Web: [www.sciencemag.jp](http://www.sciencemag.jp) , [www.aaas.org](http://www.aaas.org)

Visit the Japanese language portal today – [www.sciencemag.jp](http://www.sciencemag.jp)

Since its founding in 1848, the American Association for the Advancement of Science (AAAS) and its members have worked together to advance science and serve society. As part of these efforts, AAAS publishes *Science*, a multidisciplinary peer-reviewed journal, featuring scientific research articles and reports and providing commentaries on recent news and events from around the world.

Beyond *Science*, AAAS offers programs focused on science policy, international cooperation, science education, advancing human rights, diversity, and career development for scientists.

### IM Publications LLP

Table I

6 Charlton Mill, Charlton, Chichester, West Sussex PO18 0HY, UK.

Contact: Ian Michael ([ian@imppublications.co.uk](mailto:ian@imppublications.co.uk))

[www.imppublications.com](http://www.imppublications.com)

EJMS—European Journal of Mass Spectrometry is a peer review journal covering all areas of mass spectrometry. Whilst “European” in its publishing base, its distribution, editors and authors are truly global. EJMS provides high quality science at a fair price.

As well as regular research papers, EJMS publishes reviews, and a new series of “EJMS Protocols”, which detail practical details of how to be successful with experiments in mass spectrometry. Letters benefit from extremely rapid publication—under three weeks.

### Imtakt Corporation

Table E

Kyoto Research Park, Kyoto 600-8813, Japan

[info@imtakt.com](mailto:info@imtakt.com)

Imtakt HPLC columns have been designed with exceptional craftsmanship and decades of industry experience. Our columns give chromatographers: High Resolution; 25-50 % Lower Pressure: Novel Chemistry and Improved Selectivity. We offer a wide variety of unique stationary phases as follows: Cadenza series (High resolution and various ODS phases), Unison Family (Improved traditional C18, C8, Phenyl, Silica and Amino phases), Scherzo C18 Family (Multi-mode ODS phases), Presto (non-porous ODS for large molecules such as peptides and proteins).

### Merck Ltd.,Japan

Table A

Arco Tower 5F 1-8-1 Shimomeguro, Meguro-ku, Tokyo, Japan, 153-8927

Phone 0120-013-326, WEB <http://www.merckmillipore.jp/chemicals>

Merck Millipore, a division of Merck KGaA, Darmstadt, Germany with worldwide headquarters located in Billerica, Massachusetts, is a life sciences organization that, in partnership with its customers, creates innovative solutions for research, development and production worldwide. With a range of more than 40,000 products, Merck Millipore is a top tier supplier of tools and technologies to the life science industry..

**Mass Spectrometry Data Center, National Institute of Standards and Technology** — **Table D**

100 Bureau Drive, MS 8320  
Bldg 221, Room A111  
Gaithersburg, MD 20899-8320  
Phone: 301 975 2521  
Email: anzor@nist.gov  
Web: <http://webbook.nist.gov/chemistry/>

The NIST Mass Spectrometry Data Center (MSDC) is a part of Chemical and Biochemical Reference Data Division (CBRDD; [http://www.nist.gov/mml/chemical\\_properties/index.cfm](http://www.nist.gov/mml/chemical_properties/index.cfm) ), the Material Measurement Laboratory (MML; <http://www.nist.gov/mml/> ) within the National Institute of Standards and Technology (NIST, <http://www.nist.gov/index.html> ) . MSDC is responsible for the development of reliable reference mass spectral databases for the identification and analysis of chemical compounds by mass spectrometry. The Center is located on the NIST main campus in Gaithersburg, MD.

NIST/EPA/NIH Mass Spectral Library with Search Program (Data Version: NIST 11, Software Version 2.0g. <http://www.nist.gov/srd/nist1a.cfm> ). This database is a product of a steady, comprehensive evaluation and has been widely used for compound identification by mass spectrometry. It includes spectra from both GC-MS instruments and tandem mass spectrometers. This library encompasses four classes of data (1) a library of 243,893 electron ionization mass spectra for almost 212,961 unique compounds, (2) a gas chromatography retention index database, containing 346,757 Kovats retention index values for about 70,835 compounds covering both polar and non-polar columns, (3) an MS-MS library consisting of 95,409 spectra of over 12,568 ions obtained on qtof, HCD, triple quadrupole and ion trap mass spectrometers. (4) NIST Peptide Mass Spectral Libraries, for use in identifying peptides and their parent proteins - freely available for download (<http://peptide.nist.gov/> ).

**The Mass Spectrometry Society of Japan**  
**International Academic Printing Co., Ltd.****Table G**

4-19 Takadanobaba 4-chome, Shinjuku-ku, Tokyo 169-0075, Japan  
Web: <http://www.mssj.jp/>  
Email: [mssj-post@bunken.co.jp](mailto:mssj-post@bunken.co.jp)

The Mass Spectrometry Society of Japan (MSSJ) was established in 1953. Now a membership includes over 1,200 scientists providing an array of scientific data on relevant topics for more than half a century. The MSSJ sponsors the Annual Conference on Mass Spectrometry that is attended by more than 800 scientists, and publishes the two journals, Journal of the Mass Spectrometry Society of Japan and Mass Spectrometry. The latter one is an open access journal and available online from <http://mass-spectrometry.jp/>.

International Academic Printing Co., Ltd. (KOKUSAI-BUNKEN INSATSUSA, Tokyo) is licensed from MSSJ to publish Advances in Mass Spectrometry Vol. 19, Proceedings of 19th IMSC as well as the above two journals. If you like to order it, please contact us via E-mail ([pub-post@bunken.co.jp](mailto:pub-post@bunken.co.jp)).

**NetWell Corporation**

Table J

1-26-1 Shinjuku, Shinjuku-ku Tokyo 160-0022, Japan

Website: <http://www.netwell.co.jp/life-science/>

Email address: [bio-info@netwell.co.jp](mailto:bio-info@netwell.co.jp)

Tel, 03-5368-3459

Fax, 03- 3226-2860

NetWell shows and demonstrates three Cutting Edge Software working on Windows, two for Biological Molecular Structure Analysis using MS, MS/MS and MSn data, and one for MALDI IMS, manufactured by PREMIER Biosoft USA.

“SimGlycan®” predicts the Structure of Glycans and Glycopeptides using MS data. SimGlycan® accepts the experimental MS/MS or MSn data, matches them with its own database of theoretical fragments and generates a list of probable candidate structures. Each structure is scored to reflect how closely it matches your experimental data. In the case of glycopeptide qualitative analysis, information such as Protein ID, Protein Name, Source, peptide sequence, peptide mass etc are made available for identified glycopeptides.

“SimLipid” is a Comprehensive High Throughput Informatics Tool for Characterizing Lipids using precursors and product ions data from MS and MS/MS data.

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