Scientific Program

19th IMSC

	Main Hall	Room A	Room B-1	Room D	Room E	
15 (Sat)	**Open Lectures for General Public (in Japanese)**					**Short Course** "Fundamentals of Mass Spectrometry"(Two-day course) "Fragmentation Methods, Their Fundamentals and Application in Proteomics"(One-day course) "Introduction to Imaging Mass Spectrometry"(One-day course)
16 (Sun)						**Short Course** "Fundamentals of Mass Spectrometry"(Two-day course)
	Tutorial Lectures (Plenary) Nico M. M. Nibbering Michael L. Gross **Opening Plenary Lecture** Hiroyuki Hamada					
17 (Mon) Morning	**Plenary Lecture** David E. Clemmer					**Poster Session**
	Session 1: **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	**Session 2:** **Advances in Methods and MS Instrumentation for Biomolecule Characterization** Chair: Vicki H. Wysocki Keynote: Andrea Sinz	**Session 3:** **Structures and Dynamics of Atomic and Molecular Clusters** Chair: Fuminori Misaizu Keynote: Knut R. Asmis	**Session 4:** **Imaging I** Chair: Mitsutoshi Setou Keynote: Ron Heeren	**Session 5:** **Advances in Spray Ionization Techniques** Chair: Charles N McEwen Keynote: Kentaro Yamaguchi	
17 (Mon) Afternoon	**Session 6:** **Novel Approaches in Proteomics Analysis** Chair: Roman Zubarev Keynote: Joshua J. Coon	**Session 7:** **New Ionization Methods and Related Topics for the Next Generation** Chair: Kenzo Hiraoka Keynote: Robert Cody	**Session 8:** **Collision Dynamics and Spectroscopy Using Ion Storage Rings and Traps** Chair: Haruo Shiromaru Keynote: Steen Brøndsted Nielsen	**Session 9:** **Imaging II** Chair: Jiro Matsuo Keynote: Nick Winograd	**Session 10:** **Ion Mobility Spectroscopy Based on Instrument & Theoretical Development** Chair: Toshiki Sugai Keynote: Alexandre A. Shvartsburg	
18 (Tue) Morning	**Plenary Lecture** Albert J. R. Heck					**Poster Session**
	Session 11: **Glycomics: From Disease Markers to Therapeutic Antibody Products** Chair: Hyun joo An Keynote: Carlito Lebrilla	**Session 12:** **On-site Mass Spectrometry – Miniaturized Instruments and Allied Technologies–** Chair: Shuichi Shimma Keynote: Zoltán Takáts	**Session 13:** **Accelerator Mass Spectrometry** Chair: Hiroyuki Matsuzaki Keynote: Peter Steier	**Session 14:** **Ion–surface Collisions: Collision–induced Dissociation and Soft Landing** Chair: Jean Futrell Keynote: Julia Laskin	**Session 15:** **Mass Spectrometry for Nuclear Applications and Safety** Chair: Nobuo Takaoka Keynote: Yongzhong Ouyang	
18 (Tue) Afternoon	**Session 16:** **Glycoanalytical Technology for Systems Glycobiology and Functional Glycomics** Chair: Jane Thomas-Oates Keynote: Pauline M. Rudd	**Session 17:** **Non-Covalent Ion-Molecule Interactions** Chair: Seung-Koo Shin Keynote: Peter B. Armentrout	**Session 18:** **Advances in Resolution and Accuracy of Isotope Ratio Analyses** Chair: Takafumi Hirata Invited: Jochen Vogl	**Session 19:** **Mass Spectrometric Diagnosis** Chair: Toyofumi Nakanishi Keynote: Renato Zenobi	**Session 20:** **The Ion formation and Dissociation Mechanisms in MALDI** Chair: Myung Soo Kim Keynote: Richard Knochenmuss	
19 (Wed) Morning	**Award Ceremony** **Curt Brunnée Award Lecture**					**Poster Session**
	Session 21: **Platform Technology for Metabolomics** Chair: Yoshiya Oda Keynote: Annie Evans	**Session 22:** **Instrumentation Developments in Mass Spectrometric Imaging** Chair: Anastassios Giannakopulos Keynote: Bernhard Spengler	**Session 23:** **Gas Phase Fragmentation Mechanisms of Biomolecular Radicals** Chair: Shigeo Hayakawa Keynote: Richard A.J. O'Hair	**Session 24:** **Regulated Bioanalysis** Chair: Shinobu Kudoh Keynote: Tatsuo Kurokawa	**Session 25:** **New Approaches to Defining the Diversity of Glycans** Chair: Catherine E. Costello Key: Jane Thomas-Oates	
19 (Wed) Afternoon	**Session 26:** **Lipidomics : Recent New Techniques and Applications** Chair: Stephen Blanksby Keynote: Gavin E. Reid	**Session 27:** **Progress in Microbiology** Chair: Catherine Fenselau Keynote: Jeremy K. Nicholson	**Session 28:** **IR Spectroscopy of Gas-phase Ions** Chair: Dietmar Kuck Keynote: Philippe Maître	**Session 29:** **The Advances in Biological Mass Spectrometry in Drug Discovery and Development: Current State of the Art and Challenges** Chair: Ajai Chaudhary Keynote: Ragu Ramanathan	**Session 30:** **Data Processing and Informatics for SIMS** Chair: DaeWon Moon Keynote: David Castner	
20 (Thu) Morning	**Plenary Lecture** Hisayoshi Yurimoto					**Poster Session**
	Session 31: **Native Mass Spectrometry and Structural Biology** Chair: Satoko Akashi Keynote: Joseph A. Loo	**Session 32:** **Formation and Dissociation of Peptide Radical Ions** Chair: Dominic T.W. Chan Keynote: Roman A. Zubarev	**Session 33:** **JMS Award Symposium** Chair: Chair: Richard M. Caprioli (Editor-in-Chief, JMS)	**Session 34:** **MS Informatics for Identification and Characterization** Chair: Shigeki Kajihara Keynote: David Fenyö	**Session 35:** **Environment I** Chair: Peter Haglund Keynote: Terry Bidleman	
20 (Thu) Afternoon	**Session 36:** **Advances in Ion Mobility Mass Spectrometry** Chair: Joseph A Loo Keynote: Michael T. Bowers	**Session 37:** **Challenges in High Resolution and High Accuracy Mass Measurement Mass Spectrometry** Chair: Evgeny Nikolaev Keynote: Alan G. Marshall	**Session 38:** **Mass Spectrometry for Metabolic Diseases** Chair: Makoto Yoshino, Seiji Yamaguchi	**Session 39:** **MS Informatics for Quantitation** Chair: David Fenyö Keynote: Jürgen Cox	**Session 40:** **Environment II** Chair: Takeshi Nakano Keynote: Peter Haglund	
	Thomson Medal Award Lectures					
21 (Fri) Morning	**Plenary Lecture** Richard M. Caprioli					
	Session 41: **Chemistries of Trapped Ions and their Applications to Biological Mass Spectrometry** Chair: Gavin E. Reid Keynote: Scott A. McLuckey	**Session 42:** **New Developments in Instruments and Detectors** Chair: Takaya Sato Keynote: Evgeny N. Nikolaev	**Session 43:** **Novel Proteomics Methodologies** Chair: Yasushi Ishihama Keynote: Michael J. MacCoss	**Session 44:** **Ambient Ionization** Chair: Jentaie Shiea Keynote: Kenzo Hiraoka	**Session 45:** **Cell Biology / Cellular Pathways** Chair: Renato Zenobi Keynote: Tsutomu Masujima	
21 (Fri) Afternoon	**Closing Plenary Lecture** R. Graham Cooks					

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

TUTORIAL LECTURES (PLENARY) (Main Hall)

[Sunday Afternoon, 16th September (15:30-16:15)]

Nico M. M. Nibbering
Selected Examples of Ion Chemistry Studies

[Sunday Afternoon, 16th September (16:15-17:00)]

Michael L. Gross
Can Mass Spectrometry Play a Role in Protein Biophysics and Structural Biology?

OPENING PLENARY LECTURE (Main Hall)

[Sunday Afternoon, 16th September (17:30-18:15)]

Hiroyuki Hamada
Applied Conventional Technology- Look at Tradition for Our Future-

PLENARY LECTURES (Main Hall)

[Monday Morning, 17th September (8:00-8:45)]

David E. Clemmer
Developing Next Generation Ion Mobility/Mass Spectrometry Techniques

[Tuesday Morning, 18th September (8:00-8:45)]

Albert J. R. Heck
Tackling the Complexity of the Proteome by Mass Spectrometry

[Thursday Morning,, 20th September (8:00-8:45)]

Hisayoshi Yurimoto
Science of Asteroid Sample Return Mission "HAYABUSA"

[Friday Morning, 21st September (8:00-8:45)]

Richard M. Caprioli
Molecular Imaging of Tissues by Mass Spectrometry: Looking Beyond the Microscope

CLOSING PLENARY LECTURE (Main Hall)

[Fraiday Afternoon, 21st September (11:45-12:30)]

R. Graham Cooks
Through a Glass Darkly: Glimpses into the Future of Mass Spectrometry

List of Oral Sessions

[Monday Morning, 17th September (9:00-11:00)]

Session 1 (Main Hall):
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
"Orbitrap-based hybrid mass spectrometers: synergy of analyzers"

Scope of Session: Hybrid mass spectrometers are designed to combine the best features of different mass analyzers in order to obtain highly desirable performance characteristics and unique analytical functions that are not attainable with non-hybrid systems. The type and quality of data depends greatly on the physical characteristics of individual devices implemented on each stage. This sessions aims to present instrumental developments in tandem hybrid mass spectrometry spanning application areas from inorganic chemistry to identification of large molecules and the study of molecular complexes, and to foresee the future of this type of instruments.

Keywords: Hybrid instrumentation, Tandem mass spectrometry, Instrumental development

Session 2 (Room A):
Advances in Methods and MS Instrumentation for Biomolecule Characterization

Chair: Vicki H. Wysocki

Keynote: Andrea Sinz
"Chemical Cross-Linking and Mass Spectrometry:
A Fruitful Combination for Protein 3D-Structure Analysis"

Scope of Session: New methods and instrumentation have advanced the structural characterization of large biomolecules and complexes. This session focuses on newer methodologies that have enabled the characterization of the primary and higher order structure of biomolecules, including newer forms of dissociation techniques, ioni-zation methods, labeling strategies, and crosslinking.

Keywords: ETD, SID, Crosslinking, H/D exchange, Chemical modification, Ambient ionization techniques

Session 3 (Room B-1):
Structures and Dynamics of Atomic and Molecular Clusters

Chair: Fuminori Misaizu

Keynote: Knut R. Asmis
"Recent Advances in the Vibrational Spectroscopy
of Mass-Selected Gas Phase Cluster Ions"

Scope of Session: Size-dependent physical and chemical properties of gas-phase clusters have been investigated using various experimental techniques coupled with mass spectroscopy. The purpose of this session is to discuss recent progress in the field of structures and chemical reaction dynamics of clusters.

Keywords: Clusters, Spectroscopy, Electronic state, Geometrical structure, Reaction dynamics

Session 4 (Room D):
Imaging-I

Chair: Mitsutoshi Setou

Keynote: Ron M Heeren
"Imaging molecular signals with multimodal imaging mass spectrometry"

Scope of Session: Mass imaging technique is powerful tool to reveal molecular distribution in cells and tissues. There is still strong need for high spatial resolution and high sensitivity beyond the state-of-art. When the technology is pursued towards the limits of resolution, low abundance analytes and/or the need to sample species over a large dynamic range, issues arise that can be ignored in normal operation.

Keywords: Imaging Mass Spectrometry, Cells, Tissues, SIMS

Session 5 (Room E):
Advances in Spray Ionization Techniques

Chair: Charles N McEwen

Keynote: Kentaro Yamaguchi
"Cold-Spray Ionization Mass Spectrometry"

Scope of Session: Spray ionization has proven to offer the softest means to preserve noncovalent interactions in the gas phase including those of labile supermolecules; recently ambient ionization methods such as DESI have evolved for direct spray ionization of surfaces.

Keywords: Electrospray, Sonic spray, Non-covalent interactions, DESI

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[Monday Afternoon, 17th September (15:00-17:00)]

Session 6 (Main Hall):
Novel Approaches in Proteomics Analysis

Chair: Roman Zubarev

Keynote: Joshua J. Coon
"Instant Spectral Assignment for Rapid, High-Throughput Targeted Proteomics"

Scope of Session: Proteomics, after 15 years of explosive development, faces unexpected challenges from the next-generation sequencing methods in other omics areas. What breakthroughs can address these challenges and advance proteomics beyond the state-of-the-art?

Keywords: De novo sequencing, Novel fragmentation techniques, Novel quantification technique

Session 7 (Room A):
New Ionization Methods and Related Topics for the Next Generation

Chair: Kenzo Hiraoka

Keynote: Robert B Cody
"What is the Opposite of Pandora's Box? Direct Analysis, Ambient Ionization, and a New Generation of Atmospheric Pressure Ion Sources."

Scope of Session: Ionization plays a crucial role for mass spectrometry. This session focuses on the new ionization methods for the next-generation mass spectrometry. Ionization may be taken place under vacuum or ambient conditions.

Keywords: Ionization, Charge Transfer, SNMS, Shockwave, Tribo-Phenomenon

Session 8 (Room B-1):
Collision Dynamics and Spectroscopy Using Ion Storage Rings and Traps

Chair: Haruo Shiromaru

Keynote: Steen Brøndsted Nielsen
"Spectroscopy of firefly luciferin and oxyluciferin anions in vacuo. Color tuning by a micro-environment?"

Scope of Session: This session covers the recent drastic development of electrostatic devices, i.e. ion storage rings and ion traps. Various aspects including lifetime measurements of metastable states, action spectroscopy by laser irradiation, cross section measurements for low-energy electron collisions, and their application to bio-molecular ions will be treated. Comparison between an ion storage ring and an ion trap with keV energies as well as the traditional RF ion trap focusing on their advantages will be also discussed.

Keywords: Electrostatic ion storage ring, Ion trap, Metastable states, Laser-induced action spectroscopy, Low-energy electron collision

Session 9 ((Room D):
Imaging-II

Chair: Jiro Matsuo

Keynote: Nicholas Winograd
"Nanoscale Chemical Imaging of Biomaterials with Cluster SIMS"

Scope of Session: Mass imaging technique is powerful tool to reveal molecular distribution in cells and tissues. There is still strong need for high spatial resolution and high sensitivity beyond the state-of-art. When the technology is pursued towards the limits of resolution, low abundance analytes and/or the need to sample species over a large dynamic range, issues arise that can be ignored in normal operation.

Keywords: Imaging Mass Spectrometry, Cells, Tissues, SIMS

Session 10 (Room E):
Ion Mobility Spectroscopy Based on Instrument & Theoretical Development

Chair: Toshiki Sugai

Keynote: Alexandre A. Shvartsburg
"Pushing the frontier of high-definition ion mobility spectrometry using FAIMS"

Scope of Session: Ion mobility spectrometry (IMS) is established as a powerful tool to characterize the 3-D structure of biomolecules and nanomaterials, and new theoretical results and instrumental methods point to a yet greater potential for the IMS approach. This session focuses on recent developments in nonlinear IMS or FAIMS employing strong electric fields, improved understanding of the IMS fundamentals, and novel instrumentation, which would provide the foundation for next-generation IMS technology.

Keywords: Ion mobility Spectrometry, High-resolution Differential IMS, New instrumentation, Theoretical analyses, Applications to bio & nano related molecules and materials

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List of Oral Sessions

[Tuesday Morning, 18th September (9:00-11:00)]

Session 11 (Main Hall):
Glycomics: From Disease Markers to Therapeutic Antibody Products

Chair: Hyun joo An

Keynote: Carlito Lebrilla

"Is high throughput glycomics possible?"

Scope of Session: This session will cover new approaches for biomarker discovery and biopharmaceutical glycosylation profiling using mass spectrometry-based glycomics and glycoproteomics.

Keywords: Glycomics, Glycoproteomics, Glycobiomarker, Therapeutic antibody, Glycosylation

Session 12 (Room A):
On-site Mass Spectrometry -Miniaturized Instruments and Allied Technologies-

Chair: Shuichi Shimma

Keynote: Zoltan Takats

"In-vivo, Real-time Identification of Tissues in Human Surgical Environment by Rapid Evaporative Ionization Mass Spectrometry"

Scope of Session: This session covers the topic of promising instruments (ion traps, quadrupole mass filters, time-of-flight instruments, etc.) and related techniques to realize on-site mass spectrometry. In recent years, design and development of miniature mass spectrometers has been at the forefront of research in mass spectrometry. These instruments have widespread applications, for example, detection and identification of chemical and biological hazards for homeland security, environmental monitoring, food safety, and so forth. The miniature mass spectrometers are capable of on-site analysis of these applications. It is considered that miniature instruments would be more commonly utilized in the future. Therefore, this session will become a good opportunity to share the knowledge of the present situation and future prospects.

Keywords: Miniaturized/portable mass spectrometers, On-site detection and monitoring, On-site sampling and preparation

Session 13 (Room B-1):
Accelerator Mass Spectrometry

Chair: Hiroyuki Matsuzaki

Keynote: Peter Steier

"Accelerator Mass Spectrometry - analysis of the rarest atom species for earth and environmental science"

Scope of Session: Acelerator Mass Spectrometry (AMS) is an unique method for detection of several special rare isotopes such as ^{10}Be, ^{14}C, ^{26}Al, ^{36}Cl, ^{129}I and ^{236}U, so on. Using these isotopes, new frontier is opened in many scientific fields including Earth environmental science. This session will summarize frontier applications of AMS in various fields and anticipate future prospects.

Keywords: Accelerator mass spectrometry, Cosmogenic radio nuclides, Anthropogenic nuclides, Radiocarbon dating, Isotope system, Berylli-um-10, Iodine-129, Alluminum-26, Chroline-36, Carbon-14

Session 14 (Room D):
Ion-surface Collisions: Collision-induced Dissociation and Soft Landing

Chair: Jean Futrell

Keynote: Julia Laskin

"Ion-Surface Collisions in Mass Spectrometry: Activation, Dissociation and Soft-Landing"

Scope of Session: During the past decade key theoretical and experi-mental studies of the kinetics of ion-surface collision phenomena have established a fundamental understanding of the principal mechanisms involved in both collision-induced dissociation and soft landing. Notably, moderate energy ion collisions on self-assembled monolayer surfaces are one of the most promising techniques for sequence determination for large peptides and protein complexes. Equivalent advances in the un-derstanding of the time evolution of charge states and structures following low energy capture of ions on surfaces provide the basis for utilizing mass selected complex ions to create spatially dispersed functional devices. Several examples and instrumental advances enabling them will be de-scribed.

Keywords: Soft landing, Collision-induced dissociation, Ion-surface colli-sion phenomena

Session 15 (Room E):
Mass Spectrometry for Nuclear Applications and Safety

Chair: Nobuo Takaoka

Keynote: Huanwen Chen

"Extractive Electrospray Ionization Mass Spectrometry for Uranium Chemistry Studies"

Scope of Session: Nuclear energy has paid an important role in global energy supplies. However, the Great East Japan Earthquake and Tsu-nami has led to the accident at the Fukushima Daiichi Nuclear Power Plant, which has resulted in a significant question on nuclear energy de-velopment. The nuclear safety becomes an essential element for nuclear energy application. At the IAEA General Conference in September 2011, the IAEA Board of Governors approved and endorsed IAEA's /Nuclear Safety Action Plan/ by all 151 Member States, which is to strengthen the global nuclear safety framework. Mass spectrometry is powerful tool for both nuclear energy development and nuclear safety. The scientists and technicians who work at mass spectrometry society may contribute their efforts to fellow up the nuclear applications and safety. The 19th IMSC will set a session to discuss the issue. The following subjects are en-couraged:

1. ICP-MS, SIMS, GD-MS and other MS technologies applied to nuclear fuel and materials, water chemistry at nuclear power plant, environmental monitoring near NPP sites, global falls, sea water, sediments, remedia-tion, etc.
2.Mass spectrometries including organic & biological MS applied to the effects of nuclide and adiation on human beings and biosphere.
3.New technology of mass spectrometry for nuclear applications and safety.

Keywords: Nuclear energy development, Nuclear safety

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[Tuesday Afternoon, 18th September (15:00-17:00)]

Session 16 (Main Hall):
Glycoanalytical Technology for Systems Glycobiology and Functional Glycomics

Chair: Jane Thomas-Oates

Keynote: Pauline M. Rudd

"Glycoanalytical technologies for systems glycobiology, biomakrer discovery & therapies"

Scope of Session: The development of glycoanalytical technologies have greatly enhanced the study of glycobiology, facilitating the discovery of disease-related solutions and providing an informative view of glycosylation and its relationship with other biological disciplines in a systems biology approach. Technologies for rapid and reliable identification of glycan structure as well as the advances of computer software and glyco database are discussed.

Keywords: Glycobiology, Glycotechnology, Structural analysis, Bioinformatics, Database, Data management, Automated annotation

Session 17 (Room A):
Non-Covalent Ion–Molecule Interactions

Chair: Seung-Koo Shin

Keynote: Peter B. Armentrout

"The Thermochemistry of Non-Covalent Ion-Molecule"

Scope of Session: Non-covalent ion–molecule interactions are the building principle underlying the gathering of ions and molecules beyond the quantum mechanical description of chemical bonds. They are the driving forces behind the solvation of ions, molecular recognition of ionic species, assembly of host–guest ionic complexes, formation of metal ion–ligand complexes, and folding of DNAs and proteins in ionic environments. This session invites the presentation of ion–molecule chemistry that deals with spectroscopy, structures, energetics, conformation, and reactions. Both experimental and theoretical works are welcome to the session. Professor Peter B. Armentrout at the University of Utah will deliver a keynote speech at this session.

Keywords: Noncovalent ion-molecule interactions, Molecular recognition, Collision-induced dissociation, Host-guest complexes. Ion-mobility.

Session 18 (Room B-1):
Advances in Resolution and Accuracy of Isotope Ratio Analyses

Chair: Takafumi Hirata

Keynote: Jochen Vogl

"Advances in Isotope Ratio Mass Spectrometry and Required Isotope Reference Materials"

Scope of Session: The magnitude of many analytical problems is clearly exacerbated when trying to obtain the levels of precision required for the meaningful interpretation of isotope ratios, and this section of the analytical community is actively solving problems such as spectral interference and mass discrimination drift at new levels of sensitivity and precision. Continuous developments in inorganic mass spectrometry techniques have revolutionized the precision of the isotopic ratio measurements. Applications of the inorganic mass spectrometry in metrology or biochemistry are beginning to appear over the horizon. This session aims to present the instrumental developments for precise and accurate isotope ratio measurements and also to discuss the future direction of the techniques.

Keywords: Isotope ratio analysis, Inorganic mass spectrometry, Absolute analysis, Metrology, Imaging mass spectrometry, Mass bias, In-situ isotopic analysis, External correction

Session 19 (Room D):
Mass Spectrometric Diagnosis

Chair: Toyofumi Nakanishi

Keynote: Renato Zenobi

"Ambient Mass Spectrometry for Detecting Biomarkers in Breath"

Scope of Session: Mass spectrometry will soon take over the current diagnostic detection system to change the system to be versatile, sensitive, quantitative and qualitative. The potential of mass spectrometry for diagnosis will be discussed with basic and clinical validations.

Keywords: Disease-related biomarker, Clinical medicine, New diagnostic technology

Session 20 (Room E):
The Ion formation and Dissociation Mechanisms in MALDI

Chair: Myung Soo Kim

Keynote: Richard Knochenmuss

"MALDI and Related Desorption / Ablation / Ionization Methods:A Solved Problem or Still a Mystery?"

Scope of Session: The session will deal with two fundamental subjects in the matrix-assisted laser desorption ionization (MALDI). The first subject is the mechanism for the gas-phase ion formation from a solid sample, i.e. a matrix-analyte mixture. The second subject is the mechanism for the dissociation of polyatomic ions such as protonated peptides generated by MALDI. The session will be a forum for the fundamental aspects of the processes rather than for the detailed mechanistic pathways for individual ions. Not only the presentations of experimental results but also those of theoretical and computational results will be accommodated.

Keywords: Fundamentals of MALDI, Gas-phase ion formation mechanism, Ion dissociation mechanism

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List of Oral Sessions

[Wednesday Morning, 19th September (9:00-11:00)]

Session 21 (Main Hall):
Platform Technology for Metabolomics

Chair: Yoshiya Oda

Keynote: Annie Evans

"New generation high-field Orbitrap instrumentation in untargeted metabolic profiling"

Scope of Session: Discussion of a metabolomics global profiling technology utilizing high-throughput dual column UPLC/MS/MS2 and GC/MS analytical methods for the analysis of complex biological samples.

Keywords: Metabolomics, UPLC/MS, GC/MS, Sample preparation

Session 22 (Room A):
Instrumentation Developments in Mass Spectrometric Imaging

Chair: Anastassios Giannakopulos

Keynote: Bernhard Spengler

"High Resolution in Mass and Space: New Developments and Trends in MALDI Mass Spectrometry Imaging"

Scope of Session: Mass spectrometric imaging (MSI) links the universal detection capability of mass spectrometry with the ability to record the spatial distributions of a wide range of atoms and molecules. MSI has penetrated almost all areas of analytical science and has found uses from detecting elements in industrial applications to determining drug and biological molecule distributions in tissue. Ever increasing demand for high spatial and mass resolution is driving development in analytical instrumentation. This session aims to present recent instrumentation developments in mass spectrometric imaging with emphasis on high resolution spatial and mass spectrometric characteristics.

Keywords: Imaging mass spectrometry, Instrumental development

Session 23 (Room B-1):
Gas Phase Fragmentation Mechanisms of Biomolecular Radicals

Chair: Shigeo Hayakawa

Keynote: Richard A.J. O'Hair

"Gas Phase Chemistry of Biomolecular Radicals – An Overview"

Scope of Session: Fragmentation mechanisms of gas phase biomolecular ions have been investigated using tandem mass spectrometry with a range of excitation methods including CID, ETD, ECD, and photo-excitation. Through a combination of experiments and theoretical calculations on model systems, it has been found that radicals can play a critical role in inducing fragmentation. This session covers the fragmentation mechanism of radicals formed by various excitation methods.

Keywords: Gas phase ion chemistry, Hydrogen atom transfer, Gas phase fragmentation, Radical ion reaction, Fundamental interest, Collision induced dissociation, Electron capture or electron transfer reaction, Electron collision, Electronic excitation, Photo excitation, Electron induced dissociation

Session 24 (Room D):
Regulated Bioanalysis

Chair: Shinobu Kudoh

Keynote: Tatsuo Kurokawa

"Drug regulation and bio-analysis"

Scope of Session: Over the last 20 years, bioanalysis in drug research and development has received benefits of selectivity and sensitivity achievable by mass spectrometry (MS) in conjunction with chromatographic techniques. There are, though difficulties and problematic issues needed to be overcome or to be cared for proper results, which mostly become apparent in liquid chromatographic approaches with MS. To obtain proper results, analyses have to be conducted correctly under necessary regulations or guidelines that must be fair and scientifically correct, and are preferably acceptable globally as internationally harmonized ones in future. This session covers the recent development in regulations and guidelines, which are not exclusive for LC-MS but also for ligand binding assays. Its related topics with new ideas and practical implementations for better MS-based bioanalysis and future prospect are also discussed.

Keywords: Regulation, Guideline, EMA, FDA, PMDA, MHLW, Mass spectrometry, Chromatography, Quantitation, Qualitative analysis, Bioanalysis

Session 25 (Room E):
New Approaches to Defining the Diversity of Glycans

Chair: Catherine E. Costello

Keynote: Jane Thomas-Oates

"Development and Application of a Rapid and Sensitive Method for Screening Cellular Models of Congenital Disorders of Glycosylation"

Scope of Session: Carbohydrates and glycoconjugates are widely dispersed in nature; the importance of their roles and their broad and continuously changing structural heterogeneity are now coming to be much more appreciated in the community, yet the tools for their characterization require substantial further development. To fully determine and profile the types and distributions of glycan structures, both in the human population and throughout nature, researchers worldwide are generating novel methodologies and significant modifications of the mass spectrometry-based techniques and bioinformatics tools that facilitate peptide and protein analysis. This session will highly the dynamic research and new applications in mass spectrometry for glycobiology.

Keywords: Glycans, Glycoconjugates, Glycolipids, Glycoproteins, Glycopeptides, Ion mobility spectrometry

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[Wednesday Afternoon, 19th September (15:00-17:00)]

Session 26 (Main Hall):
Lipidomics : Recent New Techniques and Applications

Chair: Stephen Blanksby

Keynote: Gavin E. Reid

"High-Resolution 'Shotgun' Mass Spectrometry and Chemical Labeling for Comprehensive and Quantitative Lipidome Profiling of Disease"

Scope of Session: Recent advances in lipidomics have given rise to advanced methods for precise structure elucidation of molecular lipids as well as mapping their distribution within biological tissue. The structure and location of lipids have proved to be tightly connected to physiological function of specific tissues. In particular, recent advances in mass spectrometry such as ozone-induced dissociation, covalent adduct chemical ionization and high energy collision induced dissociation now allow the precise positions of carbon-carbon double bonds (and other subtle structural features such as sn-position) to be assigned online even within complex lipids. Advances in mass spectrometric methods for lipidomics and their applications will be discussed.

Keywords: Phospholipids, Molecular species, Double bond localization

Session 27 (Room A):
Progress in Microbiology

Chair: Catherine Fenselau

Keynote: Jeremy K. Nicholson

"Translating metabolic phenotyping and systems medicine into clinical Practise: Understanding gut microbial-host Interactions in personalized public healthcare problems"

Scope of Session: Reports in this session will be presented on applications of mass spectrometry to new areas of research in microbiology, and on new instrumental and chemical methods for mass spectrometry-based analysis of bacteria and viruses.

Keywords: Bacteria, Virus, Identification, Metabolome, Host-microbiome interaction

Session 28 (Room B-1):
IR Spectroscopy of Gas-phase Ions

Chair: Dietmar Kuck

Keynote: Philippe Maître

"IR Photodissociation Spectroscopy: A new dimension to Tandem Mass Spectrometry"

Scope of Session: This session would cover the exciting new field of IR spectroscopy of cold and room temperature ions with emphasis on the currently hotly debated structural issues on peptide fragments.

Keywords: Ion spectroscopy, Infrared lasers, Fragment structures, Modeling, Peptides vibrational spectra, Specific ion activation, Fragmentation modeling

Session 29 (Room D):
The Advances in Biological Mass Spectrometry in Drug Discovery and Development: Current State of the Art and Challenges

Chair: Ajai Chaudhary

Keynote: Ragu Ramanathan

"Advances in the Application of Mass Spectrometry to Drug Metabolism and Pharmacokinetics Studies"

Scope of Session: The session will focus on recent advances, applications, and challenges in the field of mass spectrometry in pharmaceutical drug discovery and development.

Keywords: Pharmacokinetics, Pharmacodynamics, Drug development, Drug discovery, Metabolite, Quantification

Session 30 (Room E):
Data Processing and Informatics for SIMS

Chair: DaeWon Moon

Keynote: David G Castner

"Image and Spectral Processing for ToF-SIMS Analysis of Biological Materials"

Scope of Session: Thanks to application of chemometrics to intricate SIMS data, information from SIMS has been expanded. For instance, subtle changes in molecular structures and distributions of biomolecules in tissues can be obtained with SIMS. In this session, brand-new SIMS studies in terms of data processing and informatics will be discussed.

Keywords: Chemometrics, Multivariate analysis, Data processing, Informatics, G-SIMS, Database

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List of Oral Sessions

[Thursday Morning, 20th September (9:00-11:00)]

Session 31 (Main Hall):
Native Mass Spectrometry and Structural Biology

Chair: Satoko Akashi

Keynote: Joseph A. Loo

"Integrating Native Mass Spectrometry and Top-Down MS for Defining Protein Interactions Important in Biology and Medicine"

Scope of Session: The analysis of noncovalent protein complexes by mass spectrometry has advanced to the study of protein-ligand and protein-protein complexes and as large as the MDa range. In this session, the structural characterization of protein complexes of importance to biology will be discussed.

Keywords: Noncovalent complexes, Electrospray ionization, Protein, Molecular machines, Ion mobility

Session 32 (Room A):
Formation and Dissociation of Peptide Radical Ions

Chair: Dominic T.W. Chan

Keynote: Roman A. Zubarev

"Formation and Dissociation of Peptide Radical Ions"

Scope of Session: This session focuses on the recent advances in the understanding and applications of tandem mass spectrometry of peptides/proteins involving radical intermediates.

Keywords: ECD, ETD, ISD MALDI, Peptide radical ions

Session 33 (Room B-1):
JMS Award Symposium

Chair: Richard M. Caprioli (Editor-in-Chief, JMS)

Scope of Session: Spectrometry Conferences. The Fifth symposium will be held in conjunction with the 19th International Mass Spectrometry Conference, Kyoto, Japan, 15 – 21 September 2012.
5 Postgraduate Awards

· 5 awards of $1500 will be made to assist the awardees in travel and attendance at the conference.
· Each winner will receive a complimentary subscription to JMS
· The postgraduate student winners will include representatives from Europe/Africa, Asia/Oceania and the Americas.
· Each winner will present a 15-minute talk on their work in the JMS Awards Symposium.
· Each winner will receive a certificate and mention in the Journal and have the opportunity to publish their paper in the journal if they choose.

Session 34 (Room D):
MS Informatics for Identification and Characterization

Chair: Shigeki Kajihara

Keynote: David Fenyö

"The value of different types of information in MS based identification"

Scope of Session: This session will cover informatics methods for the MS-based identification of molecules including proteins, peptides, and metabolites and their application to the analysis of large data sets. A special emphasis will be placed on benchmarking of methods and testing the significance of their results.

Keywords: Database searching, Spectrum libraries, de Novo Sequencing, Significance testing, PTM localization

Session 35 (Room E):
Environment I

Chair: Peter Haglund

Keynote: Terry Bidleman

"Chiral Chemicals as Tracers of Sources and Fate Processes in a World of Changing Climate"

Scope of Session: To elucidate transport and fate mechanisms for POPs on a global scale using advanced analytical tools such as congener-specific and enantioselective analysis and efficient data evaluation.

Keywords: POPs, Chiral analysis, Fate of chemicals, Enantioselection, Congener-specific determination, Source tracking, Arctic environment

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* The titles of keynote lecture may be subject to change in the final program.

[Thursday Afternoon, 20th September (15:00-17:00)]

Session 36 (Main Hall):
Advances in Ion Mobility Mass Spectrometry

Chair: Joseph A Loo

Keynote: Michael T. Bowers

"Peptide and protein aggregation: Mechanisms, inhibition and disease"

Scope of Session: Recent advances in IM-MS instrumentation have」 impacted the
analysis of a wide range of biological molecules, from lipids, carbohydrates, peptides, and nucleic acids to larger macromolecules. The development of new IM-MS instruments and their applications to chemistry and biology, including proteomics, will be presented.

Keywords: Ion mobility, Conformation, Molecular structure, Protein, Nucleic acids, Lipids

Session 37 (Room A):
Challenges in High Resolution and High Accuracy Mass Measurement Mass Spectrometry

Chair: Evgeny Nikolaev

Keynote: Alan G. Marshall

"Mass Resolution and Mass Accuracy: How Much is Enough?"

Scope of Session: Challenges in high resolution and high accuracy mass measurement mass spectrometry" will provide a forum to present and discuss research concerning mass spectrometry instrumentation, and particularly instrumentation which can be applied to modern FTMS instruments FT ICR, Orbitraps/Kingdon and Cassini traps, multiple pass TOF instruments, Zaifman traps, Applications-related topics will include: applications of ultrahigh resolution and mass accuracy, isotopic resolution of high mass proteins, fine structure of mass peaks, elemental composition determination from accurate masses, analysis of complex systems, computational modeling, and more.

Keywords: Instrumentation, High mass resolution, High mass accuracy, FTMS, FT ICR, Orbitraps/Kingdon traps, Cassini traps, Multiple pass TOF

Session 38 (Room B-1):
Mass Spectrometry for Metabolic Diseases

Chair: Makoto Yoshino, Seiji Yamaguchi

Scope of Session: Metabolic profiling to find newborn patients with metabolic diseases has long been a key technique of MS working for biochemical and laboratory medicine. Currently, tandem mass spectrometry is used for the newborn screening to detect the patients with a wide spectrum of inborn errors of metabolism, and is identifying several amino acid, organic acid and fatty acid disorders in many countries with different programs. The Japanese Society for Biomedical Mass Spectrometry (JSBMS), a pioneering society in this field, is organizing this session to include the technical and clinical aspects of MS for metabolic disorders.

Keywords: Inborn errors of metabolism, Screening, Metabolic disease, Clinical metabolomics, Clinical mass spectrometry

Session 39 (Room D):
MS Informatics for Quantitation

Chair: David Fenyö

Keynote: Jürgen Cox

"Detection of differential expression of splice variants in the MaxQuant framework for quantitative proteomics"

Scope of Session: This session will cover informatics methods to extract quantitative information from mass spectra. The main focus will be detection and correction interference, testing the significance of measured changes in
quantity, and applications of the methods to the analysis of large data sets.

Keywords: Label-free, SILAC, Interference detection, Significance testing

Session 40 (Room E):
Environment II

Chair: Takeshi Nakano

Keynote: Peter S Haglund

"Powerful GC-ToF-MS Techniques for Quantification of Legacy Pollutants and Screening and Identification of Emerging Pollutants"

Scope of Session: To develop powerful cost-efficient techniques for quantification of legacy pollutants and screening for emerging pollutants, including hyphenated techniques and various environmental applications.

Keywords: Emerging pollutants, POPs, PPCPs, Hyphenated techniques, Polutant characterization, Prioritization, Emission and exposure assessment, Risk evaluation

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List of Oral Sessions

[Friday Morning, 21st September (9:00-11:00)]

Session 41 (Main Hall):
Chemistries of Trapped Ions and their Applications to Biological Mass Spectrometry

Chair: Gavin E. Reid

Keynote: Scott A. McLuckey
"Bioconjugation in the Gas Phase: New Chemistry for Tandem Mass Spectrometry"

Scope of Session: Ion chemistry plays a critical role in the application of mass spectrometry for the structural characterization of biological molecules in the gas-phase. This session will focus on highlighting recent advances in fundamental gas-phase ion chemistry and instrumentation development, and their application to address challenges in life science research.

Keywords: Ion activation, Dissociation, MS/MS, Proteomics, Peptide, Lipidomics, Lipid

Session 42 (Room A):
New Developments in Instruments and Detectors

Chair: Takaya Sato

Keynote: Evgeny N. Nikolaev
"From supercomputer modeling to highest mass resolution in FT ICR"

Scope of Session: Mass spectrometry is a method to determine the m/z of various compounds ionized in ion source. At the beginning of the last century, the first mass spectrometer was developed for atomic and molecular physics. Since then, various types of mass spectrometer which uses different manner to achieve mass separation and detection are invented. They cover wide target application, such as from elemental analysis to protein analysis. The new ideas and improvement of separation techniques or detection technologies are expected to continue expanding range of application. This session aims to present instrumental developments in mass separation and detection techniques including simulation or making prototype equipment.

Keywords: Instrumentation, Simulation, Detector, Ion optics

Session 43 (Room B-1):
Novel Proteomics Methodologies

Chair: Yasushi Ishihama

Keynote: Michael J. MacCoss
"Shifting Proteomics from a Hypothesis Generating Workflow to a Hypothesis Testing Workflow"

Scope of Session: Rapid progress has been made in mass spectrometry-based proteomics. However it is still a challenging task to unveil proteome world even when the state-of-the-art proteomics technologies, and novel methodologies must be developed. This session will focus on the new proteomics methodologies including SRM quantitation, post-translational modifications and other methodologies applicable to proteome-wide analysis of cells and tissues.

Keywords: Proteome-wide approach, Quantitation, Post-translational modification, Protein-protein interactions, In-depth proteome analysis

Session 44 (Room D):
Ambient Ionization

Chair: Jentaie Shiea

Keynote: Kenzo Hiraoka
"Ambient desorption/ionization mass spectrometry for minimal samples"

Scope of Session: Ambient ionization mass spectrometry has evolved and grown to become one of the most important techniques for efficiently characterizing the analytes from various surfaces and matrices. This group of the techniques differs from the traditional ionization sources in that the experiment is performed under ambient conditions without sample preparation. The technique allows direct, real-time, and high-throughput analyses and has been successfully applied to different areas within the life, health and industrial sciences. With the evolution of new designs, variants, combinations and hybrids; a number of ambient ionization techniques based on the differences in sampling/desorption (ca. nebulization, laser desorption/ablation, and thermal desorption) and ionization processes (ca. electrospray ionization and atmospheric pressure chemical ionization) were developed. The main focus of this session will be on the instrumentation of ambient ionization mass spectrometry and its applications. Potential topics include, but are not limited to:

· New ambient ionization sources
· Interface for chromatograph and ambient mass spectrometry
· Principle of ambient ionization processes
· Applications related to food safety and sciences, drug analysis, forensics, environmental chemistry, homeland security, proteomic and metabolomic studies, molecular imaging, and other chemical and biochemical researches.

Keywords: Ambient, Electrospray ionization, Atmospheric pressure chemical ionization, Sampling, Desorption

Session 45 (Room E):
Cell Biology / Cellular Pathways

Chair: Renato Zenobi

Keynote: Tsutomu Masujima
"Future of Cell Analyses and Mass Spectrometry"

Scope of Session: Mass spectrometry is now a strong analytical tool for cell biology. New methods and updated applications for cellular omics, cellular pathway analyses and single cell analyses will be discussed in this session.

Keywords: Single cell analysis, Organella, Intracellular distribution, Microanalysis, Microdisection

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