28th ISMAS-WS-2014

28th ISMAS
Symposium cum Workshop
on Mass Spectrometry

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Timber Trail Heights, Parwanoo
Himachal Pradesh – 173 220, India

Editors
S.K. Aggarwal
P.G. Jaison
Arnab Sarkar

Organised by
Indian Society for Mass Spectrometry (ISMAS), Mumbai

www.ismas.org
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Invited Talks (IT)

(The underlined names are the presenting authors)

IT - 1 Homogeneous transition metal catalysis investigated in the gas phase: mechanistic studies of the Mizoroki-Heck coupling and the regioselective Diels-Alder reaction

Mathias Schäfer, Lukas Fiebig, Julian Kuttner, Gerhard Hilt, Martin C. Schwarzer, Gernot Frenking, Nils Schlörer, Hans-Günther Schmalz

IT - 2 Mass spectrometry and immunobiology: A combinatory approach to study host defense against infections

Kavitha Subramanian Vignesh, Julio A. Landero Figueroa, Aleksey Porollo, George S. Deepe, Jr., Joseph A. Caruso

IT-3 Elementary and isotopic analysis by mass spectrometry for neutronic calculation codes validations

A. Nonell, H. Isnard, M. Aubert, L. Vio, C. Bresson, F. Chartier, T. Vercouter

IT-4 Native mass spectrometry for structural proteomics

Justin L.P. Benesch

IT-5 Imaging mass spectrometry reveals complex molecular signals of disease

Ron M.A. Heeren

IT-6 Challenges in geochemical analyses by quadrupole, time of flight and magnetic sector inductively coupled plasma mass spectrometry techniques – a comparison

V. Balaram and M. Satyanarayanan

IT-7 Study of pharmaceuticals in the environment using LC-MS tools

Saranjit Singh and Kriti Jind

IT-8 Proteomics study of hemoglobinopathy

Abhijit Chakrabarti, Suchismita Halder and Shilpita Karmakar

IT-9 Elemental and isotope fractionation in LA-ICP-MS

Roland Hergenröder
IT-10 Molecular ionization from carbon nanotube paper

Rahul Narayanan, Depanjan Sarkar, R. Graham Cooks and Thalappil Pradeep

IT-11 Recent developments in pesticide residue analysis by mass spectrometry

S.K. Raza and S. Alam

IT-12 New capabilities in inductively plasma mass spectrometry and laser ablation inductively coupled plasma mass spectrometry for the analysis of particles

Detlef Günther, Olga Borovinskaya, Luca Flamigni, Joachim Koch, Hao Wang, Daniel Tabersky, Marcel Burger, Martin Tanner

IT-13 Applications of mass spectrometry in biologics drug discovery

M. Tomlinson

IT-14 Profiling of microorganisms by mass spectrometry


IT-15 Collision induced dissociation of chiral molecules using keV ion beams


IT-16 Physics with cold stored ion beams


IT-17 Multi-isotope evidence of particulate contribution to dissolved chemical budget of the Indian Ocean

Sunil K. Singh, Satinder Pal Singh, V. Goswami and V.K. Rai

IT-18 Thermal C–H bond activation of small alkanes by metal oxides in the gas phase

M. Schlangen, H. Schwarz

IT-19 Application of ICP-MS in various fields of research

B. Kovács, É. Bödi, Á. Soós, D. Andrási
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IT-20 Mass spectrometry in radioecology research – speciation of long lived manmade radionuclides

C. Walther and M. Steppert

IT-21 The application of secondary ion mass spectrometry (SIMS) and stable isotope exchange protocols in materials science

David McPhail

IT-22 Mass spectrometry based quantitative proteomics: current and future applications in cellular signalling

Kirti Sharma

IT-23 Re-visiting MALDI: going matrix free for revisiting an old technology for health-care solutions for the future

Dipankar Ghosh

IT-24 Mass spectrometry in intercepting supramolecular assemblies of small molecules in understanding organo-catalysis by ionic liquids

Asit K. Chakraborti

IT-25 Mass spectrometry of ultrafast molecular dynamics: Prospects of bond-specific fragmentation

Deepak Mathur

IT-26 Ultrafast probing of molecules by pump-probe coincidence momentum imaging and laser assisted electron diffraction

Kaoru Yamanouchi

Short Invited Talks (IT)

(The underlined names are the presenting authors)

SIT – 1 Mass spectrometry guided elucidation of reaction mechanism of cyclic-di-AMP synthesis in Mycobacterium tuberculosis

V. Sabareesh, K. Manikandan, K.M. Sinha

SIT – 2 Dried Blood Spots (DBS) blood sampling coupled with liquid chromatography, tandem mass spectrometry (LC-MS/MS) assay to investigate pharmacokinetics and pharmacodynamics of subcutaneous injection of steroid esters in an oil vehicle.

G.K. Surindar Singh, Leo Turner, Reena Desai, Mark Jimenez, David J Handelsman
Contributory Papers (CP)
(The underlined names are the presenting authors)

CP – 1 Isotope hydrological investigation to know the recharge and groundwater flow in the western part of Deccan Traps, Maharashtra

Md. Arzoo Ansari, U. Saravana Kumar, Archana Deodhar and H.V. Mohokar

CP – 2 Hydrogeologic controls on radon-222 in the hard rock fractured aquifer of Bangalore, Karnataka

U. Saravana Kumar, Md. Arzoo Ansari, Deljo Davis and R.K. Somashekar

CP – 3 Laser desorption/ionization mass spectrometric studies on Tri-iso-amyl phosphate

P. Manoravi, B. Sreenivasulu, M. Joseph, N. Sivakumar

CP – 4 Development of standalone multifunction data acquisition module for mass spectrometer

Reju K., Kuldeep D. Joshi, Meera Murali and M.M. Gulhane

CP – 5 A microcontroller based ion gauge controller for measuring ultra high vacuum in mass spectrometers and other analytical instruments

M. Gopalakrishna, S.K Gupta

CP – 6 A novel Cu-BSA nanocomposite based vapour generation approach for the rapid determination of mercury in aqueous media by cold vapour atomic absorption spectrometry (CVAAS) and on-line flow injection inductively coupled plasma mass spectrometry (FI-ICPMS)

L. Rastogi, M.V.B. Krishna, K. Chandrasekaran, D. Karunasagar

CP – 7 Comparative analyses reveal different consequences of two oxidative stress inducers, gamma irradiation and potassium tellurite, in the extremophile deinococcus radiodurans

Anaganti Narasimha, Bhakti Basu and Shree Kumar Apte

CP – 8 Automatic striking of plasma torch in ICP-MS - a step towards total automation

Sandeep Chaudhari, Nivedita Ved, Sunita Salvi, Rajendra Babu, Prakash Abhichandani and M Gopalkrishna

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Design of velocity map imaging (VMI) mass spectrometer for studying the kinetic energy release distributions (KERDS) of polyatomic molecules


Electrospray ionisation mass spectrometric studies for arsenic speciation

**P.G. Jaison, Pranaw Kumar, D. Alamelu and S.K. Aggarwal**

Study of ionization behaviour of Sm, Gd and Eu mixture in TIMS for estimation of the composition of the radioactive isobars confined in Paul Trap

**Manoj K. Joshi, D. Alamelu, A. R. Parab and Pushpa M. Rao**

Achievable accuracy precision in the determination trace amount of uranium in Plutonium Oxide samples by ID-TIMS technique using indigenous TIMS (III)

**Pawan Kumar Singh, Diganta Gogoi, S. Srinivasan, T. Kumar**

Studies on design modifications in a thermal ionization source for improved sensitivity

**Arkadip Bhasak, R.K. Bhatia, Varun K Yadav, Madhavi Sharma, Yogesh Kumar, E.Ravisankar and V.Nataraju**

Development of quadrupole DC and ion optics power supplies for inductively coupled plasma quadrupole mass spectrometer


Development of high voltage module based ion optics supply for thermal ionisation mass spectrometer


A compact reflectron time-of-flight mass spectrometer for laser spectroscopic studies


Reaction of an ion with atom: does the rate constant depend on the charge state of the ion?

**R.K. Vatsa, P.M. Badani, S. Das, P. Sharma and K.R.S. Chandrakumar**

High precision multielement analysis on geological samples by HR-ICP-MS

**M. Satyanarayanan, V. Balaram, S.S. Sawant, K.S.V. Subramanyam, G. Vamsi Krishna**
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CP – 31  Electrospray ionization mass spectrometric studies on the relative stabilities of palladium complex with thiourea, benzoylthiourea and N,N-diethyl N'-Benzoylthiourea

V.M. Telmore, Pranaw Kumar, Sumana Paul, P.G. Jaison, D. Alamelu, S.K. Aggarwal

CP – 32  Development of gel–based loading method for determination of plutonium isotopic composition by Thermal Ionization Mass Spectrometry

Sumana Paul, Raju V. Shah, A.K. Pandey, S.K. Aggarwal

CP – 33  Comparison of α-hydroxyisobutyric acid and mandelic acid for uranyl complexation by electrospray ionization mass spectrometry

Pranaw Kumar, Sumana Paul, P.G. Jaison, V.M. Telmore, D. Alamelu, S.K. Aggarwal

Research Scholars’ Presentations (RSP)

(The underlined names are the presenting authors)

RSP - 1  Nanospheres MIP as SPE sorbent for the selective extraction of urinary benzene metabolites from urine samples followed by injector port silylation and GC-MS/MS analysis

Tejasvi Bhatia, A. Chauhan, M.K.R. Mudiam

RSP - 2  Gas phase formation of nucleobases and amino sugar from CH$_3$COONH$_4$ and NaHCO$_3$

Palwinder Singh, Amrinder Singh

RSP - 3  Application of dispersive liquid-liquid microextraction and auto-injector port silylation for the simultaneous determination of polyaromatic hydrocarbon metabolites in urine by gas chromatography-tandem mass spectrometry

Manoj Kumar Gupta, R. Jain, M.K.R. Mudiam

RSP - 4  Normal-phase HPLC determination of darunavir enantiomers on rat dried blood Spots

A.M.K. Swamy, K. Guru Prasad, R. Nageswara Rao

RSP - 5  Metabolomics of pseudomonas sp. outer membrane vesicles (OMVs)

Akanksha Srivastava, Pallavi Lahiri, and Dipankar Ghosh
RSP - 6 Geographically drive chemical changes analysis in dioecious Tinospora cordifolia plant population using mass spectrometric techniques 

_V. Bajpai, A. Singh, S. Kumar and B. Kumar_

RSP - 7 High resolution precipitation records from a stalagmite of Kotumsar cave, Chhattisgarh

_Shradhha Band, M.G. Yadava, Kaushik Sree, R. Ramesh, V. J. Polyak and Y. Asmerom_

RSP - 8 Characterization of oxidative and photolytic degradation products of pimozone by using LC-MS/TOF and LC-MSn

_Pavan Kumar Raju Suraparaju, Mallikarjun Narayananam and Saranjit Singh_

RSP - 9 Tracing sources of dissolved inorganic carbon using δ¹³C in a tropical eutrophic estuary (Cochin, India)

_P.S. Bhavya, Sanjeev Kumar, G.V.M. Gupta, V. Sudheesh, Sudharma_

RSP - 10 Plasma protein binding and pharmacokinetic study of bound versus unbound fidarestat by ultrahigh-performance liquid chromatography mass spectrometry

_Murali Mohan Bhandi, Roshan M. Borkar, Ajay P. Dubey, Sanjay K. Banerjee and R. Srinivas_

RSP - 11 Identification and characterization of garlic metabolites in rat plasma by LC-MS and NMR: target identification of metabolites by in silico studies

_Roshan M. Borkar, Tarak Nath Khatua, Anvesh Jelapally, Murali Mohan Bhandi, Sanjay K Banerjee and R. Srinivas_

RSP - 12 Isotopic and geochemical studies of saline-alkaline soils, water and sediments of the ganga river system: implications to erosion and carbon cycle

_Jayati Chatterjee and Sunil K. Singh_

RSP - 13 Tracking the provenance of rain particulates from Goa using Sr and Nd Isotopes

_V. Chinni, Sunil K. Singh, Vinai K. Rai and V. Ramaswamy_

RSP - 14 Ultra performance liquid chromatography atmospheric pressure photoionization high resolution mass spectrometry for determination of multiclass pesticide residues

_Pragnay Deme and U.V.R. Vijaya Saradhi_

RSP - 15 Dissolved Sr and its isotopes in estuaries of eastern coast of India: Impact of submarine groundwater discharge

_K. Damodara Rao and Sunil K. Singh_

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Reconstructing redox conditions of mesoproterozoic-early cambrian seawater using $^{59}$Mo

Sneha Sawant, Sunil K. Singh and Vinai K. Rai

Sr isotope composition of atmospheric mineral dust at Ahmedabad: provenance and seasonal variability

A.K. Sudheer, S. K. Singh and R. Rengarajan

Ionic liquid based dispersive liquid–liquid micro extraction followed by RP-HPLC determination of saquinavir in rat serum: application to pharmacokinetics

N. Narendra Varma, Ch. Gangu Naidu, R. Nageswara Rao

Separation of isomeric betaines and dimethyl amino acids by liquid chromatography-mass spectrometry

V. Naresh Chary, B. Sudarshan Reddy and S. Prabhakar

Vendors’ Talks (VT)

(The underlined names are the presenting authors)

Overview of recent applications done with CAMECA SIMS Instruments in various fields

P. Saliot, P. Peres, F. Horreard, M. Schuhmacher

Advances in high precision isotope ratio measurements using Thermal Ionization and Noble Gas Mass Spectrometers

Zenon Palacz

The Nu Instruments PERSPECTIVE stable isotope ratio mass spectrometer

John Cantle

Dioxin Screening & confirmation by GCMSMS & HRGCMS-total workflow solutions

Hans-Joachim Huebschmann

Thermo scientific delta ray isotope ratio infrared spectrometer: field deployable CO₂ analyzer

H.J. Jost, Eric Wapelhorst, Hans-Juergen Schlueter, Oliver Kracht, Jens Radke, Andreas W. Hilkert

Poster Presentation Schedule

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