Australian and New Zealand Society for Mass Spectrometry Conference

Online, 21-25 November 2021

NOTE: All times are Australian Eastern Standard Daylight Saving (Canberra / Sydney) Time

Sunday, 21 November 2021	
	Chairs: ***Erin Humphries,*** *Children's Medical Research Institute and* ***Hyun Lee,*** *University of New South Wales*
13:00 - 15:00	Early Careers Panel ***Dr Heather Patsiouras (Waters Australia), Dr George Khairallah (Accurate Mass Scientific), Dr Gus Grey (University of Auckland), Dr Sarah Hancock (University of New South Wales)***
15:00 - 15:40	Afternoon Tea
15:40 - 16:00	**Conference Opening**
	Acknowledgement of Country & Convenor Welcome ***Dr Adam J. Carroll****, Australian National University, Canberra, Australia*
16:00 – 17:00	Opening Keynote Address ***Professor Margaret Sheil****, Vice-Chancellor and President, Queensland University of Technology, Australia*

Monday, 22 November 2021	
	Chair: *Dr Tara Pukala,* *University of Adelaide*
09:00 – 10:00	2021 Morrison Medal Presentation *Advanced Mass Spectrometry Tools for Illuminating the 'Hidden' Diversity and Structural Complexity of the Lipidome* ***Professor Gavin Reid****, Bio21 Institute, University of Melbourne, Australia*
	Advances in Instrumentation & Methods **Sponsored by** Mass Dynamics **Chair: *Dr Tara Pukala,*** *University of Adelaide*
10:00 – 10:20	Ambient Pressure Ion Funnel: Concepts, Simulations and Analytical Performance ***Associate Professor W. Alexander Donald****, University of New South Wales, Australia*
10:20 – 10:40	Internal fragment assignments enhance top-down protein sequencing experiments that are beneficial for localising post-translational modifications and protein-ligand binding sites ***Dr Muhammad Zenaidee****, Australian Proteome Analysis Facility, Macquarie University, Australia*
10:40 – 11:00	Nanosecond pulsed dielectric barrier discharge ionisation-high-resolution differential ion mobility mass spectrometry for volatile biomarker analysis ***Diana Zhang,*** *University of New South Wales, Australia*
11:00 - 11:20	Morning Tea
	Metabolomics and Lipidomics **Sponsored by** BRUKER **Chair: *Associate Professor Todd Mitchell,*** *University of Wollongong*
11:20 – 11:40	A discovery platform for fatty acids using untargeted charge-switch derivatization UPLC-OzID-MS and untargeted large-scale data analysis ***Dr. Jan Philipp Menzel****, Queensland University of Technology, Australia*
11:40 – 12:00	Broad Quantitative Lipid Profiling Using High-Throughput Targeted UHPLC-MS/MS ***Miss Monique Ryan****, Murdoch University, Australia*
12:00 - 13:00	Lunch
	Environmental and Forensic **Sponsored by** pm SEPARATIONS **Chair: *Christopher Fitzgerald,*** *Australian National University*

13:00 – 13:20	3-O-Methyldopa as an indicator of dopaminergic manipulation in equine plasma ***Miss Bethany Keen**, University of Technology Sydney, Australia*
13:20 – 13:40	Lipidomics for enhanced equine anti-doping using LC-HRMS ***Miss Kathy Tou**, University of Technology Sydney, Australia*
13:40 – 14:00	GC-MS profiling of equine urine for longitudinal assessments ***Madysen Elbourne**, University of Technology Sydney, Australia*
14:00 – 14:20	Energy-Resolved Fragmentation Aiding the Structure Elucidation of Steroid Biomarkers ***Mr Christopher Fitzgerald**, Australian National University, Australia*
14:20 – 14:40	Afternoon Tea
	Advances in Instrumentation & Methods **Sponsored by** Mass Dynamics **Chair: *Associate Professor W. Alexander Donald,** University of New South Wales*
14:40 - 15:40	2021 Bowie Medal Presentation ***Professor Michelle Colgrave**, Commonwealth Scientific & Industrial Research Organisation and Edit Cowan University, Australia*
15:40 – 16:00	FAIMS based fractionation enables proteomic/glycoproteomics analysis in a single analytical run ***Dr Nichollas Scott**, University of Melbourne, Australia*
16:00 – 16:20	Electron Activated Dissociation in Zeno-TOF Mass Spectrometer ***Takashi Baba**, Sciex, Canada*
16:20 – 16:40	Activity and Structural Screening of β-Diketonate Assemblies by High Throughput Travelling Wave Ion Mobility-Mass Spectrometry ***Mr Oscar Lloyd Williams,** University of New South Wales, Australia*
16:40 - 17:00	Development and implementation of a Multi-reflecting TOF for Spatially Resolved Metabolomics ***Dr James. I. Langridge**, Waters MS Technologies Centre, United Kingdom*

Tuesday, 23 November 2021	
09:00 – 10:00	Keynote Address: *Development and Applications of Ultraviolet Photodissociation Mass Spectrometry for Biological Applications* ***Professor Jennifer S. Brodbelt,*** *University of Texas, Austin, USA*
	Ion Chemistry and Spectroscopy **Chair: *Professor Adam Trevitt,*** *University of Wollongong* **Sponsored by** Journal of the American Society for Mass Spectrometry
10:00 – 10:20	Structural Analysis of Glyphosate and Aminomethylphosphonic Acid (AMPA) Metal Complexes using Ion Mobility-Mass Spectrometry and Computational Methods ***Olivia Rusli,*** *University of New South Wales, Australia*
10:20 – 10:40	On the mechanism of theta capillary nanoelectrospray ionisation for the formation of highly charged protein ions directly from native solutions ***Susannah Brown,*** *University of New South Wales, Australia*
10:40 – 11:00	Palladium-mediated CO2 extrusion Followed by insertion of (hetero)cumulenes for the synthesis of amidines, amides and alkenes: translating fundamental gas and solution phase mechanistic studies to develop synthetic protocols ***Yang Yang,*** *The University of Melbourne, Australia*
11:00 – 11:20	Adventures in Gas-Phase Organometallic Ion Chemistry: From Exploring Mechanisms to Inventing New Reactions. ***Professor Richard O'Hair,*** *University of Melbourne, Australia*
11:20 – 11:40	Morning Tea
	Ion Chemistry and Spectroscopy **Chair: *Professor Adam Trevitt,*** *University of Wollongong* **Sponsored by** Journal of the American Society for Mass Spectrometry
11:40 – 12:00	Isomerism of protonated para-aminobenzoic acid catalysed by a single methanol ***Mr Boris Ucur,*** *University of Wollongong, Australia*
12:00 – 12:20	Influences of Internally Oriented Electric Fields on the Protomer Specific Reactions of Quinazoline Distonic Radical Cations ***Mr. Oisin Shiels,*** *University of Wollongong, Australia*
12:20 – 12:40	Exploring substituent effects in decarboxylation of cationic zinc complexes. [(phen)Zn(O2CC6H4X)]+ ***Mr. Joshua Rand,*** *The University of Melbourne, Australia*
12:40 – 13:00	Lunch
13:00 – 14:40	**ANZSMS AGM**

14:40 – 15:00	Afternoon Tea
	Metabolomics and Lipidomics **Sponsored by** **Chair: *Associate Professor Todd Mitchell,*** *University of Wollongong*
15:00 – 15:20	Ultra-high resolution ozone-induced dissociation uncovers triacylglycerol structural diversity in human plasma ***Dr Berwyck Poad,*** *Queensland University of Technology, Australia*
15:20 – 15:40	Single-cell lipidomics by chip-based nanoelectrospray ionisation mass spectrometry ***Dr Sarah Hancock,*** *University of New South Wales, Australia*
15:40 – 16:00	Multi-omic Comparison of Growth Dependent Adaptation ***Madie Nuske,*** *University of Melbourne, Australia*
16:00 - 17:00	Keynote Address: *Isotopes in metabolic research: example of non-targeted 13C metabolite analysis to examine metabolic re-orchestration in leaves when gas-exchange conditions vary* ***Professor Guillaume Tcherkez****, Australian National University, Australia and University of Angers, France*

Wednesday, 24 November 2021	
	Chair: *Dr Matthew Taylor,* *CSIRO*
09:00 – 10:00	Keynote Address: *Quantification of Proteomic and Post-translational Changes during Kidney Injury and Protective Effects in Response to Genetic and Dietary Interventions* ***Associate Professor Birgit Schilling****, The Buck Institute, California, USA*
10:00 – 11:00	Keynote Address: Environmental and Forensic ***Professor Kimberly Prather****, Scripps Institute of Oceanography, University of California, San Diego, USA*
11:00 – 11:20	Morning Tea
	Environmental and Forensic **Sponsored by** pm SEPARATIONS **Chair: *Dr Matthew Taylor,*** *CSIRO*
11:20 – 11:40	Improving the analysis of non-conventional cationic and zwitterionic per-and polyfluoroalkyl substances in biosolids ***Mr Hyun Eui Lee,*** *University of New South Wales, Australia*
11:40 – 12:00	An Early Warning System for Illicit Drug Use: DART-MS for Trace Residue Analysis of Discarded Drug Packaging Samples and Disposed Drug Paraphernalia ***Mr. Henry West,*** *The University of Melbourne, Australia*
12:00 – 12:20	Quantifying methamphetamine in air, waste-water and house-hold furnishings, fabrics and foods to determine extent of third-hand exposure to methamphetamine (T.H.E.M). ***Associate Professor Stewart Walker,*** *Flinders University, Australia*
12:20 – 12:40	A liquid chromatography tandem mass spectrometry method for the quantification of selected analgesics and their metabolites in wastewater influent ***Fahad Ahmed,*** *The University of Queensland, Australia*
12:40 – 13:20	Lunch
	Metabolomics and Lipidomics **Sponsored by** BRUKER **Chair: *Professor Gavin Reid,*** *University of Melbourne*
13:20 – 13:40	Using LC-DAD-MS and IM-MS Methods to Characterise Anthocyanin Profiles in Novel and Commonly Consumed Plants ***Mr River Pachulicz,*** *The University of Adelaide, Australia*

13:40 – 14:00	Tightening the belt on lipid structural elucidation: the associations between glycerophospholipid sn- and DB isomers ***Mr Reuben Young,*** *Queensland University of Technology, Australia*
14:00 – 14:20	Characterization of Brain Derived Extracellular Vesicle Lipids in Alzheimer's Disease ***Huaqi Su,*** *The University of Melbourne, Australia*
14:20 – 14:40	Afternoon Tea
14:40 – 15:00	The Lipidomic Signatures of Colorectal Cancer ***Mr Tim Salita****, Bio21 Institute, University of Melbourne, Australia*
15:00 – 15:20	Development of LC-MS/MS method for quantification of Somatostatin in blood. ***Ramneek Kaur,*** *Western Sydney University, Australia*
15:20 – 15:40	Region Specific Losses of Phospholipid Derived Docosahexaenoic Acid in the Putamen of Huntington's Patients ***Miss Gabrielle Phillips,*** *University of Wollongong, Australia*
15:40 – 16:00	Refreshment Break
16:00 - 17:00	Keynote Address: Clinical and Diagnostics ***Professor Maria Fuller****, The University of Adelaide Medical School*

Thursday, 25 November 2021	
09:00 – 10:00	Keynote Address: Mass Spectral Imaging ***Dr Shane Ellis**, University of Wollongong*
	Mass Spectral Imaging **Chair: *Dr Gus Grey,** University of Auckland*
10:00 – 10:20	Imaging of nutrient and pharmaceutical transport in the ocular lens with MALDI mass spectrometry ***Dr Gus Grey,** University of Auckland, New Zealand*
10:20 – 10:40	Evaluation of Glucose uptake and metabolism in the normal bovine lens by MALDI imaging mass spectrometry ***Ali Zahraei,** The University of Auckland, New Zealand*
10:40 – 11:00	More Ions from Less Sample: Efficient Imaging of Aromatic Antioxidants Using Sequential Matrix-Assisted Laser Desorption and Resonant Photoionisation ***Ms Tassiani Sarretto,** The University of Wollongong, Australia*
11:00 – 11:20	Exploiting Laser Post-Ionisation Matrix-Assisted Laser Desorption/Ionisation (MALDI) Mass Spectrometry Imaging for Enhanced Spatial Probing of Glycosphingolipid Metabolism in Parkinson's Disease Model ***Shadrack Mutuku,** The University of Wollongong, Australia*
11:20 – 11:40	Morning Tea
	Advances in Instrumentation & Methods **Sponsored by** Mass Dynamics **Chair: *Associate Professor W. Alexander Donald,** University of New South Wales*
11:40 – 12:00	Extending differential ion mobility separation of proteoform isomers to the top-down range ***Miss Xiaojing Huang,** University of New South Wales, Australia*
12:00 – 12:20	Small-Footprint, Field-Portable LC/MS System for On-Site Analysis of Per- and Polyfluoroalkyl Substances in Soil ***Mohamed Hemida,** University of Tasmania, Australia*
12:20 – 13:40	Lunch
	Native Mass Spectrometry / Structural Biology **Chair: *Dr Tara Pukala,** University of Adelaide*
13:40 – 14:00	Biophysical characterisation of DNA triplexes for antigene technology ***Jack Klose,** University of Adelaide, Australia*

14:00 – 14:20	Hydrogen deuterium exchange mass spectrometry applied to the identification of small molecule binding sites in Escherichia coli CoaE ***Christina Spry,*** *The Australian National University, Australia and* ***Caryn Hepburn,*** *Waters Australia*
14:20 – 14:40	Afternoon Tea
	Chair: *Associate Professor W. Alexander Donald,* *University of New South Wales*
14:40 – 15:00	Rapid Response to Pandemics: Identification of novel antivirals using native mass spectrometry ***Dr Miaomiao Liu,*** *Griffith University, Australia*
15:00 – 15:20	Multiplexed screening of thousands of natural products for protein binding using native mass spectrometry ***Mr Jack Bennett,*** *University of New South Wales, Australia*
15:20 – 15:40	Native ion-mobility MS unravels the aggregation dynamics of amyloid fibril-forming proteins and their interactions with molecular chaperones ***Dr Blagojce Jovcevski,*** *University of Adelaide, Australia*
15:40 – 16:00	Break
16:00 – 17:00	Keynote Address: Native Mass Spectrometry / Structural Biology ***Professor Michal Sharon****, Weizmann Institute of Science, Israel*
17:00 - 17:30	Award Announcements and Conference Close ***Associate Professor W. Alexander Donald,*** *University of New South Wales and* ***Dr Adam J. Carroll****, Australian National University, Canberra, Australia*

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