3rd Queensland Mass Spectrometry Symposium
Delegate handbook

6-7 December 2018

Queensland University of Technology
Gardens Point Campus

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Symposium Program

Thursday 6 December 2018

Time	Activity	Venue
8:30am	**Registration**	Kindler Theatre (P421), P Block
9:00am	**Welcome and opening remarks** *Associate Professor Michelle Hill (QIMR Berghofer)*	"
9:10am	**Symposium Session 1** *Chair: Associate Professor Michelle Hill (QIMR Berghofer)* Professor Scott McLuckey (Purdue University, USA) *Novel gas-phase chemistries and mass analysis strategies using electrodynamic and electrostatic ion traps* *(40 min)* Professor Balz Kamber (QUT) *Elemental mapping with laser-ablation inductively-coupled-plasma mass-spectrometry (LA-ICP-MS): opportunities, technical developments and future applications* *(20 min)* Ms Kristina Jovic (QUT) *Correlating in-depth mechanistic understanding with mechanical properties of high-temperature resistant cyclic imide copolymers* *(20 min)*	"
10:30am	Morning tea	L4 Concourse, P Block
11:00am	**Symposium Session 2** *Chair: Dr Berwyck Poad (QUT)* Dr Brett Hamilton (UQ) *Using mass spectrometry imaging to study creatures of the sea* *(20 min)* Mr Jeremy Koelmel (University of Florida, USA) *Automated tools for lipidomic workflows and applications to environmental lipidomics* *(20 min)* Dr Tianfang Wang (University of the Sunshine Coast) *Negative ion mass spectrometry is a viable tool to study post-translational modifications of deprotonated peptides* *(20 min)*	Kindler Theatre (P421), P Block
12:00pm	Lunch	L4 Concourse, P Block
12:45pm	**Central Analytical Research Facility (CARF) tours**	L6, P Block

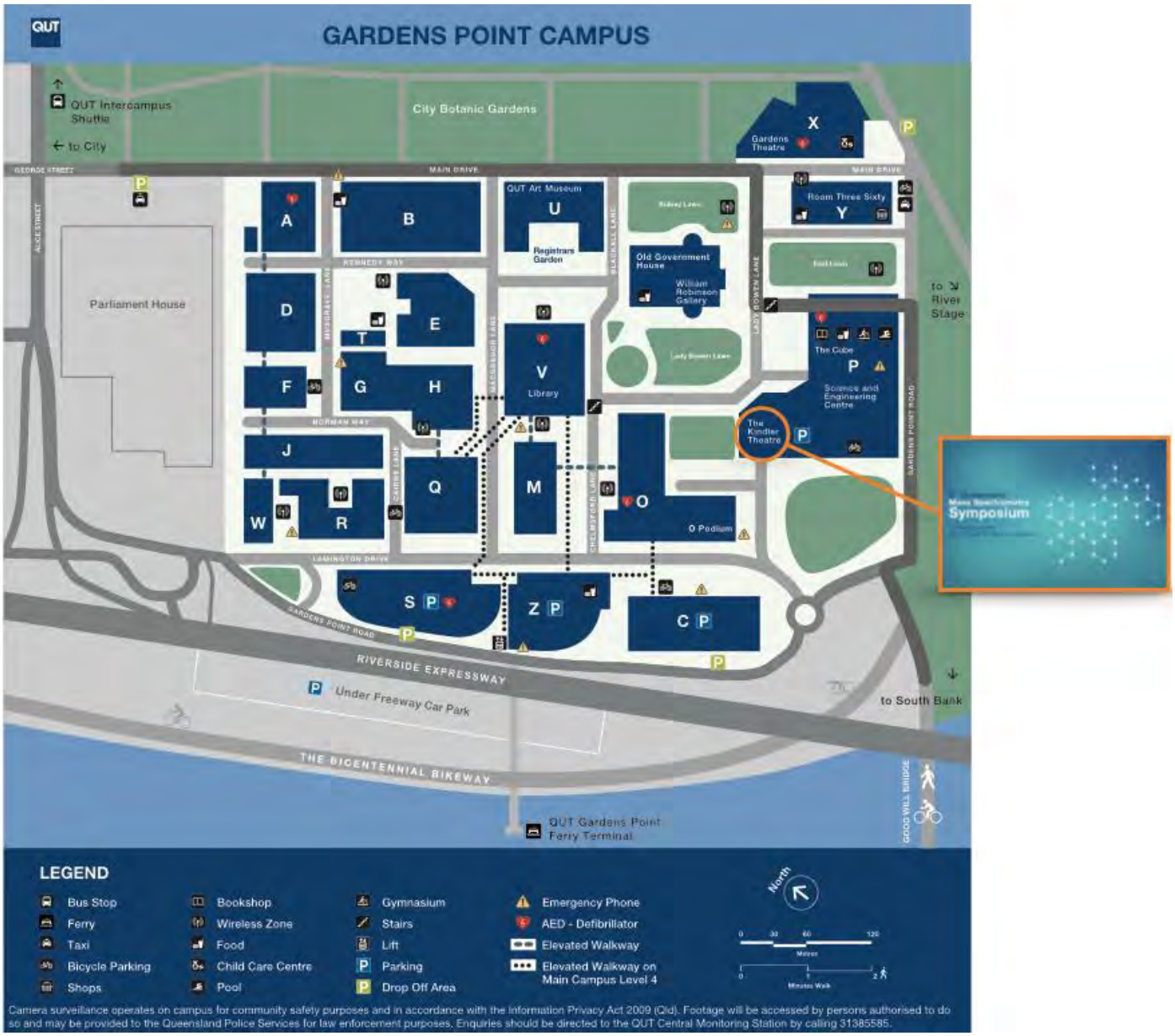
1:15pm	**Symposium Session 3** *Chair: Associate Professor Ben Schulz (UQ)* SCIEX Workshop *Dr Yves Le Blanc (Associate Chief Scientist, SCIEX)* *From EID to ECD; Alternative Fragmentation Technology for LC-MS Applications* *(45 min)* Shimadzu Workshop *Chris Bowen (Shimadzu Australia)* *Introducing the Shimadzu 9030 high sensitivity, high stability QTOF design and its implementation for untargeted DIA lipid analysis* *(45 min)*	Kindler Theatre (P421), P Block
2:45pm	Afternoon tea	L4 Concourse, P Block
3:15pm	**Symposium Session 4** Lightning Talks *Chair: Dr David Marshall (QUT)* James Carter (Queensland Health) Tobias Nitsche (QUT) Kathirvel Alagesan (Griffith University) Cassandra Pegg (UQ) John Caulfield (UQ) Utpal Bose (CSIRO) Rebecca Lane (UQ) Keshava Datta (QIMR) Edward Kerr (UQ) Zainab Noor (Macquarie University) Andreia Almeida (Griffith University) Lin Luo (UQ) (*75 min*)	Kindler Theatre (P421), P Block
4:30pm	**Poster Session**	The Cube

Friday 7 December 2018

Time	Activity	Venue
8:30am	**Registration**	Kindler Theatre (P421), P Block
9:00am	**Welcome and introduction of QUT Vice-Chancellor Professor Margaret Sheil AO** *Professor Stephen Blanksby (QUT)*	"
9:05am	**Opening remarks** Professor Margaret Sheil AO (QUT Vice-Chancellor)	
9:10am	**Symposium Session 5** *Chair: Professor Stephen Blanksby (QUT)* Mr Martin Green (Waters, UK) *A multi-function cyclic ion mobility – mass spectrometry system* *(40 min)* Dr Branka Miljevic (QUT) *From the Great Barrier Reef to Antarctica: chasing sulfuric acid using chemical ionisation mass spectrometry* *(20 min)* Mrs Cindy Giles (Biosecurity Queensland) *Determination of veterinary drug residues in animal tissues using LC-MS/MS* *(20 min)*	"
10:30am	Morning tea	L4 Concourse, P Block
11:00am	**Symposium Session 6** *Chair: Dr Pawel Sadowski (QUT)* Dr Michelle Colgrave (CSIRO) *A land-based source of omega-3 oils: how proteomics was used for safety assessment* *(20 min)* Associate Professor Ben Schulz (UQ) *Bottoms up proteomics! The dynamic beer proteome* *(20 min)* Associate Professor Michelle Hill (QIMR Berghofer) *Circulating biomarkers for early cancer detection – challenges and strategies* *(20 min)* Dr Harsha Gowda (QIMR Berghofer) *MEK activation mediates erlotinib resistance in head and neck squamous cell carcinoma* *(20 min)*	Kindler Theatre (P421), P Block
12:20pm	Lunch	L4 Concourse, P Block
12:45pm	**CARF Tours**	L6, P Block
1:30pm	**Symposium Session 7** *Chair: Dr Rajesh Gupta (QUT)*	Kindler Theatre (P421), P Block

	ThermoFisher Scientific Workshop *Steve Binos (ThermoFisher Australia)* *Novel approaches for improved small molecule identification and characterisation using Orbitrap ID-X tribrid mass spectrometer* *(45 min)* Perkin Elmer Workshop *Dr Pawel Sadowski (QUT)* *Automated Proteomics Workflows* *(45 min)*	
3:00pm	Afternoon tea	L4 Concourse, P Block
3:30pm	**Symposium Session 8** *Chair: Dr Charlotte Allen (QUT)* Dr David Beale (CSIRO) *Characterisation of environmental pollution and ecosystem health of a subtropical marine port using omics-based approaches* *(20 min)* Mr Jack Gao (UQ) *Enantiomeric profiling of amphetamine and methamphetamine in wastewater: a 7-year study in Queensland* *(20 min)* Dr Arun Everest-Dass (Griffith University) *Altered glycosylation enables increased metastasis in human colon cancer xenografts* *(20 min)*	Kindler Theatre (P421), P Block
4:30pm	**Poster Session/Facilities Showcase/Awards Session**	The Cube

QUT Gardens Point campus



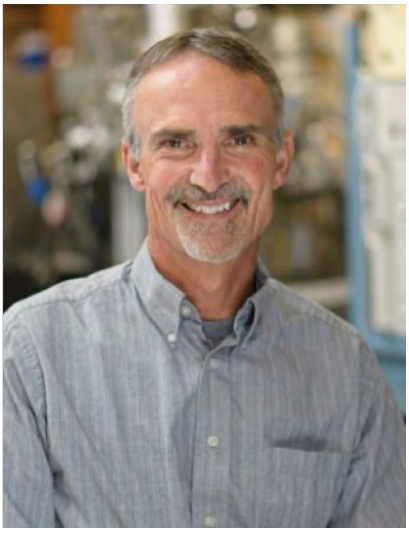
Keynote speaker

Thursday 6 December – Symposium Session 1 – 9:10am

Novel gas-phase chemistries and mass analysis strategies using electrodynamic and electrostatic ion traps

Professor Scott A. McLuckey
Purdue University, USA

Biography:



Scott A. McLuckey received his BS in Chemistry at Westminster College in 1978 and doctorate in Analytical Chemistry at Purdue University in 1982. He then served as a Postdoctoral Fellow at the FOM Institute for Atomic and Molecular Physics in Amsterdam, The Netherlands until late 1983. He was later awarded a Wigner Fellowship at Oak Ridge National Laboratory in the Analytical Chemistry Division. While at Oak Ridge, he served in such capacities as Group Leader, Organic and Biological Mass Spectrometry, and Section Head of Analytical Spectroscopy within the Chemical Sciences Division. In 2000, he moved to Purdue University as Professor of Chemistry. In June 2008, he was named the John A. Leighty Distinguished Professor of Chemistry at Purdue. He has served as an Associate Department Head for 10 years and as Head of the Analytical Chemistry Division for five years.

Dr. McLuckey's research emphases have been in the areas of gas-phase ion chemistry and instrumentation for organic and biological mass spectrometry. Fundamental aspects of ionisation, unimolecular reactions and bi-molecular reactions have been studied with the goal of improving the capabilities of analytical mass spectrometry. Ion activation, ion/molecule reactions, and ion/ion reactions have been major focal areas within the context of the mass spectrometry/mass spectrometry experiment. Instrumentation for tandem mass spectrometry has also been highlighted with emphasis on electrodynamic ion traps, electrostatic linear ion traps and ion trap/hybrid instruments. This research has been described in over 350 papers appearing in the peer-reviewed literature.

His current research focuses on the identification and characterisation of macro-molecules, primarily via whole molecule tandem mass spectrometry, ion/ion reaction chemistry and development of the electrostatic linear ion trap as a high-performance tandem mass spectrometer. Recognition for the work has included the Biemann Medal from the ASMS in 1997, the Curt Brunneé Award from the IMSF in 2000, the ACS Division of Analytical Chemistry Chemical Instrumentation Award in 2007, the ACS Field and Franklin Award in mass spectrometry in 2012, the ASMS Distinguished Contribution Award in 2016, the Thomson Medal from the IMSF in 2016 and the EAS Award in Mass Spectrometry in 2017.

Invited speakers and oral presentations

Thursday 6 December – Symposium Session 1 – 9:10am

Elemental mapping with laser-ablation inductively-coupled-plasma mass-spectrometry (LA-ICP-MS): opportunities, technical developments and future applications

Professor Balz Kamber
School of Earth, Environmental and Biological Sciences, QUT

Abstract:
The production of elemental and isotopic 'chemical' maps of diverse materials (geological, biological, engineered compounds) by LA-ICP-MS is enjoying rapidly growing popularity. The development of ablation systems built around Excimer UV lasers, the transfer of laser aerosols to the ICP torch with capillary systems and ever-more sensitive mass spectrometers have contributed to the wide applicability of the method. The most recent technical progress with laser optics and signal transfer now permits more rapid (and thus more affordable) acquisition of elemental maps and is pushing quadrupole-ICP-MS to (and one might argue, beyond) the limits of their capabilities.

In this presentation, these technical developments will be summarised for a general mass spectrometry audience and illustrated with examples, including the post-analysis extraction of quantitative data from maps. Exciting breakthroughs have been enabled, for example, in the study of environmental conditions recorded by coral growth, the delivery of fluids precipitating ore deposits, the evolution of volcanic magma feeder systems [1], and the targeting of cancer drugs in mouse tissue.

A case will be made that for many applications of LA-ICP-MS, conventional spot analysis, whereby a cylindrical volume (typical aspect ratio of width to depth >2) of material is ablated below the visible sample surface could soon be superseded with shallow (<2 microns ablation) quantitative maps [1]. If published as on-line datasets, such maps could afford a more objective means of signal integration, provide more intuitive context for readers to understand preferred data integration and offer higher value long-term data legacy. The presentation will conclude with a look to the future of trace elemental mapping, comparing Synchrotron-, Secondary Ion Mass Spectrometry and LA-ICP Time-of-Flight MS approaches and their potential untapped application areas.

[1] Petrus, J. A., D. M. Chew, M. I. Leybourne, and B. S. Kamber. "A new approach to laser-ablation inductively-coupled-plasma mass-spectrometry (LA-ICP-MS) using the flexible map interrogation tool 'Monocle'." Chemical Geology 2017, 463, 76-93, doi.org/10.1016/j.chemgeo.2017.04.027

Correlating in-depth mechanistic understanding with mechanical properties of high-temperature resistant cyclic imide copolymers

Ms Kristina Jovic
School of Chemistry, Physics and Mechanical Engineering, QUT

Abstract:
Kristina J. Jovic, Thomas Richter, Christiane Lang, James P. Blinco and Christopher Barner-Kowollik

Based on their outstanding properties, polyimides have received an increased interest for applications as advanced materials. One specific class of polyimides are poly(methacrylimides) (PMI). PMIs can exceed a mechanical stiffness (Young's modulus) of greater than 6 GPa, a Tg close to 200 °C, and feature high-temperature resistance.

So far there exists no coherent mechanistic picture that unambiguously links the thermal and mechanical properties of the generated polymers with the molecular changes along the lateral polymer chain. Based on a copolymer of tert-butylmethacrylate (t-BMA) and N-isopropylacrylamide (NIPAM), we developed an in-depth mechanistic understanding of the molecular behaviour upon thermal treatment and were able to correlate this understanding with the mechanical properties of the resulting materials.

Based on nuclear magnetic resonance (NMR), infrared (IR) spectroscopy, high-resolution mass spectrometry (HRMS) coupled to size-exclusion chromatography (SEC), tandem MS (MS/MS), thermogravimetric analysis (TGA) and nanoindentation, we correlate the time and temperature dependent cyclization process and optimize the system to achieve the highest Tg and E-modulus.

Thursday 6 December – Symposium Session 2 – 11:00am

Using mass spectrometry imaging to study creatures of the sea

Dr Brett Hamilton
University of Queensland

Abstract:
Brett R Hamilton[1,2], Karen L Cheney[3], Matthias Floetenmeyer[1], Mary J Garson[4], Bruno Madio[5], Steve Peigneur[7], Yanni K. Y. Chin[5], Sónia Troeira Henriques[5], Jennifer J. Smith[5], Ben Cristofori-Armstrong[5], Zoltan Dekan[5], Berin A. Boughton[6], Paul F. Alewood[5], Jan Tytgat[7], Glenn F. King[5], Eivind A.B. Undheim[2], Roger Wepf[1]

1. Centre for Microscopy and Microanalysis, The University of Queensland, St Lucia, 4072.
2. Centre for Advanced Imaging, The University of Queensland, St Lucia, 4072.
3. School of Biological Sciences, The University of Queensland, St Lucia, 4072.
4. School of Chemistry and Molecular Biosciences, The University of Queensland, St Lucia, 4072.
5. Institute for Molecular Bioscience, The University of Queensland, St Lucia, 4072
6. Metabolomics Australia, School of Biosciences, The University of Melbourne, Parkville, 3010
7. Toxicology and Pharmacology, University of Leuven, Leuven 3000, Belgium

Mass Spectrometry imaging (MSI) analysis of histological sections from biological specimens has, in recent years, enabled the association of specific molecules with the morphological structure of the tissue. The spatial resolution achievable using MSI, using Matrix Assisted Laser Desorption Ionisation (MALDI) as the ionisation process, is limited by the laser size and matrix crystal size. Fundamentally, MALDI imaging experiments are two-dimensional experiments, typically carried at spatial resolution of 40-100µm, although spatial resolution can be reduced to better than 10µm in certain situations.

Here I will present two examples from recent methodological developments which we have performed using understudied marine organisms. In the first study we have investigated ultrathin cryosections of high-pressure nitrogen frozen tissue by MALDI-TOF. Specifically, we have been working with the Mantle Dermal Formations (MDFs) present in the outer rim of *Chromodoris kuiteri*, a nudibranch species found in the coastal waters of Queensland. It has been hypothesised that *C. kuiteri* sequesters latrunculin-A, which is ingested from some of the sponges the nudibranch feeds upon, to the MDF structures found in the outer rim of the organism.

Sea anemones are a relatively understudied organism, despite being a repository of a large number of biologically active peptides. During this study we describe, using a combination of transcriptomic, proteomic, histological techniques, MALDI-TOF Imaging and MALDI-FT-ICR Imaging, the discovery of a new, sixth type of voltage-gated potassium channel (K_V) toxin from sea anemones. The newly discovered toxin named, κ-actitoxin-Ate1a (Ate1a), is the shortest sea anemone toxin reported to date, and it adopts a novel three-dimensional structure that we named the Proline-Hinged Asymmetric β-hairpin (PHAB) fold. It appears that Ate1a is a predatory toxin immobilising the prey via the inhibition of Shaker-type K_V channels. This activity is supported by mass spectrometry imaging and bioassay data.

Automated tools for lipidomic workflows and applications to environmental lipidomics

Mr Jeremy Koelmel
University of Florida, USA

Abstract:

Jeremy P Koelmel[1], Li Yang[2,] John A. Bowden[3], Justin E. Campbell[4], Ulrich Stingl[5], Timothy J. Garrett[1]

1. Department of Pathology, Immunology and Laboratory Medicine, University of Florida
2. BlockTEST, Boston, MA
3. Center for Environmental and Human Toxicology and Department of Physiological Sciences, University of Florida
4. Smithsonian Marine Station at Fort Pierce
5. Institute of Food and Agricultural Sciences, University of Florida

Lipidomics, the comprehensive measurement of lipids, is an emerging field with promising potential in clinical and environmental science, materials chemistry and a range of other applications. Changes in lipid concentrations can be used to determine mechanisms and/or indicators of disease and other biological perturbations. Lipids utility stem from their diversity in structure and important biological functions, as well as the fact that lipids often are more sensitive to environmental-organism interactions and phenotypical expression than proteins and genes. Increasing the coverage of identified lipids subsequently increases the likelihood of determining biomarkers and understanding biological mechanisms.

To this end, we have developed LipidMatch [1], a rule-based software for lipid identification, which contains the largest, to date, open source *in-silico* lipid fragmentation libraries. We have also developed data-acquisition strategies and scripts [2] which increase coverage of lipid fragmentation. For routine liquid chromatography high-resolution tandem mass spectrometry lipid analysis we recently released a software named LipidMatch Flow, which covers all steps in the lipidomics workflow. These steps include data conversion, peak picking, blank filtration, annotation, combining negative and positive ion mode data and statistics in a simple to use interface. Further developments include interpreting lipid changes in terms of pathway mapping and changes in membrane biophysical properties. All software is available at: http://secim.ufl.edu/secim-tools/.

In this talk, we cover software advances and applications of these workflows in the field of environmental lipidomics, with examples including accurate coverage of the insect lipidome, developing lipid biomarkers of an inflammatory disease in aquatic wildlife in Africa and lipidomics to understand remodelling of sea grass membrane under low or high phosphorus conditions. Lipidomics is gaining widespread use in the clinical science arena and we expect the same utility in the future of environmental studies.

[1] J. Koelmel, N. Kroeger, C. Ulmer, J. Bowden, R. Patterson, J. Cochran, C. Beecher, T. Garrett, R. Yost: "LipidMatch: an automated workflow for rule-based lipid identification using untargeted high-resolution tandem mass spectrometry data." *BMC Bioinformatics*. 2017 18, 331. doi: 10.1186/s12859-017-1744-3

[2] J. Koelmel, N. Kroeger, E. Gill, C. Ulmer, J. Bowden, R. Patterson, R. Yost, T. Garrett: "Expanding lipidome coverage using LC-MS/MS data-dependent acquisition with automated exclusion list generation." *Journal of the American Society for Mass Spectrometry*. 2017 28, 908. doi:10.1007/s13361-017-1608-0

Negative ion mass spectrometry is a viable tool to study post-translational modifications of deprotonated peptides

Dr Tianfang Wang
University of the Sunshine Coast

Abstract:
Tianfang Wang[1], T.T.NhaTran[2], Hayley J. Andreazza[3], Daniel Bilusich[4], Craig S. Brinkworth[5], Scott F. Cummins[1] and John H. Bowie[3]

1. Genecology Research Centre, University of the Sunshine Coast, Queensland, Australia, 4556
2. Industrial University of Ho Chi Minh City, Ho Chi Minh City, Vietnam
3. Department of Chemistry, The University of Adelaide, SA, 5005, Australia
4. Defence Science and Technology Organisation, Salisbury, PO Box 1500, South Australia, Australia, 5108
5. Defence Science and Technology Organisation, Land Division, Fishermans Bend, Victoria, Australia, 3207

The application of negative ion mass spectrometry in the backbone sequencing of deprotonated peptides in gas phase has been extensively studied [1]. Several fundamental cleavage mechanisms of (M-H)- anions of underivatised peptides have been revealed comprehensively using electrospray mass spectrometry in conjunction with theoretical calculation. The basic cleavages are the ubiquitous α- and β-backbone cleavage reactions, which provide information similar to that of the b and y ions of protonated peptides. The δ- and γ-cleavages associate with reactions initiated from side chain enolate anions of residues Asp and Asn, causing elimination reactions that cleave the backbone between the Asp (Asn) N–C backbone bond. For peptides with Glu(Gln), the δ- and γ-cleavages are initiated by attack of the side chain CO2-(CONH-) to form a lactone (lactam).

The side chains of Ser and Thr residues lose CH_2O (Ser) and MeCHO (Thr), which result in γ- and ε- processes that involve the side chain OH (of Ser or Thr) forms a hydrogen bond with the C-terminal CO2-(or CONH-), affecting a SN 2 attack at the electrophilic backbone CH of Ser with concomitant cleavage of the backbone. In addition, the negative ion mass spectrometry can be used to identify a number of posttranslational modification groups [2, 3], including kynurenine (Kyn), isoAspartate (isoAsp), pyroglutamate (pyroGlu), disulphides (both intra and intermolecular), phosphates and sulphates. For example, it allows (i) identification and positioning of the disulfide group, and (ii) sequence information of an intermolecular disulfide using CID MS3 spectra of the diagnostic disulfide cleavage ions. Besides, the quantum mechanical hydrogen tunnelling is an effect to consider when investigating these gas-phase ion reactions, as this effect might aid the proton atom transfer [3].

[1] J.H. Bowie, C.S. Brinkworth, S. Dua, Collision-induced fragmentations of the (M-H)- parent anions of underivatized peptides: an aid to structure determination and some unusual negative ion cleavages, Mass spectrometry reviews 21(2) (2002) 87-107.

[2] D. Bilusich, J.H. Bowie, Fragmentations of (M-H)- anions of underivatised peptides. Part 2: Characteristic cleavages of Ser and Cys and of disulfides and other post-translational modifications, together with some unusual internal processes, Mass spectrometry reviews 28(1) (2009) 20-34.

[3] T. Wang, T.T. Nha Tran, H.J. Andreazza, D. Bilusich, C.S. Brinkworth, J.H. Bowie, Negative ion cleavages of (M-H)(-) anions of peptides. Part 3. Post-translational modifications, Mass spectrometry reviews 37(1) (2018) 3-21.

A multi-function cyclic ion mobility – mass spectrometry system

Mr Martin Green
Waters Corporation, UK

Abstract:
Martin R Green, Jakub Ujma, Sandra Richardson, Kevin Giles

Waters Corporation, Wilmslow UK

Improvements in the performance and availability of commercial instrumentation have made ion mobility – mass spectrometry (IM-MS) a widely utilised approach for the structural analysis of ionic species as well as for separation of complex mixtures. As with any analytical technology, there is a constant drive to improve performance both in terms of resolution and added functionality. In this paper, we present an in-depth evaluation of a multi-function, quadrupole - cyclic-IMS (cIM) - time-of-flight MS research platform, capable of high IMS resolution with IMSn capability. Instrument geometry, control software, customisable functionalities and potential applications are presented.

The research platform is based on a Waters Synapt G2-Si instrument with the Triwave region modified to accept a cIM device. The cIM region consists of a closed loop, T-wave IM separator positioned orthogonally to the Synapt ion optical axis. At the interface between the ion optical axis and the cIM a planar array of electrodes provides control over the T-wave direction and subsequent ion motion. On either side of the array, there are RF/DC ion guides used for injection, ejection, storage and activation of ions. Using this multi-pass functionality IMS resolutions of greater than 500 (FWHM) are demonstrated.

In addition to standard operational modes of system, such as single and multi-pass cIM separation, the 'multi-function' instrument design enables a range of experiments to be performed such as mobility selections, activation, storage, IMSn and importantly, custom combinations of the above. The utility of IMSn with activation is demonstrated for the separation and structural analysis of a mixture of isobaric pentasaccharides. In addition, IMSn with activation is used to explore the complex unfolding pathways of populations of Ubiquitin ions.

From the Great Barrier Reef to Antarctica: chasing sulfuric acid using chemical ionisation mass spectrometry

Dr Branka Miljevic
QUT

Abstract:
Branka Miljevic, Chiemeriwo Godday Osuagwu, Luke Cravigan and Zoran Ristovski

International Laboratory for Air Quality and Health, Queensland University of Technology

Atmospheric aerosols are tiny liquid or solid particles dispersed in the air. They play an important role in regulating global climate: both directly, by scattering and absorbing incoming solar radiation; and indirectly, by acting as cloud condensation nuclei - small particles that are necessary for the formation of every single cloud droplet. However, aerosols are the least understood and constrained component of the climate system.

Sulfuric acid is one of the most climatically relevant chemical species as it can, due to its low vapour pressure, efficiently nucleate to form new particles, which can then act as cloud condensation nuclei. While in urban environments sulphuric acid is formed from SO_2 originating primarily from anthropogenic activities, the main precursor of H_2SO_4 in pristine marine environments is ocean-released dimethyl sulphide (DMS) - a metabolic product of phytoplankton and algae. Once in the air, DMS gets oxidised which ultimately leads to production of mainly sulphuric acid, but also methanesulfonic acid (MSA), dimethyl sulfoxide and dimethylsulfone. Therefore, understanding how these gases are formed from DMS, as well as their yields is important for understanding climate and predicting future climate scenarios.

H_2SO_4 as well as MSA can be detected using chemical ionisation mass spectrometry technique with $(HNO_3)_nNO_3^-$ (n = 0-2) as reagent ions. In this presentation our new Chemical Ionisation – Atmospheric Pressure Interface – Time of Flight Mass Spectrometer (CI-API-ToFMS) will be described and an overview and some results of its recent deployments onboard research vessels *Investigator* and *Aurora Australis* will be given.

Determination of veterinary drug residues in animal tissues using LC-MS/MS

Mrs Cindy Giles
Biosecurity Queensland

Abstract:
Cindy Giles, Stephen Were, Alyson Herbert, Ken Yong, Dennis Webber

Biosecurity Queensland, Department of Agriculture and Fisheries

Antimicrobial residues can be a severe barrier to trade and present a significant threat to Australia's domestic and export meat industries. It is critical that Australian laboratories develop methods that can withstand international scrutiny and remain economical enabling a meaningful number of samples to be analysed annually. A fast, specific and sensitive multi-class residue screening method was developed for use on all types of livestock. This method simultaneously allows the detection of aminoglycosides, tetracyclines, beta-lactams, cephalosporins, macrolides, quinolones, non-steroidal antiflammatory drugs and other veterinary drug residues.

Residues are extracted from tissues, usually kidney, liver or muscle using an acetonitrile/water mix. The extract is defatted and then cleaned up using dSPE. Aminoglycosides bind strongly to proteins in the sample and are extracted from the remaining precipitate using a strong acid. This acid extract is cleaned up using ion exchange SPE.

Extracts can then be analysed using a triple-quadrupole LC-MS System using positive electrospray ionisation. Each sample is injected multiple times to enable chromatography of the range of analytes with extreme differences in their chemical and physical characteristics. A HILIC column is used for chromatography of the hydrophilic compounds, the insect inhibitors cyromazine, dicyclanil and their metabolites. Heptafluorobutyric acid is used as an ion-paring reagent to enable good separation and peak-shapes of the highly polar aminoglycosides. A standard 50mm, UHPLC C18 column is used for the determination of all other analytes.

Using the speed, selectivity and sensitivity of the Shimadzu 8060 triple-quadrupole LC-MS allows this method to be a huge improvement over previous methodology, which used microbial inhibition to screen for antibiotic residues. The testing time has reduced from days to hours, the residues can now be unambiguously identified during the screening process and the method allows detection below the regulatory levels for more than 60 veterinary drugs, with this number continually increasing.

A land-based source of omega-3 oils: how proteomics was used for safety assessment

Dr Michelle Colgrave
CSIRO

Abstract:
Michelle Colgrave[1], Keren Byrne[1], Joanne Caine[2], Lukasz Kowalczyk[2], Sapna Vibhakaran Pillai[1], Bei Dong[1], Susan MacIntosh[3], Judith A. Scoble[2], James R. Petrie[1], Surinder Singh[1], and Xue-Rong Zhou[1].

1. Agriculture and Food, CSIRO
2. Manufacturing, CSIRO
3. Nuseed Americas

Omega-3s are polyunsaturated fatty acids that are important for human and fish health. Our bodies need the longer-chain omega-3s (EPA and DHA) – generally found in fish, marine animals and algae – to achieve the most significant health benefits. As we cannot make these critical nutrients, we must consume them in the foods we eat. Demand for these oils is increasing year-on-year, while existing supply from wild-caught fish oil is limited. Developing new, sustainable sources of these healthy long-chain omega-3 oils is essential.

Metabolic engineering of the omega-3 long-chain (≥C20) polyunsaturated fatty acids (ω3-LCPUFA), like eicosapentaenoic acid (EPA, 20:5ω3) and docosahexaenoic acid (DHA, 22:6ω3), in oil crops involved the transgenic expression of several fatty acid desaturases and elongases in ω3-LCPUFA biosynthesis pathway. The measurement of protein digestibility is a key step in determining the potential allergenicity of a genetically modified crop that has been traditionally accomplished using antibodies. The difficulty in expressing membrane proteins in heterologous systems means that raising antibodies may not be feasible.

In this study, LC-MS based proteomics was used to measure the in vitro protein digestibility of seven transmembrane enzymes using a two-stage digestion strategy involving pepsin followed by trypsin. The disappearance of tryptic peptide markers spanning the length of each desaturase showed that all regions were readily degraded (>95% within 5 min) and highlighted regions of the elongases that showed limited resistance to simulated gastric digestion. Traditional gel-based and Western blotting analysis of ω3-desaturase and Δ6-elongase revealed rapid hydrolysis of the intact proteins within seconds with no fragments (>3 kDa) remaining after 60 minutes, complementing the novel approach described herein. The LC-MS approach was sensitive, selective and did not require the use of purified proteins and is widely applicable to food/feed and environmental safety assessment.

Bottoms up proteomics! The dynamic beer proteome

Associate Professor Ben Schulz
University of Queensland

Abstract:
Benjamin Schulz[1], Edward Kerr[1], Toan Phung[2], Duin Mcdiarmid[2], Glen Fox[2]

1. School of Chemistry and Molecular Biosciences, The University of Queensland
2. Queensland Alliance for Agriculture and Food Innovation, The University of Queensland

Beer is one of humankind's oldest biotechnologies, and remains a key industry in Australia and internationally. The process of beer production involves agricultural ingredients with substantial varietal and environmental variability, and a series of bioprocessing steps. We have used mass spectrometry proteomics to investigate the complexity of the proteome throughout the course of beer production. This has uncovered a highly dynamic proteome with a wealth of post-translational modifications that, together with the bioprocess parameters, control the final beer proteome.

A key step in beer production is fermentation, where yeast convert sugars to ethanol and carbon dioxide. We have studied the diversity in the cell wall and global proteomes of standard brewing yeasts and wild Australian yeasts to

better understand their performance in commercial brewing settings. We see great potential for the use of MS proteomics and related systems biology approaches in understanding and improving the ancient art of beer making.

Circulating biomarkers for early cancer detection – challenges and strategies

Associate Professor Michelle Hill
QIMR Berghofer

Abstract:
Michelle M Hill[1,2]

1. QIMR Berghofer Medical Research Institute, Brisbane, Australia
2. UQ Diamantina Institute, Faculty of Medicine, The University of Queensland, Brisbane, Australia

Detection of cancers at early stages allows more effective treatment and improves cancer outcomes. With few cancer screenings currently available, there has been significant interest to discover new cancer biomarkers for early detection. Despite a multitude of published biomarker studies, few biomarker-based screening tests have been developed, likely due to limitations in existing study goals and cohort design as well as analytical techniques.

This presentation will outline the challenges of protein biomarker development for biological fluids, provide strategies, examples and learnings from our laboratory's endeavours on serum protein biomarkers over the past eight years.

MEK activation mediates erlotinib resistance in head and neck squamous cell carcinoma

Dr Harsha Gowda
QIMR Berghofer

Abstract:
Epidermal growth factor receptor (EGFR) is overexpressed in 90 per cent of head and neck squamous cell carcinomas (HNSCC). However, clinical trials with EGFR inhibitors such as erlotinib have shown a modest response in recurrent or advanced HNSCC. To investigate erlotinib resistance mechanisms in HNSCC, we characterised isogenic pair of erlotinib sensitive and resistant cell lines using exome sequencing and SILAC-based quantitative proteomics and phosphoproteomics.

Our data revealed several genomic alterations and proteomic changes associated with erlotinib resistant cells. Integrated analysis of genomic and proteomic data showed activation of MAP kinase pathway as a potential mechanism of erlotinib resistance in HNSCC. Growth inhibition studies using MAP2K1 inhibitor showed potent activity against erlotinib resistant cells. MAP2K1 inhibition can overcome erlotinib resistance in HNSCC.

Characterisation of environmental pollution and ecosystem health of a subtropical marine port using omics-based approaches

Dr David Beale
CSIRO

Abstract:
David Beale[1], Avinash Karpe[1], Joey Crosswell[2], Andy Steven[2]

1. Land & Water, CSIRO
2. Oceans & Atmosphere, CSIRO

Understanding the complex interactions between biological systems and environmental changes, natural or anthropogenic, is a significant research challenge. Traditional environmental and organism health monitoring techniques (e.g. chemical monitoring and bioassays) provide limited insight and thus, are often unsuitable for assessing subtle changes in the ecosystem and organisms' physiologies associated with low-level exposure(s).

This work presents the application of multi-omics based approaches for assessment and characterisation of bacterial community interactions with their environment. As such, the impact of several anthropogenic factors arising from point/non-point pollution sources at a subtropical multi-commodity marine port (Gladstone, Australia) and its surrounding ecosystems were studied using sediment samples from onshore (n = 5) and offshore (n = 4) sites. Sediment samples were analysed for trace metals, organic carbon, polycyclic aromatic hydrocarbons (PAH), emerging chemicals of concern (ECC) and sterols. Similarly, biological and biochemical interactions between the reef and its environment were analysed using next-generation sequencing and metabolic profiling of the bacterial community.

Multi-omics data indicated stresses on the bacterial community at all sampled sites. Especially, elevated metabolic rates were observed for fatty acid synthesis and shikimate pathway intermediates, causing generation of quinic acid-like metabolites and mycosporine-like amino acids. Such information provides an early warning sign of ecosystem degradation and demonstrates the importance of a multi-omics analysis platform for ecological assessments. This provides a comprehensive perspective of physical and chemical contaminants and, their impact on the community bacterial biome.

Enantiomeric profiling of amphetamine and methamphetamine in wastewater: a seven-year study in Queensland

Mr Jack Gao
University of Queensland

Abstract:
Jianfa Gao[1], Zeqiong Xu[2], Xiqing Li[2], Jake W. O'Brien[1], Peter N. Culshaw[3], Kevin V. Thomas[1], Benjamin J. Tscharke[1], Jochen F. Mueller[1], Phong K. Thai[1,4]

1. Queensland Alliance for Environmental Health Sciences, The University of Queensland, 20 Cornwall Street, Woolloongabba, QLD 4102
2. Laboratory of Earth Surface Processes, College of Urban and Environmental Sciences, Peking University, 100871 Beijing, PR China
3. Forensic & Scientific Services, Health Support Queensland, Department of Health, 39 Kessels Road, Coopers Plains, 4108, QLD
4. International Laboratory for Air Quality and Health, Queensland University of Technology, Brisbane, QLD 4001

Enantiomeric profiling was used in this study to investigate the consumption of amphetamine and methamphetamine in regional and urban Southeast Queensland, Australia over a period of seven years. S(+) methamphetamine was predominantly consumed in both urban and regional areas, showing a two- and threefold increase in urban and regional catchments respectively between 2011 and 2017. The ratio of amphetamine to

methamphetamine (AMP/METH) in wastewater reflected the expected excretion profile of methamphetamine consumption indicating the presence of amphetamine in this study was primarily the result of methamphetamine metabolism.

However, the occasional occurrence of R(-) amphetamine in samples containing higher AMP/METH ratios, suggested the consumption of racemic amphetamine. The R(-) methamphetamine enantiomer was also identified in several samples, possibly indicative that the phenyl-2-propanone (P2P) synthesis process rather than the more typical reduction of ephedrines was also being used to manufacture methamphetamine.

Furthermore, we identified two samples with a significantly different enantiomer ratio for the METH and AMP as well as a much lower AMP/METH concentration ratio suggesting contribution from direct disposal of methamphetamine into the sewer. This study demonstrated that enantiomeric profiling in WBE can provide valuable information for evaluating the origin of amphetamine in wastewater as either a metabolite of methamphetamine consumption or amphetamine itself.

Altered glycosylation enables increased metastasis in human colon cancer xenografts

Dr Arun Everest-Dass
Griffith University

Abstract:
Arun Everest-Dass[1], Tobias Lange[2], Mark von Itzstein[1]

1. Insititute for Glycomics, Griffith University
2. Department of Anatomy and Experimental Morphology, University of Hamburg

Patient derived xenograft (PDX) models are immunodeficient mice engrafted with patients' cancerous cells or tissues. They enable the examination of patient tumour tissue in a native environment without significantly affecting the cellular complexity, genomics and stromal architecture of the neoplasms. We observed differential expression of cancer stem cell markers CD24 and CD44 that were associated with highly metastatic human colon cancer PDX. We further investigated the metastatic behaviour with shRNA-mediated knockdown of CD24 and CD44 human colon cancer PDX. Transcriptomic analysis of these tissues indicated the alteration of several genes associated with glycan expression. To precisely identify these glycan changes, the PDX tissues were analysed using orthogonal mass spectrometry approaches.

Negative mode porous graphitic carbon (PGC) based liquid chromatography mass spectrometry (LC-MS) analysis enabled the identification and characterisation of global glycan alterations of N- and O-linked glycans from proteins, and from glycolipids. Reverse-phase LC-MS analysis and tailored electron-transfer higher-energy collision dissociation (EThcD) enabled the enriched intact glycoproteome characterization. Furthermore, the heterogeneity associated with the PDX tissues prompted the use of mass spectrometry imaging (MSI) to spatially localise the protein linked glycan alterations in formalin fixed paraffin embedded tissue (FFPE) sections.

Interestingly, the altered glycan epitopes associated with highly metastatic PDX tissues were glycan class specific. The N- and O-linked protein glycans exhibited a high expression of sialylated glycans including the non-human NeuGC residue. The glycolipid glycans were characterised by an increased expression of gangliosides and blood group A antigens. Unusually large blood group I structures were also observed that were predominantly associated with CD24 and CD44 depleted PDX tissues. Overall, our data reveal how subtle changes in glycan structures can regulate several malignancy-associated pathways and contribute to metastasis.

Facility Showcase

The Utilisation of Mass Spectrometry in Undergraduate Teaching at QUT

Dr Clare L Flakelar[1], Dr Kei Sit[1], Mr Kelvin Henderson[1]

1. Technical Services, Queensland University of Technology, Gardens Point, Brisbane

Given the nature of prospective career opportunities, value is placed at QUT on providing students with real-world experiences. The School of Biomedical Sciences and School of Clinical Sciences within the Faculty of Health (FOH) have equipped their undergraduate laboratories with a SCIEX QTRAP 4500. This instrument is currently used for mass spectrometry (MS) in undergraduate classes across several disciplines, allowing students to encounter valuable hands-on experience with MS instrumentation. An example of one such application is presented here, which involves fourth year clinical pathology students confirming the presence of controlled substances in biological samples via MS/MS.

Industrial Systems Biotechnology Platforms: Metabolomics, Proteomics, Bioinformatics, Systems and Synthetic Biology Modelling

Manuel Plan, Terra Stark, Gert Talbo, Timothy McCubbin, Robin Palfreyman, Lars Nielsen, Esteban Marcellin

Bioplatforms Australia - Industrial System Biotechnology Centre, Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland, Brisbane, QLD.

The Bioplatforms Australia (BPA) Queensland node located at the Australian Institute for Bioengineering and Nanotechnology at The University of Queensland provides analytical ‘fee for services’ to the wider scientific and research communities in Queensland and beyond. Our mission is to provide access to advanced ‘omics data generation and analysis capabilities in a high throughput manner; to both academia and industrial biotech companies.

Our core services comprise of qualitative and quantitative metabolomics including identification and quantification of amino acids, organic acids, aromatic compounds, alcohols, carbohydrates, nucleosides, nucleotides, fatty acids and vitamins. We provide proteomics analysis such as identification and quantification of targeted individual proteins as well as protein profile analysis of cell extracts. We provide bioinformatics and systems biology driven data analysis using tools such as genome-scale models with a particular emphasis on strain design for industrial biotech.

We employ an advanced suite of mass spectrometry instruments. A Shimadzu 8060 triple quadrupole and a robust SCIEX 4000 QTRAP are used for quantitative metabolomics analyses. A high resolution Thermo Q Exactive HF-X hybrid quadrupole-orbitrap is applied to proteomics and high mass accuracy analysis. Additionally, two Agilent GCMSs are utilised for open profiling and targeted analysis of metabolomics samples, especially hydrophobic analytes. Furthermore, amino acids, organic acids, aromatic compounds, carbohydrates/sugars, and fatty acids can be quantitatively analysed using Agilent HPLC and UPLC instruments.

Our bioinformatics services include multi-omics data (metabolomics, proteomics, transcriptomics and genomics) analysis and integration using computational modelling techniques to both characterise and rationally-design the phenotype of an organism. This encompasses the processing of raw data, analysis, interpretation and integration of a variety of large datasets, including that of high throughput systems, with access to range of computational power including high performance clusters.

Acknowledgements:
National Collaborative Research Infrastructure Scheme (NCRIS) an Australian Government Initiative

QUT ife Institute for Future Environments

Central Analytical Research Facility

Mass spectrometry

Analytical platforms for real world applications

QUT's Central Analytical Research Facility includes a proteomics and small molecule mass spectrometry laboratory that houses an array of cutting-edge liquid chromatography (LC-MS) and gas chromatography mass spectrometry (GC-MS) instrumentation.

Diverse expertise

Our technicians and researchers perform a range of tests, including qualitative, quantitative and structural analysis of proteins, lipids, metabolites, pesticides, pharmaceuticals and volatile organic compounds.

LC-MS instrumentation

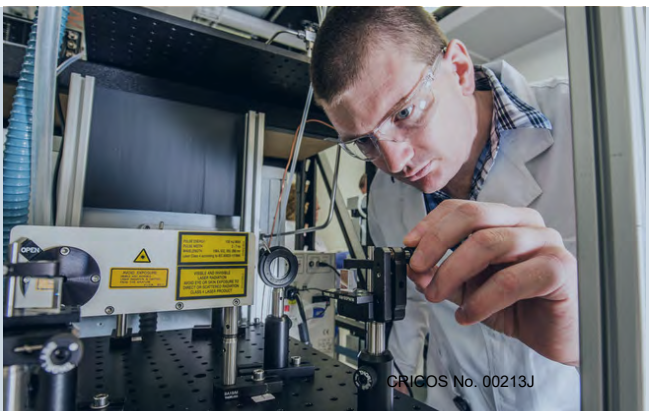
- AB Sciex TripleTOF 5600+ LC-MS/MS
- Shimadzu Triple Quadrupole 8050 LC-MS/MS
- AB Sciex QTRAP 6500 LC-MS/MS with DMS capability
- Thermo Scientific LTQ Orbitrap Elite LC-MS/MS
- Thermo Scientific LTQ LC-MS/MS

GC-MS instrumentation

- Shimadzu Triple Quadrupole 8040 GC-MS/MS
- Thermo Scientific Single Quadrupole ISQ Series GC-MS with HS, SPME and thermal desorption capabilities

Unique research capabilities

QUT is also home to a mass spectrometry development laboratory that studies isomers, their interactions with laser light and reactions with gases inside mass spectrometers. The lab is developing new ways of analysing lipids and other molecules by modifying standard mass spectrometers in unique ways.



Proteomics

We offer a 'walk-up' SWATH-MS-based protein quantitation service suitable for analysis of any number of samples of various origin (including clinical specimens). Our service covers the entire pipeline starting from study design, sample preparation, quality control measurements, optimized instrument methods, and a complete suite of bioinformatics tools. Our expert proteomics staff can also assist in post-translation modification analysis (eg. phosphorylation).

Lipidomics

We provide cost-effective lipidomics analyses using GC-MS and LC-MS. Our continuously expanding capabilities include quantitative analysis of phospholipids, glycerolipids, tri-, di- and monoglycerides, ceramides, fatty acids (via methyl esterification), lipid mediators and steroids. Using alternative ion activation methods allows us to conduct comprehensive structural elucidation of lipid isomers including double bond position determination.

Metabolomics

Our capabilities include untargeted profiling of primary metabolites (amino acids, organic acids, sugars) by TMS dervatisation and GC-MS as well as targeted analysis of purine and pyrimidine metabolites including co-factors by LC-MRM-MS.

Volatile organic compounds

Sampling using headspace, SPME and thermal desorption. Analysis of air, breath, insect and plant volatiles either directly or upon adsorption to sorbent material.

Typical research projects

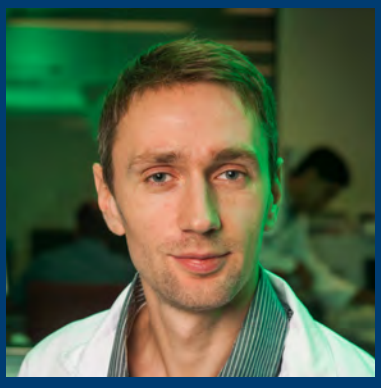
- Metabolomics approach to study effect of diet on fruit fly sexual selection
- Fruit volatiles and synthetic lure formulation [1]
- Global DNA methylation analysis into pest resistance to bioinsecticides
- Cancer lipidomics and proteomics
- Biomarkers of wound healing [2]
- Next generation veterinary proteomics
- Analysis of extractables and leachables on medical devices
- Structural lipidomics [3]

Working with us

Our equipment and services are available to QUT staff and students, external researchers and commercial clients with both self-service and full-service options. We offer comprehensive advice on study designs and sample handling. On request, we can develop individually-tailored highly sensitive and selective mass spectrometry assays targeting specific compounds.

References

[1] Cunningham et al. (2016) J Chem Ecol. 42(9): 931-940.
[2] Zang et al. (2016) Data Brief. 26(8): 1099-1110.
[3] Steiner et al. (2016) J Lipid Res. 57(7), 1194-1203.



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QUT ife Institute for Future Environments

CRICOS No. 00213J

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

CREATE CHANGE

Mass Spectrometry Facility

UQ Centre for Clinical Research

Bridging the gap between research and improved community health.

Centre for Clinical Diagnostics (CCD) is a NATA accredited research, development and evaluation facility within UQCCR. The facility allows life sciences researchers to translate their discoveries into clinical applications and commercial products faster. It reduces time-to-market for new in-vitro diagnostics and will provide training for a new generation of industry-ready researchers.

The facility houses a range of state-of-the-art platform technologies, including:

- liquid chromatography mass spectrometry,
- MALDI TOFTOF mass spectrometry
- nanoparticle tracking,
- protein solution arrays and
- real time live cell monitoring and imaging

Our facility staff are highly skilled and perform a range of services including sample preparation, data acquisition, and processing of resulting data.

The mass spectrometry facilities and services are available by appointment for use by UQ researchers, external researchers and clinicians.

Mass Spectrometry Services:

Application Area	Description of service	Instruments and Software
Protein Identification	Routine methods to identify proteins and peptides from simple and complex samples. Protein complexes are digested with an enzyme (Tryspin) and injected onto the NanoLC system that is coupled to the mass spectrometer. Ions are continually monitored in the MS until a peptide elutes, resulting in the fragmentation of the peptide (MS/MS). Once completed, the data is processed against a user-defined database to identify the proteins within the sample.	TripleTOF 5600 System (SCIEX) Eksigent NanoLC Ultra system (SCIEX) 5800 MALDI TOFTOF System (SCIEX) ProteinPilot 5.0 software (SCIEX) MASCOT software (MatrixScience)
SWATH Analysis	SWATH analysis (or data independent analysis (DIA)) is a new technique that combines the traditional MS workflows of data dependent acquisition (DDA) and MRM or targeted workflows. The advantage of this technique is that is provides a complete MS/MS profile of a biological sample that can be stored and re-interrogated at a later time.	TripleTOF 5600 System (SCIEX) Eksigent NanoLC Ultra system (SCIEX) 5800 MALDI TOFTOF System (SCIEX) ProteinPilot 5.0 software (SCIEX) PeakView software (SCIEX) SWATH acquisiton software (SCIEX) MarkerView Software (SCIEX)
Quantitation of peptides & small molecules	Targeted or Multiple Reaction Monitoring (MRM or Selective reaction monitoring (SRM)) analysis of biological samples can be used to verify and validate discovery findings such as proteins identified by protein ID and SWATH analysis, western blotting or ELISA workflows. This technique using a tandem mass spectrometer of which an ion of a specific mass (compound/ peptide of interest) is selected in the first stage of the instrument, fragmented and then a daughter ion is selected and monitored in the second stage of the mass spectrometer. Resulting data is processed using MultiQuant software for the QTRAP® 5500 system and the Insight and Post run for the LCMS 8050 system and the Qualitative Analysis program for the Agilent 6490 system.	QTRAP 5500 System (SCIEX) LCMS 8050 System (Shimadzu) Agilent 6490 System (Agilent) Nexera UHPLC Systems (Shimadzu) MicroLC 200 System (SCIEX)
Intact Protein Analysis	Intact protein analysis using mass spectrometry can be achieved using the LC MS or MALDI TOF MS systems. Non-covalent binding experiments and/or antibody drug conjugate (ADC) studies can also be conducted within the MS facility.	TripleTOF 5600 System (SCIEX) NanoLC Ultra system (SCIEX) 5800 MALDI TOFTOF System (SCIEX) PeakView software (SCIEX) BioPharmaView Software (SCIEX)
Lipidomics	Discovery based lipidomics can be completed using a screening based workflow (MSMSALL) which provides an accurate mass lipid profile. The sample is introduced by infusion or by using the TriVersa NanoMate system, and the MS/MS profile is obtained by stepping the across of mass range of interest by 1Da. The resulting data is processed uagainst a comprehensive reference library of over 25,000 lipid species characterised by head groups, fatty acid based and long chain based fragments. Targeted lipidomics workflows are best completed using triple quadrupole instruments such as the QTRAP® 5500 System, the LCMS-8050 System or the Agilent 6090 system. Precursor Ion or neutral loss experiments can be set up to monitor the lipid classes as they are detected within the systems. Samples are processed using vendor specific software. The SelexION® DMS is also available to assist in the detection and quantification of the isobaric lipid species within your samples.	QTRAP 5500 System (SCIEX) LCMS 8050 System (Shimadzu) Agilent 6490 System (Agilent) Nexera UHPLC system (Shimadzu) TriVersa Nanomate System (Advion) SelexION Ion Mobility source (SCIEX) LipidView Software (SCIEX)
Differential Ion Mobility Technology (DMS)	Differential mobility spectrometry and ion mobility spectrometry are analytical techniques used to separate hard to resolve ions based on their gas phase mobility. At UQCCR, we have recently acquired the SelexION® Differential mobility device that can be used for the following challenges: • Overcome co-eluting matrix interferences & improve quality of data in complex samples • Separate isobaric compounds for increased confidence in detection • Detect and quantify isobaric lipid molecular species • Reduce background noise that might be affecting your LOQ • Save time with simplified sample preparations.	QTRAP 5500 System (SCIEX) SelexION Ion mobilite source (SCIEX) Nexera UHPLC system (Shimadzu)

For further details, please contact:

Facility Manager: Dr Sarah Reed
Email: ccd-uqccr@uq.edu.au
Phone: +61 7 3346 5007
Postal Address: 71/ 918 Royal Brisbane Hospital, HERSTON, QLD, 4029
For further information visit: https://clinical-research.centre.uq.edu.au/services/clinical-diagnostics/mass-spectrometry-services

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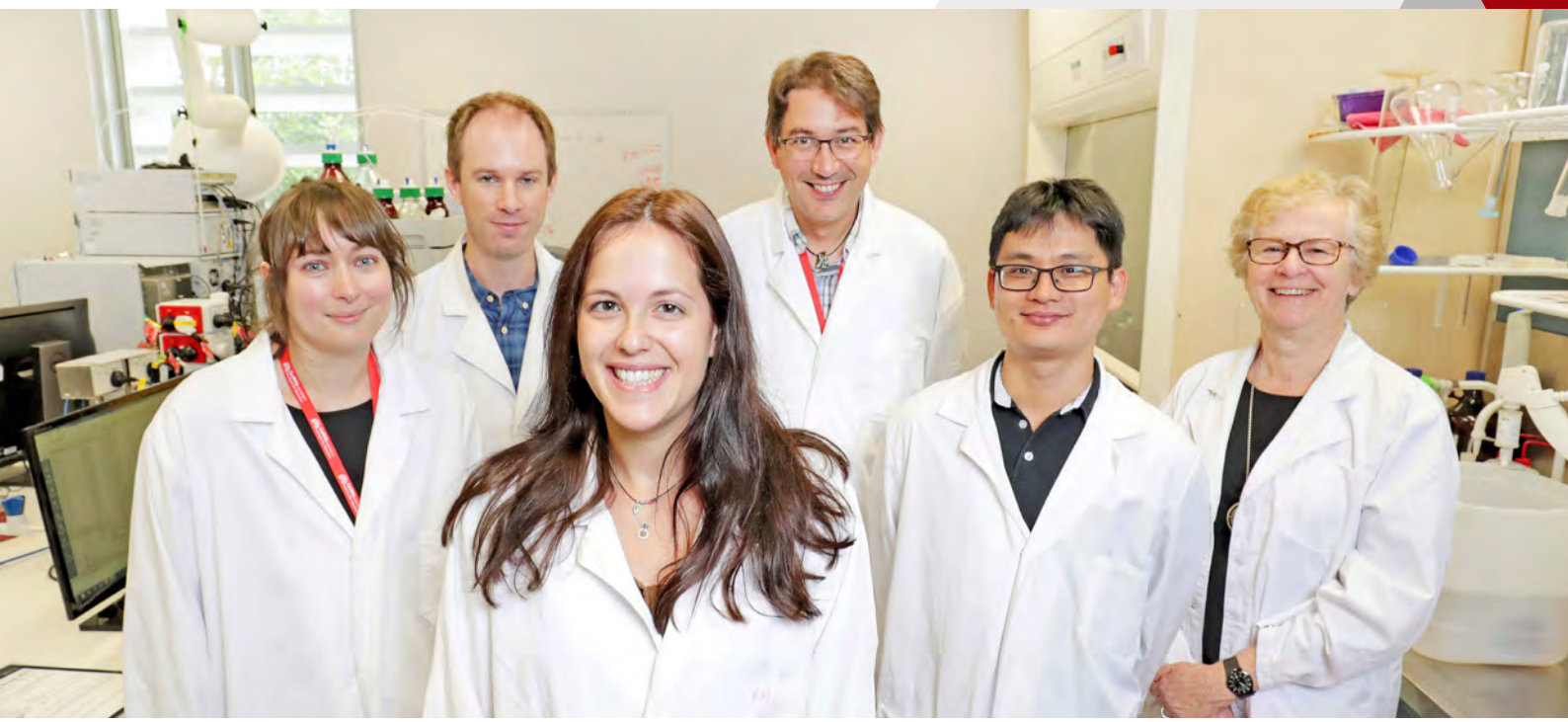
Griffith UNIVERSITY
Institute for Glycomics
Fighting Diseases of Global Impact



Australian Centre for Cancer Glycomics (A2CG)

Translating the human cancer glycome - the key to diagnosing, treating and preventing cancer.

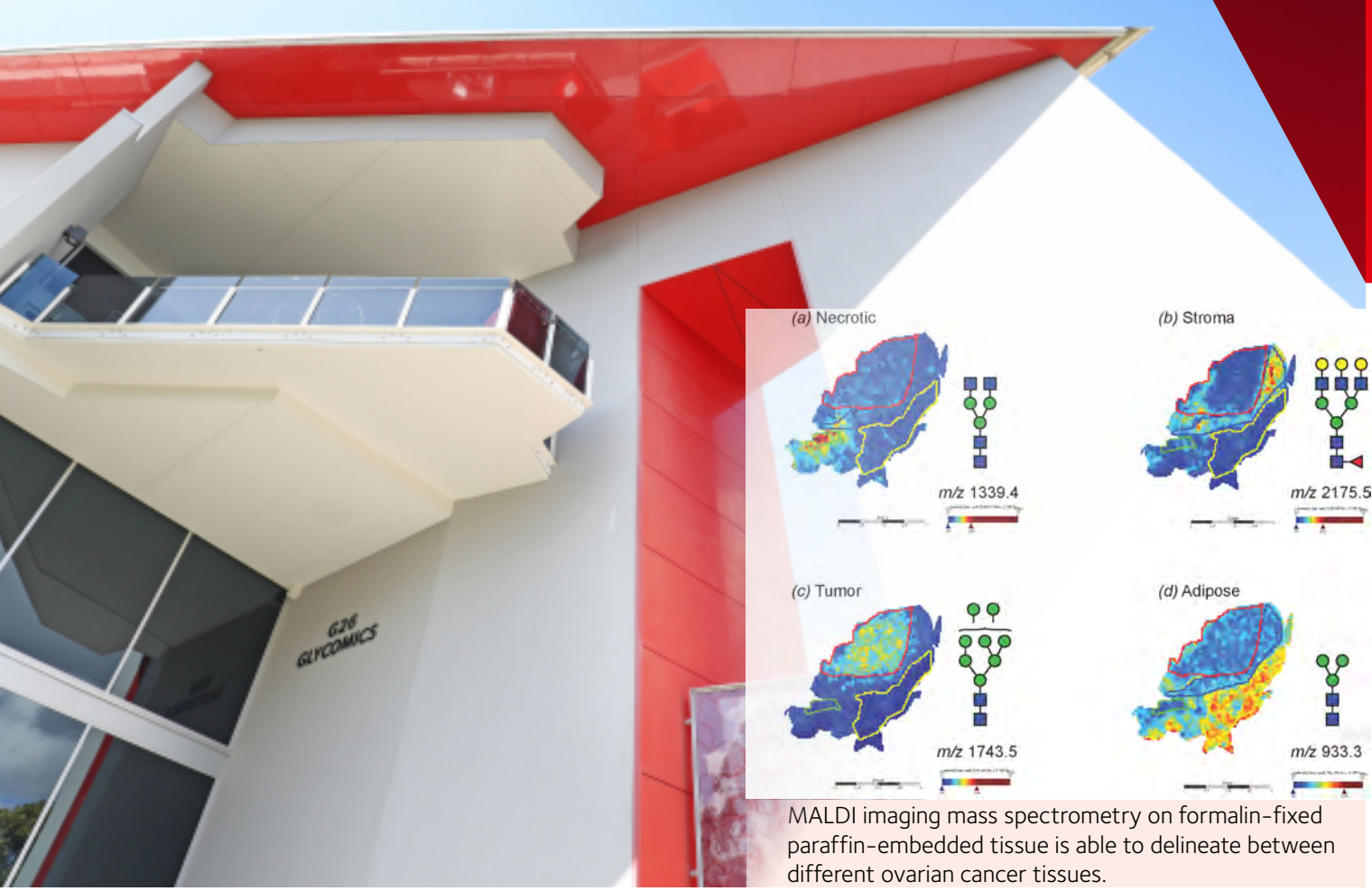
All human cells are extensively decorated with a range of complex sugar moieties (glycans), which form the host cell glycome. These glycans are utilised as receptors for a variety of carbohydrate-recognising proteins, which are also present on the cell surface. The inter-cellular interactions between glycans and proteins play an essential role in how cells communicate with each other and their environment. Not surprisingly, they also play critical roles in maintaining health and in the pathogenesis of disease, including cancers. Yet, the language of glycan interactions remains poorly understood, particularly when compared to our knowledge of the genome and proteome. **The technology required to sequence the glycome for human clinical tissue has only recently been developed, and Griffith University's Institute for Glycomics is pioneering this field.**

Extensive investment into the understanding of cancer genomics and proteomics has led to tremendous advances in cancer care. Despite this, biomarkers for many cancers remain unidentified following proteomic and genomic analyses, suggesting critical knowledge is missing. An increasing body of literature indicates that the cancer glycome is of equal importance to understanding disease pathogenesis as the genome and proteome. This is not surprising, considering the glycome's critical role in cell communication across all biological systems. **The glycome represents an underexploited aspect of cancer research, and holds the key to diagnosing, treating and preventing cancers.**

The Australian Centre for Cancer Glycomics was established at the Institute for Glycomics in May 2017. This unique national resource dedicated to cancer glycomics research, is the result of significant funding by Griffith University. The state of the art equipment and infrastructure, coupled with the brightest scientific talent in the field of cancer glycoproteomics, makes the A2CG an exciting hub of truly revolutionary research.

The Institute for Glycomics and the A2CG are taking a highly integrated, systematic approach to identifying important cancer biomarkers and tumour-associated carbohydrate antigens (TACAs), underpinned by a strategic focus geared towards **translational outcomes**. The Institute for Glycomics has a proven track record in carbohydrate drug discovery and vaccine development coupled with substantial biochemistry, structural biology and medicinal chemistry infrastructure. This demonstrates the Institute's capabilities in driving discoveries from the laboratory bench to the patient bedside.

Our team of research scientists are dedicated to understanding how cancer glycans can sketch the blueprint for the next wave of drugs, vaccines, and diagnostics. Together with a **foundation partner**, who shares our vision of harnessing this unique research platform to identify new solutions to cancer, we aim to improve the future of those living with this intractable disease.



MALDI imaging mass spectrometry on formalin-fixed paraffin-embedded tissue is able to delineate between different ovarian cancer tissues.

The A2CG Team

As the only institute of its kind in the southern hemisphere, the Institute for Glycomics is already an epicentre of glycomics research globally and houses many world-leading carbohydrate researchers. A project with the vision and scale of the A2CG requires substantial human resource, technical knowledge and specialisation. Significant investment by Griffith University has attracted the world's brightest scientific minds, including research teams led by **Professor Nicolle Packer** and **Associate Professor Daniel Kolarich**. By combining core expertise and infrastructure, the A2CG is a world-class platform for mapping the cancer glycome, and translating these discoveries into novel diagnostics and therapies.

A Call to Industry

Improving knowledge of the glycan structures present in cancer cells will lead to a better understanding of how to treat the most 'un-treatable' forms of cancer. A structured, 5-year program will systematically mine the cancer glycome; an undertaking that will remarkably transform the oncology landscape. The rapid advancement of analytical technology combined with the need for more efficacious cancer therapeutics, makes this an opportune moment for investment. With advanced technological infrastructure, knowledge and distinguished human resource, the A2CG seeks to attract a foundation partner aspiring to significantly enhance the prospects of cancer patients though innovative and revolutionary science.

Clinical Applications

The A2CG team's extensive expertise in analytical glycoproteomics affords a research program focussing on the following clinical applications:

- **Diagnostic tools** - Glycans as novel diagnostic and prognostic disease markers
- **Therapeutic potential** - TACA identification and translation to develop monoclonal antibodies and other drug candidate technologies
- **Precision medicine** - Development of specific and targeted medicines based on cancer glycan signatures
- **Advanced imaging** - Micro-section glycomics from histopathological tissue slides to bridge histopathology and molecular imaging
- **Clinical analytics** - Development of rapid, bedside diagnostic tools using focused glycomics and glycoproteomics

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SCIENCE

A FUTURE-FOCUSED COLLABORATION

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

Centre for

GEOANALYTICAL MASS SPECTROMETRY

World-class analytical equipment enabling researchers, institutions, government, industry partners and community clients to expand research across traditional boundaries.

The Centre for Geoanalytical Mass Spectrometry (CGMS) is a fully integrated research facility at The University of Queensland that is dedicated to the analysis of stable and radiogenic isotope ratios and trace element abundances in natural and man-made materials.

Radiogenic Isotope Facility (RIF)

The unique $5 million facility is a HEPA-filtered "ultra-clean" laboratory with a centrally-controlled air-handling system providing proven ultra-low analytical blank performance for highly sophisticated trace element and isotopic analysis.

Equipped with facilities to digest a variety of specimens, chemically separate and purify elements of interest, RIF houses a range of strategic mass spectrometers and a laser ablation system for various elemental/isotope analyses and dating for earth, environmental, archaeological, biological, biomedical, and forensic science research

Stable Isotope Geochemistry Laboratory (SIGL)

This is one of the most comprehensive laboratories in the Southern Hemisphere, enabling the complete cycle from preparation to analysis of stable isotopes in geological and environmental samples.

The SIGL has a long history of analysing light stable isotopes (C, H, O, N, S) and currently houses four isotope ratio mass spectrometers with online preparation systems, supporting ground breaking multidisciplinary research in the earth, environmental, biological, chemical, medical and material sciences.

Environmental Geochemistry Laboratory (EGL)

The laboratory complements the RIF by offering major and trace element analysis with ICP-OES and ICP-MS as the main analytical instruments. It hosts a range of small portable instruments and devices for field sampling and analysis of waters.

The EGL offers a specialised service for difficult samples and provides elemental analyses of environmental (rocks, sediments, waters), synthetic (slag, alloys, pharmaceuticals) and biological (blood, proteins) samples.

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Brisbane Geochronology Alliance

The Centre for Geoanalytical Mass Spectrometry has entered into a partnership with Griffith University and QUT with the creation of the Brisbane Geochronology Alliance, which aims to make Brisbane a global hub for isotope geochemistry and geochronology.

Laboratory	Equipment summary	Pricing contacts
Available to all researchers and commercial clients		

Radiogenic Isotope Facility (RIF)	• Four mass spectrometers:
	  • **Nu Plasma HR multi collector-inductively coupled plasma mass spectrometer (MC-ICP-MS)**
	  • **Nu Plasma II MC-ICP-MS** with 16 Faraday cups and 6 secondary electron multipliers
	  • **Thermo X-Series II quadrupole inductively coupled (Q-ICP-MS)**
	  • **Thermo iCAP-RQ Q-ICP-MS** for high-precision rapid multi-element analysis
	• ASI RESOlution SE laser system for in situ high-spatial resolution isotope and elemental analysis when coupled with the Nu Plasma and Thermo ICP-MS machines
	• Six positively pressured chemistry laboratories
	• HEPA and ULPA fume hoods
	• Sartorius analytical balance and Cahn microbalance
	• Acid distillation system
	• De-ionised water plant
	• Microwave digestion system
		Professor Jian-xin Zhao
		E: j.zhao@uq.edu.au
		
		Dr Yue-xing Feng
		E: y.feng@uq.edu.au

Stable Isotope Geochemistry Laboratory (SIGL)	• Four stable isotope mass spectrometers:
	  • **Isoprime-Agilent gas chromatography-combustion-isotope ratio mass spectrometer (GC-c-IRMS)** optimised for C and H isotope analysis of mixed gases
	  • **Isoprime continuous flow isotope ratio mass spectrometer (CF-IRMS)** with elemental analyser for C, N, S isotope analysis of geological and biological samples (optimised for multiple S isotope analysis)
	  • **Thermo Delta V Advantage CF-IRMS** with gas bench for DIC and thermal combustion elemental analyser for O and H isotopes on solids and liquids
	  • **Isoprime dual inlet isotope ratio (DI-IRMS)** with Multiprep for high precision H and O isotope analysis of waters and C and O isotope analysis of carbonates
	• Carbonate extraction line
	• Mineral hydrogen and fluid inclusions extraction line
	• Experimental vacuum extraction line
		Professor Sue Golding
		E: s.golding1@uq.edu.au
		
		Kim Baublys
		E: k.baublys@uq.edu.au

Environmental Geochemistry Laboratory (EGL)	• Perkin Elmer 8000 8300 ICP-OES • Agilent 7900 Q-ICP-MS • Katanax K2 Prime automatic fluxer • Balance room • Two acid resistant fume hoods • Laminar flow cabinet • Acid cleaning room • Sample preparation laboratory	**Marietjie Mostert** E: m.mostert@uq.edu.au

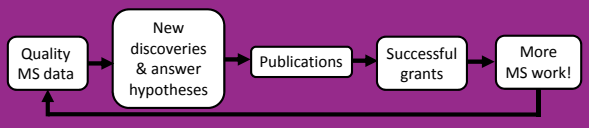
Centre for Geoanalytical Mass Spectrometry
E: sees@enquire.uq.edu.au T: +61 (7) 3365 6455
W: sees.uq.edu.au/research/analytical-facilities

Mass Spectrometry Facility

School of Chemistry and Molecular Biosciences

The University of Queensland, St Lucia

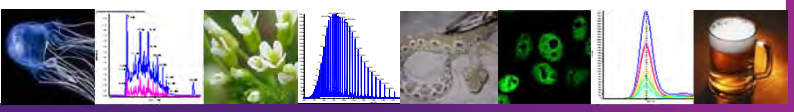
Our aim is to provide a high quality mass spectrometry facility for all researchers, including advice with sample preparation, experimental design and data analysis.



Proteomics

Extensive experience in sample preparation and identification of proteins from a wide range of sample types.

Experience in protein identification, de novo sequencing, identification of new protein products, amino acid sequence changes



Small molecule / natural product analysis

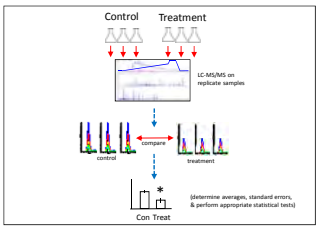
Walk up ion trap MS for first pass analysis of synthetic and purified natural products.

ESI-QTOF for high resolution / accurate mass analysis allowing confirmation of products and chemical formulas.

Analysis by infusion or by LC-MS as needed.

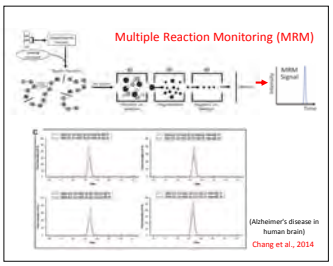
Experience with a wide range of sample types: organic and inorganic compounds, metallo-organic frameworks, metallo-supramolecular cages, dendrimers, complexes, and difficult to resolve isotopic structures

Quantitative MS



Above : General requirement for SWATH-MS analyses

SWATH-MS: Extensive experience in quantitative MS, particularly SWATH analyses on a variety of sample types and conditions.



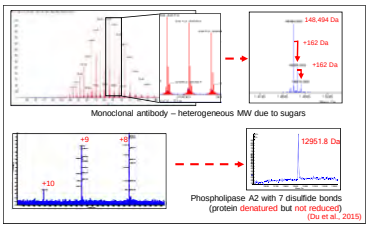
Extensive experience with Multiple Reaction Monitoring (MRM) for small molecules, peptides and metabolites

Left: MRM allows quantitation of individual proteins in samples by monitoring peak areas from individual peptides and fragment ions. MRM has been successfully utilised to monitor protein levels in Alzheimer's diseased brain vs control samples.

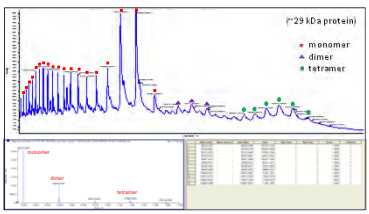
Intact mass and native mass spec

Expertise in denaturing intact mass measurements of proteins via TripleTof 5600, Orbitrap Elite, or Autoflex III MS systems as needed.

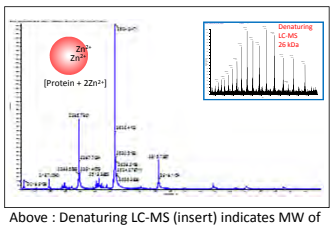
Experienced with native intact MS for analysis of protein-protein and protein-ligand interactions



Above: Intact mass analysis – both small and large proteins can be resolved, and PTMs often detected.



Above: Native MS of 29 kDa protein, indicates the presence of monomer, dimer, and tetramer.

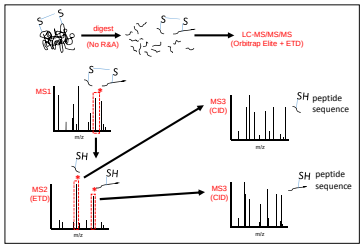


Above : Denaturing LC-MS (insert) indicates MW of protein. Native MS analysis of protein infused in NH4OAc with ZnCl2 and serine confirms the protein binds two Zn^{2+} ions.

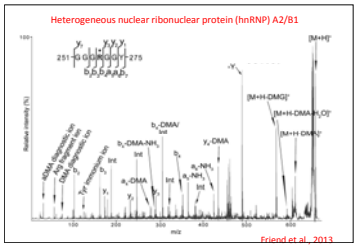
Post-translational modifications

Experience and expertise in methods for isolation / enrichment of modified peptides and characterisation by MS.

PTM analysis includes phosphorylation, glycosylation, dimethylarginine, and disulphide bond-mapping.



Above: Schematic for workflow for disulphide bond mapping using ETD and CID fragmentation.



Above: Characterisation of dimethylarginine modification, including confirmation of site of PTM and symmetry of dimethylarginine

Instrumentation

A range of instruments is available to accommodate a wide variety of projects including proteomics, metabolomics, lipidomics, small molecules & other organic, inorganic and metallo-organic compounds. Downstream software for for analysis, including identification, quantitation & deconvolution is also available.

Sample preparation equipment (HPLCs, speed vacs, freeze-driers etc) also available for facility users.

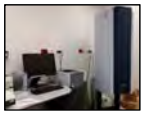
- ESI-QTOF (TripleTof 5600, Sciex)
- Automated LC-MS/MS & calibration
- For qual and quant workflows (ID, SWATH)

- ESI-QTOF (MicrOTof, Bruker)
- Accurate mass of natural and synthetic products

- ESI-QTRAP + APCI option (QTRAP 5500, Sciex)
- For quantitation of samples (Multiple Reaction Monitoring)

- ESI-QTOF (MicrOTof, Bruker)
- Accurate mass of natural and synthetic products

- ESI-Hybrid TRAP with APCI option (Orbitrap Elite with ETD, Thermo)
- ID, quant, PTMs, top-down sequencing, structural work



- MALDI-TOF/TOF (Autoflex III, Bruker – located in AIBN)
- Polymers, lipids, PEGylated proteins

Further information:
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