QUEENSLAND MASS SPECTROMETRY SYMPOSIUM 2022

The Queensland Mass Spectrometry Symposium (QMSS) serves to connect the Queensland mass spectrometry user base, and those interested in this technology across a diverse range of disciplines.

PLENARY SPEAKERS

Prof Benjamin Schulz
Better beers through mass spectrometry

Dr Leisa-Maree Toms
Human biomonitoring in Australia - Assessment of environmental pollutants

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DAY 1
THURSDAY 1 DECEMBER

8:30 - 9:30	Registration
9:30 - 9:40	Welcome
9:40 - 9:50	Silver Sponsor
9:50 - 10:30	**PLENARY: Prof Benjamin Schulz**, Better Beers through Mass Spectrometry
10:30 - 11:00	Morning Tea
11:00 - 12:30	Oral Presentations (15 Mins) **Jens Blotevogel**, Ultrahigh-resolution 21 Tesla FT-ICR mass spectrometry for suspect and nontargeted screening of PFAS **Cassandra Rauert**, Challenges with analysis of polyethylene in samples with high lipid content using pyrolysis-GCMS **Rachel Jackson**, Localisation of natural products within eucalypt flowers using mass spectrometry imaging **Jinglong Li**, A sensitive high-throughput direct injection liquid chromatography-tandem mass spectrometry method for the surveillance of antimicrobials in wastewater **Rhiannon McVeigh**, Structural elucidation of branched-chain fatty acids through charge-remote fragmentation
12:30 - 1:30	Lunch
1:30 - 2:30	Gold Sponsor - **PM Separations**
2:30 - 3:00	Afternoon Tea
3:00 - 4:00	Oral Presentations (10 Mins) **Phong Vo / Brett Hamilton**, Visualization of per- and polyfluoroalkyl substances (PFASs) distribution in concrete using Desorption Electrospray (DESI) Mass Spectrometry Imaging (MSI) **Berwyck Poad**, Revolutions in lipid isomer resolution: Applications of cyclic ion-mobility mass spectrometry to frontier challenges in lipidomics **Chang He**, Semi-quantitative characterisation of bromo-chloro paraffins and olefins in the Australian environment **Daniel Ellis**, Unravelling the diverse metabolomes of native wild yeast **Mathieu Feraud**, InSpectra – A platform for identifying emerging chemical threats
4:00	Poster Flash (5 min) **Selvam Paramasivan**, Automated proteomics workflows for high-throughput library generation and biomarker detection using data-independent acquisition **Pallav Joshi**, The role and impact of N- and O-glycosylation on surface exposed proteins and cellular lipids and metabolites **Elvis Okoffo**, Mass quantification of microplastic at wastewater treatment plants by pyrolysis-gas chromatography-mass spectrometry **Therese Fulloon**, Investigating complex mixtures of metallo-supramolecular assemblies using the Waters SELECT SERIES Cyclic IMS **Rangika Maggona Gurunnanselage**, Do beer and bread make you fat? **Cassandra Rauert**, Analysis of tyre wear particles and tyre additives in Queensland surface water **Wei Wang**, Emerging environmental contaminant para-phenylenediamine quinones (PPD-Qs): Occurrences, characteristics and health risks

DAY 1
THURSDAY 1 DECEMBER

4:45	Poster Session
	Aline De Oliveira Campos, Qualitative and spatial analysis of ganoderic acids from Australian Ganoderma fruiting bodies
	Aurelie Benfield, Cyclic tachyplesin and cyclic gomesin can overcome acquired drug resistance in BRAF mutant melanoma cells
	Bastian Schulze, Influence of SWATH-MS settings on successful identifications in a non-target workflow
	Chao (Grace) Lin, Emerging role of mass spectrometry in clinical diagnostics and toxicology at QML Pathology
	Coral Jeffries, Dietary exposure to microplastics
	David Marshall, Investigating highly reduced metallosupramolecular complexes in the gas phase
	Henry Lamb, PHGDH, a novel metabolic target in drug-resistant melanoma
	Isaac Gargett, Finding inhibitors of anti-virulence targets in Burkholderia pseudomallei
	Keith Takawira, Quantitative proteomics investigations of methane utilising bacteria and characterisation of a previously unsequenced Hyphomicrobium sp.
	Kyle Macauslane, The host subcellular proteome and glycoproteome throughout a time-course infection of influenza A virus
	Lan Chen, Metabolites and fatty acids analysis using triple quadrupole gas chromatography mass spectrometry
	Maria Elmendorp, Total carbon dioxide (TCO2) in equine plasma analysis by GCMS
	Menace Gallagher, Benchmarking the utility of open-source library-free DIA tools in the identification and quantification of glycan modifications using mass-spectrometry
	Pawel Sadowski, Automated proteomics workflows for high-throughput library generation and biomarker detection using data-independent acquisition
	Shulei Liu, Impact of site-specific N-glycosylation on yeast glycoprotein thermal stability
	Simran Kaur, Quantification and identification of microplastics in compost using Pyrolysis GC-MS method
7:00	CLOSE

DAY 2
FRIDAY 2 DECEMBER

8:30 - 9:30	Registration
9:30 - 9:40	Welcome
9:40 - 9:50	Silver Sponsor
9:50 - 10:30	**PLENARY: Leisa-Maree Toms**, Plenary: Human biomonitoring in Australia – assessment of environmental pollutants
10:30 - 11:00	Morning Tea
11:00 - 12:30	Oral Presentations (10 Mins) **Carly Beggs**, Target and suspect screening of neonicotinoids and their transformation products in environmental matrices **Michael Pfrunder**, Separation of diastereomers of metallosupramolecular cages from a dynamic mixture of interconverting species **Pradeep Dewapriya**, Non-target screening of per- and polyfluoroalkyl substances (PFAS) in cattle exposed to AFFF-contaminated groundwater imaging **Phuong Do Thi**, Programming photodegradability into vinylic polymers via radical ring-opening polymerization **Brett Hamilton**, Analysis cryo and ultrathin cryo sections by mass spectrometry imaging to reveal macro and micro scale distribution of Latrunculin-A in Chromodoris kuiteri **Stacey O'Brien**, Quantification of selected microplastics in Australian urban road dust **Luke Ney**, Endocannabinoids in saliva and hair by LC-MS/MS: New opportunities for biological exploration
12:30 - 1:30	Lunch
1:30 - 2:30	Gold Sponsor - **Sciex**
2:30 - 3:00	Afternoon Tea
3:00 - 3:40	Oral Presentations (15 Mins) **Edward Kerr**, A multi-omics approach reveals the mechanisms underlying the challenges of translating wild yeasts to industrial fermentation **Elvis Okoffo**, Identification and quantification of micro-bioplastics in environmental samples by pyrolysis-gas chromatography–mass spectrometry
3:40 - 4:30	Oral Presentations (10 min) **Natalie Turner**, Quantitative proteomics comparison of human and cow's milk-derived small extracellular vesicles by Sequential Window Acquisition of all Theoretical fragment ion Mass Spectra (SWATH-MS) **Louise Sternicki**, Developing native mass spectrometry for targeting non-coding RNAs: an emerging and challenging therapeutic target class **Yufei (Lily) Pan**, Analysis of the uptake and effects of tyre wear particles on plants **Lachlan Jekimovs**, Uncovering non-canonical unsaturated fatty acids in the brain
4:30	Facility Showcase
4:45	Awards Ceremony / Closing Comments
5:00	Social Event

PLENARY DAY 1

Better beers through mass spectrometry

Professor Benjamin Schulz[1]

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Bio:

I am Professor in Biochemistry in the School of Chemistry and Molecular Biosciences at The University of Queensland, with research interests in diverse applications of molecular systems biology in fundamental protein biochemistry, viral glycobiology, and fermented beverages. I graduated with a degree in Chemical Engineering and Science from The University of Queensland, after which I joined Proteome Systems, an Australian biotechnology company. I moved to the ETH Zurich in Switzerland for my doctoral studies, and then returned to the School of Chemistry and Molecular Biosciences as a post-doctoral research fellow, and now teaching and research academic.

Ultrahigh-resolution 21 Tesla FT-ICR mass spectrometry for suspect and nontargeted screening of PFAS

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Keywords: FT-ICR MS, PFAS, contamination, environment, forensic

Abstract:

Per- and polyfluoroalkyl substances (PFAS) are a chemically diverse family of thousands of individual species that have been ubiquitously detected in the environment from North to South Pole. Their comprehensive characterization, thus far attempted via nontargeted Orbitrap and time-of-flight mass spectrometry methods, is critical for environmental monitoring and remediation applications. 21T Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS) offers the highest available mass resolving power for complex mixture analysis, and sub-ppm mass errors across a wide molecular weight range. To explore its application to suspect and nontargeted screening, we developed a 21T FT-ICR MS method to screen for PFAS that includes suspect screening for known PFAS, molecular formula assignment with a targeted database, CF2 homologous series, 13C, 34S, and 37Cl isotopologues, and Kendrick-analogous mass difference networks (Young et al. 2022). False positive PFAS identifications in the NOM sample suggested that a minimum length of 3 should be imposed when annotating CF2-homologous series, and conflicting formula assignments at sub-ppm errors indicated the importance of using isotopologues and homologous series during formula assignment. We putatively identified 199 known PFAS in an electrochemical fluorination-derived aqueous film-forming foam sample during suspect screening, and 124 more PFAS during additional nontargeted analysis. Our results demonstrate that FT-ICR MS-based suspect and nontargeted screening methods can provide unique insights into complex PFAS compositions often encountered at contaminated sites.

References:

Young, R.B.; Pica, N.E.; Sharifan, H.; Chen, H.; Roth, K.H.; Blakney, G.T.; Borch, T.; Higgins, C.P.; Kornuc, J.J.; McKenna, A.M.; Blotevogel, J. 2022. PFAS Analysis with Ultrahigh Resolution 21T FT-ICR MS: Suspect and Nontargeted Screening with Unrivaled Mass Resolving Power and Accuracy. Environmental Science & Technology, vol. 56, no. 4, pp. 2455-2465.

Challenges with analysis of polyethylene in samples with high lipid content using pyrolysis-GCMS

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Keywords: Microplastics; Polyethylene; lipid interference; food; Pyrolysis GCMS

Abstract:

Microplastics pollution is one of the biggest environmental challenges the planet is facing. However, there is still limited understanding on human exposure, data which is further hindered by analysis challenges from complicated matrices such as food samples. This study aimed to evaluate the potential matrix interference on analysis of polyethene with Pyrolysis gas chromatography mass spectrometry from foods containing >3% fatty acid type lipids (triacylglycerols). A significant interference was observed from three types of fatty acids (saturated, monounsaturated and polyunsaturated fats) which could not be separated during instrument analysis. Subsequently, an extraction protocol was developed that included enzyme digestion coupled with sample clean up with accelerated solvent extraction that successfully removed these interferences, allowing quantification of polyethylene in a range of food samples. Finally, a simple protocol is suggested for future studies to (i) determine if an interference is present and (ii) sample processing methods to remove identified interferences (Rauert et al., 2022).

References:

Rauert, C., Pan, Y., Okoffo, E.D., O'Brien, J.W., Thomas, K.V. (2022), Journal of Environmental Exposure Assessment, 1(13), 1-12. http://dx.doi.org/10.20517/jeea.2022.04

Localisation of natural products within eucalypt flowers using mass spectrometry imaging

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Keywords: MALDI; DESI; Natural products; Eucalypt;

Abstract:

Corymbia and Angophora species are prolific sources of natural product compounds, and several isolated from the flowers are known to exhibit antimicrobial and insecticidal bioactivity. These compounds are likely to play ecological roles to aid in the host plants survival (Senadeera, S. P. D. et al., 2018).

Natural product chemists typically extract, separate, and identify the structure of complex molecules from ground biota material, offering little insight into the localisation of compounds within specific tissues and organs. To ascertain specific localisation information for compounds in tissues, Mass Spectrometry Imaging (MSI) is gradually being applied in plant biochemistry investigations. Here, MSI methods such as MALDI and DESI MSI were used to investigate the location of compounds within histological sections of flower buds and found molecules compartmentalised in oil glands and areas of nectar and pollen production, suggesting ecological relevant functions. The application of MSI techniques provide a unique cutting-edge platform to understand tissue localisation data in relation to flower bud chemistry.

Whilst MSI is still a growing field, methodologies around sample preparation are still being refined. This is particularly pertinent to plant biochemistry, where standard MSI methodology is not compatible for analysis of smaller molecular weight (100-1000 Da) natural products with standard methods often resulting in analyte signal suppression. Similarly, typical microtome slicing methods cause loss of tissue integrity for delicate floral anatomy (Boughton, B. A. et al., 2016). Here, I present low-cost method development compatible for biological samples subject to delicate anatomy as well as natural product investigations.

References:

Boughton, B. A. et al. (2016) "Mass Spectrometry Imaging for Plant Biology: A Review," Phytochemistry Reviews : Fundamentals and Perspectives of Natural Products Research, 15(3), pp. 445–488. doi: 10.1007/s11101-015-9440-2.

Senadeera, S. P. D. et al. (2018) "Antiplasmodial B-Triketone-Flavanone Hybrids from the Flowers of the Australian Tree Corymbia Torelliana," Journal of natural products, 81(7), pp. 1588–1597. doi: 10.1021/acs.jnatprod.8b00154.

A sensitive high-throughput direct injection liquid chromatography-tandem mass spectrometry method for the surveillance of antimicrobials in wastewater

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Keywords: Antimicrobial; Liquid Chromatography; Mass spectrometry; Wastewater Analysis; Direct Injection

Abstract:

Antimicrobial pollution and antimicrobial resistance pose a national and international threat to public and environmental health, yet current antimicrobial use surveillance methods are mainly limited to the clinical setting. Wastewater analysis has been identified as a promising tool for antimicrobial monitoring and the back-estimation of antimicrobial consumption, but current methods are tedious and complicated, limiting their scope for high-throughput analysis. The present study looks at the development of a sensitive direct injection method for the quantification of 78 antimicrobials, including 72 antibiotics, 2 antifungals and 4 disinfectants used for humans and animals, in raw wastewater samples using a Sciex 7500 System. The method was validated in terms of specificity, linearity, range, recovery, limit of detection (LOD), limit of quantification (LOQ), accuracy, and precision. Most analytes achieved a linearity of $R2 > 0.99$, and the quantification range was from 1 ng L-1 to 100 000 ng L-1. The filtration loss yielded recoveries from 5% to 100% for different analytes. Method LOQs were determined as low as 2 ng L-1, and accuracy and precision were achieved excellently. The method was subsequently applied to wastewater samples collected from 50 wastewater treatment plants across Australia in August 2021. In total, 39 antimicrobials were detected at concentrations ranging from 4 ng L-1 to ~100 µg L-1, from which cephalexin, sulfamethoxazole, sulfapyridine and all disinfectants had the highest concentrations. The current study provides a straightforward analytical method for antimicrobial monitoring with a fast and simple pre-treatment procedure.

Structural elucidation of branched-chain fatty acids through charge-remote fragmentation

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Keywords: Fatty acids; LCMS; plasma; lipidomics; branched-chains

Abstract:

Branched-chain fatty acids are critical as signalling molecules for various health issues and diseases. Branched-chain fatty acids are difficult to distinguish from their isomeric straight-chain counterparts by tandem-mass spectrometry strategies, with the only structural difference being a methyl group(s) at different sites along the acyl chain. The introduction of a positive fixed charge site to promote charge-remote fragmentation in the fatty acid is therefore beneficial for inducing fragmentation patterns characteristic for the carbon-carbon bonding arrangements of the acyl chain. Herein, we adopt the charge-inversion strategy of complexing straight and branched-chain fatty acid standards with the doubly-charged Magnesium tris-5-nitro-1,10-phenanthroline complex by combining the compounds in a T-infusion set up post chromatographic column separation and analysed using a Thermofisher Linear Ion Trap LTQ-XL. The non-esterified fatty acids in citrated human plasma were extracted and analysed using the same method. We demonstrate that collision-induced dissociation of these ionic complexes yields unique spectra for each fatty acid studied including the ability to differentiate between isomeric branched-chain fatty acids. The dissociation of the combined [Mg(NO2Phen)2FA]+ yields a loss of one NO2Phen ligand, and subsequent dissociation of the [Mg(NO2Phen)FA]+ produces unique spectra for each FA and allows for unambiguous identification of the branch-chain location. Enhancing charge-remote fragmentation processes maximises the structural information obtained in the analysis and enables chain branching assignment for even low abundant fatty acids, including branched chain fatty acids in human plasma. Combining this technique with chromatographic separation of a wider range of branched-chain fatty acids will allow for further investigation into plasma.

References:

Randolph, CE, Foreman, DJ, Betancourt, SK, Blanksby, SJ & McLuckey, SA 2018, 'Gas-Phase Ion/Ion Reactions Involving Tris-Phenanthroline Alkaline Earth Metal Complexes as Charge Inversion Reagents for the Identification of Fatty Acids' Analytical Chemistry, vol. 90, no. 21, pp. 12861-9.

Pikulski, M, Aguilar, A & Brodbelt, JS 2007, 'Tunable Transition Metal-Ligand Complexation for Enhanced Elucidation of Flavenoid Diglycosides by Electrospray Ionization Mass Spectrometry' American Society for Mass Spectrometry, vol. 18, pp. 422-31.

Visualization of per- and polyfluoroalkyl substances (PFASs) distribution in concrete using Desorption Electrospray (DESI) Mass Spectrometry Imaging (MSI)

Phong H.N. Vo[1], Brett R. Hamilton[2], Roger A. Wepf[2], Trent A. Key[3], Thi Minh Hong Nguyen[1], Phong K. Thai[1], Kevin V. Thomas[1], Jochen F. Mueller[1]

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Keywords: AFFFs; PFASs; DESI; MSI; concrete

Abstract:

Per- and polyfluorinated substances (PFASs) including perfluorooctane sulfonate (PFOS) and perfluorohexane sulfonate (PFHxS) have become ubiquitous pollutants. They were a key component of aqueous film forming foams (AFFFs) for firefighting which has led to widespread contamination of firefighting training grounds (FFTGs) (Moody and Field, 2000). Little research has been carried out on distribution of PFASs in the impacted concrete. A key issue is to identify the heterogenicity and vertical distribution of PFASs in the concrete at FFTGs. Works to date only focused on analysis of drilling material from different depth along concrete cores (Baduel et al., 2015; Thai et al., 2022). The second approach that was investigated was the use of a mass spectrometry imaging (MSI) to determine if PFOS and PFHxS could be mapped in relatively flat vertical transects of concrete core samples. The aim of this presentation is to evaluate desorption electrospray ionization mass spectrometry (DESI) as a tool for providing a vertical-spatial distribution of PFASs in concrete from a firefighting ground without extraction. The results showed that the PFOS/PFHxS mapping observed using DESI MSI matched well with the extraction results analysed by liquid chromatography mass spectrophotometry (LC-MS). Yet, the drilling visualization provides a much less detail and its resolution at the top surface is insufficient to assess the distribution of PFASs for leaching out during run off events. Taken together both techniques allow for a complete picture of the PFOS/PFHxS distribution/penetration into solid and porous samples such as concrete.

References:

Baduel, C., Paxman, C.J., Mueller, J.F., 2015. Perfluoroalkyl substances in a firefighting training ground (FTG), distribution and potential future release. J. Hazard. Mater., 296, 46-53. https://doi.org/10.1016/j.jhazmat.2015.03.007

Moody, C.A., Field, J.A., 2000. Perfluorinated Surfactants and the Environmental Implications of Their Use in Fire-Fighting Foams. Environ. Sci. Technol., 34(18), 3864-3870. 10.1021/es991359u

Thai, P.K., McDonough, J.T., Key, T.A., Thompson, J., Prasad, P., Porman, S., Mueller, J.F., 2022. Release of perfluoroalkyl substances from AFFF-impacted concrete in a firefighting training ground (FTG) under repeated rainfall simulations. Journal of Hazardous Materials Letters, 3, 100050. https://doi.org/10.1016/j.hazl.2022.100050.

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Revolutions in lipid isomer resolution: Applications of cyclic ion-mobility mass spectrometry to frontier challenges in lipidomics

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Keywords: ion mobility; lipidomics; isomers

Abstract:

Despite increases in sensitivity, many families of lipid isomers remain unresolved by contemporary liquid chromatography-mass spectrometry leading to an underestimate in structural diversity within the lipidome. Ion-mobility coupled to mass spectrometry has been identified as a potential means to address this challenge through providing an additional means of resolving lipid isomers. Previous exploration of drift-, travelling-wave and differential-mobility technologies for resolving lipid isomers have shown some promise but also demonstrate that some isomers require resolving power beyond the capabilities of conventional mobility platforms. Here we present results from the application of ultra-high resolution travelling-wave ion mobility for the resolution of simple and complex lipid isomers that differ in the location of a single carbon-carbon double bond, the stereochemistry of the double bond (i.e. cis or trans) or –for glycerolipids– the relative substitution of acyl chains on the glycerol backbone (i.e., sn-position). These preliminary findings suggest that high resolution ion-mobility has exciting potential for isomer-resolved lipidomics and it is attractive to consider future integration of cIMS with other modes of ion-activation, including ozone-induced dissociation, to bring together advanced separations and structure elucidation to complete the lipidome.

Semi-quantitative characterisation of bromo-chloro paraffins and olefins in the Australian environment

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Keywords: Persistent Organic Pollutants (POPs); α-bromo-chloro alkenes; atmosphere; dust; sludge

Abstract:

A semi-quantitative high-resolution mass spectrometry method was developed and applied to assess the occurrence of bromo-/chloro paraffins (BCPs) and olefins (BCOs) in the environment. More than 400 possible BCPs and BCOs congener groups were detected in dust, air, and sewage sludge samples collected from Australia. Median chain analytes with the number of halogen atoms <7 (CnHmClxBry, 14≤n≤17, x+y<7) prevailed in the dust and sludge samples, while short chain analytes (CnHmClxBry, 10≤n≤13, x+y<7) predominated the air samples. The estimated concentrations of ∑BCPs and ∑BCOs in dust and sludge were approximately 20% that of the chlorinated paraffins (CPs) present, with the median concentrations of 5.4 μg/g (dust) and 0.18 μg/g (sludge) for ∑BCPs, and 22 μg/g (in dust) and 0.50 μg/g (sludge) for BCOs. In the air samples, the concentrations of BCPs (0.020 pg/m3) and BCOs (0.032 pg/m3) were 3-4 orders of magnitudes lower than the concentrations of CPs (790 pg/m3). Significant correlations (P<0.001) were found between the concentration of CPs, BCPs and BCOs in all the matrices.

Unravelling the diverse metabolomes of native wild yeast

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Keywords: Metabolomics; Yeast; Beverages

Abstract:

The production and consumption of fermented beverages has been carried out for millennia by numerous cultures, and today represents a vast global industry of diverse products. Saccharomyces yeasts have traditionally dominated this industry, however, consumer demands for new products with varying sensory profiles and actual or perceived health benefits is driving the use of non-Saccharomyces yeasts in fermented beverage production. The influence of non-Saccharomyces yeasts on fermented beverage sensory characteristic diversity is, in large part, due to the diverse metabolites they produce. The use of metabolomic analyses allows for the exploration of the impact non-Saccharomyces yeasts have on fermented beverage sensory qualities. Here we have used a suite of untargeted DIA-LC-MS/MS and HS-GCMS approaches to identify and quantify the different metabolites produced by yeasts from our library of native non-Saccharomyces yeasts. We identified significant differences in metabolite production between our native wild yeasts and when compared to US05, a commercial S. cerevisiae brewing yeast.

InSpectra – A platform for identifying emerging chemical threats

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Keywords: HRMS; non-target; suspect screening; open-access; processing; archiving

Abstract:

Non-target analysis employing high-resolution mass spectrometry (HRMS) coupled with liquid chromatography is increasingly being used to identify chemicals of biological and environmental relevance. Often such HRMS datasets are both large and complex meaning that identifying potentially relevant chemicals is extremely challenging. Furthermore, HRMS data are recorded in vendor-specific formats meaning that to interpret them, users are often reliant on vendor-specific software that may not accommodate the advancements in HRMS data processing techniques.

Here we present InSpectra, an automated early warning social network to systematically detect newly identified emerging chemical threats. InSpectra is a web-based open-source open-access software platform that provides vendor-independent complete non-target analysis and suspect screening workflows. As a cloud-based platform, InSpectra takes advantage of parallel computing and ability to archive all data and associated metadata with a focus for sharing and community curation of HRMS data. This will allow rapid retrospective analysis to optimise the way emerging chemical threats are identified. Additionally, InSpectra is completely modular with a future vision to incorporate state-of-the-art algorithms and tools. Current InSpectra workflows will be demonstrated using case studies to showcase its capabilities including sample matrix and temporal trend comparisons.

Automated proteomics workflows for high-throughput library generation and biomarker detection using data-independent acquisition

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Keywords: Proteomics

Abstract:

Recent developments in mass spectrometry data acquisition underpinned by advanced bioinformatics offer a framework for comprehensive analysis of proteomes and the discovery of robust biomarkers. Specifically, Sequential Window Acquisition of all THeoretical fragment ion spectra (SWATH) has proven to be a reliable approach for measuring the abundance profiles of thousands of proteins in large numbers of replicate samples. However, the lack of a generic sample preparation platform to tackle the heterogeneity of material collected from different sources may be a limiting factor to the broad application of this technique. Universal and fully automated sample preparation workflows have been developed for clinical specimens that support high-throughput library generation and label-free quantification of proteins across virtually any number of replicates without compromising reproducibility. When applied to various bovine tissues and body fluids representing healthy animals, the workflows enabled in-depth characterization of their proteome, in many cases for the first time. The application to an ovine model of myocardial infarction revealed significant changes associated with injury. Gene regulatory networks inferred from protein abundance data supported by microarray profiling of miRNA and mRNA expression resulted in the identification of three master regulatory genes that were previously shown to be diagnostic for infarcted cardiac tissue, thereby validating the automated workflows for clinical applications and in different animals.

POSTER FLASH

The role and impact of N- and O-glycosylation on surface exposed proteins and cellular lipids and metabolites

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Keywords: Glycosylation; Lipidome; Metabolome; Ost3; Pmt1

Abstract:

N- and O-Glycosylation plays a variety of roles in the eukaryotic cells. The structure of proteins influences their functions, and macromolecules like glycans can significantly alter the structure of a protein. Glycosylation also plays a very important role in lipid metabolism, assisting in ER protein quality control, lipid homeostasis, and peroxisome biogenesis (William James et al., 2019). While it is well known the role and impact N- and O-glycosylation has on the proteome and the effect glycosylation deficient has on the proteome, the exact effect of N- and O-glycosylation have on the lipidome, and metabolome is poorly understood. In this study, we compare the lipidome, metabolome, and proteome of BY4741 (wild type Saccharomyces cerevisiae) to glycosylation deficient S. cerevisiae strains, Dost3 and Dpmt1 and BY4741 grown with tunicamycin. Ost3 & Pmt1 genes encode for regions of different protein complexes that helps with N- and O-glycosylation respectively (Zatorska et al., 2017). Several significant deviations in the abundance of secreted proteins, surface-exposed proteins, metabolites, and cellular lipids have been observed. Finally, this study attempts to explain how changes in the glycosylation of proteins affect the lipidome and metabolome of the yeast cells.

References:

William James, A., Ravi, C., Srinivasan, M. & Nachiappan, V. 2019. Crosstalk between protein N-glycosylation and lipid metabolism in Saccharomyces cerevisiae. Scientific Reports, 9, 14485.

Zatorska, E., Gal, L., Schmitt, J., Bausewein, D., Schuldiner, M. & Strahl, S. 2017. Cellular Consequences of Diminished Protein O-Mannosyltransferase Activity in Baker's Yeast. International Journal of Molecular Sciences, 18, 1226.

POSTER FLASH

Mass quantification of microplastic at wastewater treatment plants by pyrolysis-gas chromatography-mass spectrometry

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Keywords: Plastics; Microplastic Mass concentrations; Wastewater treatment; Removal efficiency; Pyr-GC/MS

Abstract:

Municipal wastewater treatment plants (WWTPs) are a central point of collection of plastic particles from households and industry and for their re-distribution into the environment. Existing studies evaluating levels of plastics in WWTPs, and their removal rates have reported and used data on polymer type, size, shape, colour, and number of plastic particles, while the total mass concentration of plastic particles (especially >1 µm) remains unclear and unknown. To address this knowledge gap, raw influent, effluent, and reference water samples from three WWTPs in Australia were collected to analyse the mass concentrations and removal rates of seven common plastics (>1 µm in size) across the treatment schemes. Quantitative analysis was performed by pressurized liquid extraction followed by pyrolysis coupled to gas chromatography mass spectrometry. Results showed that the total plastic content in the WWTPs raw influent samples was between 840 and 3,116 µg/L, resulting in an inflow of between about 2.1 and 196.4 kg/day of the total measured plastics. Overall, >99% by mass of the plastics entering the three WWTPs from the raw influent was removed during the pre-treatment stages, presumably ending up in the sewage sludge, which means emissions (via treated effluent) from the treatment plants are low. Compared with the raw influent, the plastic mass concentrations in the treated effluents (i.e., Class C, A, and final effluent) from the three WWTPs, as well as the reference water samples within their catchments were below the limits of reporting. Of the five quantified plastic types, polyethylene (PE, 76.4%), and polyvinylchloride (PVC, 21%) dominated by mass, while polyethylene terephthalate (PET, 1.9%), polypropylene (PP, 0.4%) and polymethyl methacrylate (PMMA, 0.3%) accounted for a small proportion of the total. Overall, this study investigated the mass concentrations of plastic particles above 1 µm in wastewater and their removal, which provided valuable information regarding the pollution level and distribution characteristics of plastic polymers in Australian WWTPs.

POSTER FLASH

Investigating complex mixtures of metallo-supramolecular assemblies using the Waters SELECT SERIES Cyclic IMS

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Keywords: Waters Cyclic IMS; Metallo-Supramolecular Assemblies; Separating Isomers

Abstract:

Metallo-supramolecular assemblies have unique structures which have applications in drug delivery, catalysis and guest recognition (Pullen, Tessarolo and Clever, 2021). In the past, the majority of research has explored symmetrical assemblies, subsequently limiting potential structures and applications. It is only recently that asymmetric structures have been investigated, with most structures minimising complexity by focusing on the formation of a single product. This reticence to study complex mixtures could be attributed to limitations in characterisation techniques, where NMR often provides insufficient data resolution to confidently and efficiently analyse these mixtures. Ion mobility mass spectrometry (IM-MS) is a specific type of MS which allows the clear resolution of different species based on their mass, shape and charge (Chan et al., 2009). This project investigates the synthesis of complex mixtures of discrete metallo-supramolecular cages and their characterisation using the Waters SELECT SERIES Cyclic IMS.

References:

Chan, Y., Li, X., Soler, M., Wang, J., Wesdemiotis, C. and Newkome, G., 2009. Self-Assembly and Traveling Wave Ion Mobility Mass Spectrometry Analysis of Hexacadmium Macrocycles. Journal of the American Chemical Society, 131(45), pp.16395-16397.

Pullen, S., Tessarolo, J. and Clever, G., 2021. Increasing structural and functional complexity in self-assembled coordination cages. Chemical Science, 12(21), pp.7269-7293.

POSTER FLASH

Do beer and bread make you fat?

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Keywords: Lipidomics; shotgun; yeast

Abstract:

Rationale
Mass spectrometry-based shotgun lipidomics has enabled comprehensive and quantitative assessments of the cellular lipid composition of yeast. Saccharomyces cerevisiae is a well-known yeast used to make products derived from fermentation. (e.g., bread, beer, wine, cider) The aroma profile constitutes a vital quality parameter of bread, and the aromas can be derived from the oxidation of lipids. S. cerevisiae produces fatty acids during alcoholic fermentation, which influence the aromatic profile of the wine. Nevertheless, ethyl esters formed by medium chain fatty acids (MCFAs) are responsible for fruity and floral aromas. This project deals with the lipidome of two Saccharomyces cerevisiae strains, one used in baking and the other in the brewing industry.

Methods
Herein, one Baker's and one Brewer's yeast strains of Saccharomyces cerevisiae were compared based on their cellular lipidome. Lipids were extracted using procedures identical to those published by Matyash et al. and quantified using deuterated lipids (SPLASH Lipid-o-Mix) and a deuterated palmitic acid as internal standards. (hexadecanoic acid-d31). Lipid extracts were analyzed by mass spectrometry using an Orbitrap Elite high-resolution mass spectrometer equipped with a robotic nanoflow ion source Triversa Nanomate.

Results
The most abundant lipid classes in both strains are: phosphocholine, phosphatidylethanolamine, phosphatidylinositol, phosphatidylserine, phosphatidic acid, triacylglycerols, Ergosterol and the respective lyso-derivatives. Differences were observed between the two yeast strains concerning total lipid content and lipid composition.

Conclusion
Regarding the results obtained, it was possible to differentiate between Baker's and Brewer's yeast based on their lipid composition.

References:

Mbuyane, L. L., Bauer, F. F. & Divol, B. 2021. The metabolism of lipids in yeasts and applications in oenology. Food Res Int, 141, 110142.
Heitmann, M., Zannini, E. & Arendt, E. 2018. Impact of Saccharomyces cerevisiae metabolites produced during fermentation on bread quality parameters: A review. Crit Rev Food Sci Nutr, 58, 1152-1164.

POSTER

Analysis of tyre wear particles and tyre additives in Queensland surface water

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Keywords: Tyre wear; tyre additives; LC-MS/MS; Pyrolysis-GCMS; Microplastics

Abstract:

Tyre road wear particles (TRWPs) are now recognised as one of the largest sources of microplastics to the urban environment. Whilst being a significant source of microplastics they also contain a wide range of chemicals and recently the chemical 6PPD-quinone (a transformation product of the common tyre rubber antiozonant 6PPD) has raised concerns due to acute toxicity towards certain salmonoid species (Tian et al., 2021). There is little to no data on environmental concentrations of TRWPs or tyre additives in the Australian environment. This study used the complimentary techniques of Pyrolysis gas chromatography mass spectrometry and liquid chromatography tandem mass spectrometry to quantify both TRWPs and 15 tyre additives in surface water from 5 urban centres in Queensland. Tyre additives were ubiquitously detected with concentrations approaching the LC50 for coho salmon during severe storm events (Rauert et al., 2022a). Concentrations of TRWPs were correlated with concentrations of additives during storm events suggesting stormwater road runoff is a primary source of these pollutants to the monitored ecosystems. A traffic source related additive profile is also suggested (Rauert et al., 2022b) that may assist with designing future targeted sampling campaigns.

References:

Tian, Z., Zhao, H.N., Peter, K.P., Gonzalez, M., Wetzel, J., Wu, C., Hu, X., Prat, J., Mudrock, E., ... Kolodziej, E.P. (2020). Science, 371(6252), 185-189. https://doi.org/10.1126/science.abd6951

Rauert, C., Charlton, N., Okoffo, E. D., Stanton, R. S., Agua, A. R., Pirrung, M. C., & Thomas, K. V. (2022a). Environmental Science and Technology, 56(4), 2421–2431. https://doi.org/10.1021/acs.est.1c07451

Rauert, C., Vardy, S., Daniell, B., Charlton, N., & Thomas, K. (2022b). Science of the Total Environment, 852, 158468. https://doi.org/10.1016/j.scitotenv.2022.158468

POSTER FLASH

Emerging environmental contaminant para-phenylenediamine quinones (PPD-Qs): Occurrences, characteristics and health risks

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Keywords: HRMS, suspect screening, emerging contaminants, air pollution

Abstract:

In 2021, Science has revealed the cause of "urban runoff mortality syndrome", i.e., acute and widespread mortality of coho salmon in streams/rivers during rainfall events. N-1, 3-dimethylbutyl-N'-phenyl-p-phenylenediamine quinone (6PPD-Q), an oxidation product of the widely adopted tire rubber additive 6PPD, was identified to induce acute mortality to coho salmon at lower doses (24-h semi-lethal concentration of 95 ng/L). Since then, research interests in the environmental behaviours and toxicities of para-phenylenediamine quinones (PPD-Qs) have greatly arisen. Herein, by applying high-resolution mass spectrometry-based suspect screening strategy, we have first identified a series of novel PPD-Qs and revealed their occurrences in the ambient environments of Hong Kong and mainland China. Using synthesized standards, their environmental levels and compositional profiles were specifically characterized, which provided comprehensive data on their multi-route exposures and related human intake doses. Besides that, the environmental characteristics of such emerging contaminants in atmospheric particulate matter (PM2.5) including potential sources, influencing factors, and spatiotemporal variations were investigated with a total of 133 intra- and intercity samples collected over one year. Additionally, health risks regarding the oxidative potential, i.e., ability to induce oxidative stress, of PPD-Qs were evaluated for the first time through an acellular dithiothreitol (DTT) assay. These investigations have provided insights into the occurrences, characteristics, and health risks of emerging PPD-Qs.

References:

Tian, Z., Zhao, H., Peter, K. T., Gonzalez, M., Wetzel, J., Wu, C., Hu, X., Prat, J., Mudrock, E., Hettinger, R., Cortina, A. E., Biswas, R. G., Kock, F. V. C., Soong, R., Jenne, A., Du, B., Hou, F., He, H., Lundeen, R., Gilbreath, A., Sutton, R., Scholz, N. L., Davis, J. W., Dodd, M. C., Simpson, A., Mcintyre, J. K. & Kolodziej, E. P. 2021. A ubiquitous tire rubber-derived chemical induces acute mortality in coho salmon. Science, 371, 185-189;

Tian, Z., Gonzalez, M., Rideout, C. A., Zhao, H. N., Hu, X., Wetzel, J., Mudrock, E., James, C. A., Mcintyre, J. K. & Kolodziej, E. P. 2022. 6PPD-Quinone: Revised Toxicity Assessment and Quantification with a Commercial Standard. Environmental Science & Technology Letters, 9, 140-146;

Cao, G., Wang, W., Zhang, J., Wu, P., Zhao, X., Yang, Z., Hu, D. & Cai, Z. 2022. New Evidence of Rubber-Derived Quinones in Water, Air, and Soil. Environ Sci Technol, 56, 4142-4150;

Wang, W., Cao, G., Zhang, J., Wu, P., Chen, Y., Chen, Z., Qi, Z., Li, R., Dong, C. & Cai, Z. 2022. Beyond Substituted p-Phenylenediamine Antioxidants: Prevalence of Their Quinone Derivatives in PM2.5. Environmental Science & Technology, 56, 10629-10637;

Wang, W., Cao, G., Zhang, J., Chen, Z., Dong, C., Chen, J. & Cai, Z. 2022. p-Phenylenediamine-Derived Quinones as New Contributors to the Oxidative Potential of Fine Particulate Matter. Environmental Science & Technology Letters, 9, 712-717.

POSTER

Qualitative and spatial analysis of ganoderic acids from Australian Ganoderma fruiting bodies

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Keywords: Ganoderma; Triterpenoids; high-resolution mass spectrometry; UHPLC-MS/MS

Abstract:

Ganoderma is a genus of saprotrophic cosmopolitan bracket fungus known for its health benefits. Commercial extracts from G. lucidum and members of G. lucidum complex are rich in bioactive ganoderic acids (GAs) and other lanosterol-derived triterpenes. The bioactivity of these compounds comes from its ability to modulate the immune system, leading to effects that include anti-aging, anti-cancer, and anti-inflammatory activity. Some of these medicinal compounds can be found in other Ganoderma species, such as G. orbiforme, G. zonatum, and G. australe. The structural similarity between GAs hinders the efficient separation and analysis of Ganoderma compounds. However, high-performance liquid chromatography associated with mass spectrometry (HPLC-MS) has demonstrated to be a powerful tool to analyse such metabolites. In this study, the triterpenoids of 23 Ganoderma fruiting bodies originated from Australia have been qualitatively analysed through HPLC-MS. Additionally, tissues from different regions of the same fruiting body were compared for their triterpenoid concentration and diversity. Based on fragmentation, retention time, and mass, 22 GAs were tentatively identified, including GA-AM1, GA-F, and GA-G, that have demonstrated anti-tumour activity (Gong et al., 2019). These GAs accumulated mostly in the cap and pore tissue, as opposed to the context. Commonly, secondary metabolites like GAs act protecting the organism against environmental hazards, which may explain their higher accumulation in external tissues (Demain & Fang, 2000). This work provides important data regarding the chemical composition of Ganoderma in Australia, as well as relevant information regarding triterpenoid accumulation within the fruiting body.

References:

Demain, A. L. & Fang, A. 2000. The natural functions of secondary metabolites. History of modern biotechnology I, 1-39.

Gong, T., Yan, R., Kang, J. & Chen, R. 2019. Chemical Components of Ganoderma. In: LIN, Z. & YANG, B. (eds.) Ganoderma and Health. Advances in Experimental Medicine and Biology: Springer Nature Singapore Pte Ltd.

POSTER

Cyclic tachyplesin and cyclic gomesin can overcome acquired drug resistance in BRAF mutant melanoma cells

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Keywords: anti-cancer peptides; drug-resistance; membrane lipid; cell surface charge; lipid metabolism

Abstract:

Melanoma is a deadly cancer due to its metastatic nature. The overall survival rate of patients with metastatic melanoma has greatly improved over the last decade thanks to targeted therapy and immune check points inhibitors. However, approximately half of the patients are irresponsive, or develop drug-resistance within 6-10 months of treatment. Therefore, alternative drugs with distinct mechanisms of action to treat melanoma patients are needed. We investigated the use of cyclic peptides inspired by host defence peptides from spider and horseshoe crab with a beta-hairpin structure as an alternative therapeutic option to kill drug-tolerant and drug-resistant melanoma cells. We explored the activity of these anti-melanoma peptides and characterised the lipidome and proteome of untreated melanoma cells and ones that have acquired drug-resistance to dabrafenib, a small molecule inhibitor used to treat patients with BRAF V600E metastatic melanoma. We discovered that the cell membrane lipid composition of melanoma cells changed while acquiring resistance to dabrafenib, that both peptides could kill metastatic melanoma cells during each stage of developing drug resistance and metastatic melanoma cells did not acquire resistance to tested peptides. These host defence peptides are therefore well suited as templates to design novel therapeutic leads to target drug-resistant metastatic melanoma cells and/or as a co-treatment option with small molecule drugs.

POSTER

Influence of SWATH-MS settings on successful identifications in a non-target workflow

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Keywords: non-target analysis; quality assurance; quality control; SWATH-MS

Abstract:

Non-target analysis (NTA) using high resolution mass spectrometry (HRMS) is a comprehensive approach to characterise untargeted, suspect and unknown chemicals including chemicals of emerging concern and has seen a steady increase recently.

Given the relative novelty of this type of analysis, robust quality assurance and quality control (QA/QC) measures are imperative to ensure quality and consistency of results. Due to fundamental differences to established targeted workflows, one goal of QA/QC must be to understand which information regarding the analysed chemical space (i.e., the totality of all chemicals in a specific environment/sample) is lost. Therefore, it is important to know how parameters and settings influence the acquired data; with the goal of minimizing the risk of losing information on potential substances of interest (i.e., false negatives) or introducing contamination (i.e., false positives), which can happen during each step of an analytical workflow.

Here we present how different mass spectrometric settings influence the ability to obtain confident identifications of as many components in river water as possible. For this, we first investigated the ideal number of SWATH windows (a way of data independent acquisition) for different matrices, before assessing several other parameters that were considered essential for successful identifications (including declustering potential and collision energy), using a central composite design (CCD) approach. This was done for each SWATH window (and therefore m/z range) individually.

POSTER

Emerging role of mass spectrometry in clinical diagnostics and toxicology at QML Pathology

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Keywords: Pathology; Clinical MS; Toxicology;

Abstract:

Liquid chromatography-tandem mass spectrometry (LC-MS/MS) has seen enormous growth in clinical pathology laboratories during the last 10–15 years. It offers analytical specificity superior to that of traditional immunoassays and conventional high performance/pressure liquid chromatography (HPLC) for low and high molecular weight analytes and has higher throughput than gas chromatography-mass spectrometry (GC-MS).

Queensland medical laboratory (QML) is a NATA accredited GX multi-disciplinary reference laboratory functioning under the Healius Limited umbrella, with a network of pathology laboratories around the Australian continent deploying state-of-the-art technology and assays to cater to the growing demands of precision diagnostics.

Of particular interest is the pioneering role of LC-MS/MS tool for assaying wide variety of disease markers at QML Pathology. The proposed poster showcase the details of the growing portfolio of LC-MS/MS based assay menu in the clinical mass spectrometry and drug toxicology space in our Biochemistry Dept, with special emphasis on how industry like ours has successfully assimilated this technology in a highly regulated environment while addressing its limitations, and seeking innovative and collaborative efforts to allow accessible, cost-effective, high-throughput, and high-quality assays for novel molecular targets/ biomarkers used for pathology applications available to Australian public.

POSTER

Dietary exposure to microplastics

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Keywords: Food, diet, microplastics, ASE, pressurised liquid extraction, Pyrolysis-GCMS

Abstract:

Food and beverage products can be contaminated with microplastics at any stage of the food production process and consumption of microplastics through the diet is recognised as a major pathway of human exposure (Yates et al. 2021). Concerns are growing internationally around the potential health impacts of ingesting microplastics and despite increased research in this area over the last 10 years, there is insufficient data available on commonly eaten foods to reliably determine total dietary exposure (World Health Organisation 2022). This study analysed 30 different food and beverages from the 10 most regularly consumed food groups as identified by the Australian Health Survey (Australian Bureau of Statistics, 2014). Identification and quantification of seven different plastics was undertaken using pressurised liquid extraction (ASE) together with double-shot pyrolysis gas chromatography–mass spectrometry. Concentrations determined in the food products were used to calculate average dietary exposure of the Australian population.

References:

Australian Bureau of Statistics (2014) 'Australian Health Survey: Nutrition First Results - Foods and Nutrients', Australian Bureau of Statistics, accessed 27 January 2022

World Health Organisation (2022) 'Dietary and inhalation exposure to nano- and microplastic particles and potential implications for human health' World Health Organisation, accessed 22 September 2022

Yates J, Deeney M, Rolker, HB, White, H, Kalamatianou, S and Kadiyala, S (2021) 'A systematic scoping review of environmental, food security and health impacts of food system plastics', Nature Food, 2: 80 – 87, doi: 10.1038/s43016-021-00221-z

POSTER

Investigating highly reduced metallosupramolecular complexes in the gas phase

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Keywords: electron transfer; supramolecular complexes; ion chemistry

Abstract:

Transition metal complexes with accessible low oxidation states are central to catalysis. Investigating the intrinsic properties of such complexes beyond their conventional oxidation state(s) is complicated by an inability to cleanly isolate a pure population, as well as their propensity to react with solvent or ambient air. Using electron transfer dissociation (ETD) in conjunction with ion mobility mass spectrometry, we show that highly reduced metal complexes can be prepared, isolated, and investigated (Pfrunder et al., 2022). The effect of precursor ion charge state, ligand structure, and guest encapsulation on the reaction products and rates is explored.
ETD of isolated supramolecular complex cations yielded intact, charge-reduced species, with products associated with up to 14 reduction steps detected. No change in molecular mass or collisional cross-section was observed, indicating that the coordination complex remains intact despite the significant reaction exothermicity. Repeating the experiment with an encapsulated fullerene guest inside the complex further confirmed that the structural integrity of the complex was retained. In both cases, the reaction kinetics could be modelled as a series of stepwise, single electron transfers under pseudo-first order conditions. Further, the reactivity of the reduced complexes was investigated by re-isolation of each product ion in the presence of adventitious O2.

The selectivity of mass spectrometry enables the isolation and interrogation of transient species, including highly reduced complexes. This work opens an avenue to further investigations of these elusive species by interfacing the current method with gas-phase chemical or spectroscopic methods.

References:

Pfrunder, M. C., Marshall, D. L., Poad, B. L. J., Stovell, E. G., Loomans, B. I., Blinco, J. P., Blanksby, S. J., Mcmurtrie, J. C. & Mullen, K. M. 2022. Exploring the Gas Phase Formation and Chemical Reactivity of Highly Reduced M8L6 Coordination Cages. Angewandte Chemie International Edition.

POSTER

PHGDH, a novel metabolic target in drug-resistant melanoma

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Keywords: Melanoma; lipidomics; peptides; Serine metabolism

Abstract:

The incidence of melanoma in Australia and New Zealand is amongst the highest in the world. When diagnosed early, melanoma has an overall survival (OS) rate of 100%. However, stage 4 melanoma has an OS of 26% and is amongst the lowest survival rates for stage 4 metastatic cancers. Resistance to targeted therapies, such as MAPK pathway inhibitors, leads to changes in melanoma cell morphology, metabolism and behaviour and can lead to cross-resistance to immunotherapy. Therefore, Identification of novel targets that can help resensitise drug-resistant melanoma to standard therapies may improve patient outcomes. Phosphoglycerate dehydrogenase (PHGDH) is the rate limiting enzyme of the serine synthesis pathway and is reportedly upregulated in drug-resistant melanoma. The serine synthesis pathway is important for the use of serine in glutathione and one-carbon metabolism, sphingolipid and phosphatidylserine synthesis, glycine and alpha-ketoglutarate production. We have designed linear peptide sequences to target the oligomeric state of PHGDH and disrupt its function, in an enzymatic assay. The secondary structure of linear peptide sequences will be analysed using circular dichroism (CD) spectroscopy. Furthermore, we will investigate the effect of PHGDH inhibition in drug-resistant melanoma by incubating drug-resistant melanoma cells with a small molecule PHGDH inhibitor. We propose the continual inhibition of PHGDH in drug-resistant cells will lead to changes in the cell membrane lipid composition, especially Phosphatidylserine and Sphingomyelin. In addition, the susceptibility of drug resistant melanoma cells to dabrafenib and their ability of melanoma to migrate will be affected.

POSTER

Finding inhibitors of anti-virulence targets in Burkholderia pseudomallei

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Keywords: Fragment Based Drug Discovery, Native Mass Spectrometry, Burkholderia pseudomallei

Abstract:

With no targeted treatments available, the rare tropical disease melioidosis continues to infect and kill. With an average of 10 cases in Australia annually, it is most often diagnosed at a late stage of infection where harsh bactericidal antibiotics are no longer effective, resulting in a mortality rate of 20%. The bacterium responsible; Burkholderia pseuodmallei; presents a challenge in developing new targeted anti-microbials due to its innate drug-resistance. Drugs that target virulence rather than bacterial viability offer an alternative to bactericidal antibiotics, that limits the development of acquired drug-resistance.

Cyclophilins ppiA and ppiB natively expressed by Burkholderia pseudomallei have been identified as essential for virulence. Their deletion leads to anti-virulence effects due to their function in the cis/trans isomerization of proline residues in virulence factors. Exploring ppiA and ppiB as drug targets could lead to a targeted therapy, whereby their inhibition disarms the bacterium, allowing the hosts immune system to elicit a more effective response.

Fragment-based drug discovery (FBDD) is a fast-growing high-throughput innovation that allows novel drug leads to be uncovered. Applying this technique to the search for targeted melioidosis therapeutics allows a large area of chemical space to be explored, leading to a diverse range of potential drug leads.

This poster will discuss the utility of native mass spectrometry (nMS) in our FBDD approach towards developing novel anti-virulence drug leads against melioidosis. Central to our approach is to study the ppiA and ppiB proteins protein-fragment interactions against the CSIRO 720-member fragment library stored at Compounds Australia.

POSTER

Quantitative proteomics investigations of methane utilising bacteria and characterisation of a previously unsequenced Hyphomicrobium sp.

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Keywords: Pan-Proteomics, Hyphomicrobium, Genome-Sequencing. Degradation

Bio:

Increasing levels of methane correlate with increased atmospheric temperatures that have adverse effects in the environment such as global warming. This has led to the importance of identifying solutions to remove methane from the environment, a potential solution is using bacteria that utilise methane. In the Great Artesian Basin there are a number of novel putative methanotrophs that have been discovered. The assembly of their genomes is currently been conducted. Bacterial taxonomy is aided by the use of Mass Spectrometry (MS). Sequential Window Acquisition of all Theoretical Mass Spectrometry (SWATH-MS) proteomics has been identified as vital application for quantitative characterisation of different organisms such as bacteria. SWATH-MS is utilised to confirm the accuracy of the genome assemblies and identify potential methane degradation pathways of the previously uncharacterised species of Hyphomicrobium including CS1GBMeth 3 and NDB2Meth4 isolated from bore water wells located at the Great Artesian Basin. Sequences are processed and annotated using massPix MS package. In conclusion, FASTA files that contain protein sequences from each genome assembly will be used to produce in-silico spectral libraries which allows for the extraction of peptide SWATH data using DIA-NN package.

POSTER

The host subcellular proteome and glycoproteome throughout a time-course infection of influenza A virus

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Keywords: Proteomics; Glycoproteomics ; Virology ; Influenza ; Cellular Biology

Abstract:

Influenza A virus infections account for substantial morbidity and mortality, particularly amongst the elderly, young children, and pregnant women. Given the fact that current therapeutic strategies remain inadequate, it is imperative that we further develop our understanding of viral-host protein interactions.

The host proteome during influenza A virus infection is well characterised at a global level, however little attention has been given towards both the host subcellular proteome and glycoproteome. It is suspected that the influenza A virus glycoprotein neuraminidase, as a sialidase, alters glycosylation of host glycoproteins during infection, and viral-host protein interactions likely further contribute to perturbations of the host glycoproteome.

We developed a LC-MS/MS based protocol using tandem mass tag (TMT) labelling, and HILIC enrichment, to identify and quantify the dynamic changes in protein abundance, and glycosylation throughout the course of infection with two influenza A virus strains representative of the two subtypes predominating infections in humans: the H1N1 virus A/PR8/8/34 and the H3N2 virus A/X31.

We applied this protocol to infected human A549 cells at several timepoints, analysing four subcellular fractions relevant to influenza virology: the organelle, nuclear, cytosolic, and secreted protein fractions. Using this protocol, we are able to discern the dynamic host subcellular proteome and glycoproteome in influenza A virus infection, and we are further able to discern strain-specific host responses in infection with the two subtypes.

POSTER

Metabolites and fatty acids analysis using triple quadrupole gas chromatography mass spectrometry

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Abstract:

New platforms on metabolites and fatty acids analysis are now available on Shimadzu TQ 8050NX. Metabolites analysis provides ready-to-use methods for over 500 primary metabolites. Combination of full scan and MRM scan methods created from Shimadzu Trimethylsilylated (TMS) Metabolites Libraries. To start analysis without an investigation of measurement conditions, use full scan and/or MRM scan suited to the analysis aims. Protocol includes TMS derivatisation through AOC 6000plus auto-sampler.

Fatty acids platform provides the methods for characterization of unsaturated fatty acids structures and quantitative total fatty acid profile. Characterization of unsaturated fatty acid structures uses Shimadzu solvent-mediated chemical ionization unit to implement covalent adduct chemical ionization. CACI-MS/MS yield unique diagnostic ions that enable structural characterization of most FAMEs with no need for standard solution. Quantitative total fatty acid profile uses full scan either EI-MS and/or CACI-MS suited to detect fatty acid methyl esters (FAMEs).

A few examples analysis demonstrated these methods would be beneficial for research in the field of health science, and food science1,2,3, etc.

References:

1. Zang, T; Heath, K; Etican, J; Chen, L; Langley, D; Holland, A. J.A.; Martin, L; Fear, M; Parker, T. J.; Kimble, R; Wood, F; Cuttle, L; Wound Rep Reg. 2022; 30: 560-572
2. Wang, DH; Wang, C; Cortright, J.R.; Le, K P; Liu, L; Kothapalli, K.S.D.; and Brenna, J.T.; Anal.Chem. 2020, 92, 8209-8217
3. Wang, DH; Brenna J.T.; Shimadzu technical report

POSTER

Total carbon dioxide (TCO2) in equine plasma analysis by GCMS

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Keywords: plasma analysis; gcms; carbon dioxide; mass spectrometry; equine

Abstract:

Alkalizing substances administered to horses in the racing industry have the potential to be a significant issue in sporting integrity. The administration of alkalizing substances in horses is detected through the analysis of the total carbon dioxide concentration (TCO2) in their plasma. Currently TCO2 is measured using a Beckman-Coulter DxC600. In March 2022 Beckman stopped supporting this instrument, which required a change in approach to how TCO2 was measured in our laboratory. This has led to our development of a method on a Shimadzu GCMS 8050NX.
The objectives of this study are to verify the new GCMS method is comparable to the previously used DxC600 and move towards a more modern analysis technique eliminating the reliance on the DxC instrument.

The new GCMS method measures TCO2 in equine plasma samples though the liberation of CO2 from the sample into the gas phase by acidification, heating and agitation. The samples are then analysed by headspace analysis. Comparison data was gathered by analysing paired samples on both instruments, in order to determine effectiveness and accuracy of the GCMS method.
The results of the comparison data indicated the two methods produced directly comparable results, with the GCMS demonstrating superior repeatability, comparable run time, and improved RSDs.
This comparison shows that the uses of gas chromatography coupled to a mass spectrometer is a reliable technique to replace ion selective electrodes for TCO2 analysis in plasma.

POSTER

Benchmarking the utility of open-source library-free DIA tools in the identification and quantification of glycan modifications using mass-spectrometry

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Keywords: glycoproteobioinfomatics; glycomics; library-free DIA

Abstract:

Data Independent Analysis (DIA) has been recently established as a robust and reproducible peptide quantification and identification technique in the field of proteomics, overcoming the limitations of Data Dependent Analysis (DDA). Recent advancements in library-free analysis methods streamline DIA workflows, bypassing the need for DDA library generation, which makes savings on time, resources, and sample volumes. This has made DIA a valuable analysis pathway for fields where DDA based library generation is not practical, however the utility of these tools for the identification of post-translational modifications (PTMs) has not been thoroughly established.

We aim to establish the utility of existing library-free DIA tools to the field of glycoproteomics and compare against DDA based glycan identification methods.

Using in-house generated proteomic/glycoproteomic data as well as datasets available from online repositories we assess the most-current versions of the open-source software;
DIA-NN, DIA-Umpire (MaxQuant), OpenSWATH, Skyline, and FragPipe, and set a baseline for glycoform identification using the proprietary DDA software Byonic. We initially use a known glycoprotein mixture of IgG, lactalbumin, and fetuin, followed by vigorous testing across HeLa lysate, human serum, and human saliva. Each software is assessed on the basis of reproducibility, quantification linearity, and number of proteins and PTMs identified, with a particular focus on O- and N- linked glycosylation.

We compare these key metrics against existing DDA workflows, summarise the relative performance of each tool and discuss possible refinements to DIA workflows to maximise their utility for the field of glycoproteomics.

POSTER

Automated proteomics workflows for high-throughput library generation and biomarker detection using data-independent acquisition

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Keywords: Automation; Filter aided sample preparation; Data-independent acquisition; Myocardial Infarction; Biomarker discovery

Abstract:

Sequential window acquisition of all theoretical mass spectra (SWATH-MS) underpinned by advanced bioinformatics offer a framework for comprehensive analysis of proteomes and the discovery of robust biomarkers. However, the lack of a generic sample preparation platform to tackle the heterogeneity of material collected from different sources may be a limiting factor to the broad application of this technique. We have developed universal and fully automated workflows using robotic sample preparation platform, which enabled in-depth and reproducible proteome coverage and characterization of bovine and ovine specimens representing healthy animals and a model of myocardial infarction. In the case of infarcted tissue, proteomics data were validated using mRNA and miRNA profiling to infer gene regulatory networks and identify master regulatory genes previously associated with diagnostic markers. The findings suggest that automated workflows can be employed for various clinical applications across different animal species and animal models of health and disease.

POSTER

Impact of site-specific N-glycosylation on yeast glycoprotein thermal stability

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Keywords: Protein thermal stability; Site-specific N-glycosylation; quantitative MRM-MS; thermal proteome profiling; secreted eukaryotic glycoproteins

Abstract:

Glycosylation is a crucial protein post-translational modification (PTM) that affects both the physical properties and biological roles of proteins. N-glycosylation is particularly important for glycoprotein stability on account of its role in protein folding in the Endoplasmic Reticulum (ER) and in the stabilization of mature glycoproteins. However, the effects of site-specific glycosylation on glycoprotein stability are not well understood. To assess protein stability we used thermal proteome profiling (TPP) with thermal perturbation to cause protein denaturation and aggregation, followed by quantitative proteomic analyses. Using yeast genetics and chemical perturbation of glycosylation, together with TPP and MRM-MS analysis, we aimed to discover the roles of specific N-glycosylation sites on the thermal stability of secreted eukaryotic glycoproteins.

POSTER

Quantification and identification of microplastics in compost using Pyrolysis GC-MS method

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Keywords: Microplastics, Compost, Microplastics extraction, Microplastics quantification, Pyrolysis-GCMS

Abstract:

The contamination of the environment with microplastics has emerged as a global challenge. Compost has been widely used for land-use application to maintain and improve soil fertility, but little is known about microplastics in composts (Braun et al., 2021). Hence, to quantify and investigate the prevalence of microplastics in commercial composts, this study used Pyrolysis coupled with gas chromatography and mass spectrometry (Py GC-MS). Application of Py-GC-MS technique revealed that the compost samples contained plastic particles, such as polyethylene (PE), polypropylene (PP), and polyvinyl chloride (PVC), in detectable amounts. A few research studies have reported compost as a primary microplastics source in the terrestrial environment, influencing various structural and physicochemical changes in the soil biome (Watteau et al., 2018; Vithanage et al., 2021). The presence of microplastics within compost is an alarming environmental issue as there may be both environmental and human health-related risks associated with it. Thus, this preliminary study, presenting the findings of quantitative research of microplastics in compost will further provide the basis for conclusions about compost as a carrier of microplastics in the terrestrial environment.

References:

Braun, M., Mail, M., Heyse, R. and Amelung, W., 2021. Plastic in compost: Prevalence and potential input into agricultural and horticultural soils. Science of The Total Environment, 760, p.143335. https://doi.org/10.1016/j.scitotenv.2020.143335

Vithanage, M., Ramanayaka, S., Hasinthara, S. and Navaratne, A., 2021. Compost as a carrier for microplastics and plastic-bound toxic metals into agroecosystems. Current Opinion in Environmental Science & Health, 24, p.100297. https://doi.org/10.1016/j.coesh.2021.100297

Watteau, F., Dignac, M.F., Bouchard, A., Revallier, A. and Houot, S., 2018. Microplastic detection in soil amended with municipal solid waste composts as revealed by transmission electronic microscopy and pyrolysis/GC/MS. Frontiers in Sustainable Food Systems, 2(Article 81), pp.14-p. https://dx.doi.org/10.3389/fsufs.2018.00081

Human biomonitoring in Australia – assessment of environmental pollutants

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Bio:

Dr Leisa-Maree Toms is a researcher and senior lecturer in the School of Public Health and Social Work at Queensland University of Technology (QUT), Brisbane, Australia. Leisa-Maree has a PhD from the Queensland Alliance for Environmental Health Sciences (formerly the National Research Centre for Environmental Toxicology), The University of Queensland and specialises in the study of sources and exposure pathways of environmental pollutants, such as persistent organic pollutants (POPs) in human and environmental matrices. She is especially interested in the temporal trends of human body burdens of flame retardants and per- and poly-fluoroalkyl substances (PFAS) since regulation to decrease exposure. She is part of a team of researchers who have been carrying out human biomonitoring of POPs in Australia since 2002..

Target and suspect screening of neonicotinoids and their transformation products in environmental matrices

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Keywords: Neonicotinoids; LC-MS/MS; HRMS; Transformation products

Abstract:

Neonicotinoids are a group of moderately to highly water-soluble insecticides, with a broad range of applications in urban and agricultural settings. Over 400 agricultural and domestic neonicotinoid containing products are registered for use in Australia. Globally, neonicotinoids have attracted research and media attention for their adverse effects on honeybee populations across North America and Europe. However, less attention has been paid to the detection of neonicotinoids in environments which can cause harm to non-target organisms. The aquatic environment is a major sink of neonicotinoid insecticides from sources such as agricultural and runoff, and wastewater treatment plant (WWTP) effluents released into environmental waters, putting aquatic species at increasing risk of neonicotinoid poisoning.

Little is known about the presence of neonicotinoids in Australian aquatic environments. Popular neonicotinoid insecticide Imidacloprid is occasionally included in environmental monitoring programs, though few peer-reviewed studies have documented the presence of some neonicotinoids in Australian waters (Sánchez-Bayo and Hyne, 2014, Hook et al., 2018). To our knowledge, the presence of neonicotinoid transformation products (TPs) in Australian aquatic environments has not previously been investigated. Here, we have developed and validated a sensitive method by QTRAP LC-MS/MS for the target analysis of seven neonicotinoids in various environmental matrices including water, soil and biota. Previously established suspect screening workflows by QTOF HRMS have been optimised for the qualitative assessment of neonicotinoid TPs in environmental waters.

References:

Hook, S. E., Doan, H., Gonzago, D., Musson, D., Du, J., Kookana, R., Sellars, M. J. & Kumar, A. 2018. The impacts of modern-use pesticides on shrimp aquaculture: An assessment for north eastern Australia. Ecotoxicology and Environmental Safety, 148, 770-780.

Sánchez-Bayo, F. & Hyne, R. V. 2014. Detection and analysis of neonicotinoids in river waters – Development of a passive sampler for three commonly used insecticides. Chemosphere, 99, 143-151.

Separation of diastereomers of metallosupramolecular cages from a dynamic mixture of interconverting species

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Keywords: Cyclic ion mobility; supramolecular; ion mobility; dynamic equilibrium

Abstract:

Metallosupramolecular cages are 3-dimensional assemblies that often feature internal cavities and have myriad applications including enantio- and regioselective catalysis, molecular sensing, stabilisation of reactive species and drug delivery (Clegg 2017). These species are notoriously difficult to unambiguously characterise on account of their dynamic behaviour in solution, such as isomer interconversion, reversible guest binding and other structural rearrangements. While traditional techniques including nuclear magnetic resonance, single crystal X-ray crystallography and electrospray ionisation mass spectrometry (MS) are typically employed to achieve this end, another technique, namely ion-mobility MS, has begun to grow in popularity (Rissanen 2019) as it can provide information about the shape and size of many co-existing species simultaneously without requiring the growth of single crystals. By utilising the separating power of cyclic ion-mobility, we have extracted and resolved diastereomers of a series of M4L6 cages from a mixture of kinetically labile interconverting molecules. We have also extended this methodology to investigate cages containing paramagnetic ions such as octahedral Ni2+ revealing information regarding the equilibrium ratio of isomers that is not possible to discern using traditional techniques. The potential applications for this technique as both a specialist tool and a standard characterisation technique for the analysis of metallosupramolecular cages will be explored and our progress to date on this will be discussed.

References:

Brock A, Al-Fayaad H, Pfrunder M & Clegg J 2017 'Functional Supramolecular Materials: From Surfaces to MOFs', The Royal Society of Chemistry.

Kalenius E, Groessl M & Rissanen K 2019, 'Ion mobility–mass spectrometry of supramolecular complexes and assemblies', Nature Reviews Chemistry, vol. 3, no. 4, pp 4-14.

Non-target screening of per- and polyfluoroalkyl substances (PFAS) in cattle exposed to AFFF-contaminated groundwater

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Keywords: per- and polyfluoroalkyl substances; PFAS; Non-target Screening; Firefighting foam

Abstract:

Aqueous Film-Forming Foam (AFFF) used for firefighting and military purposes has been the primary source of per- and polyfluoroalkyl substances (PFAS) contamination of groundwater and soil. Leaching PFAS from a firefighting training area situated in a small town in the State of Queensland, Australia, has also resulted in extensive contamination of groundwater and nearby farmlands. A previous study on serum samples collected from the cattle held in these contaminated farmlands showed a significantly high concentration of PFAS. This study presents a comprehensive non-target analysis of blood and sera from the cattle exposed to contaminated groundwater. Pooled blood (n=8) and serum (n=6) samples were analysed via high-resolution mass spectrometry (HRMS) using liquid chromatography-quadrupole time-of-flight mass spectrometry (LC-QTOF/MS) in both positive and negative electrospray ionisation modes (ESI+ and ESI−). The features detected were prioritised based on feature intensity, mass-defect filtering and case-control approach. The prioritised features were identified via suspect screening with a PFAS suspect list specific to aqueous film-forming foams (AFFFs) and PFAS spectral library search. A range of perfluoroalkyl sulfonates and sulfonamides that were not reported in the target analysis such as perfluoropropane sulfonate (PFprS), perfluoropentane sulfonate (PFPeS), perfluoropropane sulfonamide (FprSA) and perfluorobutane sulfonamide (FBSA) were identified from the samples. This study suggests that AFFF-derived short-chain sulfonamides, which are not currently being monitored in many PFAS biomonitoring studies, are potentially bioaccumulative.

Programming photodegradability into vinylic polymers via radical ring-opening polymerization

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Keywords: Photodegradable polymer; Radical ring-opening polymerization; Ion mobility mass spectrometry; SEC-MS

Bio:

Degradation of polymers by cleaving photoresponsive groups in polymer backbones plays an important role in many polymeric systems. However, current methods to incorporate photolabile linkages into the polymer main chain are still confined to step-growth polymerization, while radical polymerization is the staple polymerization method of industry and fundamental research. Herein, we report a new strategy to program efficient photodegradability into vinylic polymer chains using radical ring-opening polymerization (rROP). A macrocyclic monomer was synthetically accessible through intramolecular dimerization of coumarin terminated allylsulfide linear monomer. The intramolecular cyclisation was confirmed by morphological change from linear to cyclic monomer with the ionized cyclic monomer displayed a shorter drift time (i.e. smaller collision cross-section) compared to the linear analogue in ion mobility- mass spectrometry analysis. Upon copolymerization of methyl acrylate (MA) with the cyclic monomer, the photolabile coumarin dimer moieties from the cyclic monomer were imbedded into the copolymer through rROP of the monomer. The photodegradation of obtained polymer was triggered by UVB light at which the photodissociation reaction of coumarin dimer was anticipated to occur, leading to scission of the polymer main chain. The degradation products were analyzed by size-exclusion chromatography coupled high-resolution mass spectrometer (SEC-HRMS). The proposed rROP and degradation mechanism was evidenced by chemical structure of degraded MA oligomers with putative coumarin end groups identified by SEC-HRMS. Mass spectrometry analysis with other complementary characterization techniques afforded a comprehensive understanding for the photodegradable polymer synthesis developed herein, paving the way to integrating a range of photoresponsive groups into vinylic polymer backbones.

Analysis cryo and ultrathin cryo sections by mass spectrometry imaging to reveal macro and micro scale distribution of Latrunculin-A in Chromodoris kuiteri

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Keywords: Mass Spectrometry Imaging; Microscopy; metabolites

Abstract:

In this study, we have examined the nudibranch specie, Chromodoris kuiteri (Cheney et. al., 2016), using mass spectrometry imaging (MSI). The samples were prepared using regular cryostat sectioning to produce 10 - 20 micron sections for macroscopic spatial distribution, and ultrathin cryosectioning following high-pressure freezing to produce 200 nm sections to allow for further investigation of the microscopic sub-cellular features. During this study we utilised high accuracy orthogonal TOF, with and without post ionisation (Soltwisch et. al, 2020), and axial MALDI TOF instruments to show that latrunculin-A was being specifically stored by Chromodoris kuiteri in the mantle dermal formations in outer rim of the organism. This combination of approaches has the potential to contribute towards more routine methodologies for sub-cellular MSI.

References:

Cheney, K.L., White, A., Mudianta, I.W., Winters, A.E., Quezada, M., Capon, R.J., Mollo, E., Garson, M.J. Choose Your Weaponry: Selective Storage of a Single Toxic Compound, Latrunculin A, by Closely Related Nudibranch Molluscs. Plos One. 2016, 11(1): e0145134

Soltwisch, J., Heijs, B., Koch, A., Vens-Cappell, S., Hoehndorf, J., Dreisewerd, K. MALDI-2 on a Trapped Ion Mobility Quadrupole Time-of-Flight Instrument for Rapid Mass Spectrometry Imaging and Ion Mobility Separation of Complex Lipid Profiles. Anal Chem. 2020, 92, 8697-8703

Quantification of selected microplastics in Australian urban road dust

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Keywords: Microplastic; Dust; Pyr-GC/MS; Quantification; Road traffic

Abstract:

Microplastics (1 - 5000 µm) are pervasive in every compartment of our environment. However, little is understood regarding the concentration and size distribution of microplastics in road dust, and how they change in relation to human activity. Within road dust, microplastics move through the environment via atmospheric transportation and stormwater run-off into waterways. Human exposure pathways to road dust include dermal contact, inhalation and ingestion. In this study, road dust along an urban to rural transect within South-East Queensland, Australia was analysed using Accelerated Solvent Extraction followed by pyrolysis Gas Chromatography-Mass Spectrometry (Pyr-GC/MS). Polypropylene, polystyrene, polyethylene terephthalate,
polyvinyl chloride, poly (methyl methacrylate) and polyethylene were quantified. Microplastic concentrations ranged from ~0.5 mg/g (rural site) to 6 mg/g (Brisbane city), consisting primarily of polyvinyl chloride (29%) and polyethylene terephthalate (29%). Size fractionation (< 250 µm, 250–500 µm, 500–1000 µm, 1000–2000 µm and 2000–5000 µm) established that the < 250 µm size fraction contained the majority of microplastics by mass (mg/g). Microplastic concentrations in road dust demonstrated a significant relationship with the volume of vehicles (r2 = 0.63), suggesting traffic, as a proxy for human movement, is associated with increased microplastic concentrations in the built environment..

Endocannabinoids in saliva and hair by LC-MS/MS: New opportunities for biological exploration

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Keywords: LC-MS/MS; Endocannabinoids; Saliva; Hair

Abstract:

Endocannabinoids are a lipid signalling system that are increasingly recognised to be heavily involved in many disease states. However, quantitative methods for endocannabinoids are limited and have not been developed in many human matrices. In the present work, we developed an LC-MS/MS method for sensitively quantifying arachidonoyl ethanolamide (AEA), 2-arachidonoyl glycerol (2-AG), and oleoylethanolamide (OEA) in human saliva and hair at less than 1pg/mL for AEA, 100pg/mL for 2-AG and 2pg/mL for OEA. Our methods are linear, precise, and show minimal matrix effects. The methods involve simplified sample preparation using acetone-based protein precipitation for saliva and isotope dilution for both hair and saliva. Mobile phases include 2mM ammonium acetate (A) and acetonitrile (B) and the runtime of the method is 12 minutes. Application of the method in over 150 healthy participants suggests that endocannabinoids in saliva are part of the sympathetic nervous system, are stress and exercise responsive, and do not correlate with endocannabinoid levels found in plasma. Further, similar to blood endocannabinoids, salivary endocannabinoids show ex vivo generative properties, suggesting that they should be frozen immediately after sampling. The present work has produced new methods for understanding endocannabinoid biology and can be used by researchers using human participants.

A multi-omics approach reveals the mechanisms underlying the challenges of translating wild yeasts to industrial fermentation

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Keywords: Proteomics; Yeast; Stress; Lipidomics, Multi-omics

Abstract:

Historically, wild, non-Saccharomyces yeasts have also been frequently used in mixed culture fermentations to provide interesting and unique flavours to beer. However, brewing using mixed cultures or by spontaneous fermentation makes reproducing flavours and beer styles extremely difficult. Previously, we isolated a suite of wild yeast and characterised a single isolate to produce a reproducible beer with interesting flavours. Key to this successful commercialisation was uncovering that the stress created by maltose and hydrostatic pressure had a significant effect on the growth of wild yeast isolates. We found that relieving maltose as a stressor with the addition of glucoamylase to digest maltose into glucose, industry scale fermentation was possible. Here, we use proteomics, metabolomics, and lipidomics to reveal the mechanisms underlying the challenges of translating wild yeasts to productive fermentation at an industrial scale. We performed a series of stress-based growth assays and identified proteins related to lipid membrane remodelling, proton pumps, and nutrient transporters central to our wild yeast's stress response. We also identified significant changes in presence of sphingolipids and glycerophospholipids in response to stress. This work helps unravel the complex stress response in yeast and provides the tools to produce commercial and reproduce fermentation using wild yeast.

Identification and quantification of micro-bioplastics in environmental samples by pyrolysis-gas chromatography–mass spectrometry

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Keywords: Pyrolysis, Bioplastics, Micro-bioplastics, Quantification, Extraction, Pyr-GC/MS

Abstract:

Bioplastics are materials that are biobased and/or biodegradable, but not necessarily both. Concerns about environmental plastics pollution is constantly growing with increasing demand for substituting fossil-based plastics with those made using renewable resource feedstocks. For many conventional bioplastics to completely decompose/degrade, they require specific environmental conditions that are rarely met in natural ecosystems, leading to rapid formation of micro-bioplastics. As global bioplastics production and consumption/use continues to increase, there is growing concern regarding the potential for environmental pollution from micro-bioplastics. However, the actual extent of their environmental occurrence and potential impacts remains unclear, and there is insufficient mass concentration-based quantitative data due to the lack of quantitative analytical methods. This study developed and validated an analytical method coupling pressurized liquid extraction and pyrolysis gas chromatography–mass spectrometry combined with thermochemolysis to simultaneously identify and quantify five targeted micro-bioplastics (i.e., polylactic acid, polyhydroxyalkanaoate, polybutylene succinate, polycaprolactone and polybutylene adipate terephthalate) in environmental samples on a polymer specific mass-based concentration. The recovery of spiked micro-bioplastics in environmental sample (biosolids) ranged from 74 to 116%. The limits of quantification for the target micro-bioplastics were between 0.02 and 0.05 mg/g. PLA and PBAT were commonly detected in wastewater, biosolids and sediments samples at concentrations of between 0.07 and 0.18 mg/g. The presented analytical method enables the accurate identification, quantification, and monitoring of micro-bioplastics in environmental samples. This study quantified five micro-bioplastic types in complex environmental samples for the first time, filling in gaps in our knowledge about bioplastics pollution and providing a useful methodology and important reference data for future research.

Quantitative proteomics comparison of human and cow's milk-derived small extracellular vesicles by Sequential Window Acquisition of all Theoretical fragment ion Mass Spectra (SWATH-MS)

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Keywords: Extracellular vesicles; mass spectrometry; proteomics; milk; infant formula

Abstract:

Background: The global infant formula (IF) market was valued at US$ 58.84 billion in 2021 and is predicted to reach US$ 125.2 billion by 2030. Most IF has a protein base derived from cow's milk (CM), however the difference to human milk (HM) is not well-understood. Small extracellular vesicles (sEVs) are nanoparticles of 50 – 200 nm in size (Théry et al., 2018); sEVs are present in all biofluids including milk (Vaswani et al., 2017) and have been successfully recovered by our group from numerous IF products (unpublished data). Here, we developed a proteomic workflow to compare sEVs derived from HM and CM. Methods: sEVs were isolated from pooled HM and CM by sequential differential centrifugation and size-exclusion chromatography. sEV-enriched samples were processed for quantitative proteomics analysis by sequential window acquisition of all theoretical fragment ion mass spectra (SWATH-MS) (technical replicates; n = 3/group). Mass spectrometry (MS) data were processed in DIA-NN (False discovery rate = 0.01) and output files were imported and processed in R Studio. Results: An average of 307 ± 45 and 1057 ± 44 proteins were detected in HM and CM samples, respectively. Of these, 216 were common to both groups, with 143 differentially abundant between HM and CM (126 up-regulated and 17 down-regulated in HM). Discussion: The workflow captured species-specific differences, thus demonstrating potential for future characterisation of milk-derived sEVs relating to infant health. Additionally, sEVs have loading capabilities that could be exploited to package desirable compounds and further boost nutrition in infants with impaired gut health.

References:

Théry, C. et al. (2018) 'Minimal information for studies of extracellular vesicles 2018 (MISEV2018): a position statement of the International Society for Extracellular Vesicles and update of the MISEV2014 guidelines', Journal of Extracellular Vesicles, 7(1). doi: 10.1080/20013078.2018.1535750.

Vaswani, K. et al. (2017) 'A method for the isolation and enrichment of purified bovine milk exosomes', Reproductive Biology. Elsevier, 17(4), pp. 341–348. doi: 10.1016/j.repbio.2017.09.007.

Developing native mass spectrometry for targeting non-coding RNAs: an emerging and challenging therapeutic target class

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Keywords: native MS; RNA targeting; drug discovery; screening; ion mobility

Abstract:

Native mass spectrometry (nMS) allows the observation of biomolecules in their folded states. Through precise control of instrument parameters, gentle conditions are utilised to maintain noncovalent interactions. This positions nMS as a suitable biophysical approach for drug discovery. Routine screening of soluble proteins or protein complexes by nMS to identify noncovalent ligand modulators is well established. However, challenging target classes and new therapeutical modalities are emerging to provide novel mechanisms for disease intervention, including via small molecule targeting of non-coding, structured RNAs. The biomolecules that underpin these modalities and targets present new analytical challenges, which nMS can overcome.

Structured, noncoding RNA targets have been identified to play important roles in disease, and the large proportion of non-coding RNA in the genome (approximately 98%) presents many alternate drug targets for modulating disease compared to conventional protein targets. Small, structured RNA aptamers, namely the theophylline, kanamycin B and tobramycin aptamers, were utilised as example systems to study the binding of small molecules by nMS. Selective binding was observed for a small panel of literature ligands, with binding responses correlating across the range of literature affinity measurements (μM to nM). Ion mobility nMS allowed the structural investigation of RNA aptamer folding under different conditions and with the binding of ligands. The methods to establish nMS for characterising and screening non-coding RNAs as an emerging and challenging therapeutic target class will be presented.

Analysis of the uptake and effects of tyre wear particles on plants

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Keywords: Tyre wear; Plant; LC-MS/MS; Pyrolysis-GCMS; Microplastics

Abstract:

Microplastic pollution is a well-recognised problem around the world and tyre wear particles (TWP) are a significant source of environmental microplastics. Currently, there is little to no data on environmental concentrations of TWPs or tyre additives in the Australian environment and the implications on the ecosystems remain largely unknown. Research has shown that microplastics are able to enter plants from root cells and be transported to other parts of the plant (Mateos-Cárdenas et al., 2021), though this has rarely been studied with TWPs. On the other hand, tyres are also known to contain additives including a range of aromatic amines, benzothiazoles and benzotriazoles (Rauert et al., 2022). The leachate of TWP had raised concerns due to its acute toxicity towards aquatic species (Capolupo et al., 2020; Tian et al., 2021). This study investigated the uptake of TWPs, and the effect tyre leachate has on lab-cultivated common duckweeds (Lemna minor), and the presence of TWPs in plants growing in a contaminated creek. Scanning electron microscopy and pyrolysis gas chromatography mass spectrometry were both used to identify the presence of TWPs absorbed by the plants. Liquid chromatography tandem mass spectrometry was used to quantify tyre additives in the leachate. This project improves our understanding of how TWPs affect the ecosystem particularly the primary producers.

References:

Mateos-Cárdenas, A, van Pelt, FNAM, O'Halloran, J & Jansen, MAK (2021). Environmental Pollution, 284, 117183. https://doi.org/10.1016/j.envpol.2021.117183

Rauert, C., Charlton, N., Okoffo, E. D., Stanton, R. S., Agua, A. R., Pirrung, M. C., & Thomas, K. V. (2022). Environmental Science and Technology, 56(4), 2421–2431. https://doi.org/10.1021/acs.est.1c07451

Capolupo, M., Sørensen, L., Jayasena, K. D. R., Booth, A. M., & Fabbri, E. (2020). Water Research (Oxford), 169, 115270. https://doi.org/10.1016/j.watres.2019.115270

Tian, Z., Zhao, H.N., Peter, K.P., Gonzalez, M., Wetzel, J., Wu, C., Hu, X., Prat, J., Mudrock, E., ... Kolodziej, E.P. (2020). Science, 371(6252), 185-189. https://doi.org/10.1126/science.abd6951

Uncovering non-canonical unsaturated fatty acids in the brain

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Keywords: LC-MS; Lipids; Lipidomics; OzID; Brain

Abstract:

By weight, the human brain is made up of 50% lipid. Despite its major contribution to the mass of the brain, at the molecular level, the brain lipidome remains incompletely described and the functions of many of the species identified to-date are unknown. Recently for example, the presence of unsaturated fatty acids with carbon-carbon double bonds in positions outside those usually described in mammalian lipid metabolism were identified in mouse brain. Technological impediments to the detection and tracing of such non-canonical fatty acids present a frontier challenge to understanding the underlying metabolism and their biological function(s). Free fatty acid stable isotope tagging (FFAST) was employed with reverse phase liquid chromatography ozone-induced dissociation mass spectrometry (LC-OzID-MS) to uncover stimulation-driven changes in unsaturated FFAs within PC-12 cells. In parallel, desorption electrospray ionisation was deployed in combination with OzID to search for complex lipids carrying non-canonical fatty acids within rat brain sections. Application of the FFAST-OzID method revealed the presence of abundant populations of the non-canonical species FA16:1(n-10) and FA18:1(n-10) in extracts from PC-12 cell lines. Neither of these FFAs have previously been reported in neurons or neurosecretory-like cells, with both demonstrated to increase 2-3-fold in abundance upon stimulation of the cells. Surveying the complex lipids in rat brain revealed the presence of double bond positional isomers with different spatial distributions within canonical phosphatidylcholine lipids of composition PC 34:1. Preliminary evidence also shows the presence of the non-canonical monounsaturated PC 34:1 in rat brain, albeit at significantly lower abundance than its canonical isomers.

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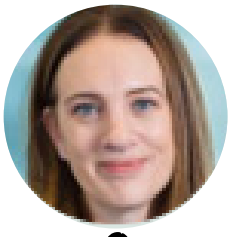

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