27th ANNUAL
RACI R&D TOPICS CONFERENCE

TOPICS 2019

1-4 DECEMBER
ADELAIDE, SOUTH AUSTRALIA

raci
Royal Australian Chemical Institute

ANALYTICAL & ENVIRONMENTAL CHEMISTRY DIVISION

Welcome

to Adelaide and the 27th RACI R&D Topics Conference on behalf of the 2019 committee.

We recognise that Flinders operates on Indigenous peoples' traditional lands and waters and acknowledge their continued responsibility to care for country at the University's various teaching locations, including the lands and waters of the following peoples: Kaurna, Arrernte, Boandik, Bungarla, Gunditjmara, Jawoyn, Larrakia, Nauo, Ngarrindjeri, Peramangk, Wurundjeri, Yolgnu.

Conference Chairs

Jennie Bartle Kelly-Anne Stark

Public Relations

Shaun Johns

Committee Members

Callum Bonnar Tristan Fraser Samantha Pandelus

Simone Madaras Claire Lenehan

Special Thanks

Dr. Zoe Smith Mrs Mary Pappa Mrs Robyn Taylor

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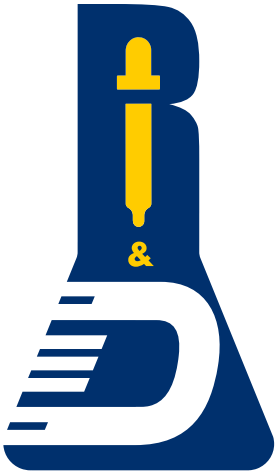

TOPICS 2019

About R&D Topics

The RACI Research and Development Topics conference was founded in 1992 by Professor Neil W. Barnett of Deakin University. Based initially on the Analytical Research Forum run by the Royal Society of Chemistry in the UK, RACI R&D Topics was first held in 1993 at Deakin. It has since grown to include sixteen universities from across Australia, attracting in excess of 100 delegates annually.

RACI R&D Topics conference is organised primarily by postgraduate students of the hosting university. It is focused on giving postgraduate students the opportunity to share their research with a national audience of students and academics. For many students, this is their first opportunity to network with academics and students from around the country in a research-oriented environment.

We invite Honours, MSc and PhD students, and young scientists from government/ industry (up to 4 years post BSc. or equivalent degree), to submit oral presentations and/or poster presentations. We also invite postdoctoral fellows (up to 3 years post PhD) to submit poster presentations. We welcome all supervisors and other researchers that wish to attend the conference to hear the latest research and innovation from the next generation of scientists in analytical and environmental chemistry in Australia, in addition to guest lectures from invited speakers and the recipients of the three medals awarded annually by the RACI Analytical and Environmental Chemistry Division as well as trade displays from industry sponsors.

In its 27th year the RACI R&D Topics conference continues to showcase the current and developing research of Australia's newest scientific minds in Adelaide, South Australia.

We greatly appreciate the financial support offered by the following sponsors

PLATINUM SPONSORS

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Congratulations

to the 2018 and 2019 Analytical & Environmental Chemistry Division Award Recipients

Graeme Batley Medal

2018 Recipient Stephen Blanksby, Queensland University of Technology
2019 Recipient TBD

The Graeme Batley medal (formerly known as the Doreen Clark Medal) is awarded for excellence in pure or applied scientific work in Australia that involved substantial analytical chemistry, or for service to Analytical Chemistry in Australia, over the prior fifteen years.

Paul Haddad Medal

2018 Recipient Mark Hackett, Curtin University
2019 Recipient Dario Arrua, University of South Australia

The Paul Haddad Medal (formerly known as the Peter W. Alexander Medal) is awarded annually for excellence in pure or applied scientific work in analytical chemistry in Australia, and for service to Analytical Chemistry. This award specifically recognises these contributions from individuals within the first 10 years of that person's career.

Environmental Chemistry Medal

2019 Recipient Ed Butler, The Australian Institute of Marine Science

The medal will be awarded annually for excellence in scientific work in Australia that has involved substantial environmental chemistry, or for service to Environmental Chemistry in Australia, over the past ten years.

Original Research Publication Award

2019 Recipient Giang Nguyen, University of New South Wales

This annual Division award recognizes research publications from higher degree research students that are lead author on a peer-reviewed research manuscript. The purpose of the award is to encourage students to publish their research and to assist and encourage them to participate in scientific meetings early in their research careers. The research must have a significant impact (or potential impact) in the field of analytical and/or environmental chemistry.

Analytical and Environmental Division Citation

2018 Recipient Ashley Townsend, University of Tasmania

The Division Citation is awarded for the 'Outstanding service to the Division of Analytical and Environmental Chemistry of the Royal Australian Chemical Institute'.

Orientation & General Information

Location & Travel

This year the conference is being held at Flinders University's Victoria Square building, at 182 Victoria Square in the heart of the Adelaide CBD. This location can be reached on foot relatively easily from most parts of the city.

A free city loop bus service operates from early morning until 7:15pm, there is a tram stop at Victoria Square, and tram services within the CBD from The Entertainment Centre to the South Terrrace tram stop is free, and further public transport options are available throughout the city.

For Adelaide Metro timetables, Metrocards or further information please visit adelaidemetro.com.au.

While there is no dedicated parking onsite, there are many paid parking options within 500m of the venue.

All presentations, including posters and trade displays, are scheduled to take place on Level 2 of the building. Lunch and morning/afternoon tea will be served in the sponsor room 2.1. We ask that all attendees are mindful of those who are currently presenting when moving through common spaces.

Maps of both the Adelaide CBD and the conference space have been included for your convenience.

Oral Presentations

Oral presentations will be held in the combined rooms 2.2 and 2.3. Delegates presenting talks are requested to contact a conference committee member during the registration period at the beginning of each day to have their presentations uploaded onto the computer. This will assist in smooth transitions between speakers.

Poster Presentations

A poster session will be held in the same room as the oral presentations on Monday December 2, between 12:40pm and 1:20pm. Delegates with posters are asked to hang their poster on the designated poster board on Sunday or first thing Monday morning. Poster locations will be labelled with the number corresponding to the abstract number in this book. Authors presenting posters are requested to be in attendance at their poster for the duration of the session.

Name Badges

Please wear name badges at all conference sessions including morning/afternoon tea and lunch sessions. Members of the organising committee will be also be indicated by their name tags, should you need their help during the conference.

Rear of Badge

2019 R&D Topics Conference Prizes

1st, 2nd and 3rd place oral and poster prizes will be awarded to presenters according to an independent judging panel of academic and industry representatives. This year the best student oral presentation is sponsored by Agilent Technologies. Prizes will be awarded at the close of the conference on Wednesday 4 December.

Internet Access

Wifi is available throughout the building using the inter-university Eduroam program.

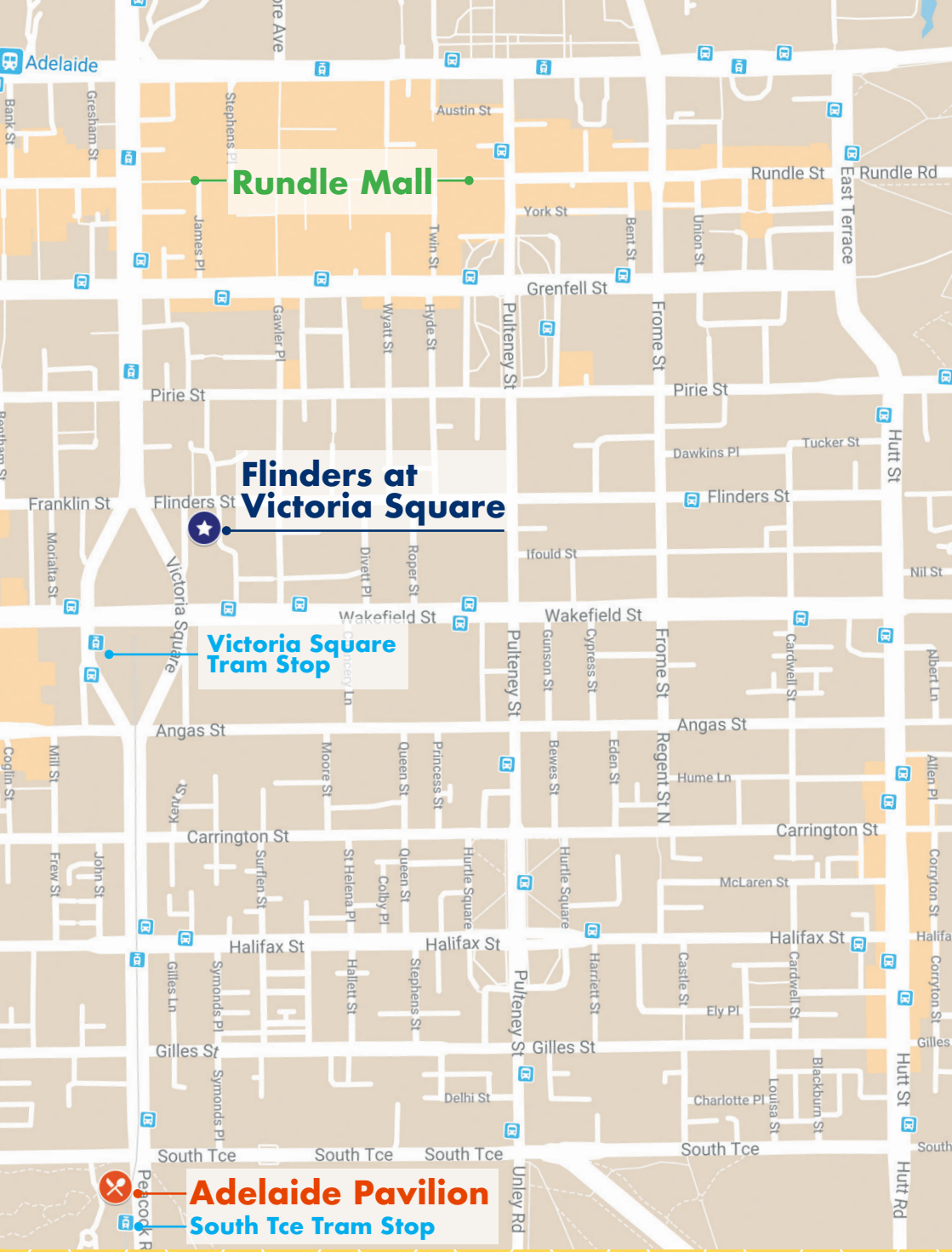
Emergency

Flinders University Victoria Square Concierge: (08) 7221 8686

Flinders University Victoria Square Building Security: (08) 7221 8694
**press security speed dial button from an internal phone or 0427 611106 from a mobile.*

Emergency Services: 000 Police Non-Emergency: 131 444
Poisons Information: 131 126

ADELAIDE CBD


Adelaide
Rundle Mall
Flinders at Victoria Square
Victoria Square Tram Stop
Adelaide Pavilion
South Tce Tram Stop
Austin St
Rundle St
Rundle Rd
East Terrace
York St
Grenfell St
Frome St
Pirie St
Dawkins Pl
Tucker St
Hutt St
Flinders St
Franklin St
Wakefield St
Angas St
Carrington St
Halifax St
Gilles St
South Tce
Pulteney St
Victoria Square
Hurtle Square
Regent St N
McLaren St
Hume Ln
Ely Pl
Delhi St
Charlotte Pl
Unley Rd
Hutt Rd
Bank St
Gresham St
Stephens Pl
James Pl
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Union St
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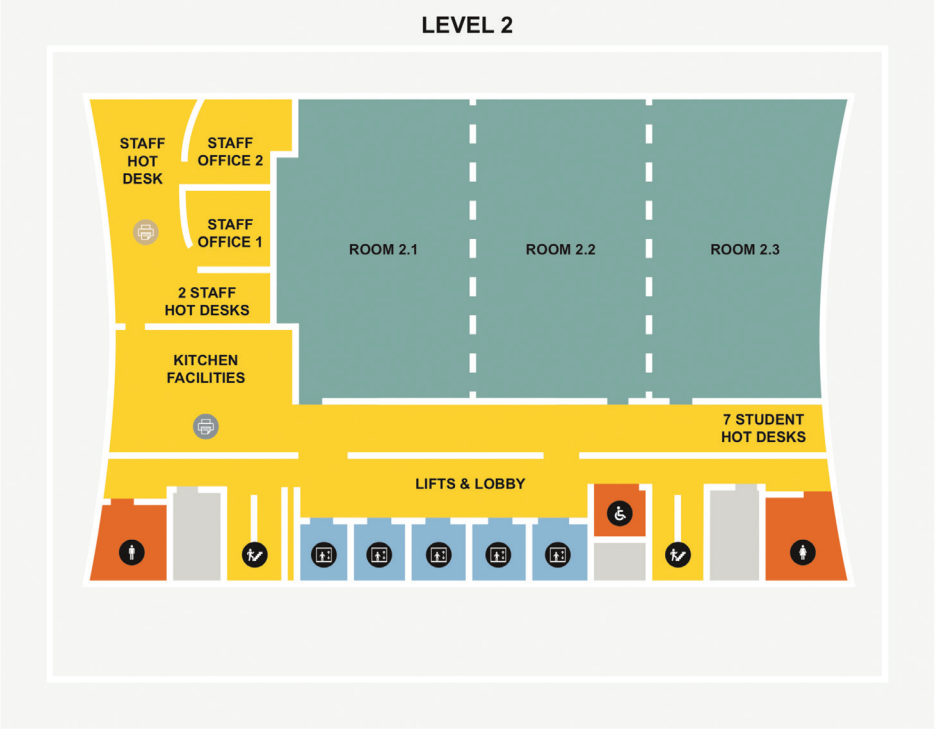
John St
Surflen St
St Helena Pl
Colby Pl
Harriett St
Castle St
Corryton St
Gilles Ln
Symonds Pl
Hallett St
Stephens St
Blackburn St
Louisa St
Peacock Rd

Venue Map


LEVEL 2
STAFF HOT DESK
STAFF OFFICE 2
STAFF OFFICE 1
2 STAFF HOT DESKS
KITCHEN FACILITIES
ROOM 2.1
ROOM 2.2
ROOM 2.3
7 STUDENT HOT DESKS
LIFTS & LOBBY
TEACHING ROOMS
COMMON AREAS
PLANT/EQUIPMENT
TOILETS
FEMALE TOILETS
MALE TOILETS
ACCESSIBLE TOILETS
STAFF TOILETS
LIFTS
STAIRS

Social Activities Program

Arrival & Pre-Mixer

Sunday December 1

Venue: Flinders University Victoria Square campus, Level 2
Time: 15:30 – 18:30 Cost: Included in registration

Come and break the ice at the social pre-mixer where you will get the chance to informally mingle with other attendees and the organising committee. This is a great opportunity for all delegates to socialise with their peers and get to know your fellow academics in a comfortable setting.
Food and drinks will also be provided with an assortment of non-alcoholic and alcoholic beverages. So come down, say hello, grab a bite to eat and get to know your fellow attendees.

Quiz and Games Night

Monday December 2

Venue: Flinders University Victoria Square campus, level 10
Time: 17:30-21:30 Cost: Included in registration

After the first day of conference, it's time to party with games and a quiz night! Food and beverages will be provided and, more importantly, fantastic PRIZES! Come along to chat, test your knowledge, socialise, and maybe pick up a wonderful prize. We will make sure you are fully charged for Tuesday's schedule.

Formal Conference Dinner

Tuesday December 5

Venue: The Adelaide Pavilion Cost: Included in registration
Time: 18:30–22:30 drink service from 19:00

Three-course meal with choice of two options for each.
Beverage package is included. More information coming soon.
Dress Code: Smart casual attire

Conference Schedule

Sunday 1 December	Monday 2 December	Tuesday 3 December	Wednesday 4 December
	8.00-9.00am Registration Open		
	9.00-9.10am Conference Opening	8.00-9.00am Registration Open	9.30-10.00am Registration Open
	9.10-9.40am Welcome	9.00-9.30am 2019 Paul Haddad Medallist Dario Arrua	10.00-10.30am 2018 Paul Haddad Medallist Mark Hacket
	9.40-10.40am Oral Session 1	9.30-10.30am Oral Session 4	10.30-11.30am Oral Session 7
	10.40-11.10am Morning Tea/Trade Display	10.30-11.00am Morning Tea/Trade Display	11.30am-12.00pm Morning Tea/Trade Display
	11.10-11.40am 2019 Environmental Chemistry Medallist Edward Butler	11.00-11.30am 2018 Division Citation Award Ashley Townsend	12.00-1.00pm Oral Session 8
	11.40am-12.40pm Oral Session 2	11.30am-12.50pm Oral Session 5	
	12.40-1.20pm Poster Session	12.50-1.10pm Waters Australia Trade Talk	1.00-1.20pm Syrris Ltd. Trade Talk
	1.20-2.20pm Lunch/Trade Display	1.10-2.10pm Lunch/Trade Display RACI Divisional AGM	1.20-2.20pm Lunch/Trade Display
	2.20-2.50pm 2018 Graeme Batley Medallist Stephen Blanksby	2.10-2.40pm 2019 Original Research Publication Award Giang Nguyen	2.20-3.20pm Oral Session 9
	2.50-3.50pm Oral Session 3	2.40-4.00pm Oral Session 6	
3.30-6.30pm Registration Open Conference Pre-mixer	3.50-4.10pm Agilent Technologies Trade Talk		3.20-3.40pm Afternoon/Trade Display
	4.10-4.40pm Afternoon Tea/Trade Display	4.00-4.20pm Afternoon Tea/Trade Display	4.00pm Conference Closing
	5.30-9.30pm Quiz Night	6.30-10.30pm Conference Dinner Adelaide Pavillion	

Oral Presentation Topics

DAY 1

Session 1 **9.40am** Chair Callum Bonnar

Brooke Mansell

Downscaling liquid chromatography for ICP-MS detection: Effects on sensitivity

Mohammad Shafiqur Rahman

3D optical data storage: A nanocrystal approach

Dominique Scott

Clinical Production and Quality Control Testing of [^{68}Ga] Gallium-Exendin-4 for the Localisation and Detection of Insulinomas at the Royal Brisbane and Women's Hospital

Session 2 **11.40am** Chair Amber Brown

Jennie Bartle

The Influence of Birnessite Crystal Structure on its Oxidative Reactivity

David Hartnell

Spectroscopic Alterations in Lipofuscin during Ageing

Erin Humphries

Bad Hair Day: Detecting Athlete Drug Use

Session 3 **2.50pm** Chair Georgia Sinclair

Ashley Hollings

Spectroscopic Studies of Brain Zinc Homeostasis and Its Role During Cognitive Decline and Ageing

Laura de Wal

Polymeric monoliths for the characterization of intact proteins

Alisha Deo

Profiling the Seasonal Variability of Decomposition Odour from Human Remains in a Temperate Australian Environment

DAY 2

Session 4 9.30am Chair Dominique Scott

M. M. Chayan Mahmud
Aroma Compounds in Coffee-Beverages and the Relationship with Consumer Acceptance

Sepideh Keshan Balavandy
Portable 3D Printed Colorimetric Sensor for Remote Soil Measurement

Charles Croft
Column separation of lanthanide ions from electronic waste

Session 5 11.30am Chair Ester Lumbomirsky

Monique G. de Mello
Considerations for multiplexed Immuno-Mass Spectrometry-Imaging

Jan Klouda
Minimising Fouling During Dopamine Detection at Carbon Electrodes Hydrogenated by Aromatic Organosilanes

Rhiannon Boseley
Using Synchrotron Sourced Microscopy to Explore Fingermark Chemistry

Fidelis Nitti
Development of a 3D-printed flow-through passive sampler for the monitoring of Zn2+ in freshwaters free of environmental effects

Session 6 2.40pm Chair Raymond Yu

Callum Bonnar
Ambient Ionization Mass Spectrometry: Benefits, Challenges and Practical Observations

Amber Brown
Profiling volatilomes as a novel forensic method used to distinguish the species identity of confiscated specimens from the Illegal Wildlife Trade

Céline Burnier
ATR-FTIR spectroscopic studies of condom lubricants: An investigation into the international market from a forensic perspective

DAY 3

Session 7 10.30am Chair Charles Croft

Ester Lubomirsky
Hierarchically Porous Polymer Monoliths for Separation Science

Mayisha Ahmedullah
Delivering Antibiotics Using Nanomeshes

Raymond Yu
Open-tubular admicellar electrochromatography of charged analytes

Session 8 12.00pm Chair Erin Humphries

Georgia Sinclair
Using Metabolomics to Understand Effects of PFAS in Invertebrates

Karina Khambatta
Development of Spectroscopic Protocols to Study the Relationship between Epicuticular Surface Chemistry and Flora

Shuzhi Zhao
Development of a polymer inclusion membrane for the separation of Co(II) from Ni(II)

Session 9 2.20pm Chair Ashley Hollings

Rima Chakrabarty
For Research Use Only: Quality Testing Fitness Drugs Purchased Online

Gabriela Paniagua-Cabarrus
Continuous particulate removal for capillary electrophoresis applications

Sharni Collins
Human Decomposition Fluids and Clothing Degradation

MEDALLIST & INVITED SPEAKER ABSTRACTS

SUMMARY

MONDAY

2019 Environmental Chemistry Medallist

Edward Butler 11.10am
The mutuality of analytical and environmental chemistry - some learnings and reflections

2018 Graeme Batley Medallist

Stephen Blanksby 2.20pm
On the path to analytical utopia through the resolution
of isomers by mass spectrometry

Agilent Technologies Trade Talk **3.50pm Benjamin Davies**
Agilent's New 8890 Gas Chromatograph & 7250 Quadrupole
Time of Flight Mass Spectrometer

TUESDAY

2019 Paul Haddad Medallist

Dario Arrua 9.00am
Porous polymers for separation science

2018 Division Citation Award

Ashley Townsend 11.00am
Determination of trace elements in open ocean seawater samples using NOBIAS resin with SF-ICP-MS detection. Method development and example applications from Heard Island

Waters Trade Talk **12.50pm Caryn Hepburn**
Select Series Cyclic IMS: A novel ion mobility enabled mass spectrometer

2019 Original Research Publication Award

Giang Nguyen 2.10pm
Perfluorinated alkylsubstances of significant environmental concern can potently inhibit human carbonic anhydrase isozymes

WEDNESDAY

2018 Paul Haddad Medallist

Mark Hackett 10.00am
Multi-Modal Spectroscopic Imaging to Study Brain Disease:
Ions, Metals, Memory Loss and More!

Syrris Ltd. Trade Talk **1.00pm Chinh Nguygen**
Exploiting segmented flow chemistry in modern compound library synthesis ,

2018 Graeme Batley Medallist

On the path to analytical utopia through the resolution of isomers by mass spectrometry

Stephen J. Blanksby[1]
stephen.blanksby@qut.edu.au

[1]*Central Analytical Research Facility, Institute for Future Environments, Queensland University of Technology, Brisbane, QLD, Australia*

Advances in mass spectrometry over recent years have significantly improved the mass-resolving power of modern instrumentation and the speed with which high mass-accuracy data can be acquired. These advances have underpinned increased confidence in compound identification in complex mixtures and opened up entirely new means of data acquisition including the next generation of data-independent analytical workflows. While powerful, an inherent limitation in all these analytical approaches lies in the discrimination of isomers which, by definition, share the same elemental composition and thus the exact same mass. Conventional approaches to isomer discrimination have relied on chromatographic separations prior to mass analysis and tandem mass spectrometry however, this has proven a limited tool box for structurally similar isomers (e.g., regioisomers) and can significantly extend analysis times. Fortunately, exciting new developments in ion-mobility and ion-activation technologies are emerging to tackle the challenge of isomer-discrimination by mass spectrometry. This presentation will address the latest developments in these rapidly emerging technology areas in the context of lipidomic analysis with examples illustrating effective discrimination of regio- and even stereo-isomers.

Agilent Trade Talk

Agilent's New 8890 Gas Chromatograph & 7250 Quadrupole Time of Flight Mass Spectrometer

Benjamin Davies[1]

[1]*GC and GCMS Product Specialist, Agilent, Australia & New Zealand*

The 8890 Gas Chromatograph (GC) continues Agilent's legacy of proven GC systems. It is the most flexible and configurable GC and exceeds expectations for uptime and accuracy.

The 8890 GC features built-in intelligence that enables remote connectivity using a browser interface suited to PCs as well as mobile devices. Autonomous and user-initiated system checks monitor system health. Guided maintenance provides users with step-by-step instructions on common maintenance procedures.

The 8890 GC can be coupled with the 7250 Quadrupole Time of Flight Mass Spectrometer (QTOF) to deliver full-spectrum, high-resolution, accurate-mass data with a wide dynamic range for identifying and quantifying GC-amenable compounds. This high-resolution GCQTOF enables accurate mass screening and enhanced compound identification through tandem mass spectroscopy (MSMS), low energy electron ionization and complimentary chemical ionization techniques.

Whether being used in complex metabolomics studies, pesticide screening in challenging matrices, or compound identification in herbal extracts, quadrupole time-of-flight mass spectroscopy delivers the ultimate in performance.

Agilent Technologies

2018 Division Citation Award

Determination of trace elements in open ocean seawater samples using NOBIAS resin with SF-ICP-MS detection. Method development and example applications from Heard Island

Ashley Townsend[1]
Ashley.Townsend@utas.edu.au

[1]*Central Science Laboratory, University of Tasmania, Hobart, TAS, Australia*

The determination of ultra-trace elements in open ocean seawater samples is a challenging task considering the analyte concentration levels expected (pM to nM), presence of dominant salt matrix, and the risk of contamination at all stages of sample collection and analysis. Direct determination of seawaters by atomic spectroscopic methods is usually not possible, with sample pretreatment (i.e. analyte separation and preconcentration) typically required for accurate and precise measurements. Solvent extraction or coprecipitation methods have traditionally been applied, while recently the use of chelating resins has grown in popularity. Sohrin et al.[1] demonstrated the application of NOBIAS resin (containing immobilised ethylenediaminetriacetic acid and iminodiacetic acid groups) resulting in the successful analysis of trace metal ions in seawaters. This pioneering work showcased the affinity of this resin for a broad range of key elements of relevance to oceanography.

Over the past five years work in our laboratories has considered and applied this resin for the extraction and preconcentration of ultra-trace elements in samples collected from the Southern Ocean. Both in-house[2] and commercial (seaFAST, Elemental Scientific, USA)[3] systems have been considered, with (offline) detection using Sector Field ICP-MS (offering superior sensitivity and interference free measurement). A particular focus has been the extensive and critical evaluation of the seaFAST system, including experimental parameters such as extraction pH, column efficiency, range of target analytes, preconcentration factors, achievable blank and detection limits, as well as tolerance to sample salinity. Method validation results will be presented for ten important trace elements (Cd, Co, Cu, Fe, Ga, Mn, Ni, Pb, Ti and Zn)[3], along with example application results considering samples collected near Heard Island during the Heard-Earth-Ocean-Biosphere Interactions (HEOBI) voyage in Jan.-Feb. 2016[4,5].

More recently, we have investigated the use of NOBIAS resin as a cost effective, time saving sample pretreatment approach for the simultaneous separation and preconcentration of Rare Earth Elements (including Nd) and 230, 232Th from seawaters[6]. These elements and associated isotopes are often used as oceanographic tracers, and in the case of samples collected near Heard Island, were expected to provide information as to potential lithogenic sources to nearby waters. Tailored extraction parameters were investigated, while detection was made possible using a Desolvating Neubuliser (DSN) sample introduction system to the SF-ICP-MS (particularly for Th isotopes). Considering large volume samples (10L) blank levels in the fM-pM range were achieved, although contamination issues for La were initially encountered. Method parameters and preliminary results from the analysis of samples collected near Heard Island will be discussed.

[1]*Sohrin, Y. et al. Analytical Chemistry, 2008, 80, 6267-6273*
[2]*Queroue, F. et al. Analytical Methods, 2014, 6, 2837-2847*
[3]*Wuttig, K. et al. Talanta, 2019, 197, 653-668*
[4]*Holmes, T. et al. Marine Chemistry, 2019, 211, 1-14*
[5]*van der Merwe, P. et al. Frontiers in Marine Science, 2019, 6, article 332*
[6]*Perez-Tribouillier, H. et al. Talanta, 2019, 202, 600-609*

Waters Trade Talk

Select Series Cyclic IMS: A novel ion mobility enabled mass spectrometer

Caryn Hepburn[1]

[1]*Application Support Specialist, Waters Australia*

Since releasing the first commercially available Travelling Wave Ion Mobility enabled mass spectrometer in 2006, Waters has continued to develop the technology and enabled leading researchers to unlock the potential in scientific discoveries. Released in 2019, the Select Series Cyclic IMS introduces the latest development in ion mobility separations for the structural analysis of ionic species as well as for separation of complex mixtures. In this presentation we will explore the unique geometry of the cyclic ion mobility device and the extended scope of multi-function Ion mobility experiments it provides. The multi-function capabilities are demonstrated through some application examples to illustrate how these unique experiments are used in solving analytical challenges.

2019 Original Research Publication Award

Perfluorinated alkylsubstances of significant environmental concern can potently inhibit human carbonic anhydrase isozymes

Giang T. H. Nguyen[1], Alessio Nocentini[2,3], Andrea Angeli[2], Paola Gratteri[3], Claudiu T. Supuran[2,*] and William A. Donald[1,*]

claudiu.supuran@unifi.it; w.donald@unsw.edu.au

[1]*School of Chemistry, University of New South Wales, Sydney, NSW, 2052, Australia*
[2]*Department NEUROFARBA-Pharmaceutical and Nutraceutical Section, University of Firenze, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Firenze, Italy*
[3] *Department NEUROFARBA-Pharmaceutical and Nutraceutical Section, Laboratory of Molecular Modeling Cheminformatics & QSAR, University of Firenze, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Firenze, Italy*

Perfluorinated alkyl substances (PFASs) have been extensively used since the 1950s as fluorosurfactants in numerous household products, in fire fighting foams, and many industrial processes. Such compounds are ubiquitous in the environment, readily bioaccumulate, and some PFASs have been identified to be toxic to mammals. However, the origins of PFAS toxicity and the specific proteins and protein functions that are affected by such compounds remain unclear. Here, we demonstrate that PFASs can directly interact with human carbonic anhydrases and inhibit their enzymatic activity for the first time. Fifteen PFASs, including the widely used perfluorooctanoic acid (PFOA), perfluoroctanesulfonic acid (PFOS) and perfluoroctanesulfonamide (PFOSA), were tested for their inhibitory effects on human carbonic anhydrase I, II, IX, and XII, which are ubiquitous enzymes that play key roles in regulating pH and many other functions, and are highly abundant in the blood, tissues, and organs of mammals. Native mass spectrometry was used to directly identify specific protein-ligand interactions and key interactions were modelled using docking simulations in combination with X-ray crystal structures that are available in the literature. These results indicate that some PFASs can inhibit some carbonic anhydrase isozymes with low nM to low μM. These results were in excellent agreement with the results from native mass spectrometry and can be rationalised based on molecular docking simulations. Overall, this research indicates that PFASs can interact strongly with carbonic anhydrases and inhibit their catalytic activity, which may play an important role in the mechanism of PFAS toxicity.

2018 Paul Haddad Medallist

Multi-Modal Spectroscopic Imaging to Study Brain Disease: Ions, Metals, Memory Loss and More!

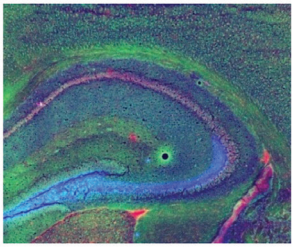
Mark Hackett[1,2]

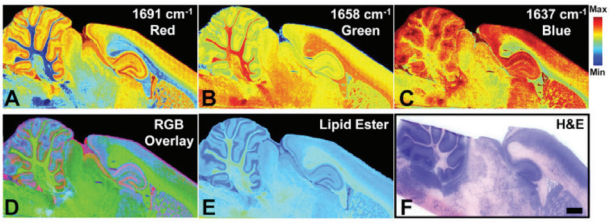
[1]*Curtin Health Innovation Research Institute*
[2]*Curtin Institute for Functional Molecules and Interfaces*

Neurodegeneration during brain disease or following brain injury is a major health and economic concern with limited treatment options. The lack of effective therapies can be attributed to incomplete understanding of the chemical mechanisms that are essential for healthy brain function, and an incomplete understanding of how injury or disease perturbs brain chemistry.

Advanced imaging technologies such as synchrotron X-ray fluorescence microscopy (XFM) and micro X-ray absorption spectroscopy (μXAS) are making an important contribution to our understanding of brain function and malfunction. This is due to their capability to directly image diffusible ions (K^+, Ca^{2+}, Cl^-) and transition metals (Fe, Cu, Zn) at cellular resolution. Integration of XFM and μXAS alongside vibrational spectroscopy and traditional histochemical methods in a multi-modal approach enables association between cell physiology, altered metal ion homeostasis, protein aggregation, oxidative stress, and disturbed brain metabolism.

My presentation will highlight recent research advances with respect to optimisation and application of the above spectroscopic techniques for direct in situ imaging within ex vivo tissue sections of animal models of neurodegeneration (specifically stroke and dementia). In addition to neuroscience, the multi-modal spectroscopic approach is well suited to a range of other analytical applications, such as forensic fingermark detection and in vivo monitoring of plant physiology, which I will also briefly discuss.





CURTIN HEALTH INNOVATION RESEARCH INSTITUTE

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Curtin University
INSTITUTE FOR FUNCTIONAL MOLECULES AND INTERFACES

Syrris Ltd. Trade Talk

Exploiting segmented flow chemistry in modern compound library synthesis

Chinh Nguygen[1]

[1]*Syrris Ltd, United Kingdom*

The pharmaceutical industry continues to go through changes both in its approach to drug discovery and in the way, it uses new enabling technologies. The constant demand to deliver new drugs to market is the driver to adopt new strategies to improve the speed through early discovery to production and to the point of care. One of the major challenges faced today in drug discovery programs is the increasing demand to deliver a continuous supply of active compounds, generally novel and structurally diverse, in increasing numbers and in shorter timelines.

During the past two decades, there has been considerable effort to develop chemically diverse libraries to successfully meet this challenge with advances in automation, miniaturization and high-throughput methodologies. With the advancement of computational tools and high throughput screening the bottle neck has shifted more towards the synthesis step.

The process of drug discovery is a complex process that relies on the iterative learning cycle of molecular design, synthesis, testing and analysis. The traditional approach to this leads to time delays between the design and ultimately the screening results of these compounds. Traditional methods of synthesising compound library are restricted to scale and the chemistries available often delivering low yielding and unreliable reactions and require extensive re-optimization during subsequent re-synthesis and scale-up. The time-consuming purification needed after each reaction step wastes resources and delays the delivery of the final compounds. This has a huge impact on the timelines and success rates of the drug discovery process. The adoption of continuous flow in the drug discovery process has made a significant impact in overcoming these issues.

The use of these enabling techniques to the chemical synthesis of libraries allows the exploration of novel reaction windows to deliver a wider chemical space and more compound diversity over traditional methods. The technique enables the rapid optimization of synthetic protocols, access to reactions that were formerly avoided because of scale or safety concerns, telescoped reactions avoiding purification between steps and ready-made scale-up strategies. The ability to harness these advantages with fully automated systems has led to the rise in these techniques being adopted.

This presentation illustrates how flow chemistry technology has enabled the synthesis of a range of structurally diverse compounds across a range of chemistries with the benefits of automation and reaction control.

ORAL PRESENTATION ABSTRACTS

Downscaling liquid chromatography for ICP-MS detection: Effects on sensitivity

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Liquid chromatography-inductively coupled plasma-mass spectrometry (LC-ICP-MS) is an essential tool for studying elements in biological samples. ICP-MS possesses the isotope specificity, multi-elemental detection capability, sensitivity, and large linear range needed for the detection of bio-elemental species. ICP-MS is, however, subject to a number of disadvantages as an LC detector, most of which are related to sample introduction and ionisation. While chromatographic downscaling (reducing the internal diameter (ID) of the column used) is known to be beneficial for molecular detection techniques such as LC-MS, the response is less thoroughly studied for mass-based detectors like ICP-MS.[1]

Here we systematically examined the effects of reducing column ID by determining absolute and relative limits of detection as a measure of sensitivity without altering any unrelated parameters. Limits of detection for the narrowest ID column were similar to or lower than those of the larger columns. The improved absolute limits of detection were expected due to the smaller injection volume, however improvement in relative limits has previously only been observed after modifications to post-column sample transport and introduction into the ICP,[2,3] whereas these results can be attributed directly to the chromatographic downscaling. Improvements in peak sensitivity overcome the reduced mass load reaching the detector, providing an avenue to further improve the separation and detection of biomolecules with complementary elemental and molecular detection techniques.

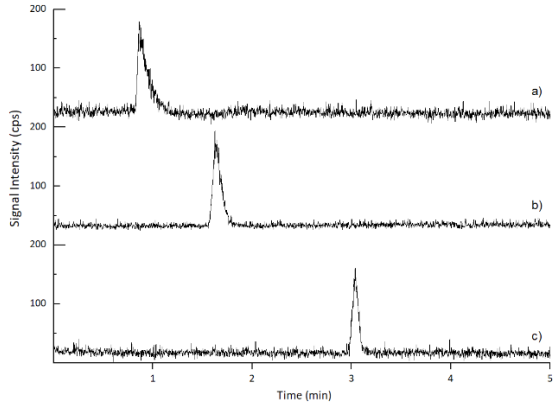

Figure 1. *Chromatograms of a 15 ng mL^{-1} cyanocobalamin obtained with a) a 1.0 ID column, b) a 2.0 mm ID column, and c) a 4.6 mm ID column.*

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3D optical data storage: A nanocrystal approach

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The dramatically growing amount of information generated has created an urgent demand for new and improved data storage devices [1-2]. Sm doped BaFCl nanocrystals have excellent optical storage properties with potential to be used for 3D memory. 3D memory requires the nanocrystals to be embedded in a transparent matrix. We have used PMMA as the matrix and developed techniques for dispersing nanocrystals in the medium. The BaFCl:Sm in the matrix allows data to be encoded by changing the fluorescence spectrum [3-6]. We have synthesized transparent BaFCl:Sm nanocrystal doped PMMA nanocomposites by ex-situ polymerization as shown in Fig. 1. The main challenge was agglomeration of the nanocrystals. To overcome this, long-term stirring was performed to get improved dispersion within the matrix. The pre-polymerization of monomers forms oligomers which allows for nanocrystal dispersion in the solid matrix because of the creation of an initial cross link polymer network. The dispersion of nanocrystals in the nanocomposite was investigated by transmission electron microscopy and the average nanoparticle size was found to be 90nm.

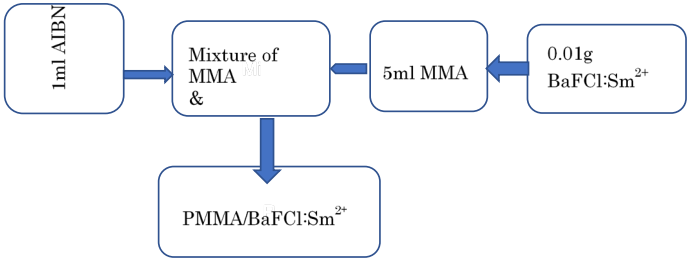

Figure 1. *Flow diagram of the synthesis of PMMA/BaFCl:Sm^{2+} nanocomposites*

[1]Gu, M; Qiming, Z.; Simine L. Nanomaterials for optical data storage, *Nature Reviews Materials*, **2016**, 12, 16070.

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Clinical Production and Quality Control Testing of [^{68}Ga] Gallium-Exendin-4 for the Localisation and Detection of Insulinomas at the Royal Brisbane and Women's Hospital

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Insulinoma is a rare type of neuroendocrine tumour (NET) that develops in the pancreas and affects approximately 1 - 4 people per million per year (1,2) but is also one of the most common tumours of the pancreatic islet (3). Benign insulinoma tumours can cause patients to suffer from mild to severe symptoms of hypoglycaemia (4) and could result in death.

[^{68}Ga]Gallium-exendin-4 is a radiopharmaceutical which specifically targets the glucagon-like peptide-1 receptors (GLP-1R) commonly overexpressed on the tumour. This presentation will describe the radiolabelling process from two E&Z IGG100 ^{68}Ge/^{68}Ga generator input on the Scintomics GRP® module utilising commercial reagent and hardware kit for synthesis of ^{68}Ga peptides (SC-01, ABX).

Product specifications used for the clinical batches of [^{68}Ga]Gallium-exendin-4 are adapted from the monograph for [^{68}Ga]Gallium-DOTA TOC. QC testing will be presented, which includes, pH, chemical and radiochemical purity through HPLC testing, radiochemical purity through iTLC testing, HEPES quantification through HPLC, residual solvents testing on the GCMS, radionuclide identification through multi-channel analyser and half-life assay, radionuclide purity, filter integrity, sterility, and bacterial endotoxin testing.

We have found the production of [^{68}Ga]Gallium-exendin-4 difficult with respect to meeting pre-defined acceptance criteria (radiochemical purity) due to larger amounts (>10%) of impurity, thought to be radiolabelled oxidised exendin-4. Communication with other sites, nationally and internationally, revealed [^{68}Ga]Gallium-exendin-4 was being used satisfactorily for clinical imaging with this impurity present, in up to 30%.

Clinical validation of this PET imaging agent for clinical use (3 consecutive productions of [^{68}Ga] Gallium-exendin-4) has been completed and will be summarised in this presentation.

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The Influence of Birnessite Crystal Structure on its Oxidative Reactivity

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Birnessite $Na^{+}(Mn^{3+}\ Mn^{4+})_2O_4 \cdot 1.5H_2O$, is a common manganese dioxide mineral found in soils and has been found to have many applications such as catalysis[1], oxidation[2] and environmental remediation[3]. It is known that the mineral structure impacts on its catalytic and oxidative performance[4]. The crystal structure of birnessite can vary in several ways; i) the main birnessite structure can either be triclinic or hexagonal, ii) it can contain different interlayer cations and iii) it can have varying degrees of crystallinity or layer disorder. Various birnessite synthesis methods have been reported and used in the literature, however most result in poorly crystalline materials that are not well characterised. This work compares four literature synthesis methods for the resulting birnessite crystallinity, purity and reactivity. The effect of post synthesis treatment of birnessite with various alkali and alkaline metals salts on the birnessite crystallinity, purity and reactivity was also investigated. The different synthesis methods were found to form birnessites with varying structures, crystallinity and reactivity. Post synthesis treatment of birnessite with potassium chloride over time was found to increase the crystallinity and purity of birnessite product but had no effect on the materials reactivity. Finally, the interlayer cation was observed to be an important factor for driving the material reactivity. This knowledge of the impact of the synthesis methods on birnessite properties will allow researchers to carefully design a material that is more suitable for their end application.

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Spectroscopic Alterations in Lipofuscin during Ageing

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Lipofuscin deposits are bundles of oxidised, cross-linked and aggregated nucleic acid, lipid and protein residues formed in lysosomes[1]. Found commonly in brain cells, and considered a waste product, their interaction with the cellular environment, and correlation with ageing and neurodegenerative disease has fuelled further studies into their characterisation over the course of ageing. Lipofuscin is auto-fluorescent and easily observed inside cells using fluorescence microscopy, however, characterising the chemical composition of lipofuscin and identifying changes in lipofuscin chemical composition during ageing is more difficult. Application of direct spectroscopic methods in combination with fluorescence microscopy may enable the chemical composition of lipofuscin to be studied in more detail during the ageing process, which could provide important insight into altered intracellular chemical environments that occur during ageing.

HYPOTHESIS: Lipofuscin deposits interfere with autophagic processes, causing increased accumulation of damaged cellular components, and increased cellular vulnerability to oxidative stress.

AIM: Characterise the biochemical profile of lipofuscin *in situ*, to determine if markers of increased oxidative stress occur during the ageing process.

METHODS: Tissue was generated from the senescence accelerated mouse prone strain 8 (SAMP8) from mice aged 4, 20 and 40 weeks. Raman spectroscopy was used to image individual brain neurons *in situ* within tissue sections, at sub-micron spatial resolution to reveal tissue-autofluorescence and biochemical composition.

RESULTS: Raman spectroscopic analysis revealed the size, abundancy and chemical composition of lipofuscin deposits change during ageing. Specifically, the biochemical profile of lipofuscin appears to be enriched in nucleic acid material in young SAMP8 mice, with data indicating a transition towards protein accumulation in older SAMP8 mice.

CONCLUSIONS: Our data shows unique, direct biochemical insight into the biochemical composition of lipofuscin during ageing. The increased accumulation of protein aggregates in aged SAMP8 mice is consistent with elevated protein oxidation and decreased function of the proteasome.

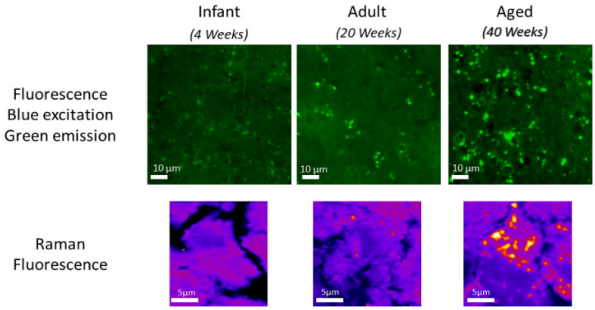

Figure 1. *Raman and fluorescence microscope images highlighting accumulation of lipofuscin during ageing*

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Bad Hair Day: Detecting Athlete Drug Use

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Hair is a popular matrix in criminal investigations, workplace drug testing and postmortem toxicology for the detection of drugs of abuse and drugs associated with crime.[-3] The major advantage of hair testing is the longer window of drug detection, up to several months after drug administration. By segmenting the hair into smaller pieces, a retrospective calendar of an individual's possible drug use over time can be established and used to distinguish between acute and chronic drug use. Despite these advantages, hair testing has yet to become a routine matrix for human antidoping investigations.

The aim of this project was to develop and validate a multitargeted initial testing procedure for the trace level detection of performanceenhancing drugs in human scalp hair. A liquid chromatography highresolution mass spectrometry method was developed for the detection of 38 drugs; predominately anabolicandrogenic steroid esters and other anabolic agents. Literature extraction protocols were then evaluated before a new protocol was developed. This new protocol was validated as a qualitative screening method with picogram per milligram limits of detection. In a practical application, a performanceenhancing drug was successfully detected in a horse administration study sample and a human hair sample.

This validated initial testing procedure allows the Australian Sports Drug Testing Laboratory to conduct sensitive and reliable hair testing of athletes. This has provided a strong deterrent for athletes considering or already taking performance enhancing drugs due to the greatly extended window of drug detection.

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Spectroscopic Studies of Brain Zinc Homeostasis and Its Role During Cognitive Decline and Ageing

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The greatest risk factor for dementia is ageing. With no cure or effective therapies to slow progression, and with an ageing population, dementia has reached crisis levels in Australia. The content and distribution of metals such as Fe, Cu, Zn is known to change in the ageing brain (metal dis-homeostasis)[1, 2] and thus, increased understanding of the mechanistic role of metal dis-homeostasis may illuminate new therapeutic strategies. Specifically, Zn homeostasis and dis-homeostasis appears to be a potent modulator of memory function[3, 4], yet, the exact chemical form(s) of Zn that are vital to memory function are unknown[5, 6]. Development of new spectroscopic methods to image different chemical forms of Zn may help increase understanding of Zn-modulated memory function and dysfunction. There are currently no available imaging protocols to differentiate between different chemical forms of Zn, however, substantive evidence supports that X-ray absorption techniques could provide such capability[7, 8]. Recently, our group has utilised X-ray absorption spectroscopy (XAS) to build a spectroscopic library of Zn compounds that reflects the chemical forms of Zn likely to be present in the brain. Preliminary analysis has revealed that XAS is able to differentiate between multiple Zn compounds across anatomically separate brain regions. Future experiments hope to reveal which Zn compounds change, in which brain regions, during ageing or neuorodegenerative disease. Such insights into whether specific types of zinc are affected with ageing may reveal mechanisms contributing to cognitive decline, in turn presenting potential pathways for targeted therapeutic interventions.

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Polymeric monoliths for the characterization of intact proteins

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Polymeric monolithic stationary phases are well suited for the separation and characterization of large structures using different chromatographic modes like hydrophobic interaction chromatography or ion exchange chromatography. Polymeric monolith stationary phases show higher efficiencies and resolution for the separation of proteins.[1]

In order to preserve the higher order structure of proteins, chromatographic methods as hydrophobic interaction chromatography (HIC) or ion exchange chromatography (IEC) are of great value to obtain information about the intact structure of proteins. However, traditional approaches use high concentrations of non-volatile salts, which makes them not suitable to couple to mass spectrometry (MS). To overcome this challenge to characterize intact proteins with LC-MS, a successful HIC or IEC method needs to be developed with a low concentration of MS-compatible salts. Here, polymeric monolithic stationary phases are used to increase the affinity between the proteins and the stationary phase to a point that proteins are retained and eluted using a maximum salt concentration of 1M of a MS-compatible salt.[2]

Two different polymeric monolith structures were prepared, for hydrophobic interaction chromatography it was based on an acrylate-based PEGDA (poly(ethylene glycol) diacrylate) monomer and for ion-exchange chromatography a monolithic structure based on a SPE (*N,N*- dimethyl-*N*-methacryloyloxyethyl-*N*-(3-sulfopropyl) ammonium betaine) zwitterionic monomer was prepared.[3,4] Both capillary columns showed good results when traditional salts were used. Research is still on going for finding appropriate methods with new salts. Promising is the separation of immunoglobulins with the SPE zwitterionic stationary phase where proteins can be separated based on a pH gradient with only a low concentration of buffer in the mobile phase.

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Profiling the Seasonal Variability of Decomposition Odour from Human Remains in a Temperate Australian Environment

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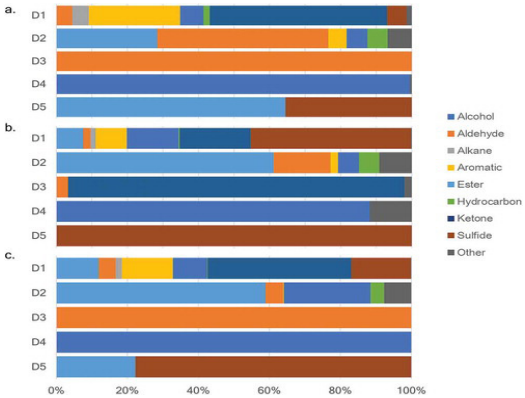
Determining time since death (TSD) during a crime investigation can provide vital information to law enforcement. One area of research used to determine TSD is volatilome profiling in which the volatile organic compounds (VOCs) emitted from decomposing cadavers are collected and analysed. Previous research into volatilome profiling as an indicator of TSD has relied on the use of human analogues (*i.e.* pigs) due to the ethical and legal restrictions surrounding research on whole human cadavers. Further, these studies are often restricted to summer and winter seasons, as these seasons mark the greatest variation in visual decomposition changes. The aims of this project were to analyse human decomposition volatilomes as a function of TSD from whole human cadavers across various seasons.

Volatilomes were collected from five cadavers over the course of one year at the Australian Facility for Taphonomic Experimental Research (AFTER). Samples were collected periodically using dual sorbent tubes (Tenax TA and Carbograph 5TD) for a sample size (n=22-24) per cadaver. Samples were analyzed using two-dimensional gas chromatography – time-of-flight-mass-spectrometry (GCxGC-TOFMS). Resulting data was normalized against VOCs of control plots and Principal Component Analysis (PCA) was conducted on resulting whole volatilomes.

Results demonstrated that cadavers placed in warmer conditions showed higher variety and abundances of chemical compounds compared to cadavers placed during cooler weather. These variances were also clearly differentiated in the PCA analyses. All seasonal trials showed differences, illustrating the variation of volatilome profiles in relation to decomposition and environmental temperatures. This can be seen through Figure 1, in which the variation in chemical class abundances during the stages of decomposition for each cadaver can be visualised. This information will be useful in future forensic work as it has demonstrated variability in decomposition compound abundances related to environmental conditions.



Deo, A., et al. (2019). "Profiling the seasonal variability of decomposition odour from human remains in a temperate Australian environment." Australian Journal of Forensic Sciences: DOI: 10.1080/00450618.2019.1637938.

Figure 1*: Relative percentages of chemical class abundances during (a) early, (b) middle and (c) late decomposition stages for each cadaver. D1 refers to donor 1, D2 refers to donor 2, D3 refers to donor 3, D4 refers to donor 4 and D5 refers to donor 5 (Deo, Forbes et al. 2019).*

Aroma Compounds in Coffee-Beverages and the Relationship with Consumer Acceptance

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In addition to coffee's stimulation effect, the complex aroma is the main driver of coffee consumption. Coffee aroma is not result of a single compound, but a combination of thousands compounds, however, not all of them influence consumer liking. To identify the important aroma compounds in coffee beverages, nine iced-coffee samples were formulated with different fat (0g, 3.7g and 7.4g /100g) and coffee (0.67g, 2g and 6g / 100g) concentration. A consumer panel (n = 231), using 9-point hedonic scale, assessed their overall liking, and overall aroma liking of those nine formulated iced-coffee beverages. Next, Head Space Solid Phase Micro-extraction (HS-SPME) in combination with Chromatography Mass spectrometry Olfactometry (GCMS/O) was used for aroma analysis. A trained panel (n = 6) used Modified Frequency (MF) method to provide the intensity and aroma description for each aroma compound during GCMS/O analysis. Partial Least Squares Regression (PLSR) was performed to associate the consumer liking data with instrumental data. A total of 52 aroma compounds were tentatively identified based on the mass spectral information, retention index and aroma description from panellists. Aroma compounds such as Isobutyraldehyde (caramel, cocoa, malt), Methyl isovalerate (apple, fruit, pineapple), Furfural (almond, floral, bread, candy), 2, 5-Dimethyl pyrazine (roasted nut, cocoa) etc. were positively correlated with aroma liking, while compounds such as Hexanal (grass, green), 4-Methylthiazole (green, nut, roasted meat), 2-Furanmethanol (cooked, solvent, wood) etc. were negatively correlated with consumer liking of aroma of iced-coffee. In this presentation, I will describe the approach taken to identify key aroma compounds that influence consumer acceptability of coffee flavoured beverages.

Portable 3D Printed Colorimetric Sensor for Remote Soil Measurement

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Simple and portable colourimetric devices for determination of soil nutrients in the field has always been highly demanding. However, the existence of high loads of suspended solids present in the sample matrix is a bottleneck for the application of microfluidics requiring extra steps of sample preparation like filtration, or centrifugation. Many approaches have been used to incorporate functional units in microfluidic devices, most of which involve laborious and time-consuming fabrication processes to create leakage-free devices [1-5]. To overcome this issue, we report single-material 3D printing for membrane integration enabling direct soil measurements, with the ability to print more than 1100 fully bonded and sealed devices in 18 hr (63 s per device) at a cost of $2.50 each. Based on previous designs [3], commercially available transparent build material (Veroclear-RGD810) was used to print the body of the device by a PolyJet 3D printer (Objet Eden 260VS Stratasys, Eden Prairie, MN, USA), with water-soluble support materials (SUP707) filling the channels. After removal of the support material, a porous structure was left at the interface between the build and support material. The properties of this filter could be tuned by simply varying the fabrication orientation of the print head to the direction of the channel and the design width (Figure 1). The printed device was evaluated for the determination of iron Using hydroxylammonium chloride for the reduction of Fe^{3+} to Fe^{2+}, 1-10 phenanthroline as a colourimetric reagent, and a cell phone camera for signal acquisition.

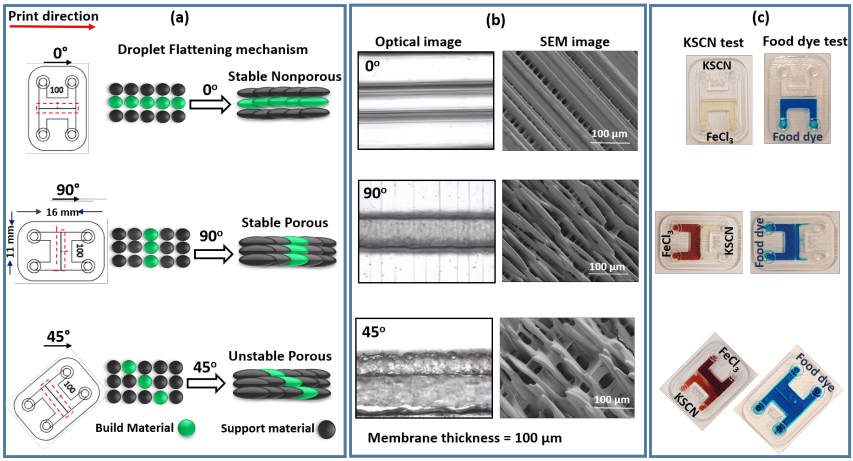

Figure 1: *(a) Design, orientation and illustration of 3D printed support and build material droplet flattening mechanism to create integrated filtration membranes in 3D printed devices. (b) Light microscopic images and scanning electron microscopy (SEM) images of the surface of the 3D printed membranes. FeCl3 and KSCN formation test (c)*

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Column separation of lanthanide ions from electronic waste

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Lanthanide elements are an integral part of our daily lives, with applications in the latest electronic, medical and research technologies. The increasing demand and diminished supply of these elements has prompted research to focus on recycling end of life electronics as a way of satisfying future requirements, and to make sourcing more sustainable.[1, 2] It's estimated that only 1% of lanthanide elements are currently recycled.[2] Suggested sources of lanthanide elements include computer hard drive disks, fluorescent lights and NiMH batteries, however, no effective green separation methods have yet been developed.[1,2]

On an industrial scale, lanthanide elements are usually separated using solvent extraction (SX), a process which involves the use of large quantities of toxic, volatile and flammable solvents thus posing a risk to human health and causing significant environmental impact.[3] In the past 20 years, separation based on polymer inclusion membranes (PIMs) has been proving to be a suitable solvent-free alternative to SX, including lanthanide separation.[4] However, PIMs have a relatively low specific surface area which can sometimes make the extraction performance slow or impractical.

Micro polymer inclusion beads (μPIBs) are a new form of polymer inclusion materials, which are manufactured using a novel microfluidic technique.[5] Due to their higher specific surface area they provide faster rates of extraction than PIMs of the same composition, and their bead format also opens the possibility to a variety of applications (e.g., column separation). Previous research has shown that μPIBs composed of 60 wt% di-(2-ethyl hexyl) phosphoric acid as the extractant and polyvinyl chloride or Poly(vinylidene fluoride-co-hexafluoropropylene) as the base polymer, can be effectively produced and are stable under the acidic lanthanide extraction conditions. Hence, in the present work these μPIBs were packed into a column in order to perform on-line separation of lanthanides. Subsequent extraction and back-extractions were effective under the previously described sulphuric acid conditions.[4] Preliminary studies also showed that the μPIBs were able to separate lanthanide ions form one another.

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Considerations for multiplexed Immuno-Mass Spectrometry-Imaging

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Determining the abundance and location of multiple low-expression proteins using standard techniques such as Western blot and immunohistochemical imaging is complicated due to issues including low signal sensitivity and specificity, poor protein solubility, absence of external standards and fluorescent signal crossover. Immuno-mass spectrometry imaging (iMSI), a subset of elemental bio-imaging (EBI), is a new approach for quantitative biomolecule imaging based on the combination of laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) and immunohistochemistry (IHC). Protein quantification using iMSI takes advantage of the high resolution, sensitivity and isotopic analysis of LA-ICP-MS and the specificity of immunohistochemistry to simultaneously provide the location and amount of multiple biomolecules. A number of multiplexed iMSI applications have been developed with up to 32 proteins simultaneously imaged on a single biopsy, however to date none have investigated the potential for steric interactions between antibodies preventing reproducible quantitative binding to the analytes.

Here we describe a protocol for examining steric interferences in multiplexed iMSI using the muscle proteins, dystrophin, sarcospan, and myosin as our model. Anti-dystrophin, anti-sarcospan, and anti-myosin antibodies were labelled with Gd-158, Dy-163, and Nd-142 respectively, before histological application to mouse quadriceps sections using standard IHC protocols, and imaged with LA-ICP-MS. The antibodies were applied to 9 sections individually, and to 9 sections multiplexed before statistical comparisons to determine differences. No significant differences were seen using either pairwise t-tests, or multivariate ANOVAs between the concentrations of the antibodies measured in the individual samples or the multiplexed samples. These analyses provide a framework for ensuring reproducibility during multiplexed iMSI, which will allow quantitative exploration of protein-protein interactions and provide a greater understanding of fundamental biological processes during healthy and diseased states.

Minimising Fouling During Dopamine Detection at Carbon Electrodes Hydrogenated by Aromatic Organosilanes

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In this work, we have studied the effect of phenyl rings sterically positioned on a carbon electrode surface, by the reduction of phenylsilane and diphenylsilane, against fouling during the detection of neurotransmitter dopamine *in vitro*. Dopamine is a predominant monoamine neurotransmitter associated with motivation and reward behaviour.[1] It is involved in neural signalling during substance abuse and is also linked to pathological conditions such as Parkinson's disease, schizophrenia or Tourette's syndrome.[2,3] External to the central nervous system, it plays multiple roles in cardiovascular function, hormone secretion, renal function and gastrointestinal motility.[3]

Electrochemical detection of dopamine has been extensively studied owing to its ease of oxidation.[4] Additionally, availability of miniaturised sensing electrodes has also made electrochemical detection of dopamine *in vivo* possible. However, a common problem encountered in such experiments is electrode fouling, where intra- and extracellular species including amphiphilic peptides, proteins and lipids adsorb on the electrode surface and hinder dopamine oxidation. This generates diminishing transient dopamine signals, which jeopardise the long-term electrode stability. Recently, boron-doped diamond electrodes with a hydrophobic sp^3-carbon surface were demonstrated to show antifouling characteristics because of less favourable adsorption of fouling species.[5]

A hydrogenation method involving phenylsilane and diphenylsilane was exploited in this work to develop electrodes with an sp^3-carbon rich surface, followed by evaluation of their antifouling capability during dopamine detection *in vitro*. In this hydrogenation method, C=O bonds on the carbon surface are converted to C–H bonds, but phenolic groups are converted to siloxane dendrimers.[6] These dendrimers were previously shown to prevent a close contact of amphiphilic biomolecules on the hydrophobic electrode surface, leaving the surface for dopamine oxidation. The phenyl groups are hypothesised to sterically protect the electrode surface against fouling. Electrochemical detection of dopamine *in vitro* will be used to evaluate the relative antifouling effectiveness of the hydrogenated carbon electrodes.

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Using Synchrotron Sourced Microscopy to Explore Fingermark Chemistry

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The successful detection of latent fingermarks is a valuable tool for forensic investigation, however current detection methods can be hindered by variation in response or lack of robustness. Studies of fingermark chemistry aim to provide explanation for the effectiveness or lack thereof for current detection methods, as well as driving the development of improved techniques to increase detection capabilities.

We have used synchrotron sourced Fourier-Transform Infrared (FTIR) and X-ray Fluorescence Microscopy (XFM) to probe the spatial distribution of the molecular and elemental components within latent fingermarks. FTIR enabled us to determine that fingermarks have a complex heterogeneous distribution of eccrine and sebaceous material. Our research has focused primarily on visualising the lipid and amino acid distribution at both the macro and sub-micron scale.[1] More recently we have carried out time-course studies to investigate the rate freshly deposited fingermarks lose water. Our findings reinforce the heterogeneity of the chemical composition of latent fingermarks at the micron level and also demonstrate how differences in chemical composition appear to influence the rate of water loss and chemical redistribution of lipid material during drying.

We used XFM to explore the inorganic components within fingermark residue. The distribution of trace metals including endogenous trace metals (Fe, Cu, Zn), diffusible ions (Cl^-, K^+, Ca^{2+}), and exogenous metals (Ni, Ti) were successfully imaged across multiple donors.[2] Further experiments have also explored the effects of the external environment on these metals post deposition, and the transfer of exogenous metals prior to deposition. Using this technique, our research allows a better understanding of the chemical complexity and chemical transfer processes associated with latent fingermarks. Such insight provides the necessary fundamental understanding for the development of new, improved detection methods or to identify chemical traits within the fingermark.

We gratefully acknowledge funding provided by ANSTO, funded by the Australian Government.

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Development of a 3D-printed flow-through passive sampler for the monitoring of Zn^{2+} in freshwaters free of environmental effects

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Passive sampling is an important tool for monitoring the presence and concentration of heavy metals in environmental waters. The passive sampling accumulation, however, depends strongly on several environmental factors such as flow-pattern, matrix and temperature, which often lead to unreliable results[1]. Previously, we have developed a 3D-printed flow-through passive sampler (PS) that could eliminate the effect of flow-pattern using Zn^{2+} as the model analyte. The proposed PS consisted of an acrylic 3D-printed flow-through compartment, a glass vessel containing the receiving solution (RS) and a polymer inclusion membrane (PIM) as the semipermeable membrane separating the RS from the controlled flowing stream of the source solution (SS)[2].

In this research, the same device was used to study the effect of the interfering matrix and temperature. PIMs containing dinonylnaphthalene sulfonic acid (DNNS) or di(2-ethylhexyl) phosphoric acid (D2EHPA) as the extractant were compared for their Zn^{2+} accumulation performance using synthetic SS spiked with 100 mg L^{-1} Zn^{2+} and other major interfering cations (i.e., Na^{+}, K^{+}, Ca^{2+}, and Mg^{2+}) in concentrations significantly higher than Zn^{2+} [3,4]. The results demonstrated that the PS using the D2EHPA-based PIM as the semi-permeable barrier accumulated 50% more Zn^{2+} in the RS in comparison to that of the PS using the DNNS-based PIM. However, the accumulation of Zn^{2+} was significantly affected by the co-transport of other major interfering cations present in the SS when using 1 M HNO_3 as RS. Nevertheless, it was observed that this effect was reduced as the concentration of acid in the RS was increased, and 4 M HNO_3 was found to accumulate the same amount of Zn^{2+} irrespective of the concentration of the other major cations. Under these conditions the pH at the membrane-SS interface was about 3, which is known to be ideal for the selective extraction of Zn^{2+} [5]. The PS was then calibrated at different temperatures (10 – 25 °C). A linear relationship was obtained between the concentration of Zn^{2+} in the RS and in the SS for SS concentrations within the range of 10-200 µg L^{-1}.

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Ambient Ionization Mass Spectrometry: Benefits, Challenges and Practical Observations

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Mass spectrometry is well-recognised as a powerful analytical tool, especially when combined with separation techniques. However it is often necessary to carry out extensive preparation to get each sample into a form that can be accepted by traditional laboratory instruments, and long chromatographic runtimes can limit throughput of high-volume testing.

Ambient ionisation, as the name suggests, covers a collection of technologies that allow for the generation and detection of ions from a sample at ambient temperature and pressure (1,2). These techniques have the potential to allow for extremely rapid non-destructive analysis, from in-situ surfaces, and at high sensitivity and specificity. Therefore it has been explored in literature for applications such as drug identification, explosives detection, and food safety and medical screening (3-5).

Conversely the open and versatile nature of these techniques can also create drawbacks; the sensitivity of the method can be significantly affected by matrix suppression and trace atmospheric contaminants. Using smokeless (gun) powder as an example, this talk will compare two plasma-based ambient ionisation instruments and their potential for use in a forensic detection role.

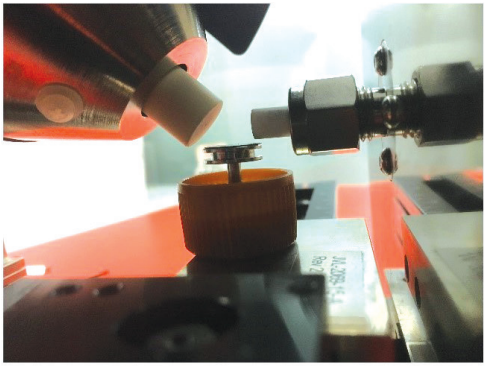

Figure 1. *Direct Analysis in Real-Time (DART) Sampling Inlet*

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Profiling volatilomes as a novel forensic method used to distinguish the species identity of confiscated specimens from the Illegal Wildlife Trade

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Volatile organic compounds (VOCs) are low molecular weight compounds that create unique odour profiles (*i.e.* volatilomes). Volatilomes have been described as individual or species specific due to dietary, genetic, and metabolic factors. The project aim was to determine whether volatilomes could be used to determine the species identity of animal parts often confiscated from the Illegal Wildlife Trade (IWT). Volatilomes of elephant ivory (known n=7; unknown n=8) provided by the Department of Environment and Energy were compared to outgroup samples provided by the Australian Museum. Outgroup selection criteria included samples of the same biological composition as ivory (*e.g.* dentine: dugong, n=4; sperm whale, n= 2), common fakes (*e.g.* bone: cow, n=5; koala, n=4; sheep n=1) or parts of elephants (tooth n=1) that are not often traded. Samples were individually placed into either 20 mL solid phase micro-extraction (SPME) vials or sealed stainless-steel tins based on size. Prior to extraction, samples were heated for 30 minutes at 80 °C. A 50/30 mm divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) 24 Ga Stableflex SPME fibre was exposed to the headspace for 45 min and volatilomes were extracted. Samples were analysed using comprehensive two-dimensional gas chromatography (GC×GC) coupled with time of flight mass spectrometry (ToFMS). The resulting volatilomes were normalized to sample blanks and analysed using principal component analysis (PCA). VOCs were manually classified into chemical classes, averaged, and compared. Discriminant analyses was conducted on ivory vs dentine products and ivory versus bone products. The PCAs revealed distinct separation between items, which was supported by differences in average chemical compound classes. The discriminant analyses distinguished ivory from dentine products with 71.4% accuracy whereas ivory could be distinguished from bone products with 75% accuracy. This preliminary data reveals the potential of volatilome profiling as a screening method to identify the composition and species identity of confiscated wildlife specimens.

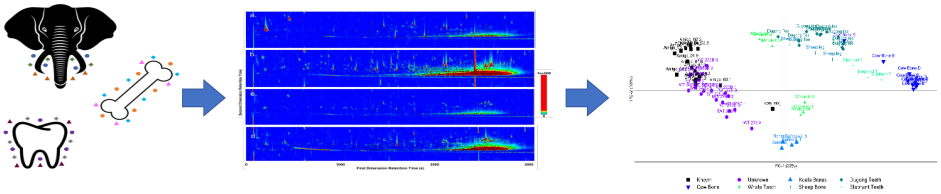

Figure 1: *Succession of wildlife specimen volatilome profiling and analyses*

ATR-FTIR spectroscopic studies of condom lubricants: An investigation into the international market from a forensic perspective

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In sexual assault and rape cases, DNA evidence recovered from the victim's genital area can be critical to identifying the perpetrator[1]. However, the last 10 years has seen a significant increase in cases where no DNA was found [2,3]. The presence of condom traces could explain the absence of the perpetrator's DNA in such cases, several of which have been reported in the literature[4-6]. For forensic purposes, it is important to establish whether condom lubricants can be distinguished from each other, or from other personal hygiene products[5]. Although the forensic analysis of condom evidence is usually performed on 'real' samples within a biological matrix, it is important to first establish whether products can be distinguished based on the analysis of bulk reference samples.

In this study, ATR-FTIR spectroscopy was used to obtain chemical profiles of a large set of 162 condoms, lubricants, oils, personal hygiene products and creams found on the Australian, New Zealand and Swiss markets. Visual inspection of the spectra determined that several qualitative chemical profiles could be readily identified based on the characteristic peaks from PDMS, PEG, glycerine and oily component. Subsequent chemometric analysis of the spectra dataset was then carried out using Principal Components Analysis, which revealed additional patterns in the data. The presentation will conclude with an evaluation of the forensic significance of the results obtained in this study.

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Hierarchically Porous Polymer Monoliths for Separation Science

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Size defines physical, chemical and biological properties of macromolecules such as proteins, polysaccharides, and synthetic polymers. Macromolecules separation and characterization are essential for industrial, clinical and research purposes. Size Exclusion Chromatography (SEC) is a liquid chromatographic technique in which analytes are separated by its size. The retention mechanism is quite simple, large analytes are excluded from the pores in the stationary phase and will elute first, while small analytes can enter the pores and will be retained (see **Figure 1**). SEC has been widely used not only for separation of analytes in a complex sample, but also for quantitative and qualitative analysis as it allows the determination of molecular weight of the analytes and its distribution.

However, current technologies for chromatographic size separations, based on particulate materials, have some drawbacks. In the search for higher efficiencies, smaller particles can be used as mesopores are more accessible for analytes, but that also implies high back pressures for analysis, which may cause stationary phase damage and bleeding as well as analytes decomposition[1].

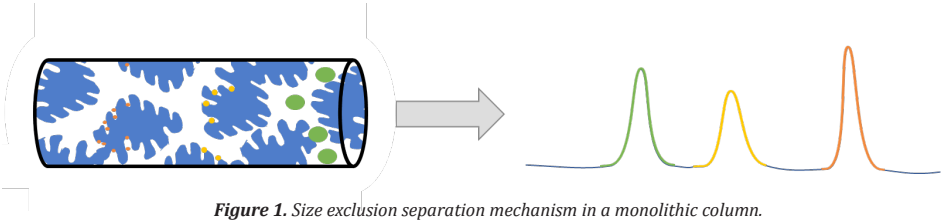

Figure 1. *Size exclusion separation mechanism in a monolithic column.*

Monoliths, porous polymers synthesized in one piece, can overcome current challenges with SEC columns, as they provide a network where pores are accessible for the analytes, column bleeding is avoided and convective flow is promoted trough the interconnected pore channels, achieving low back pressures. A monolithic column for SEC requires macropores (over 50nm) to achieve high permeabilities as well as mesopores (2-50nm) to provide the sites for inclusion/exclusion of the analytes. However, having both macro and mesopores at the same time have not been yet achieved for organic monoliths. Here, a novel way to obtain organic monoliths with a bimodal pore distribution is proposed. Reversible Addition-Fragmentation Chain Transfer (RAFT) polymerization is proposed to obtain mesopores and the addition of an inert polymer in the reaction mixture is proposed to achieve simultaneous macropores[2].

[1]Janco, M; Alexander IV, J. N; Bouvier, E. S; Morrison, D. Ultra-High Performance Size-Exclusion Chromatography of Synthetic Polymers: Demonstration of Capability. *Journal of Separation Science*, **2013**, 36, 2718-2727

[2]Saba, S. A; Mousavi, M. P; Buhlmann, P; Hillmyer, M. A. Hierarchically Porous Polymer Monoliths by Combining Controlled Macro- and Microphase Separation. *Journal of the American Chemical Society*, **2015**, 137, 8896-8899

Delivering Antibiotics Using Nanomeshes

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Antibiotic loaded polymer nanomeshes were fabricated by electrospinning a biocompatible polymer, polycaprolactone (PCL) with 12.5% w/w colistin. The antibiotic of choice, colistin, is regarded as the last-in-line therapeutic agent shown to be effective in the treatment of infections caused by multidrug-resistant gram-negative bacteria. The nanomeshes, prepared using previously optimised parameters, featured homogenous nanofibres without any visible defects upon the loading of colistin.[1] The nanomeshes act as scaffolds for the loaded antibiotic, making them suitable for drug delivery purposes. The effect of different pH and temperature conditions on the drug release from the nanomesh was studied. The antibiotic release under different pH conditions did not show significant differences. The nanomeshes exposed to different temperature conditions, however, displayed different release profiles. The highest sustained release of colistin occurred at a temperature of 4˚C for a 5 mg, 1.5 cm^2 nanomesh.

The release of colistin from the nanomeshes was quantified using a UV-spectrophotometric method which was validated in accordance with the guidelines provided by the International Council for Harmonization and National Association of Testing Authorities, Australia. This UV quantification method was optimised for the appropriate solubility and stability conditions for the polypeptide drug in terms of the pH, ionic strength and temperature which were determined to be a pH of 4, ionic strength of 0.025 M and temperature of 25˚C. Under these conditions the stability, specificity, linearity, accuracy and precision of the UV quantification method were all found to be in agreement with the recommended guidelines. These colistin loaded nanomeshes (Fig 1.) have the potential to be used for the specific delivery of antibiotics to the infection site in localised infections such as wounds.

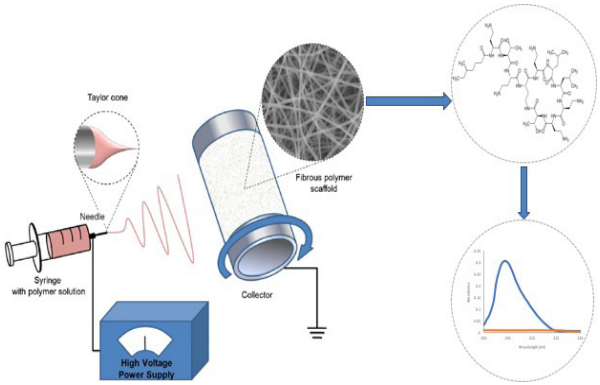

Figure 1. *Schematic of the electrospinning process for the fabrication of polymer nanomeshes loaded with colistin and the drug release measured using a validated UV-spectrophotometric method.[2]*

[1]Fuller, M.A.; Carey, A.; Whiley, H., Kurimoto, R., Ebara, M.; Köper, I. Nanoparticles in an antibiotic-loaded nanomesh for drug delivery. *RSC Advances,* **2019,** *9*(52), pp.30064-30070

[2]Rim, N.G.; Shin, C.S.; Shin, H. Current approaches to electrospun nanofibers for tissue engineering, *Biomedical Materials*, **2013**, 8(1), p.014102

Open-tubular Admicellar Electrochromatography of Charged Analytes

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Fundamental studies on the separation of cationic and anionic analytes in open-tubular admicellar electrochromatography (OT-AMEC) using cetyltrimethylammonium bromide (CTAB) and fused silica capillaries are presented. OT-AMEC was compared with open-tubular admicellar liquid chromatography (OT-AMLC) by running the two methods using the same mobile phases. The mobile phases were buffered at pH > 6 and contained a low concentration (above the critical surface aggregation concentration and below the critical micelle concentration) of CTAB. The stationary pseudophase of CTAB admicelles were formed at the solid surface and liquid interface inside the capillary by simply conditioning the capillary with the mobile phase. Separations were performed in a 30 cm (21.5 cm to UV detector) long and 50 µm inner diameter capillary, using low pressure (50 mbar) in OT-AMLC and high voltage (15 kV at negative polarity) in OT-AMEC. The appropriate equations for the experimental estimation of retention factor (*k*) values of analytes were discussed. For anionic analytes, *k* in OT-AMEC were carefully determined by considering the observed interaction between CTAB monomers and tested analytes. The calculated *k* for each analyte was found similar in OT-AMLC and OT-AMEC, although the mechanism of retention was not entirely different due to the contribution of electrophoresis in OT-AMEC. Studies on the addition of a typical (*i.e.*, acetonitrile) and atypical modifier (*i.e.*, nonyl-β-glucoside) into the mobile phase, and sample focusing with >10x improvement in peak height under isocratic conditions were also conducted[1].

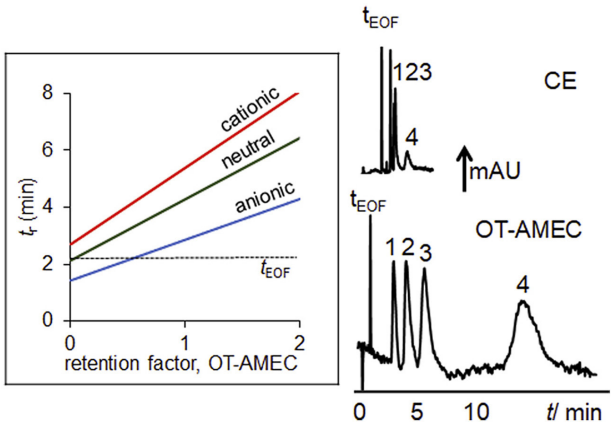

Figure 1. *(left) theoretical plot of t_r of analytes vs k in OT-AMEC; (right) comparison of separation of cationic analytes in CE vs OT-AMEC.*

[1]Yu, R.B.; Quirino, J.P., Open-tubular admicellar electrochromatography of charged analytes. Talanta, 2020, 208, 120401.

[†] Permanent address: Department of Pharmaceutical Chemistry, College of Pharmacy, University of the Philippines Manila, Corner Taft Avenue and Pedro Gil Street, Ermita 1000 Manila, Philippines

Biochemical effects following exposure to PFAS on model organisms

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Poly/ perfluoroalkyl substances (PFAS) are a diverse group of man-made, synthetic chemicals. They have been in use since the 1950s for a wide variety of industrial and commercial applications due to their unique properties. PFAS has since been detected globally in substrates and within tissues of organisms. This has led to strict restrictions on the use of PFAS and considerable concern over potential health impacts. Despite the growing concern, there is little to no detailed information that provides consistent evidence determining the levels PFAS exposure needs to be to cause adverse effects on humans and animal health. Therefore, more information on the mechanisms of PFAS toxicity and the doses at which such toxicity occurs is required. Such knowledge is important for managing PFAS properly, this is what the proposed project will provide, using a biochemical technique known as metabolomics.

Metabolomics is a large-scale study of small molecules, known as metabolites, that are the product of normal metabolism. The approach can deliver information on the interactions between organisms and their environments whilst also providing an overview of contaminant exposure. Changes in metabolites due to stress are often detected before other toxicological endpoints are apparent (i.e. reproduction, growth and mortality) (Figure 1).

This research aims to develop appropriate analytical methods for both metabolites and PFAS chemicals. The project will explore the biochemical changes induced by low doses of PFAS exposure on model organisms in controlled laboratory and semi-controlled field exposures to determine the metabolomic stress response. The next stage will be to sample species from the field to look for signature PFAS stress response previously identified. The project's objective is to identify the dose of PFAS exposure that causes adverse stress effects in ecosystems benefiting guidelines and applications worldwide.

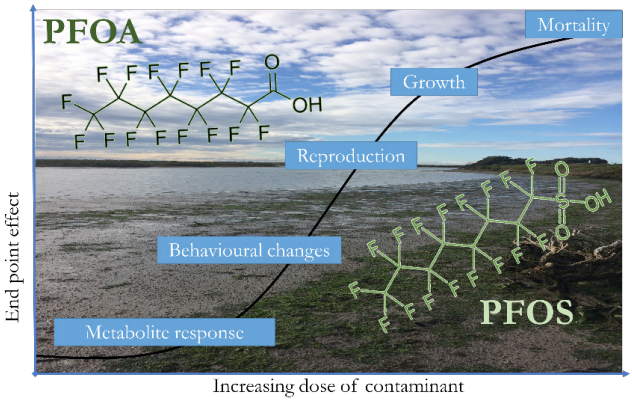

Figure 1. *Endpoint detection, with increasing concentration of PFAS compounds. This infographic highlights the sensitive initial detection of metabolomic endpoints compared to other more common endpoints*

Development of Spectroscopic Protocols to Study the Relationship between Epicuticular Surface Chemistry and Flora

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With an increasing global population and rising temperatures associated with climate change it is important to monitor and mitigate the effects of environmental stress on both native flora and agricultural crops.

The wax coating on the surface of plant leaves (epicuticular waxes) holds important physiological functions to protect against environmental stress, for example; minimising water loss, UV protection, protection from disease, as well as acting as an anti-feedent.[1] Studying the composition and distribution of epicuticular waxes on the surface of plant leaves can provide valuable insight into plant fitness and the presence of environmental stressors. Current methods to study plant waxes require extraction of the wax from the leaf surface.[2] This approach reveals substantial insight into chemical composition of plant waxes; but, destroys valuable information relating to the spatial distribution of waxes on the leaf surface. The development of analytical methods that can directly image epicuticular waxes across the surface of plant leaves is therefore, sought after to complement existing bulk analyses.

I will present my initial work on the development, adaptation and validation of direct spectroscopic imaging methods, specifically Fourier transform infrared (FTIR) and Synchrotron ATR-IR spectroscopy[3], and FTIR-reflectance spectroscopy, to enable the *in situ* and *in vivo* investigation of epicuticular wax distribution on the surface of plant leaves. This research hopes to develop the technical methodology that can then be used by the agricultural and environmental industry sectors to help monitor changes in plant health and fitness of native flora populations and crops.

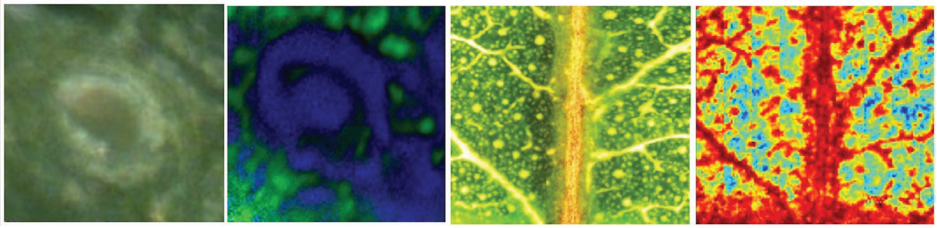

Figure 1. *Synchrotron ATR-IR (Left) and FTIR images (Right) with complementary visual images.*

[1]Buschhaus, C; Herz, H; Jetter, R; Chemical Composition of the Epicuticular and Intracuticular Wax Layers on Adaxial Sides of Rosa canina Leaves. Annals of Botany. 2007; 100(7):1557-1564. DOI:10.1093/aob/mcm255.

[2]Lara, I; Belge, B; Goulao, LF. A Focus on the Biosynthesis and Composition of Cuticle in Fruits. Journal of Agricultural and Food Chemistry. 2015; 63(16):4005-4019. DOI:10.1021/acs.jafc.5b00013.

[3]Vongsvivut, J; Pérez-Guaita, D; Wood, B; Heraud, P & Khambatta, K. et al. (2019). Synchrotron macro ATR-FTIR microspectroscopy for high-resolution chemical mapping of single cells. The Analyst, 144(10), 3226-3238. DOI: 10.1039/c8an01543k

Development of a polymer inclusion membrane for the separation of Co(II) from Ni(II)

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The separation of Co(II) and Ni(II) remains a challenge in industry, mainly because the chemical and physical properties of these elements are very similar. The most efficient method for the separation of Co(II) and Ni(II) reported so far involves the use of Aliquat 336 as an anionic-exchanger for the selective extraction of Co(II) as a chlorocomplex, taking advantage of the inability of Ni(II) to form such complexes.[1] However, a very high concentration of chloride (~7 mol L^{-1} HCL or LiCl) is necessary, which in a large scale industrial separation can either cause safety issues or equipment damage. Moreover, solvent extraction, which is the most commonly used separation method in industry, involves the use of large amounts of toxic, volatile and flammable diluents which are often expensive and dangerous.[2]

With the aim of developing a greener and safer alternative for the separation of Co(II) from Ni(II), the ionic liquids trihexyltetradecylphosphonium bis(2,4,4-trimethylpentyl) phosphinate (Cyphos IL 104) and trihexyltetradecylphosphonium chloride[3] (Cyphos IL 101) were studied for their suitability as the extractants in a polymer inclusion membrane (PIM). PIMs are extracting polymeric membranes which are diluent free. The mechanism of extraction of Co(II) into the two Cyphos-based PIMs was studied. The results indicated that, in the presence of a low concentration of thiocyanate, Co(II) was extracted into the Cyphos IL104-based PIMs as $Co(SCN)_4^{2-}$ and Co-phosphinate while as $Co(SCN)_4^{2-}$ only into the PIMs containing Cyphos IL 101 as the extractant. The PIMs were applied to solutions containing both Co(II) and Ni(II), and good selectivity towards Co(II) was observed.

[1]Paimin, R. and R.W. Cattrall, The extraction of cobalt(II) from hydrochloric-acid solutions by Aliquat 336 dissolved in chloroform. *Australian Journal of Chemistry*, **1983**. 36(5): p. 1017-1020.

[2]Jonsson, J.A. and L. Mathiasson, Liquid membrane extraction in analytical sample preparation I. Principles. *Trac-Trends in Analytical Chemistry*, **1999**. 18(5): p. 318-325.

[3]Rybka, P. and M. Regel-Rosocka, Nickel(II) and Cobalt(II) Extraction from chloride solutions with quaternary phosphonium salts. *Separation Science and Technology*, **2012**. 47(9): p. 1296-1302.

For Research Use Only: Quality Testing Fitness Drugs Purchased Online

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The use of performance and image enhancing drugs (PIED) in the community is increasingly apparent. The type of drugs taken are evolving from anabolic-androgenic steroids to selective androgen receptor modulators and metabolic modulators. The toxicity and drug-drug interactions of these newer drugs are unknown. However, they are easily accessible online.[1]

A survey of 111 liquid PIED products designed for oral administration was conducted by liquid chromatography-high resolution tandem mass spectrometry and gas chromatography-tandem mass spectrometry validated to assess the contamination and concentration of the PIED products. This revealed that while most products correctly labelled the main active pharmaceutical ingredient, few correctly reported its concentration, and almost half of the products studied were contaminated with one or more other PIEDs.

These results were compared against the presentation of the products on their websites and their labels, to assess the current status of PIED products on the market since their purchase in 2017.

This research shows that PIED products purchased online are often misrepresented by their label and are fraught with contamination with other PIEDs. The health and safety of people using these drugs are at risk due to the quality issues with these products. These results will enable PIED users to make informed choices, and highlight the urgency for better regulation of these products.

1. Brennan, B. P.; Kanayama, G.; Pope Jr., H. G., Performance-Enhancing Drugs on the Web: A Growing Public-Health Issue. *Am. J. Addict.* **2013,** *22* (2), 158-161.

Continuous particulate removal for capillary electrophoresis applications

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Water quality has become a global issue of concern as human populations grow, industrial and agricultural activities expand, and climate change threatens to cause major alterations to the hydrological cycle. Detection of nutrients in aquatic systems is crucial in understanding water quality. Portable analytical devices have been developed in recent decades to detect these nutrients on site and avoid the problem of sample loss, time consumption and transport logistics when analysed off site. However, most of the portable systems developed include membrane filters which need to be changed regularly, thus making the possibility of an autonomous analysis difficult. Here, we developed a sample preparation micro device, without a membrane filter, that is able to remove particulate matter above 1 µm size continuously from a flowing water sample for six weeks. This device was incorporated into a portable homemade capillary electrophoresis system with a C4D detector. Separation and identification of anions such as Cl^-. NO_3^-, ClO_4^- and SO_4^{2-} in a simulated water sample containing particulate matter up to 100 µm was successfully performed. Limit of detection (LOD) values of 0.9 to 2 ppm of the anions were obtained. The developed device is simple to fabricate, low cost, easy to operate and can work autonomously.

[1]Gray, S.; Hanrahan, G.; McKelvie, I.; Tappin, A.; Tse, F.; Worsfold, P. Flow Analysis Techniques for Spatial and Temporal Measurement of Nutrients in Aquatic Systems. Environ. Chem. 2006, 3 (1), 3–18.

[2]Alhusban, A. A.; Breadmore, M. C.; Gueven, N.; Guijt, R. M. Capillary Electrophoresis for Automated On-Line Monitoring of Suspension Cultures: Correlating Cell Density, Nutrients and Metabolites in near Real-Time. Anal. Chim. Acta 2016, 920, 94–101.

[3]Gaudry, A. J.; Guijt, R. M.; Macka, M.; Hutchinson, J. P.; Johns, C.; Hilder, E. F.; Dicinoski, G. W.; Nesterenko, P. N.; Haddad, P. R.; Breadmore, M. C. On-Line Simultaneous and Rapid Separation of Anions and Cations from a Single Sample Using Dual-Capillary Sequential Injection-Capillary Electrophoresis. Anal. Chim. Acta 2013, 781, 80–87.

Human Decomposition Fluids and Clothing Degradation

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The discovery of human remains is often concomitant with the recovery of clothing material. Traditionally, the study of clothing textiles has been a focus area of archaeological and anthropological practices, providing fundamental insight to the history of humans all over the globe[1,2]. In a forensic context, textiles can be a valuable source of physical evidence or a host for biological fluids or DNA[3], giving additional information to law enforcement agents during crime events.

The aim of this study was to use attenuated total reflectance – Fourier transform infrared (ATR-FTIR) spectroscopy to indirectly detect and monitor changes in the decomposition chemistry of human remains. This technique is non-destructive, and it enables the class of molecules encountered during decomposition (primarily lipids and proteins) to be investigated and monitored over time. This study was conducted at the Australian Facility for Taphonomic Experimental Research (AFTER) and reports the findings of biological fluids collected in clothing retrieved from decomposing human remains donated through the UTS Body Donation Program. A preliminary examination of the clothing textiles revealed that lipids and proteins, and their corresponding by-products could be identified and linked to the stages of decomposition.

These results demonstrate that investigating clothing materials, associated with human remains, can aid in the vital estimation of time since death. Subsequently, this knowledge can provide victims' families with closure and a sense of justice by understanding the fate of their loved ones.

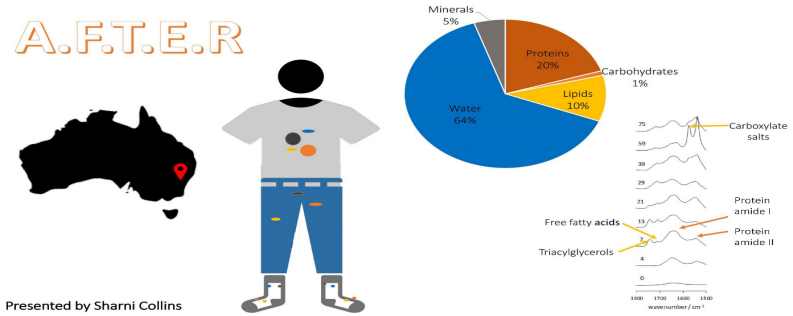

Figure 1. *Graphical overview of the investigation of human decomposition fluid collected in clothing in a temperate Australia environment*

[1]Taupin, J & Cwiklik, C. Scientific Protocols for Forensic Examination of Clothing, **2011**, Taylor and Francis; Boca Raton.
[2]Bier, C & Dusenbury, M, Textiles. In: Pearsall, D.M. (ed.), *Encyclopaedia of Archaeology*, **2008,** Elsevier; Amsterdam, 2119-2125.
[3]Van Amber, R. Apparel and Household Textiles and Their Role in Forensics. In: Carr, D (ed.), *Forensic Textile Science*, **2019**, Elsevier Science & Technology.

POSTER PRESENTATION ABSTRACTS

SUMMARY

1 **Kelly-Anne Stark** Characterisation of Xylitol Pentanitrate

2 **Sorour Shahbazi** Detection of Latent Fingermarks using Luminescent Core-Shell Quantum Dots in Aqueous Solution

3 **John Adeola Adegoke** Quantification and detection of malaria infection in Plasmodium infected red blood cells using miniature NIR spectrometer

4 **Meg Willans** Investigating diversity in polymer-based identification cards using ATR-FTIR spectroscopy and chemometrics

5 **Joshua D'Uva** Preliminary investigations into the source attribution of party sparklers using trace elemental analysis and chemometrics

6 **Natalie Uhlikova** Measuring Total Inorganic Nitrogen (TIN) by Microfluidic Paper-based Analytical Devices (μPADs)

7 **Samantha Pandelus** Identification of radionuclide uptake mechanisms by native flora in the vicinity of uranium mines in arid South Australia

8 **Tristan Fraser** Shinning A Light on The Photolysis of Tattoo Pigments

9 **James Chan** Isolation of Malaria Parasites using Polymer Monoliths

10 **Simone Madaras** Towards elucidation of the reaction mechanism between lawsone and amino acids

11 **Charles Croft** The fabrication of Micro Polymer Inclusion Beads (μPIBs) using green solvents

Characterisation of Xylitol Pentanitrate

Kelly-Anne S. Stark[1], Dr. Mark Fitzgerald[2], Dr Chad Prior[2], Prof. Claire E. Lenehan[1], Prof. K. Paul Kirkbride[1]

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Nitrate ester explosives are well-known for their use as improvised explosives and in the military industry worldwide. Some of the well-known nitrate esters, such as nitroglycerin (NG), erythritol tetranitrate (ETN), and pentaerythritol tetranitrate (PETN) have been widely studied for their explosive performance, and physical and chemical properties. Characterisation data for these compounds have been published using a wide variety of analytical techniques, such as gas chromatography-mass spectrometry (GC-MS), infrared spectroscopy (IR) and Raman.

A lesser known nitrate ester, xylitol pentanitrate (XPN), was first isolated as a crystalline product in 1960 and is similar in structure to NG and ETN.[1] Due to the recent prevalence of its precursor, xylitol, as a sugar alternative and the simplistic method of nitration, it is possible to encounter XPN as an improvised explosive. Although literature references for NG, ETN and PETN are prolific, there are few mentions of XPN. A partnership between Flinders University and the Defence Science and Technology Group has revealed the crystal structure and theoretical explosive performance of XPN.[2] However, there is still a gap in literature in regards to the characterisation of XPN. This information is crucial to inform the practices of first responders, forensic laboratories and the military.

Characterisation data, such as GC-MS, liquid chromatography (LC), electrospray ionisation-mass spectrometry (ESI-MS), IR, Raman and nuclear magnetic resonance spectroscopy (NMR) have been collected for XPN and compared to data for other nitrate ester explosives.

[1]Wright, I. G.; Hayward, L. D., The Pentitol Pentanitrates. *Can. J. Chem.* **1960,** *38*, 316-319

[2]Stark, K. A. S.; Alvino, J. F.; Kirkbride, K. P.; Sumby, C. J.; Metha, G. F.; Lenehan, C. E.; Fitzgerald, M.; Wall, C.; Mitchell, M.; Prior, C., Crystal Structure, Sensitiveness and Theoretical Explosive Performance of Xylitol Pentanitrate (XPN. *Propellants Explos. Pyrotech.* **2019,** *44*, 541-549

Detection of Latent Fingermarks using Luminescent Core-Shell Quantum Dots in Aqueous Solution

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The detection of latent fingermarks for forensic science can be considered to be a form of chemical imaging, and in a similar fashion to other areas of analytical science there is demand for ever more sensitive techniques. There has been significant interest in recent years into the use of luminescent nanoparticles for the detection of latent fingermarks, in order to negate the interferences exhibited by dark, multi-coloured or patterned substrates. Here we present our recent studies into the use of aqueous solutions of core-shell quantum dots to detect latent fingermarks on non-porous surfaces. A simple, fast, green and inexpensive nanoparticle-based technique was developed to overcome complications associated with current methods such as multiple step, lengthy procedures, expensive reagents, high background and toxicity. This novel approach involved the synthesis of red-near infrared luminescent and heavy-metal-free Cu-In-S/ZnS quantum dots, which were subsequently applied to the detection of latent fingermarks on a range of surfaces (Figure 1).

Following previous studies,[1] a mixture of copper, indium and sulfur precursors in water was heated at low temperatures (<100˚C) to produce the Cu-In-S core, and then a zinc precursor was added to form the shell around the cores. N-acetylcysteine was added as a post-treatment step to the solution to enhance stability, increase safety, and heighten interactions between quantum dots and lipids and amino acids present in fingermark secretions. The coated quantum dots were applied to the successful development of latent fingermarks deposited on a variety of non-porous surfaces including the sticky side of adhesive tape as a common and challenging substrate found at crime scenes.

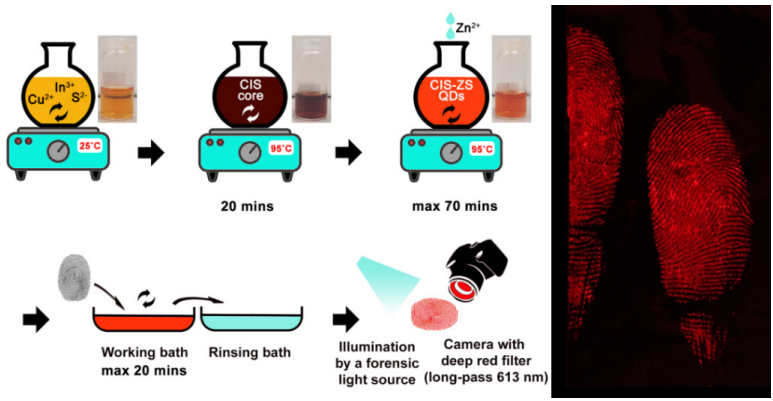

Figure 1. *Synthesis and application of Cu-In-S/ZnS quantum dots for the detection of latent fingermarks*

Raevskaya, A et al. Non-stoichiometric Cu–In–S@ZnS nanoparticles produced in aqueous solutions as light harvesters for liquid-junction photoelectrochemical solar cells. *RSC Advances*, **2016**, 6, 100145-100157.

Quantification and detection of malaria infection in *Plasmodium* infected red blood cells using miniature NIR spectrometer.

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New diagnostics which are sensitive to low parasitemia, easy to use in field settings and affordable for the developing world are urgently required to meet the World Health Organization's objective of reducing malaria cases and related life losses by at least 90% globally on or before 2030. In this study, ultra-cheap miniaturized near infrared spectrophotometer was used to first characterize the major biomarkers of malaria infection including haemozoin, lipid and haemoglobin. Secondly, in combination with chemometrics applied to detect and quantify malaria infection *in vitro* from isolated dried red blood cells using a fingerpick volume (15-25µl) of blood down to 0.5% parasitemia for the first time. No sample preparation was involved except for the centrifugation steps used in obtaining isolated RBCs and a single spectrum was acquired within two seconds consequently reducing the analysis time drastically and eliminating the complicated laboratory routine associated with current methods. This technique relies on detecting the distinct changes associated with the NIR spectroscopic signatures of the associated biomarkers in the overtone and combination region showing good separation and parasitemia prediction with PCA and PLS-R respectively. This work demonstrates the potential of the low cost ultra-portable NIR device to diagnose malaria, future research using wet blood samples and development of robust calibration model will undoubtedly set a pace for a rapid non-invasive testing of malaria infections.

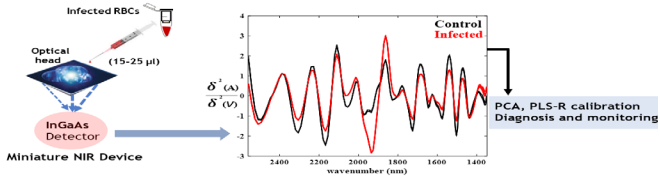

Figure 1: *Proposed straight-forward approach for malaria diagnosis using ultra-portable NIR spectrometer*

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Investigating diversity in polymer-based identification cards using ATR-FTIR spectroscopy and chemometrics

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Polymer cards such as driver's licences are used extensively as identification documents, and as such are common targets for counterfeit production. A rapid screening method for counterfeit cards would be useful in "front line" situations where personnel may have limited document examination training, or as a complementary approach to current document examination processes. Attenuated Total Reflectance - Fourier Transform Infrared spectroscopy (ATR-FTIR) was chosen to characterise the composition of the cards, as it provides chemical specificity, is non-destructive, and can be made readily portable.

The approach for this study needed to be non-destructive, reproducible, produce spectra representative of all layers in the card, and be operationally simple to perform. Preliminary work involved manually holding the cards onto the ATR crystal, leading to concerns regarding the reproducibility of the spectra[1]. A custom-made jig was subsequently developed and found to give acceptable reproducibility, whilst also making collection of spectra easier to perform.

Spectra were then collected from a population of Australian and international polymer cards consisting of polyvinylchloride (PVC) or polycarbonate (PC). Principal component analysis was applied to explore the chemical diversity in the population. The significance of these results will be discussed in the context of potential forensic document examination applications.

McGann, J; Sauzier, G; Hackett, MJ; Lewis, SW; McGinn, J; Trubshoe, T; et al. ATR-FTIR spectroscopic studies of polymer-based identification cards. *ChemRxiv*, **2019**, Available at: doi.org/10.26434/chemrxiv.7593032.v1

Preliminary investigations into the source attribution of party sparklers using trace elemental analysis and chemometrics

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Inorganic based homemade explosives (HMEs) are frequently used in explosive attacks as the precursors are often readily available and easily accessible. Whilst many inorganic substances present within explosive residue can be detected, there has been little prior attempt to identify their origin as well as distinguish one source of the same substance from another. Party sparklers are commonly used as an initiator or as the primary oxidising agent within HMEs. They are easily obtainable, inexpensive and are rich in nitrate salts such as barium or potassium nitrate. The aim of this study is to demonstrate the potential of using trace elemental profiling coupled with chemometric and other statistical techniques to link a variety of different sparklers to their origin. A similar methodology has been performed on other common inorganic precursors, however sparklers are yet to be explored.[1,2]

A series of analyses using Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) were first performed on one type of sparkler to determine the most appropriate extraction method. Extracting the ground up sparkler residue in 10% nitric acid for 4 hours was found to give the most reliable quantification. ICP-MS was then used to determine the concentration of 56 elements in 48 samples from 8 unique sparklers. ANOVA based feature selection and degree of class separation was used to develop an elemental profile which consists of the detected elements that give the greatest amount of separation between each class. The collected data was then analysed using Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA), to explore whether the sparkler samples classified into distinct groupings.

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Measuring Total Inorganic Nitrogen by Microfluidic Paper-based Analytical Devices (μPADs)

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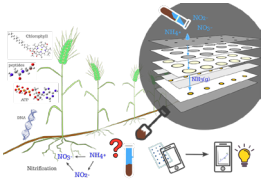
Nitrogen is an essential plant macronutrient. Being part of peptides, nucleic acids, ATP and chlorophyll makes it the second most abundant element in plant cells[1], accounting for 3-4% of plant above-ground tissues.[2,3] In soils of temperate or subtropical climate, plants uptake nitrogen throughout roots predominantly in the form of nitrate, and to a lesser extent as ammonium or as soluble organic nitrogen (amino acids).[7,8] These forms of nitrogen are termed as plant-available nitrogen.[9]

A sufficient supply of plant-available nitrogen throughout the crop growing cycle is crucial for the plants' healthy development and high content of grain protein. Ammonium phosphate and urea are amongst the most commonly applied fertilisers in Australia. Reports from the Australia Bureau of Statistics state that in 2014-2015, approximately 108 kg of fertilisers were applied per hectare of agricultural land, of which 66% is attributed to nitrogen-based fertilisers alone.[10] Fertilisation is beneficial for achieving high crop yields, although the excess not taken by crops poses a danger to the environment. Agricultural runoff rich in nutrients leads to eutrophication causing a significant damage to aquatic ecosystems.



To maintain sufficient nutrition for plants and to prevent environmental damage, it is vital to accurately monitor the levels of nitrogen in soils. An ideal analytical procedure should be fast, low cost, portable, feasible to perform on-site, and reliable. Paper-based microfluidic analytical devices (μPADs) meet many of these criteria, which is why μPADs are attractive analytical tools worth of further investigation for soil nutrient analysis. Nitrate reducing agents utilised in common detection methods are zinc[21], cadmium[22], zinc-cadmium[23], copperised cadmium[24,25] in column form, enzymes[26] and Devarda alloy. The study intends to incorporate these into a μPAD and examine its suitability for measuring total inorganic nitrogen.

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Identification of radionuclide uptake mechanisms by native flora in the vicinity of uranium mines in arid South Australia

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Environmental risk assessments for radiological contamination follow internationally accepted methods including use of the Environmental Risk from Ionising Contaminants: Assessment and Management (ERICA) tool. Concentration ratios are an essential input for these models. However, the available international input data are primarily from temperate Europe and North America, and may not apply in arid conditions. It has previously been shown that Australian native species accumulate higher amounts of radionuclides from their environment when compared to similar species from other climates.[1,2] This research aims to develop a concentration ratio dataset relevant for U and Th series radionuclides in arid and semi-arid conditions. Two uranium mines are the focus of the research. Olympic Dam (BHP, South Australia) is the largest mine in SA, utilising underground mining with the ore being processed on site. Beverley (Heathgate, South Australia) is an in-situ recovery uranium mine. The two mines offer different conditions when considering the natural background radiation and the type of mining operations. Samples of flora and surrounding soil have been collected and concentration ratio data has been developed. Analysis has included gamma-ray spectroscopy, neutron activation analysis, alpha-particle spectroscopy and inductively coupled plasma mass spectrometry.

The Diffusive Gradients in Thin-film (DGT) technique has been applied to determine the bioavailability of radionuclides and metals within the soil for uptake within native flora. Alpha track analysis, using a nuclear emulsion gel layer, has been used to identify radionuclide accumulation and spatially-resolve its location within structures of the leaves. Overall this research provides a better understanding of the behaviour of radionuclides in an arid environment and provides data on the mechanisms of radionuclide uptake in flora. It augments existing international data for use in models in Australia and other localities with similar arid environments.

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Shinning A Light on The Photolysis of Tatt Pigments

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Tattoos are a rising trend, especially amongst the younger generations, despite concerns about dangers of the tattoo ink components.[1] In the past, tattoo inks used inorganic compounds, such as cinnabar (mercury sulphide), as pigments however these compounds have been mostly been replaced with organic pigments to reduce health risks and improve lifespan.[2, 3] In Australia, regulation concerning the composition of tattoo inks is limited and refers to the European Council ResAP(2008) which outlines a number of components that should not be permitted in tattoo inks, primarily metal salts and the azo based organic pigment Red 22. Recent research has shown that azo based pigments will degrade, into potentially hazardous compounds, when irradiated with UV and visible light., This includes Red 22 along with other yellow, orange and red azo based pigments that are commonly used in tattoo inks.[4-6] However, the literature rarely mentions the pigments used to produce green, blue and purple tattoo inks. These are usually formed from phthalocyanine based, and polycyclic, pigments.

This project is investigating the stability and chemistry of these blue, green and purple pigments when irradiated by UV and Visible light. The irradiation of the tattoo inks will be performed by exposure to solar light and laser light to mimic natural fading from sun exposure and tattoo laser removal, respectively. The irradiated sample will then be analysed using techniques such as mass spectrometry and nuclear magnetic resonance imaging to identify the photolytic products. The results are intended to aid in the formation of regulations for the composition of tattoo inks and laser removal protocols.

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Isolation of Malaria Parasite using Polymer Monoliths

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Malaria disease, a global health burden that affects millions of lives each year, is primarily caused by *Plasmodium falciparum*[1]. Many discoveries and extensive studies were made since the introduction of the in-vitro culture system for malaria parasites. However, there are still much more to learn about the disease. Challenges remain in finding a straightforward method to isolate ring-stage malaria parasites for research and diagnostic purposes[2]. The aims for this study were; firstly, to develop a highly portable, economical and user-friendly device, secondly, to investigate the selectivity of using polymer monoliths to isolate different maturation stages of *P. falciparum.*

Here, an approach of using poly(HEMA-co-EDMA) polymer monolith prepared in a pipette tip format, that has been successfully used for separation of plasma from whole blood was described. Additionally, the porous morphology of the polymer monolith was chemically modified and then applied for the separation of different maturation stages of *P. falciparum*.

The principle of separation here was based on the red blood cell membrane deformability[3]. Studies had shown that the red blood cell membrane loses its ability to deform when it became infected by *P. falciparum* (**Figure 1**). The red blood cell membrane ability to deform decreases as the parasite matures.

Overall, the findings showed that isolation of *P. falciparum* was successful using polymer monoliths in pipette tip format. Additionally, a highly portable, economical and straightforward method of isolating malaria parasites has been made. Furthermore, polymer monoliths can be upscaled to a larger version for higher throughput and shorter turnaround time. In addition, this approach is label-free and does not require additional additives that may hamper the growth of the parasites.

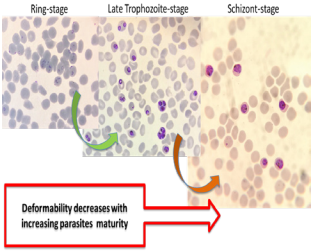

Figure 1. *Different stages of Plasmodium falciparum infected red blood cells. Red blood cells membrane deformability decreases as parasite maturation increases.*

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Towards elucidation of the reaction mechanism between lawsone and amino acids

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Naphthoquinones, such as lawsone (2-hydroxy-1,4-naphthoquinone), are compounds of interest due to their antibacterial, anti-cancer, analgesic, and anti-inflammatory properties[1]. They are commonly used as scaffolds to form derivatives and analogues that may exhibit more enhanced properties. Recent studies reported the use of lawsone as a reagent to elucidate latent fingermarks based on the presence of fluorescent red/purple marks that were left on paper substrates[2]. The researchers suggested that the fluorescent red product would form following a mechanism similar to the ninhydrin reaction with amino acids, and that the final product would comprise a lawsone dimer with a central amine linker.

This work establishes that the structure of the red fluorescent product, shown in Figure 1, is not that as previously suggested. Instead, the dimeric structure incorporates two lawsone molecules connected via an amine linker and a carbon linker. Research examining the reaction mechanism by which the dimer is formed has suggested that the amine is incorporated into the structure via direct substitution of the amino acid to the lawsone molecule at the -OH position. We have demonstrated that the carbon linker originates from the alcohol used as solvent, however the mechanism is not immediately obvious. Studies into possible intermediates via which the product is formed are presented.

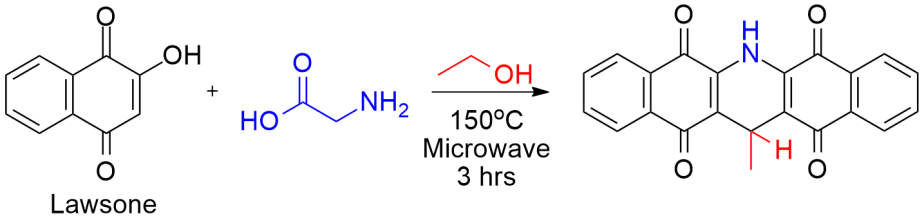

Figure 1. *Identified structure of compound resulting from the reaction between lawsone and amino acids.*

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The fabrication of Micro Polymer Inclusion Beads (μPIBs) using green solvents

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Green chemistry has become a prominent area of research in the last decade due to the large amounts of environmentally harmful chemicals being used in areas, such as, separation science and analytical chemistry. Therefore, the development of solvent-free alternatives for separation methods such as solvent extraction (SX) (a method which requires large volumes of toxic and harmful organic solvents) is considerable interest. Separation based on polymer inclusion membranes (PIMs) has proven to be highly suitable as an alternative to SX, not only for analytical purposes but also for the clean-up or separation of a wide range of chemical species (e.g., metal ions, small organic compounds)[1].

Micro polymer inclusion beads (μPIBs) are a newly developed form of polymer inclusion materials with a different range of applications that have not been previously available to PIMs. μPIBs have higher versatility due to their physical shape and higher surface area. However, the current method for manufacturing mPIBs requires dissolving the reagents in tetrahydrofuran (THF), which is a harmful and non-sustainable solvent.

This project thus aims to investigate whether the green solvents, ethyl acetate and Cyrene™, are suitable for the fabrication of poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP)- and cellulose triacetate (CTA)-based μPIBs, respectively. The flow conditions of the microfluidic system[2] (i.e. flow rate and tube diameter) were reoptimized and at appropriate flow rates, desired size and uniformity of μPIBs were obtained as illustrated in Figure 1.

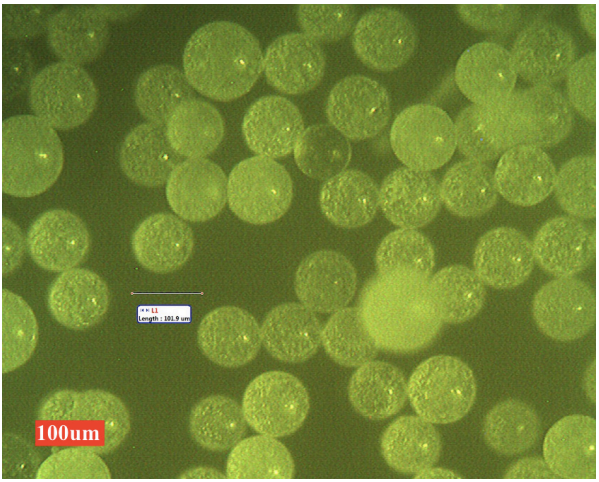

Figure 1. *Uniform μPIBs fabricated with ethyl acetate as the green solvent (100 μm in diameter). Experimental conditions: produced at 100 μL min^{-1} of 2 wt% PVDF-HFP solution and 3 mL min^{-1} of 15 wt% NaCl.*

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Notes