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Abstracts (Oral Presentation)

Monday 2nd December

(Section 1 & 2)

3-D Printed Microfluidic Devices for In-Field Colorimetric Measurement of Soil Macronutrients

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To sustain soil fertility for crops cultivation, intervention by fertilizer application needs to be performed expeditiously. Current analysis of soil Nitrate are laboratory-based, though reliable; are both time consuming and costly. Thus the need for a low-cost, in-field device that provides accurate measurements in real time. The application of 3-D printed microfluidic devices offers opportunities with the potential to fulfill these requirements for agriculture.

A dual layered 3-D printed microfluidic device was developed using a glass-like “simulated PMMA material” to measure Nitrate in soil via colorimetry using the Griess Reagent. The device includes self-calibration as a core requirement to improve measurement accuracy by using standard addition to eliminate variances in soil properties and ambient lighting. The flow processes involve, injecting a soil sample solution into the device where it traverses through a network of modified bifurcating channels, and then distributed uniformly into multiple independent channels . The distributed solutions would flow through the modified Tesla micro-mixer valves that serve as both mixing and calibrant immobilising features. Finally, the sample solution reaches the colorimetric detection zone and reacts with the pre-impregnated Griess reagent to produce a colorimetric reaction that will be quantified using a smartphone software application. The highlighted features in the design of the detection zone are the reagent immobilisation pockets, multi-depth pathlengths to enable colorimetric measurements for different saturations and an upward slope that is used to entrap air bubbles at the uppermost corner.

The capability of this design to produce a distinct colour gradient denoting standard addition in the detection zones has been successfully demonstrated to industrial representatives, who were also provided with hands-on experience in using this device. Satisfactory feedback was received especially on the ergonomics and ease of use. use. Since then, our developments have been focused on evaluating the accuracy and repeatability of the device for Nitrate measurements. A filtered 1:2 ½ soil: water ratio suspension for four different soil samples were compared for cuvettes as a reference with the microfluidic devices. Subsequent RGB colorimetric analysis was carried out using a camera and the photographic image was quantified using an image processing software “ImageJ”. The results were promising as the measurements were nearly comparable to the concentrations measured in cuvettes as shown in the graph. Hence, indicating a step in the right direction for more in-depth evaluations.

High-resolution 3D printing and applications: Development of a microfluidic device for the detection of nitrate in water

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The increasing accessibility of high-resolution 3D printers has cemented 3D printing as a versatile method for small form factor fabrication. This is particularly evident in the field of microfluidics, where highly complex and minute devices can be realised within hours. High-resolution stereolithography (SLA) 3D printing eliminates many of the problems previously associated with the fabrication of microfluidic devices both by other 3D printing methods and traditional manufacturing methods. [1]

Microfluidics is a key component of micro total analysis systems (µTAS) whose small scale allows for portability, quicker analysis response times and reduced reagent and sample use leading to lower costs. Here we will present a brief review of different 3D printing methods, and the development of a 3D printed microfluidic colorimetric monitoring device for the detection of nitrate in water. Nitrate levels are of interest as a marker of water health as higher concentrations are not only detrimental to aquatic life but also humans, leading to methemoglobinemia, particularly in infants. [2]

The developed microfluidic chip is a complex multilayered design with integrated fluidic splitters, mixers and gradient generator and has a range of absorbance path lengths from 0.5 mm to 4mm. This path length range aims to avoid issues with both colour saturation (for high analyte concentrations) and faint colour signal (for low analyte concentrations) and so increases the linear range of the device.

Nitrite is detected at µM concentration using the Griess reaction. Colorimetric detection is semi-automated and performed by the image processing of a photograph taken by a mobile phone camera and analysed for intensity. The sample is quantified via standard addition. This chip will be integrated into a µTAS unit and deployed for in-field environmental monitoring. Further, other nutrients could be assayed with the same chip by changing the reagents used.

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Photodegradation of tattoo pigments: Assessment of degradation product toxicity

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Tattoos are increasingly popular; however, a significant part of the tattooed community has second thoughts and regret their tattoo. Consequently, laser tattoo removal therapy has seen an increase in demand over the years. This practice is relatively unregulated in Australia. Prior research indicates the photodegradation of tattoo pigments with laser therapy can produce potentially carcinogenic and acutely toxic compounds [1]. Therefore, identifying these degradation products is essential for creating safer guidelines for laser tattoo removal, and improving safer patient outcomes.

This research examined the ex-situ photodegradation of a suite of organic pigments found in tattoo inks. Pigments were subject to either i) photodegradation using replicated laser removal conditions a removalist would use during removal, or ii) pyrolysis-mediated thermal degradation method to replicate the thermal cleavage of pigment bonds during laser removal.

The degradation products generated upon laser removal were examined using gas chromatography – mass spectrometry (GCMS). A range of potentially harmful compounds were identified, including benzene. We are now working with laser tattoo removalists and individuals to examine the exposure of these compounds (and their potential metabolites through the analysis of human urine collected before and after the removal procedure. The results from this research will provide insights into what types of degradation products someone might be exposed to during laser removal therapy, as well as how the body metabolises and eliminates these foreign chemicals. This research will aid in laser removal strategies and help in the regulations of removal procedures.

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Unravelling Key Aroma Compounds in (shelf-stable ready-to-eat) Butter Chicken

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Convenience foods are becoming increasingly popular. Ready-to-eat meals can be considered as one such convenient food option. Among the factors that influence consumer preferences, flavour plays a pivotal role. Research indicates that 72% of Australian consumers rank flavour as the number one driving factor influencing their purchasing decisions [1]. Therefore, understanding how flavour changes during storage in shelf stable ready-to-eat meals is essential for product development and processing optimisation.

In this study, flavour changes in butter chicken will be examined over time. Flavour extraction was performed using automated solvent assisted flavour evaporation technique with modified glassware [2]. The chemical fingerprint of the flavour extract was analysed using GC–TOFMS (Gas Chromatography-Time of Flight Mass Spectrometry), allowing for detailed identification of the chemical compounds present. Additionally, aroma compounds were identified using GCMS–O (Gas Chromatography-Mass Spectrometry-Olfactometry) and Aroma Extract Dilution Analysis (AEDA) was conducted to identify the key aroma compounds that contribute significantly to the overall aroma profile of butter chicken. The GCMS–O analysis revealed approximately 50 aroma compounds present in the butter chicken flavour extract. Among these, compounds with higher Flavour Dilution (FD) factors were selected as the key compounds that are most responsible for the overall aroma of butter chicken. Ultimately, these findings are critical in developing shelf-stable ready to eat meals ensuring optimal flavour throughout the storage.

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SUITABILITY OF POST-CONSUMER RECYCLED PLASTIC AS A FOOD CONTACT MATERIAL

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The widespread use of plastic and low recycling rates has sparked concerns about plastic waste, environmental pollution, and sustainability. In response, many organizations are working to increase the proportion of post-consumer recycled (PCR) content in their overall plastic packaging. In Australia, the 2021 National Plastics Plan stated, one of the National Packaging Targets for industry is "including 50% of recycled content in packaging by 2025" [1]. The AS 2070-1999 prohibited the utilisation of PCR material for direct contact with food, but this standard was withdrawn in 2021. At present, no standard has been introduced to replace AS 2070-1999, meaning there is no established guideline for the use of PCR as a food contact material in Australia. However, in 2019, Coca-Cola Amatil had achieved a milestone by introducing a carbonated soft drink bottle made entirely from 100% recycled plastic into the market, marking a pioneering achievement in Australia [2].

While food safety in relation to food contact materials has been extensively researched, there remains a significant knowledge gap concerning aroma compounds in PCR plastic. This study aims to develop and optimise the solid-phase microextraction (SPME) method coupled with gas chromatography-mass spectrometry (GC–MS) to identify volatile compounds from a model plastic. Followed by aroma-active compounds screening with aroma extract dilution analysis (AEDA) approach by using gas chromatography with olfactometry detection (GCO).

A plastic-packaged fabric softener was purchased at a local grocery in Australia. The American Society for Testing and Materials (ASTM) washing method was applied to wash the model plastic to ensure the compounds detected were from plastic instead of detergent. Volatile compounds from plastic were extracted by the SPME method in which the extraction method was optimised using a statistical design of experiments (DoE). The volatiles extracted by SPME were analysed by AEDA to find the most potent odorants.

The optimised conditions included incubation temperature of 45°C and extraction time of 60 min. Under these conditions, the chromatogram exhibited the maximum number of peaks. AEDA results yielded more than 30 aroma-active regions with flavour dilution factors ranged from 4 to $\geqslant$2048. This developed method provided a sensitive and reliable approach for the analysis of volatile compounds in model plastic. It allowed for the comprehensive identification of 'residual' compounds still present from the plastic even after washing. It will also be applied to determinearoma-active compounds in real recycled plastic in next study.

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Optimising IR Polymer Identification for Weathered Marine Plastics: Addressing Library Limitations and Weathering Effects

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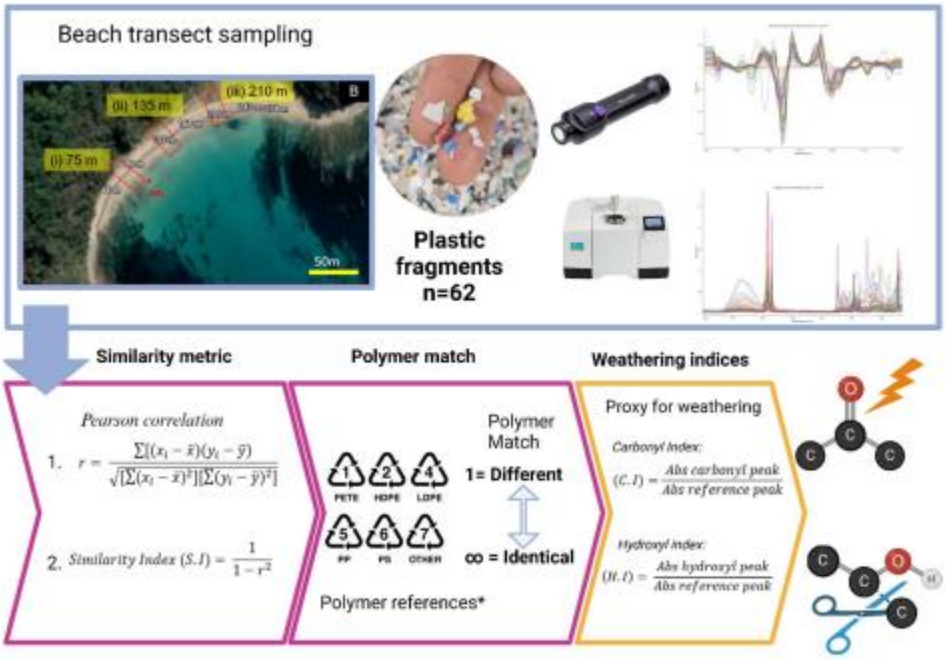
Abstract:

Plastic pollution is a growing environmental crisis, with over 10 million tonnes of plastic waste entering oceans each year. It remains in the marine environment where it is subjected to weathering processes, fragmenting into smaller plastics, often washing up on shores. Identifying these altered marine plastic fragments is challenging, Fourier Transform Infrared (FTIR) and Near-Infrared (NIR) spectroscopy are widely used for polymer identification, typically relying on spectral matching against reference libraries[1]. However, environmental weathering disrupts the structural integrity and chemical composition of plastics, leading to inconsistencies in the spectral fingerprints of the polymer. In response, some spectral libraries—both proprietary and open-source—have expanded to include spectra of weathered plastics, theoretically improving match accuracy[2]. However, expanding libraries can increase the risk of incorrect matches, particularly in open-source repositories where propagation of misidentified spectra can occur. This study investigates the impact of library limitations and weathering on spectral matching accuracy for marine plastic identification. We assess the use of a non-linear Similarity Index (S.I), to evaluate spectral similarity between weathered marine plastics and reference polymers. Additionally, two well-established weathering indices—the Carbonyl Index (C.I.) and Hydroxyl Index (H.I.)—are employed as proxies for oxidation, offering insights into degradation influence spectral matching reliability[3]. Our results reveal that heavily weathered plastics consistently produce low similarity matches with standard reference spectra, highlighting a strong correlation between low S.I. values and advanced oxidation, as indicated by elevated C.I. and H.I. values. We also observe frequent spurious correlations, where specific weathered plastics are misclassified due to overlapping spectral characteristics. This study further explores the application of NIR spectroscopy for rapid, field-based polymer identification. By examining these variables, we propose improvements to spectral matching practices for marine plastics, advocating for curated libraries that integrate weathered spectra and adjusted matching metrics to enhance accuracy in marine environments.



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Determination of residual chemicals in bio-derived solvents using liquid chromatography - mass spectrometry

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Cyrene™ (dihydrolevoglucosenone) is an innovative bio-based solvent derived from cellulose, recognised as an eco-friendly alternative to conventional organic solvents due to its low toxicity and reduced environmental impact.[1] With excellent solvating properties, Cyrene™ is a promising option for inorganic/organic synthesis, nano-material synthesis, and pharmaceutical industry-. [2] As with other biosolvent or biochemical manufacturing processes, residual impurities may be present in the final product. Therefore, developing an analytical method to detect and quantify these chemical species is essential.

This study presents a rapid and straightforward liquid chromatography- mass spectrometry (LCMS) based method for the analysis of impurities in commercial Cyrene™. The significance of this method lies in its enhanced sensitivity for high molecular weight, non-volatile, and/ thermo-mobile compounds without requiring derivatisation. The LC separation was completed in under 10 minutes using a flow rate of 1 mL/min in gradient mode on a C18 column -ODS Hypersil (150 mm × 4.6 mm, 5 µm) maintained at 25°C. The mobile phase consisted of 2 mM ammonium acetate in acetonitrile as the organic modifier and 2 mM ammonium acetate in water as the aqueous phase, the new method developed allowed the separation of more than 20 impuritiesand the quantification of three major residual impurities: Levoglucosenone (LGO), 2-methoxyphenol, and sulfolane. Direct UV-VIS absorbance detection was performed at 200 nm, 224 nm, and ⩽200 nm for Cyrene™, LGO, and 2-methoxyphenol, respectively. Sulfolane was quantified via positive ESI-MS full-scan acquisition mode, based on its characteristic ammonium adduct at 138 m/z. LODs obtained for LGO, 2-methoxyphenol, and sulfolane were 0.02 mg/mL, 0.02 mg/mL, and 0.07 mg/mL, respectively. Intra- and inter-day repeatability for all analytes were under 3% and 10%, respectively. The results obtained from the developed LC-MS method were cross-validated against an established gas chromatography-mass spectrometry (GC-MS) method, demonstrating excellent agreement with percentage difference errors in the range 0.5%-10%.

The newly developed method enables the rapid identification and quantification of residual impurities in bio-derived solvents, supporting process optimisation and ensuring production quality compliance.

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Abstracts (Oral Presentation)

Monday 2nd December

(Section 3 & 4)

Development of ruthenium complex-based thin film-based sulphate sensors

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Sulphate (SO_4^{2-}) is one of the anions that possesses the highest hydration energy. [1,2] Consequently, it is hard to separate and filter SO_4^{2-} especially in water purification processes. Because of that, SO42- has been used as an indicator for validating reverse osmosis membranes. [3] In this study, a SO42- sensor was developed using ruthenium complex within thin film-solid contact sensor technology. Herein, the thin film as a $SO_4$2- transfer mediator was made from a solution composed by polyurethane, plasticiser 2-Nitrophenyl octyl ether (NPOE), supporting electrolyte ETH 500, synthesised redox transducer ruthenium (pod)(pob) (Haga group, Japan) and synthesised ionophore T.Thio.bisCF3 (Jolliffe group, Sydney, Australia). This solution was spin-coated onto glassy carbon electrodes. The electrochemical properties of the thin film were studied by cyclic voltammetry using conventional three electrode cells. Voltammetric behaviour and response for SO_4^{2-} of the thin film were investigated. As a result, the thin film possessed 6 nmol.cm-2 of electroactive species (Ru(pod)(pob)) which controls the SO_4^{2-} transfer with a transfer rate 0.38 s-1. Linear response was achieved within the SO_4^{2-}- concentration range of 1 µM – 100 mM, with a limit of detection of 0.2 µM. The selectivity for SO_4^{2-} was high after testing the sensor's response to other anions (Cl^- and NO_3^-), showing a promising SO_4^{2-} sensor response.

Keywords: sulphate, ruthenium complex, thin film, electrochemical behaviour, voltametric response

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Anti-fouling electrochemical sensors for Bisphenol A based on ionic liquid and poly(ionic liquid) films

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Bisphenol A (BPA) is used in the production of polycarbonate, unsaturated polyester, epoxy resin, and polystyrene resins, which are utilized in plastic containers. As a result, BPA can be found in food and beverages. Exposure to BPA, even at trace levels, has been linked to serious health effects, including infertility, diabetes, brain damage, and various types of cancer. Among the various analytical techniques to detect BPA, electrochemical methods become the preferred choice due to low-cost instrumentation, fast response times, durability and portability. A significant challenge involved in the electrochemical detection of BPA is the electrode fouling that results from polymer formation from phenoxy radicals during the irreversible oxidation of BPA.[1]

In this work, we used gel-like mixtures containing the ionic liquid (IL) 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C_2mim][TFSI]) and the poly(ionic liquid) (PIL) poly(diallyldimethylammonium) bis(trifluoromethylsulfonyl)imide ([PDADMA][TFSI]) as an electrolyte. The gel was used with a miniaturized electrode to prepare an electrochemical sensor for BPA that showed a promising antifouling effect (Figure 1). Under optimized experimental conditions, the oxidation peak current was linearly proportional to BPA concentration with a coefficient of determination (R^2) of 0.997. The sensor was able to overcome electrode fouling with good reproducibility. Also, we demonstrate that the addition of Fe_3O_4 nanoparticles enhanced the current signal while maintaining the anti-fouling effect.

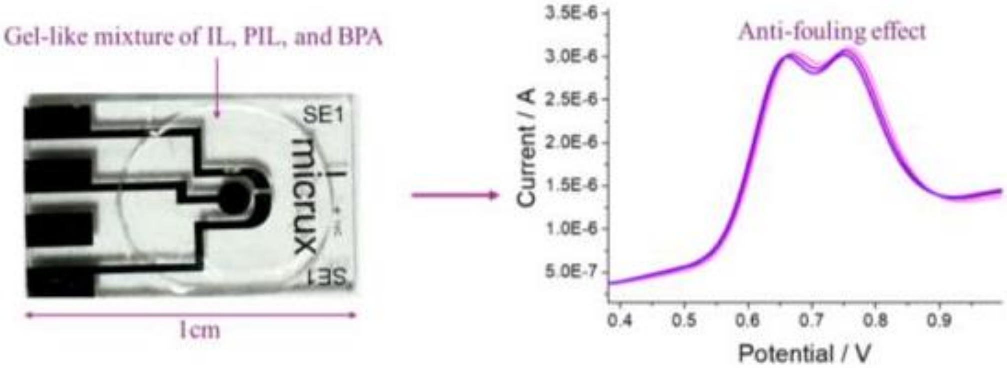

Figure 1. (left) Platinum thin-film electrodes with gel-like mixture of IL, PIL, and BPA; (right) Squarewave voltammetry curves of BPA in a gel-like electrolyte.

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Quantification of small organic molecules in sustainable biosolvent production processes using offline and online monitoring techniques.

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Biosolvents from renewable feedstock provide a sustainable alternative to fossil-fuel-based solvents. Circa Group AS has recently launched Cyrene™, a novel biosolvent with excellent solvating properties, produced using the patented Furacell™ process[1, 2]. The complex production of Cyrene™ necessitates the development of sophisticated offline and online process analytical technology (PAT) to provide accurate and real-time characterisation of primary and secondary products within the FuracellTM process. Developed PAT will improve monitoring of compositional changes at various stages of the process, enabling operators to obtain real-time information as well as ensuring effective and optimal operations.

This study presents a novel method for the simultaneous quantification of formaldehyde, methanol, acetic acid, and formic acid in Furacell™ process samples, utilising gas chromatography coupled with mass spectrometry (GC-MS).This method features simple sample preparation and achieves baseline separation of target analytes in complex sample matrices in under 15 minutes using a DB-WAX-UI column, which provides improved resolutionfor polar compounds. Data acquisition was conducted in single ion monitoring (SIM) mode to obtain high sensitivity in quantification and in full scan mode to facilitate untargeted monitoring. Achieved instrumental LODs were 0.09, 0.04, 0.02, and 0.03 µg mL^{-1} for formaldehyde, methanol, acetic acid, and formic acid, respectively. Repeatability intra- and inter-day were always below 5% and 12%, respectively. The method was applied to the analysis of 28 Furacell™ process samples collected at two sample points along the production line, over the course of a month.

Moreover, NIR spectra of the above samples were recorded using a benchtop NIR instrument to develop an online, real-time monitoring platform. Prediction models were generated implementing partial least squares (PLS) regression analysis to obtain the concentrations of target analytes. Developed models, and the selection of spectral regions important for analyte prediction, will be applied for the development of a portable device equipped with NIR LEDs to provide chemometric-supported quantitative analysis. Outcomes of this project will enhance laboratory staff's ability to quantify various by-products offline and access real-time process information.

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Spiral Inertial Microfluidics for Sorting, Separation and Real-time Detection of Bacteria

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Pathogenic bacteria cause a range of diseases and public health crisis from foodborne illnesses to waterborne diseases which are a serious concern world-wide [1]. Traditional methods for bacterial separation and detection, are effective though often time-consuming, expensive, and labour-intensive [2]. In recent years, microfluidic technologies have emerged as powerful tools for bacterial separation and detection. Microfluidics refers to the circulation of small volumes of fluids, typically in the microliter to nanolitre range, within microchannels. This technology offers several advantages over traditional methods, including reduced sample and reagent consumption, shorter processing times, and the ability to perform complex analyses on a single platform [3].

This study aims to develop a high-throughput spiral inertial microfluidic chip for efficient bacteria separation from wastewater with application in a portable water monitoring device. Our research goal presents a unique challenge as water potentially contains particulate matter and a range of sizes of particles under 1 µm. Initially, the plan is to design a spiral microfluidic chip with backward flow direction, meaning the flow will be injected from the centre of the spiral, and the outlet will be at the end of the spiral. The total spiral loop will be six for ensuring effective separation by providing higher conduits length. A pre-filter will be designed to hinder penetration of comparatively large size particles inside the microchip to protect potential blocking of micro-channels. Separation experiments will be validated using coloured/fluorescent polystyrene particles before progressing to bacterial samples. Based on the results from the trial phase, experiments will be conducted with cultured bacteria, varying the cross-sectional areas of the channel and different loop settings to finalize the microchip design for efficient bacterial separation. This process will focus on separation efficiency and various flow rates, as maintaining appropriate flow rates is crucial for the continuity and realistic implementation of separation technology in a portable device. The final stage involves integrating the entire setup, including the pre-filter and the designed microchip, into a portable device called enPhytobox. This integrated system will be validated and tested using real-life samples from local wastewater to evaluate the design setup and measure bacterial separation efficiency in complex, real-world conditions.

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Lubricin (PRG-4) anti-fouling coating for surface-enhanced Raman scattering biosensing: Towards a hierarchical separation system for analysis of unprocessed samples

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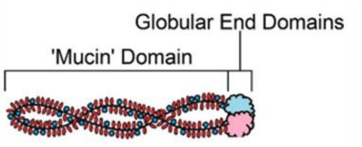
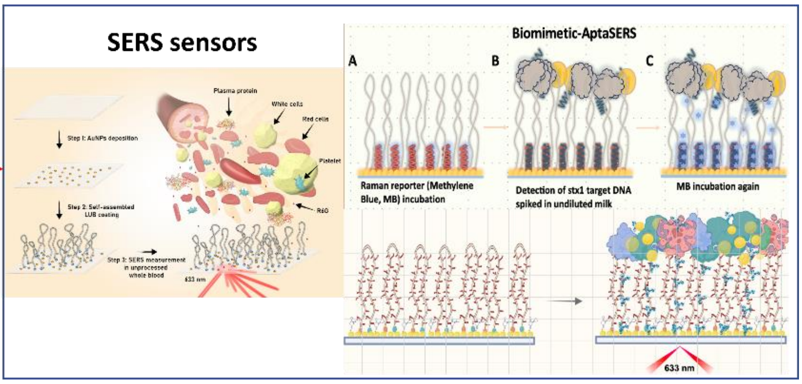
Surface-enhanced Raman Spectroscopy (SERS) is a powerful optical sensing technique that amplifies the signal generated by Raman scattering by many orders of magnitude. Although the extreme sensitivity of SERS enables an extremely low limit of detection, even down to single molecule levels, it is also a primary limitation of the technique due to its tendency to equally amplify ‘noise’ generated by non-specifically adsorbed molecules at (or near) optically active interfaces. Eliminating system noise is thus critically important to SERS biosensing and typically involves onerous extraction/purification/washing procedures and/or heavy dilution of biofluid samples. Consequently, direct analysis within biofluid samples or in vivo environments is practically impossible. In this study, an anti-fouling coating of recombinant human Lubricin (LUB) was self-assembled onto AuNP-modified glass slides via a simple drop-casting method. A series of Raman spectra were collected using rhodamine 6G (R6G) as a model analyte, which was spiked into NaCl solution or unprocessed whole blood. It was demonstrated for the first time that LUB coating can mitigate the deleterious effect of fouling in a SERS sensor without compromising the detection of a target analyte, even in a highly fouling, complex medium like whole blood. In addition to the detection of R6G in unprocessed whole blood, real analytes such as L-cysteine, vancomycin, and Shiga toxin 1 DNA spiked in milk samples were also successfully detected without any pre-separation or dilution. This feat is achieved through a molecular sieving property of LUB that separates small analytes from large fouling species directly at the sensing interface resulting in SERS spectra with low background (i.e., noise) levels and excellent analyte spectral fidelity. These findings indicate the great potential for using LUB coatings together with an analyte-selective layer to form a hierarchical separation system for SERS sensing of relevant analytes directly in complex biological media, aquaculture, food matrix or environmental samples.



- **Self-assembly**
- **Anti-adhesive and anti-fouling**
- **Size-selective**



Abstracts (Oral Presentation)

Tuesday 3rd December

(Section 5 & 6)

Near infrared spectroscopy as a tool for rapid assessment of peatland condition

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Degradation, coupled with growing global pressure to improve the C sequestration capacity and overall health of peatlands, are creating demand for improved peatland condition monitoring. Near Infrared (NIR) spectroscopy offers the advantages of speed, ease of use, accuracy, and cost-effectiveness for peatland monitoring. In addition, this method is objective and does not rely on monitoring personnel to have plant identification or other background expertise to collect reliable data. Despite these advantages, the application of NIR spectroscopy to study peatlands is limited and no study has yet explored its potential for monitoring peatland condition. Thus, we investigated the potential of NIR spectroscopy to assess peatland condition. Peat soils from degraded and intact peatlands were analysed in situ and in the laboratory with a portable, handheld MicroNIR. Peat samples collected from the surface and from the depth profile of three intact and degraded peat areas were also analysed to determine the scanning strategy that yielded the best results. Our results show that NIR spectroscopy was able to effectively differentiate between samples from intact and degraded surface peats ($p< 0.05$), with 68% of this variation explained by PC1 and PC2. The water and C-H (hydrocarbon) regions of the NIR spectra were identified as the key factors contributing to the separation of results from the intact and degraded peats, which aligns with our understanding of biogeochemical peatland degradation mechanisms. Overall, these findings demonstrate that NIR spectroscopy has strong potential as a valuable tool for the rapid assessment of peatland condition by identifying the extent of degradation and monitoring the effectiveness of restoration interventions over time.

Comprehensive Analysis of Paleoclimatic Proxies in Ice Cores via Dual Capillary Ion Chromatography-Mass Spectrometry: Targeted and Untargeted Approaches

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The trapped dissolved and particulate matter in ice cores is invaluable for understanding past atmospheric composition and paleoclimatic conditions. Research often targets proxies like inorganic ions and organic acids such as methanesulfonic acid (MSA) to track past changes in sea ice extent, terrestrial dust variability, and atmospheric aerosol transport. Herein, we present an improved dual Cap-IC-MS method for the simultaneous quantification of fluoride, acetate, formate, MSA, chloride, nitrite, nitrate, bromide, sulphate, oxalate, phosphate, sodium, ammonium, potassium, magnesium, and calcium in ice core and snow samples. This method requires a direct injection of only 190 µL of sample, 35 times less than standard ion chromatography methods. Limits of detection (LODs) for all analytes determined using conductivity detection were similar to those of standard IC methods. The dual Cap-IC system was hyphenated with mass spectrometry detection for targeted ion identity confirmation, lowering LODs, and untargeted screening analysis to broaden knowledge of the organic aerosol chemical composition in ice cores. The new developed method was applied to analyse ice core samples from Antarctica, demonstrating its applicability and laying the groundwork for future research within the significant 'Million Year Ice Core' (MYIC) project

Comparing levoglucosan and mannosan ratios in sediments and corresponding aerosols from recent Australian fires

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The monosaccharide anhydrides levoglucosan, mannosan, and galactosan are known as ‘fire sugars’ as they are powerful proxies used to trace fire events. Despite their increasing use, their application is not completely understood, especially in the context of tracing past fire events using sediment samples. There are many uncertainties about fire sugar formation, partitioning, transport, complexation, and stability along all stages of the source-to-sink pathway. While these uncertainties exist, the efficacy of fire sugars as fire tracers remains limited. This work compared high-resolution fire sugar fluxes in freshwater sediment cores to known fire records in Tasmania, Australia. Past fire events correlated with fire sugar flux increases down-core, with the magnitude of the flux inversely proportional to the distance of the fires from the study site. For the first time, fire sugar ratios (levoglucosan/mannosan, L/M) in aerosols were compared with those in sediments from the same time-period. The L/M ratio in surface sediments (1.42–2.58) were significantly lower than in corresponding aerosols (5.08–15.62). We propose two hypotheses that may explain the lower average L/M of sediments. Firstly, the degradation rate of levoglucosan is higher than mannosan in the water column, sediment-water interface, and/or sediment. Secondly, the L/M ratio of non-atmospheric emissions during fires may be lower than that of atmospheric emissions from the same fire. Due to the uncertainties about transport partitioning (atmospheric versus non-atmospheric emissions) and fire sugar degradation along all stages of the source-to-sink pathway, we advise caution when inferring vegetation type (e.g. softwood, hardwood, or grasses) based purely on fire sugar ratios in sediments (e.g. L/M ratio). Future investigations are required to increase the efficacy of fire sugars as a complimentary, or standalone, fire tracer in sediments.

Challenges in the determination of surfactants in complex industrial wastewater samples

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Industrial wastewater frequently contain a diverse array of toxic contaminants which can be of significant environmental concern. Among these contaminants are surfactants which are increasingly being discharged directly or indirectly into the environment through industrial processes or from wastewater treatment plants.[1] The persistence of anionic surfactants, which are commonly used in detergents and other cleaning products, can drastically alter water quality parameters. Consequently, their presence in the environment not only poses a toxicological risk to ecosystems and human health, but also raises challenges in the treatment of the wastewater.2Hence it is important to monitor the concentration of surfactants in industrial wastewater to ensure appropriate management and treatment strategies can be implemented.

This work explores the practical challenges in the analysis of industrial wastewater, particularly when small sample volumes are available. This involves factors including the matrix composition and consequent matrix interferences as well as large variations in analyte concentrations between samples. In this study, the complexities in the analysis of industrial wastewater matrices have been considered for the determination of anionic surfactants. A standard spectrophotometric method for the determination of anionic surfactants concentrations in wastewater has been modified and validated for significantly reduced sample volumes. A liquid-liquid extraction of the sample is followed by UV-spectrophotometric measurements of the anionic surfactant-methylene blue ionic pair at 652 nm. The method offers a simple and reliable method of determining anionic surfactant concentrations in complex water samples where sample volumes are often limited. The challenges associated with the analysis of such samples and results will be further discussed in detail in the presentation.

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The Bioaccumulation and Biodistribution of Mercury Species in a Demersal Marine Fish (Lutjanus Sebae)

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Oil and gas infrastructure have the potential to release residual mercury if decommissioned in situ in the northwest shelf of Western Australia.[1, 2] Mercury's toxicity to biota has led to changes in the use of mercury as required by the Minamata Convention. With Australia ratifying the convention, the potential impacts of anthropogenic sources of mercury to marine life need to be researched, and initial data on how background mercury biomagnifies up marine food webs is required before impacts from oil and gas infrastructure can be assessed. This thesis validates methods of mercury analysis to establish a baseline dataset for background mercury concentrations in a demersal marine fish (*Lutjanus sebae*) with mercury total and speciation analysis.

The optimal method had total mercury recoveries (84.9 ± 5.0%) and MeHg speciation recoveries (81.0 ± 4.4%), validated against a fish tissue certified reference material. Here we show that MeHg was the primary species of mercury present in muscle tissue with a positive correlation between the fork length of *L. Sebae* and the concentration of MeHg analysed ($n = 9$, $R^2 = 0.80$). $\delta^{13}C$ and $\delta^{15}N$ stable isotope analyses suggested that the primary uptake of mercury for *L. sebae* is through dietary exposure ($n = 9$, $R^2 = 0.80$). The highest concentrations of inorganic mercury (IHg) were in the liver and kidney.

Selenium has the capacity to detoxify mercury through the formation of mercury selenide, so totalselenium concentrations were analysed to inform mercury detoxification potentials in *L. Sebae*. The highest concentrations of selenium were found in the liver and kidney. [tSe] in muscle tissue was independent of the concentration of MeHg present. The analysis of *L. sebae* establishes data on background concentrations of mercury and aids our understanding of mercury biomagnification in marine food webs.

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Water-Activated Silica-Based Solid Phase Extraction for Extracting Steryl Glucoside in Biodiesel

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Steryl glucosides (SG) are problematic byproducts in biodiesel production, contributing to filter blockages in diesel engines despite their low concentration in biodiesel[1]. Quantifying SG presents challenges due to their limited presence. Solid phase extraction (SPE), a prevalent pretreatment method for SG analysis, traditionally employs hazardous solvents like chloroform for activation or preconditioning[2]. This study focuses on optimizing SPE for SG pretreatment in crude biodiesel before analysis using high-performance size exclusion chromatography (HPSEC) with a 100-Å Phenogel column. Aiming for a more environmentally friendly approach, water (0.05-0.5 mL) was utilized as a solvent for preconditioning the Strata silica-based SPE. The method involved recovering adsorbed SG in the SPE through heptane washing and elution with acetone/methanol (9/1, v/v). Results demonstrate that minimal water content (0.075 mL) significantly improved SG extraction (106.29 µg/mL) compared to non-preconditioned (27.06 µg/mL), heptane-preconditioned (53.70 µg/mL), and acetone: methanol-preconditioned (76.73 µg/mL) methods. The limit of detection (LOD) and quantification (LOQ) for SG on a 100-Å Phenogel column were determined as 8.0735 µg/mL and 24.4651 µg/mL, respectively. In conclusion, the addition of a small amount of water balanced the SPE polarity, resulting in enhanced SG extraction efficiency.

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Enhanced Glucose Sensing through Tailored Enzyme-Inspired Substrate Channels on Electrode Surface

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Sensitive and selective quantification of analytes in complex biofluids, such as blood, remains a significant challenge in biosensing. To overcome this issue, we developed an array of isolated carbon nanochannels on a flat gold electrode, designed to function as molecular sieves that significantly reduce protein fouling and eliminate the need for antifouling coatings. We investigated nanochannels with various diameters and lengths specifically for glucose sensing applications.

Employing a two-step pulsed electrochemical method, we initiated the process with a reductive pulse that effectively removed negative interferences and fouling molecules[1, 2]. This was followed by an oxidative pulse to facilitate glucose oxidation at both the bottom of the nanochannels and the gold surface. The unique nanoconfined environment provided by the upper carbon nanochannel layer, combined with the redox-active properties of the gold catalyst, promotes the generation of hydroxide ions, thereby creating a higher pH environment that enhances glucose oxidation efficiency.

Our results demonstrate that increasing channel lengths enhances sensitivity up to an optimal point, beyond which sensitivity declines due to mass transport limitations of glucose and restricting of the underlined Au surface. In contrast, varying channel diameters did not significantly impact sensitivity. This study highlights the importance of channel diameter and channel length modulation on flat surfaces, providing valuable insights into catalytic activity and potential applications beyond glucose sensing. These findings pave the way for advanced wearable biosensing technologies capable of operating in complex biological environments, ultimately enhancing diagnostic capabilities for real-time monitoring of analytes in clinical settings.

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Methamphetamine contamination and distribution in cars

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Methamphetamine can be manufactured, transported or smoked in cars leading to contamination. People occupying the car post manufacture or after smoking could then be exposed by inhalation, skin adsorption, or ingestion routes.[1,2] This thirdhand contamination may result in symptoms including headaches, respiratory problems, and behavioural issues.[3] Therefore, to protect public health it is important to determine methamphetamine contamination levels.[4] Commonly, smooth, non-porous surfaces are wipe sampled following the National Institute for Occupational Safety and Health (NIOSH) 9111 method.[5] However, this sampling method may not be ideal for porous or rough surfaces as the drug could become embedded in a material. This sampling method also does not consider levels in the air.

This study presents the extent and distribution of methamphetamine contamination in two cars. One car was found contaminated, while the other was contaminated from a simulated smoking session. Air sampling was performed using two different sorbent tubes connected to sampling pumps. Surface wipe sampling of approximately 100 cm^2 was performed for areas such as air vents using methanol-wetted gauze. Bulk material cuttings were taken from porous materials such as roof linings, and seat fabrics and underlying foams. All samples were extracted in 0.1 M sulfuric acid then analysed using a Thermo Vanquish Horizon system coupled with an ISQ EC Single Quadrupole Mass Spectrometer. The LC-MS method was adapted from the NIOSH 9111 method used for analysing methamphetamine from wipes.[5]

Results demonstrated that methamphetamine can be detected in the air and on non-porous and porous surfaces. The drug was also detected after second and subsequent wipe sampling events of a plastic surface. Methamphetamine was detected from bulk material samples and from the underlying foam layers indicating drug penetration into materials. These results indicate a need for further research on methamphetamine testing and remediation in cars, which is ongoing.

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Abstracts (Oral Presentation)

Wednesday 4th December

(Section 7 & 8)

Nanomaterials for 3D Printing Nano- and Micro-Porous Silicon-based Glass and Ceramics

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3D printing of silicon-based glass and ceramics is gaining increasing interest in various socio-economic sectors. This is owing to the exceptional properties of these materials (high chemical resistance, temperature stability, and mechanical robustness) and the unique capabilities of additive manufacturing methods (rapid development, ease of customisation, and low setup and operating cost). Conventionally, complex manufacturing processes associated with glass and ceramics limited their use from developing intricately detailed structures. However, the advent of 3D printing is bringing a paradigm shift in research and industry-scale manufacturing, offering the potential for more extensive utilisation of these high-performance materials. The presentation will delve into our recent work on developing novel materials and technologies for 3D printing silicon-based glass and ceramics with precisely controlled hierarchical porosity. The employed methodology facilitates the fabrication of intricate structures, such as micro-needle arrays and biomimetic replicas of natural elements like leaves and butterfly wings. Precise control over pore size and distribution is achieved, and the versatility extends to generating structures with diverse pore patterns using conventional 3D printers. The approach has been extended to various high-interest materials, such as silica, silicon carbide, conductive and non-conductive black glass, and polydimethylsiloxane (PDMS). This groundbreaking technique enables the creation of bespoke structures with minute features, thereby unlocking avenues for developing nature-inspired sensors, filters, and energy storage and generation systems

The bio-inspired heterogeneous single-cluster catalyst Ni100–Fe_4S_4 for enhanced electrochemical Conversion of CO2-to-CH_4: A DFT Study

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Electrochemical conversion of CO_2-to-CH_4 is a process of converting the inert greenhouse gas into energy molecules. It offers great promise for the transformation of carbon-neutral economy. However, achieving high CH_4 activity and selectivity remains a major challenge because the electrochemical reduction of CO_2-to-CH_4 is accompanied by various C_1 intermediates at the catalytic site, involving multiple proton-coupled electron transfer processes. Herein, different from the traditional designing strategy, we propose a bio-inspired theoretical design approach to construct a heterogeneous single-cluster catalyst Ni100–Fe_4S_4 at the atomic level, which may show high CO_2 electroreduction performance.[1] Combined with the crystallographic data and theoretical calculations, Ni100–Fe_4S_4 and CO dehydrogenase exhibit highly similar catalytic geometric active centers and CO_2 binding modes. By exploring the origin of the catalytic activity of this biomimetic structure, we found that the activation of CO_2 on Ni100–Fe_4S_4 theoretically exceeds that on natural CO dehydrogenase. Density functional theory calculations reveal that the dehydrogenase enzyme-liked Fe–Ni active site serves as an electron enrichment 'electro-bridge' (an electron-rich highly active catalytic site), which can activate CO2 molecules efficiently and stabilize various intermediates in multistep elementary reactions to selectively produce CH_4 at a low overpotential (0.13 eV). The calculated CO_2 electroreduction pathways are well consistent with the nickel-based catalytic materials reported in experimental studies. Our work showcases and highlights the rational design of high-performance catalytic materials via the biomimetic methodology at the atomic level.

Literature:

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Synthesis and Characterization of Eugenol-Derived Compounds as Biobased Plasticizers

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The incorporation of plastic across various industries becomes increasingly unavoidable and the escalating production of plastic correlates with a significant rise in plastic waste, leading to the potential leaching of toxic chemical additives and plasticizers into the environment [1]. In 2023, the plasticizer market was valued at USD 17.98 billion with phthalates leading the market [2]. However, regulatory frameworks are shifting the focus toward less harmful non-phthalate alternatives [3]. Consequently, the development of green renewable materials as plasticizers - that are also safe and inexpensive - without adversely affecting performance has become a critical area of focus. In this study, eugenol from clove oil was used in the preparation of four different plasticizers. Eugenol was combined with various fatty acids to obtain 4 different bio-based esters. Plastic blends with each of the four compounds were prepared to test their thermostability and plasticization capabilities using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The results obtained from the TGA and DSC analysis for the eugenol-based plasticizers suggested good thermostability, plasticization, and compatibility with the polymer matrix. Collectively, the results show the plasticization efficiency of these new plasticizers and their potential as biobased alternative to phthalates.

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Redox-Mediated Enhancement and Quenching of Co-Reactant Electrochemiluminescence

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Electrochemiluminescence (ECL) is a highly selective and sensitive mode of detection whereby electrochemically generated reactants form electronically excited species that emit light upon relaxation to the ground state.[1] By far, the well-documented $[Ru(bpy)_3]^{2+}$/tri-n-propylamine (TPrA) coreactant system has been the most extensively explored and, to date, is the most widely used in commercial assays involving clinical diagnostics, environmental monitoring, and forensic detection protocols.[1] Most analytical ECL systems employ a bead-supported assay format, where the target analyte selectively binds to a 'capture' molecule that is immobilised on a magnetic bead, and a 'detection' molecule to which the luminophore is attached (**Figure 1a**, from reference).[2]Importantly, however, this has proximal limitations in that the vast majority of the $[Ru(bpy)_3]^{2+}$ luminophore is bound at distances from the electrode that do not permit its direct oxidation. Therefore, only the coreactant TPrA is oxidised (**Figure 1b**).[3]In such systems, the fate of oxidised TPrA diverges. In the first mechanism, the amminium radical cation species that is generated ($TPrA^{\bullet+}$) may deprotonate to form a strongly reducing radical species which interacts with the luminophore to form $[Ru(bpy)_3]^{+}$. In the second, $TPrA^{\bullet+}$ persists and, therefore, may act as a sufficiently strong oxidant to generate the excited state luminophore from reduced $[Ru(bpy)_3]^{+}$. However, the latter pathway is limited by the former, and so signal output is diminished. As such, in this work, we focus on the enhancement of this pathway through addition of iridium(III) complexes possessing stable redox states. In solution, these species may operate as 'redox mediators,' where they effectively replace $TPrA^{\bullet+}$ to generate the excited $[Ru(bpy)_3]^{2+*}$ electrochemiluminophore (**Figure 1c**).[4]

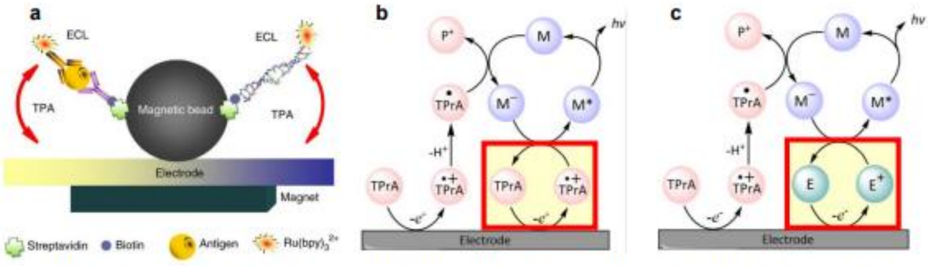

Figure 1. (a) Magnetic bead supported ECL assay format. Image from Zhou *et al.* (b) Conventional ECL 'indirect' pathway in the co-reactant system. (c) Our proposed pathway, where 'E' is an iridium(III) complex possessing suitable redox properties for facile generation of the excited state electrochemiluminophore.

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Heterojunction photocatalysts for liquid phase CO2 reduction

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Climate change mitigation requires innovative and scalable technologies for CO_2 capture, storage and utilisation [1]. The latter transformation of CO_2 into carbon containing and chemicals is particularly desirable to support sustainable chemical manufacturing and the circular economy [2]. Photocatalytic CO_2 reduction to C_1-C_3 molecules driven by visible light over inorganic semiconductors has attracted great academic attention but suffers from low quantum efficiency and materials instability [3]. Here we discuss the synthesis, characterisation and application of heterojunction nanocomposites [4], comprising UV-absorbing TiO_2 and visible light-absorbing graphitic carbon nitride (g-C_3N_4) for the aqueous phase photoreduction of CO_2 to CO, CH_4 and methanol (**Fig. 1**), and apply quantum mechanical (DFT) modelling to explore the role of copper co-catalysts. Photophysical properties, including the density, mobility, and transport of photoexcited electrons and holes across the TiO_2/gC_3N_4 interface are correlated with catalyst performance.

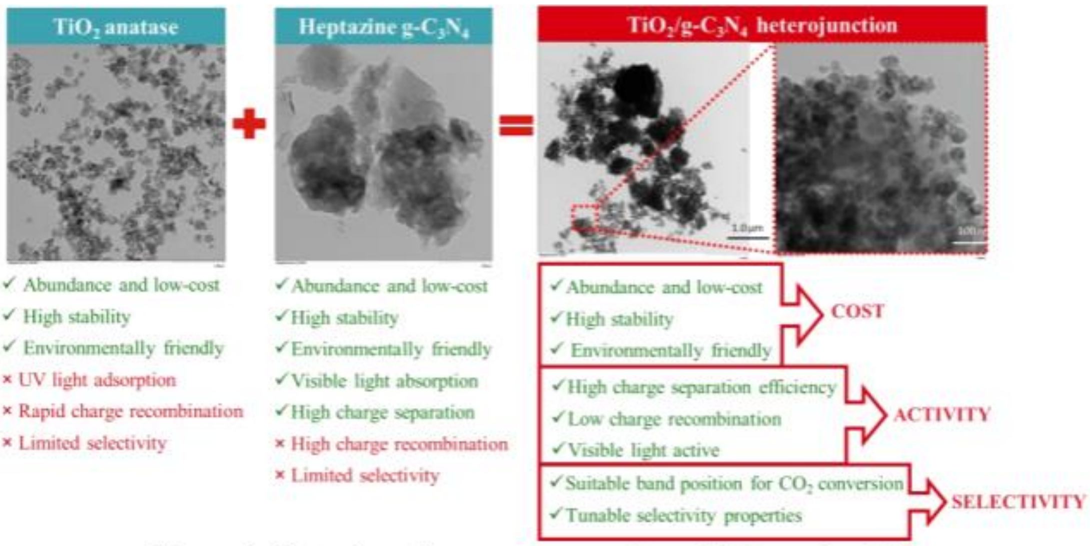

Figure 1. Heterojunction nanocomposites of TiO_2 and g-C_3N_4 for photocatalytic CO_2 reduction.

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Synthesis and electrochemical characterisation of a Y-doped barium cerate zirconate proton conductor for hydrogenation and dehydrogenation applications

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Ceramic proton conductors have drawn significant attention in various green hydrogen related fields such as hydrogen production from hydrogenated chemicals such as water, ammonia, methanol, and dimethyl ether, as well as hydrogen storage by synthesising these chemicals as H-carriers in-situ,[1] including natural gas upgrading; combing heat and power applications. These proton conducting ceramics operate at temperatures ranging from 400 to 600 °C, at such, low cost waste heat from other industrial processes can be directly utilised, reducing the carbon footprint associated with their production, by lowering their energy cost and by using green hydrogen as reactant.[2]

In this study, we investigate the synthesis and properties of a Y-doped barium cerate zirconate perovskite oxide (BCZY), a promising proton-conducting electrolyte, prepared via the modified Pechini sol-gel method.[3] Structural, morphological, and compositional analyses were conducted using XRD, SEM, EDS, and ICP-OES, while electrochemical impedance spectroscopy (EIS) assessed the ionic conductivity of sintered pellets.

Our results reveal how the phase of BCZY evolves with calcination temperature, and how this impacts on crystallite and particle size, sinterability, and densification of the electrolyte pellets. These structural properties, along with operation parameters, strongly influence the material's final electrochemical performance, demonstrating how the conductive properties of BCZY can be optimised to make it potential candidate as solid electrolyte for efficient ammonia production.

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Synthesis and Characterization of Biopolymers from Wood-Derived Compounds

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The huge concern of plastic pollution is due to use of excessive use of fossil fuel-based synthetic polymers. Even though polymers are necessary for modern living and the global economy, over 90% of today's synthetic polymers derive from fossil fuels, and 87% of these substances end up in landfills after single use.[1] The production of goods based on fossil fuelbased polymers is surging worldwide, even as awareness about climate change and the environment is growing.[2] Significant efforts are being made all around the world to change from the current economy, which is dependent on fossil fuels, to a more sustainable bioeconomy.[3] The development of highly effective and economical processing of biological feedstocks into a variety of bio-based products will enable bridging the gap between economic growth and environmental sustainability.

To synthesize sustainable organic molecules that can compete with or eventually replace those obtained from fossil fuels, one approach is to use cellulose-derived sustainable compounds because it is the world's most important renewable bio-feedstock each year. In this research project, initially the sustainable compound levoglucosenone (LGO), a bicyclic ketone, which is derived from cellulose by pyrolysis has been utilized to synthesize various forms of novel monomers bearing alkene functional groups. These monomer derivatives of LGO were subsequently cured via ultraviolet (UV)-initiated radical thiol-ene “click” chemistry with commercially available multifunctional thiols to obtain colourless, optically transparent cross-linked thermosets. The monomers prepared in this work are unique due to utilising the internal double bond of the LGO ring during polymerization as part of the cross-linked network. The thermal and mechanical properties along with the degradation of these thermosets were studied. These thermosets had glass transition temperatures between 0.3 and 37.4 °C, and good thermal stability of up to 300 °C.

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Abstracts (Poster Presentation)

Impact of Temperature and Concentration eluent on Retention Behavior of Inorganic Analytes in Hydrophilic Interaction Liquid Chromatography (HILIC)

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Hydrophilic interaction liquid chromatography (HILIC) is widely used for separating and analyzing polar compounds, especially those challenging to retain in nonpolar stationary phases. Its effectiveness with highly hydrophilic analytes makes HILIC valuable across fields like environmental analysis, clinical research, and inorganic chemistry[1, 2]. Recently, studies have demonstrated the retention of highly polar species, such as inorganic ions, using 100% aqueous eluents on commercial HILIC phases—a technique termed "reversed-HILIC" or "per-aqueous" liquid chromatography. Building on this approach, our study explores high-performance inorganic ion separations on novel fused-core silica particle-based hydrophilic columns (HALO 90 Å Penta-HILIC, 2.7 µm), employing low-concentration ammonium formate buffers (1.0–2.5 mM, pH 3.0) under varying temperature conditions. Efficient separation of inorganic anions was achieved and monitored using UV absorbance, demonstrating the effectiveness of this optimized HILIC method for high-resolution analysis of polar inorganic analytes.

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Deep low-frequency Raman spectroscopy for the characterisation of buried apatites

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The current method for classifying breast microcalcifications involves a routine mammogram with a subsequent invasive needle biopsy. However, only around 20% of needle biopsies of microcalcifications result in a cancer diagnosis meaning a majority of microcalcifications are benign.[1] Microcalcifications are broadly classified into 2 classes being Type I (Calcium Oxalate) which are benign and Type II (Calcium Hydroxyapatite) which can either be benign or malignant.[2] Further to this there is established literature that correlates substitution of other ions (Metals and Carbonate) into the hydroxyapatite lattice as potential diagnostic tools.[3-5]

Therefore, there is a clear need for the development of non-invasive, diagnostic tools that can classify these microcalcifications in situ with great precision. Key metrics that have been used in the literature to discriminate between subclasses of type 2 calcifications surround crystallinity and carbonate content.[3, 4, 6] As such, commonplace techniques such as X-ray diffraction (XRD) and vibrational spectroscopy which can probe these factors have been applied rather easily, to already extracted specimens. Where the literature lacks however is both a single catch all technique to assess both carbonate content and crystallinity as well as its ability to detect these factors both in situ and non-invasively.

Two such relatively recently developed techniques that can be combined are low frequency Raman which probes phonon modes related to the long-range order of molecules as well as spatially offset Raman which has the ability to collect a Raman spectrum below an external layer. Therefore, this project sets out to explore the application of spatially offset low frequency Raman spectroscopy (SOLFRS) along with a machine learning approach as a catch all diagnostic tool. Preliminary results surround the comprehensive characterisation of substituted apatites and the construction of a free space low-frequency Raman system

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Compositional Analysis of Commercially Sourced Cyrene™ Using Advanced Gas Chromatography Mass Spectrometry Techniques

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The shift towards using renewable resources and biomass for chemical feedstocks is essential for creating a greener, more sustainable chemical industry with reduced reliance on fossil fuels. This transition, particularly in the development of bioderived solvents, aligns with the Twelve Principles of Green Chemistry and is driven by the need to replace toxic petroleumbased solvents. Cyrene™ is a biosolvent produced by hydrogenation of levoglucosenone, a major product of wood pyrolysis. Produced from a naturally sourced biomass, Cyrene™ bears similar properties to dipolar aprotic solvents such as N,N-dimethylformamide (DMF), Nmethyl-2-pyrrolidone (NMP), and dimethyl sulfoxide (DMSO). Impurities in Cyrene™ can play a major role depending on its application as Cyrene™ is used in different applications such as environmental applications, synthetic chemistry and more closely regulated pharmaceutical industry.[1]

Headspace gas chromatography-mass spectrometry (HS-GCMS) is a powerful technique for analysis of very volatile organic compounds (VVOCs) in natural products, environmental samples, and samples obtained from industrial processes. In addition to HSGCMS analysis of VVOCs, volatile and semi-volatile organic compounds (VOCs and SVOCs)are determined using liquid injection gas chromatography mass spectrometry (LI-GC-MS)

In this research, both HS-GC-MS and LI-GC-MS have been employed to characterise VVOCs, VOCs and SVOCs in commercially sourced Cyrene™ biosolvent. Both techniques showed good repeatability, with relative standard deviation for VVOCs being lower than 7%, and for VOCs and SVOCs, being lower than 10%. Utilising these two techniques, more than 30 compounds, previously not being reported in commercially sourced Cyrene™, have been detected with more than 20 being positively identified. Furthermore, LI-GC-MS have been employed to identify VOCs and SVOCs and perform their quantitative analysis. Levoglucosenone, 2-methoxy phenol, sulfolane and p-cresol were identified as the major volatile and semi-volatile impurities in Cyrene™. Developed method for the quantitative analysis of these analytes showed good intra-day and inter-day repeatability, being < 5% and < 10%, respectively, reaching limits of detection and quantification below 500 ng/mL.

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Novel Super critical fluid chromatography – High-resolution mass spectrometry interface development

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Non-targeted analysis (NTA) using high resolution mass spectrometry (HRMS) has improved detection and identification of environmental contaminants. However, it has also brought to light the gap in what chemicals can be detected by common analytical techniques. Polar, ionic and zwitterionic compounds are particularly difficult to detect with conventional chromatographic separation. Super critical fluid chromatography (SFC) has re-emerged in the scientific space for its relevance in filling this gap, bringing novel selectivity through the use of supercritical CO^2 ($scCO^2$) [1,2].

A novel interface between HRMS and SFC is proposed for application to identifying environmental contaminants in groundwater. It is benefitted by novel selectivity usually requiring both normal and reverse phase liquid chromatography in a single chromatography method [2]. The interface consists of Ultra performance convergence chromatography (UPC^2), a binary make-up solvent pump and the 120 Exploris Orbitrap. Method development has been conducted using a number of environmental contaminants, pharmaceuticals, pesticides and contaminant indicators including sugars. This range of compounds has allowed for precise development of a UPC^2 method that expands on the polar and ionic compounds that can be separated using chromatography. Multiple parameters were optimised for the separation of polar compounds. Flow rates between 0.8 and 1.5 mL/min were tested, with the lower density supercritical CO_2 allowing for higher flow rates to be reached on an analytical grade column. The use of $scCO_2$, polar cosolvents and a polar Torus diol column allowed for high polar compound retention and the use of a cosolvent gradient prevented the need for long run times. Optimisation of ionisation parameters allowed standard compounds to be detected in both ionisation modes. Further improvements are needed to decrease peak broadening and improve ionisation sensitivity in mass detection. This interface is novel for NTA and has not been reported previously in literature for application to polar compound separation.

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Assessing the Impact of Tattoo Ink Laser Degradation Products on Skin Cell Viability: A Toxicological Investigation

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Tattoos have long been a feature of human culture. However, as the number of people getting tattoos grows, so does the number of people wanting to remove their tattoos. Laser tattoo removal is the most effective procedure, as it works by breaking down pigments into smaller particles, which are then transported away from the skin [1,2]. A limited number of studies have been conducted to specifically assess the toxicity of the chemicals in tattoo inks, and even fewer studies assess the toxicity of the products that are formed when tattoos are removed by laser treatment. Some research has identified hazardous, poisonous, and carcinogenic particles such as benzene, benzonitrile, hydrogen cyanide, and aniline [3].

In this research, pigments and tattoo inks were irradiated with QS Nd:YAG laser irradiation. GCMS and UV-Vis were used to characterise tattoo pigments, tattoo inks, and their laser products. Subsequently, the cytotoxicity of the tattoo inks and their laser fragments were assessed using HaCaT skin cells as a model, and cell viability was determined using the MTT assay.

The results obtained from the GC-MS and UV-Vis showed that o-toluidine and o-toluene isocyanate were the predominant fragments produced during laser treatment of pigments and inks. The MTT assay illustrated that cell viability decreased in a dose-dependent manner. Unirradiated pigments and inks decreased the cell viability to around 50%. In contrast, a significant cytotoxicity was observed at higher concentrations (50-150µg/mL) of irradiated pigments and tattoo inks. These results highlight potential health risks associated with laser tattoo removal, as the irradiation of tattoo inks, particularly at higher concentrations, significantly increases cytotoxicity, which may pose dangers to skin cells and overall tissue health.

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Preliminary data analysis for calibration and structure-property-activity relationships

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Calibration in analytical chemistry [1] establishes the relationship between a response (usually provided by an instrument as a signal) and known concentrations of an analyte, serving various purposes, including accuracy and reliability of measurements, compensations for instrument drift and variations and quantification of unknown samples. Structure-Property/Activity Relationships[2] are build on a similar principle, expressing a property and/or an activity as a function of chemical structure. In both instances, linear regression plays a pivotal role, not only because it is the simplest case of association, or because it is the most studied case, or because are available the most developed tools for analysis, but also because it is the most often encountered case in practice.

In most of the instances, because it is so simple, people forgot to check implicit assumptions regarding to the data, which include the normality of the data. Visually, normality is manifested by a bell shape of the data distribution, with symmetry around the mean value. However, a numerical analysis must accompany the preliminary analysis of the data, conducted with statistical tests. A combined use [3] of 8 statistical tests is reported here. Two sets of experimental data (from [4] and [5]) measured on pyrrolyl-acetic acid derivatives regarding their inhibitory activity serve as computational examples for preliminary data analysis.

In all cases under analysis, the assumption of normality of the data could not be rejected with 5% risk of error, which indicated that the posterior linear regression analysis was appropriate and valid regression models were obtained. The presence of outliers and/or extreme values leverages the regression [6] and should be disallowed from inclusion.

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Deep eutectic solvents (DES): A green method for the preparation of functional hydrogel-based materials

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Deep eutectic solvents (DESs) are a class of mixtures that are receiving much attention for their recent applications in sustainable materials synthesis.[1, 2] Similar to ionic liquids, DESs can possess a low melting point, exhibit low vapour pressures and are chemically and thermally stable. A noticeable advantage they hold over ionic liquids is their tunability – the ratio of constituent reagents can be tuned to precisely elicit desired physicochemical properties. They are also easily prepared with reagents from renewable sources.

This work investigates the development of eutectogels (hydrogels prepared from a DES) based on the methacrylic derivative of choline chloride. These gels were photo-polymerised under visible light using a xanthene dye. After polymerisation, the gels were purified via dialysis in water. The resultant eutectogels showed high swelling ratios, conductivity and antibacterial activity among other properties. These hydrogels do not require solvents to be prepared allowing them to be reagent-efficient (100% atom economy) with no waste, making them a green alternative to current preparation methods.

Physicochemical properties of both the DES-based resins and the resulting gels have been investigated including rheological properties, glass transition phenomena, thermal stability and their swelling capacity. Furthermore, eutectogel curing exhibited more rapid kinetics than the aqueous equivalent, suggesting 3D printing as a promising future direction.

We present this work for its possible future applications, indicating analytical and environmental chemistry via novel direct ink writing. This can be expanding into areas such as wearable sensors, in-field monitoring devices, and point-of-care applications.

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Towards more effective decontamination: Development of a bespoke test apparatus to analyse vapour from residual toxic chemical contamination

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Chemical warfare agents (CWAs) pose a threat to military personnel; both directly through contact or inhalation, and indirectly through degradation to operational tempo. In order to reduce the hazard of CWA contamination, effective methods to decontaminate military equipment and platforms are required. Defence Science and Technology Group (DSTG) plays a vital role in assessing and improving decontamination techniques. Historically, decontamination effectiveness has been assessed through analysis of residual contaminant remaining on a surface post decontamination. However, this only captures contact hazard. Secondly, contamination may become entrained in features of military equipment and vehicles that form capillaries (i.e. overlapping panels, screw threads, latches and etc.).

While entrainment of contamination may temporarily decrease contact hazard, it is unknown what the effect of vapour hazard is on military personnel. DSTG requires a test method that both captures potential vapour hazards and can effectively simulate CWA interaction with complex features.

DSTG have developed a bespoke testing apparatus to meet the above criteria. The test rig involves a small-scale chamber under steady state conditions. Constant flow of nitrogenenters the chamber where a test piece is spiked with a simulant for a toxic chemical. The gas flow through the chamber is then interrogated with atmospheric pressure mass spectrometry to determine the relative concentration of vapour caused by the residual contamination simulant in near real time. This allows for test and evaluation of decontamination technique and an assessment of vapour hazard. The development of this test rig and initial results involving small-scale test pieces that are both coated and uncoated will be discussed. Results indicate that surface coatings play a critical role in reducing the time it takes for contamination to evaporate from a surface. Further work is planned involving more intricate test pieces to emulate real-world features and material commonly found on military equipment

Soil Health Chip: A Cost-Effective and Portable Device for Precision Agriculture

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Nitrogen is the 2nd largest plant nutrient. It is essentially required for high-yielding and nutrient-exhaustive crop varieties. Therefore, maintaining the adequate soil-N level is imperative. However, injudicious application of N-fertilizers, without soil testing, has serious economic and environmental repercussions. The increased cost of crop production, rise in global temperature due to GHG emissions from agriculture, and algal blooms due to eutrophication are some of the examples of mismanagement of N in agriculture sector. Conventional soil testing techniques are costly, time consuming and labour-intensive. This study aims to develop a miniaturized device which will help to estimate soil ammonium level and urease enzymatic activity in the field, quickly, accurately and cheaply. The device developed using additive manufacturing (3D printing) could reduce the cost of crop production by better management of N fertilisers. It would also help to reduce leakage of excessive N to the environment by precise and site-specific application of N fertilisers.