10th Conference for Analytical Sciences in Ireland 2025

3rd and 4th July 2025
Devere Hall, UCC

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

School of Chemistry
Scoil na Ceimic

Book of Abstracts CASi 2025

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

School of Chemistry

Welcome

Welcome to the **10th Conference for Analytical Sciences in Ireland (CASi)**, at University College Cork (UCC). On behalf of the Royal Society of Chemistry Analytical Division, Republic of Ireland Sub-Region and the School of Chemistry here at University College Cork, it is with great pleasure that we can host the event in 2025. We are also celebrating 25 years since CASi first started back in 2000!

About CASi

CASi will take place in the Devere Hall, UCC on Thursday and Friday, 3rd and 4th July 2025. This will be the 10th CASi event where around one hundred and fifty researchers from across Ireland and beyond will meet to discuss advances in this interdisciplinary field, bridging the life sciences with Analytical chemistry. The conference will feature several international keynote and invited speakers, as well as contributed talks from Irish researchers and industry. There is also a significant poster session covering a broad range of Analytical topics with 32 posters being presented this year.

Many of the main universities and research institutes on the island of Ireland are well represented, in addition to international guests and participants. We have incredible sponsorship support from industry and a significant presence at the conference with talks and exhibitions.

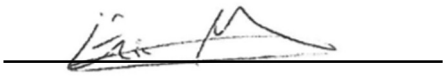
The programme reflects topics of interest to the Irish Analytical Community and speakers will represent experts across a variety of fields with a unique forum to discuss challenges and future opportunities within the academic, industrial and state agency sectors. QR code links to online pdf version.

Topics for CASi 2025 include:

- Green Analytical Chemistry
- Sensors, Actuators & PAT
- Separation Science
- Environmental Analysis
- Forensic Analysis
- Bioanalytical Chemistry
- Virtual Laboratories

Finally, none of this is ever possible without the generosity of our sponsors Royal Society of Chemistry, Cork Convention Bureau and our Gold, Silver and Bronze industry level sponsors

We hope you enjoy the event,



Steering Committee: RSC Analytical Division, Republic of Ireland Sub-Region

- Eric Moore, University College Cork (Chair)
- John Clancy, Henkel
- Aoife Morrin, Dublin City University
- Eithne Dempsey, Maynooth University
- Donal Leech, University of Galway
- Blanaid White, Dublin City University
- Aidan Dineen, Metrohm
- Ciara Machale, Eli Lilly
- Kevin Ryan, University of Limerick
- Eoin Gillespie, Atlantic Technological University Silgo
- Siobhan Moane, Technological University of the Shannon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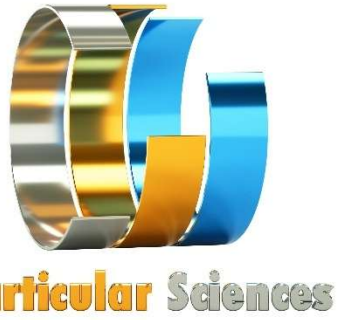

Particular Sciences


SCIENTIFIC
LABORATORY
SUPPLIES


Glantreo


Lilly

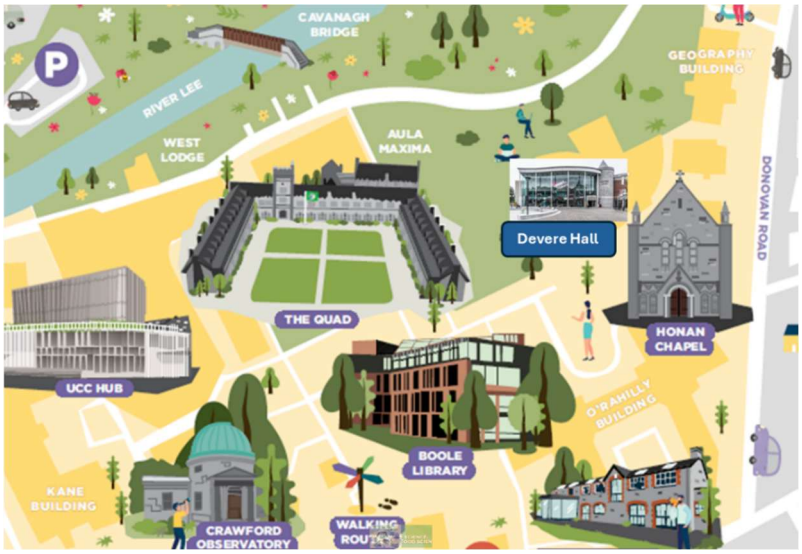

Labster


Eurachem
Ireland


ROYAL SOCIETY
OF CHEMISTRY


Johnson&Johnson

Maps, Directions & CASi 2025 Internet Access

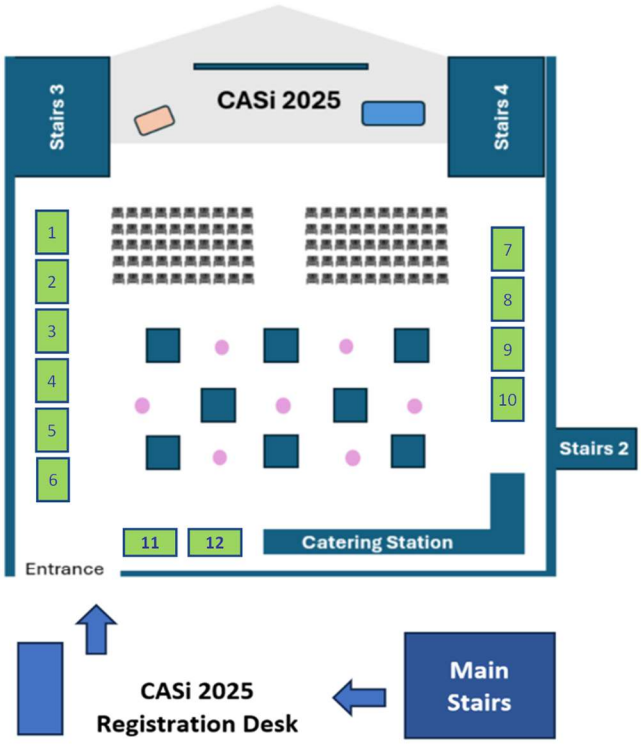


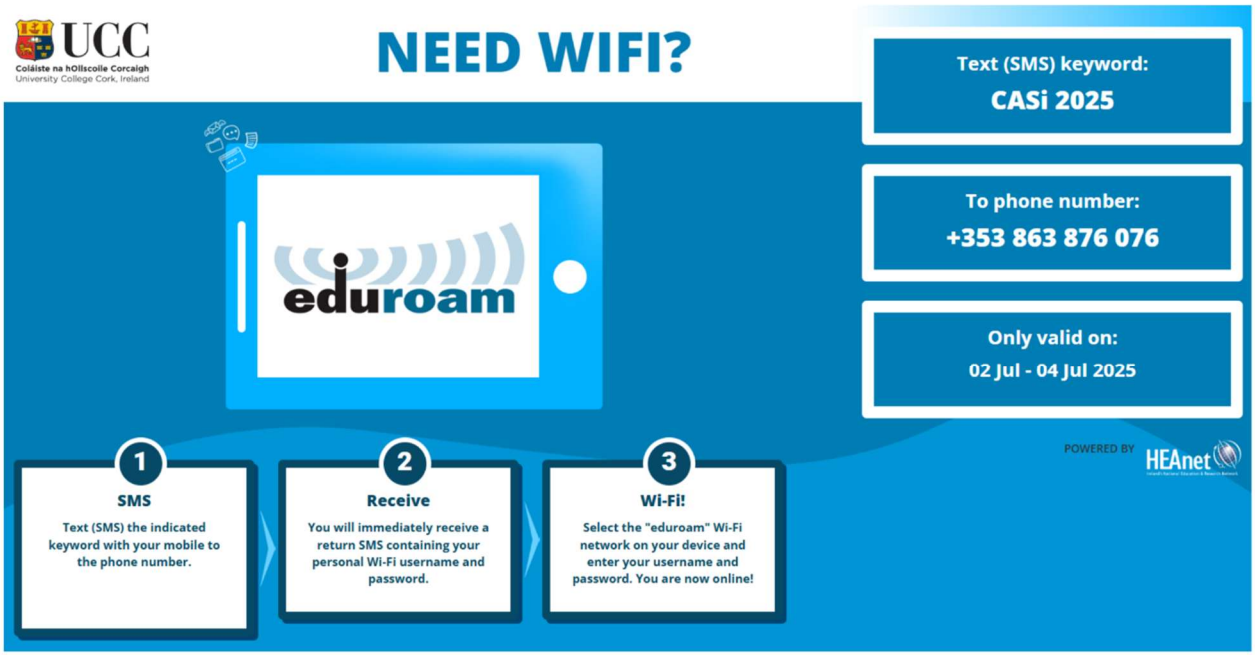
Map of UCC Campus – Venue for CASi 2025 is the Devere Hall

Devere Hall Floor Plan

Industry Exhibitor Booths

1. Labster
2. Anton Paar
3. Eli Lilly
4. Johnson & Johnson
5. Glantreo
6. Water Technology
7. Particular Sciences
8. MSD Brinny
9. Pfizer
10. Agilent
11. SLS Ltd
12. Avantor





Keynote Speakers

Green Analytical Chemistry (Session sponsor – RSC Separations Science Group)

Dr Ruth Godfrey (Associate Professor in Liquid Chromatography Mass Spectrometry, Medical School, Swansea University)
Ruth is an innovation academic, supporting the R&D of multinational companies, government agencies and SMEs. Her research focuses on analytical technologies and method development for medical/chemical analysis, with her most recent work concerning environmental medicine, mass spectrometry and sample preparation technology development. She has received grant funding (UKRI, EU, industry, charities etc), supervised postgraduate research students (MRes, MPhil and PhD) and performed consultancy work in separation science and mass spectrometry.

Biosensing and Sensors (Session sponsor – Johnson & Johnson)

Dr Marion Kennefick (Associate Director, Johnson & Johnson Innovative Medicine)
Marion currently serves as the Associate Director at Johnson & Johnson Innovative Medicine, where she leads a scientific team focused on Separation Sciences, specializing in method transfer, release, and stability testing for the JNJ clinical portfolio. With extensive experience as a subject matter expert in host cell proteins, Marion has overseen stability initiatives for advanced therapy clinical and commercial programs and has implemented laboratory automation for analytical techniques. With 15 years of experience in the biopharmaceutical industry, Marion holds a PhD in Microbiology, a MSc in Biotechnology, and a BSc in Zoology from University College Cork.

Forensic Analysis (Session sponsor – Agilent)

Mr Johnathan Spencer (LC-MS Applications Scientist, Agilent)
Jonny studied BSc Natural Sciences at the University of Nottingham, where he divided his studies between chemistry and biochemistry. He went on to study MSc Forensic Science at Sheffield Hallam University. Following graduation, he spent 2 years as a Confirmatory Analyst in an anti-doping and forensic toxicology lab, before joining Agilent as an LC-MS Applications Scientist. At Agilent, he focuses on small molecule applications using LC-TQ and LC-QTOF in fields like food, forensic and environmental analysis.

Environmental Analysis (Session sponsor – Particular Sciences)

Prof. Brett Paul (University of Tasmania)
Brett is a BSc, PhD and DSc graduate of the University of Plymouth, U.K. and a Professor of Analytical Chemistry at the University of Tasmania. His research sits at the interface of materials and analytical science, with a focus on analytical platform technologies to explore industrial and environmental systems. Brett is currently Director of the ARC Training Centre for Hyphenated Analytical Separation Technologies (HyTECH), a multi-partner industry supported research centre focussed on analytical technology development to meet complex end-user challenges.

RSC INTEREST GROUP SEPARATION SCIENCE

Agilent

Johnson&Johnson

Particular Sciences

Separation Science (Session sponsor – Pfizer)

Prof. Melissa Hana-Brown (Chair Analytical Chemistry, University College Cork)

Melissa's profile has combined a sandwich of academic and industrial research with a generous dose of professional society/board roles. She started her career in King's College London (Pharmacy) as a separation science lecturer before moving to Pfizer in 2006 where she had various roles (most recently as global Analytical Technology & External Strategic Innovation Lead) and simultaneously taught separation science Masters students as a Visiting Full Professor since 2011. During that same period, she had roles including President of the RSC Analytical Division, Member of RSC Council and she led the Pfizer Analytical Quality by Design work including representing Pfizer in the EFPIA efforts contributing to the recently introduced ICH Q14 guidance. In 2024, Melissa joined UCC as the Futures Pharmaceuticals Chair of Analytical Chemistry and is working hard on re-establishing her academic career, research group (and funding). Melissa's research focus is on separations method development and specifically the journey from 'molecule to green method'.

Bioanalytical Chemistry (Session sponsor – Eli Lilly)

Dr Mark Milford (Director Analytical, Eli Lilly)

Mark is an analytical scientist with over 25 years of industrial experience in the protein analytical field. Having gained a PhD from the University of Southampton (UK), Mark's industrial experience has spanned analytical roles in development, commercialization and routine manufacture of biopharmaceuticals, most recently in the analytical testing of monoclonal antibody products. Currently holding a position of Director - Analytical with Eli Lilly, based at the Kinsale manufacturing facility, Mark has technical oversight of analytical aspects of new product introduction and commercialization for biopharmaceutical drug substances, overseeing the analytical method lifecycle and driving analytical control strategy. Mark has a particular interest in analytical procedure development, validation and post-approval lifecycle from a large molecule perspective. As such, Mark holds the position of Industry Expert on the ICH Implementation Working Group for ICHQ2(R2) / ICHQ14, as well as Deputy Topic Lead for the EFPIA ICHQ2(R2) / ICHQ14 Support Group. Mark also holds a position on the EDQM Expert Group 6 – Biological and Biotechnological products, providing regular support for authoring and maintenance of European Pharmacopoeia monographs.

Virtual Labs (Session sponsor – Labster)

Prof. Eric Moore (School of Chemistry, University College Cork)

Eric heads the Separation and Sensing research group in the School of Chemistry at University College Cork focused on chemical and bio-sensing and separation. He leads a multi-disciplinary team of researchers whose principal research activities are focused on developing integrated bio/sensor platforms, separation techniques, surface attached chemistry, electrochemical analysis and micro-fluidics. He is an Academic member within the Life Science Interface group at Tyndall National Institute and a Principal Affiliate at the Environmental Research Institute, University College Cork. He has extensive linkages with the pharmaceutical, biopharmaceutical, biomedical device, environment and food/beverage sectors. He has championed postgraduate education, especially at the MSc level and is dedicated to providing high calibre industry ready graduates. He is currently the Vice Dean for Graduate Affairs in the College of Science, Engineering and Food Science.

Pfizer Lilly Labster

10th Conference for Analytical Sciences in Ireland 2025

Wednesday 2nd July

Special Remembrance Event for Prof. Jeremy Glennon
2:30-4:30pm in the Aula Maxima, UCC

- Prior to event special Tree Planting Ceremony at 1:15pm
- Lifetime Achievement Award presented to Family of Prof. Glennon at 4:15pm

Tours
4:30-6:30pm (depart from Aula Maxima)

- 2 tours (one at 4:30pm and other at 5:30pm)
- Short tours of the Science Studio between 4-6pm

RSC Analytical Division, Republic of Ireland Sub-Region Committee Meeting 6-7pm Northwing Conference Room

CASi Reception
6:30-9pm in the Aula Maxima, UCC

- CASi pre-registration from 6:30pm in the Aula Maxima
- Welcome video at 7pm
- Music from 7:15pm (Traditional Irish Music – Uillean Ceoil)
- Drinks and finger food reception from 7:30pm

10th Conference for Analytical Sciences in Ireland 2025

Thursday 3rd July

Welcome & Opening of Conference Day 1	
08:30 – 09:10	Registration, Poster display and Industry Exhibitor setup
09:10 – 09:20	Welcome (Prof. Eric Moore, Conference Chair, UCC) and Welcome Video
09:20 – 09:30	Opening Address (Prof. Anita Maguire, Head of School, Chemistry, UCC)

Session 1 – Green Analytical Chemistry	Chair: John Clancy (Henkel)
09:30 – 10:00	**Keynote Speaker:** Ruth Godfrey, University of Swansea. "Sustainable Analytical Science: Future-Proofing Methods From Bench to Field"
10:00 – 10:15	**Oral 1:** Christopher Kent, University College Cork. "Optimizing parameters for solar electrolysis of water to yield green H2 using Broadband Acoustic Resonance Dissolution Spectroscopy"
10:15 – 10:30	**Oral 2:** Pankaj Kumar, Teerthanker Mahaveer University. "Graphitic Carbon Nitride-ZnO Nanocomposites as Efficient Cold Field Emission in Green Energy Applications"
10:30 – 10:45	**Oral 3:** Jessica Smith Osorio, University of Limerick. "Advancing Quantification Standards: Coulometric Titration Validation for Potassium Hydrogen Phthalate"
10:45 – 11:00	**Oral 4:** Niamh O'Mahony, University College Cork. "Rapid determination of the active pharmaceutical Ingredient (API) content of suspension formulations using Broadband acoustic resonance dissolution spectroscopy (BARDS)"
11:00 – 11:30	Tea/Coffee, Networking and Poster Viewing

Session 2 – Biosensing and Sensors	Micheal Scanlon (University of Limerick)
11:30 – 12:00	**Keynote Speaker:** Marion Kennefick, Johnson and Johnson. "An Overview of Host Cell Proteins in Manufacturing and Analytical Processes"
12:00 – 12:15	**Oral 5:** Mohamed Sharafeldin, University College Cork. "Accessible Hepatitis C Virus (HCV) Diagnostics via Unamplified Nucleic Acid Detection"
12:15 – 12:30	**Oral 6:** Atieh Mousavi, Tyndall National Institute. "Enabling early detection of ovarian cancer using a novel electrochemical sensing platform"
12:30 – 12:45	**Oral 7:** Dinakaran Thirumalai, Dublin City University. "A sensitive non-enzymatic lactate sensor based on pulse electrodeposited nickel oxide on carbon electrode"
12:45 – 13:00	**Oral 8:** Justina Ugwah, Tyndall National Institute. "A pilot study evaluating the performance of a prototype impedance sensor integrated on a biopsy needle for breast cancer detection"
13:00 – 14:00	Lunch, Networking and Poster Viewing

Session 3 – Forensic Analysis	Chair: Elizabeth Gilchrist (University College Cork)
14:00 – 14:30	**Keynote Speaker:** Johnathan Spencer, Agilent. "Next Generation Forensic Screening using Accurate Mass High Resolution Mass Spectrometry"
14:30 – 14:50	**Invited Speaker:** Anjan Roy, Coherent Corp (USA). "Applications of THz-Raman spectroscopy"
14:50 – 15:05	**Oral 9:** Yineng Wang, Tyndall National Institute. "Development of a mobile CE workstation with a C4D detector for rapid detection of organophosphates under CBRN field conditions"
15:05 – 15:20	**Oral 10:** John Moran, Forensic Science Ireland. "Using a portable Near-Infrared Spectroscopy (NIRS) instrument with chemometrics for rapid drugs analysis: A recent evaluation at Forensic Science Ireland"
15:20 – 15:35	**Oral 11:** John Moriarty, Department of Agriculture. "Veterinary Toxicology and Geochemical Risk"
15:35 – 16:00	Tea/Coffee, Networking and Poster Viewing

Session 4 – Environmental Analysis	Chair: Eithne Dempsey (Maynooth University)
16:00 – 16:30	**Keynote Speaker:** Brett Paul, University of Tasmania. "Taking Chromatographs out into the Field"
16:30 – 16:50	**Invited Speaker:** Isabelle Ourliac-Garnier, Nantes University. "Unravelling Sterol Biosynthesis in Fungi: Where Analytical Chemistry Meets Medical Mycology"
16:50 – 17:05	**Oral 12:** Micheal Scanlon, University of Limerick. "Electrosynthesis of Free-Standing Conducting Polymer Thin Films at a Polarized Liquid|Liquid Interface for Electroanalytical Applications"
17:05 – 17:20	**Oral 13:** Dean Venables, University College Cork. "Chemical analysis of the atmosphere — Towards sensitive, fast, and lower cost spectroscopic sensors"
17:20 – 19:30	Drink Reception, Networking and Poster Viewing

Conference Social Event

Mardyke Entertainment Complex 8-10pm

- Fun interactive evening with table tennis, pool, darts and shuffle board
- Finger food and refreshments

Mardyke Entertainment Complex, Sheares Street, Cork (T12 CX7A)

10th Conference for Analytical Sciences in Ireland 2025

Friday 4th July

Welcome & Opening of Conference Day 2	
08:30 – 09:20	Registration, Poster display and Industry Exhibitor setup
09:20 – 09:30	Welcome (Prof. Eric Moore, Conference Chair, UCC) and Announcements

Session 5 – Separation Science	Chair: Donal Leech (University of Galway)
09:30 – 10:00	**Keynote Speaker:** Melissa Hanna-Brown, University College Cork. "Pills, Pressure, and Parting Ways: Innovative Separation in Modern BioPharma"
10:00 – 10:20	**Invited Speaker:** John Lough, University of Sunderland. "Eiroshell™-Enabled Extension to LC Method Development Screening Approaches"
10:20 – 10:40	**Invited Speaker:** Ryan Osborne, Pfizer. "An Approach to Method Development in SFC Leveraging Machine Learning for the Development of a Late-Stage Oncology Drug Candidate"
10:40 – 10:55	**Oral 14:** Ilaria Neri, University of Naples Federico II. "Biomimetic chromatography-based investigation of environmental contaminants toxicity and biological barrier permeation"
10:55 – 11:30	Tea/Coffee, Networking and Poster Viewing

Session 6 – Bioanalytical Chemistry	Chair: Ciara MacHale (Eli Lilly)
11:30 – 12:00	**Keynote Speaker:** Mark Milford, Eli Lilly. "The Mystery of the Disappearing Excipient: An Analytical Case Study, Investigating a Reduction in Polysorbate Content in a Monoclonal Antibody Drug Substance"
12:00 – 12:15	**Invited Speaker:** Ruchi Gupta, University of Birmingham. "Hydrogel Lollipops for Early Detection of Cancer"
12:15 – 12:30	**Oral 15:** Aine O'Brien, Maynooth University. "Chemoenzymatic Glycoengineering of Monoclonal Antibodies"
12:30 – 12:45	**Oral 16:** Alan Ryder, University of Galway. "Polarized Excitation Emission Matrix (pEEM) spectroscopy for the rapid, non-destructive analysis of proteins"
12:45 – 13:00	**Oral 17:** Somali Dhal, Tyndall National Institute. "Optical Evaluation of the Impact of Filtration on Diagnostic Salivary Components"
13:00 – 14:00	Lunch, Networking and Poster Viewing

Session 7 – Virtual Labs	Chair: Aoife Morrin (Dublin City University)
14:00 – 14:30	**Keynote Speaker:** Eric Moore, University College Cork. "Future Proofing Learning and Teaching through Gamification and VR Laboratories"
14:30 – 14:50	**Invited Speaker:** Charlotte Hamblet, Labster. "What If Your Toughest STEM Courses Became Your Students' Success Stories?"
14:50 – 15:05	**Oral 18:** Janine Boertjes, University College Cork "Development of a Virtual Reality Capillary Electrophoresis Experiment for Postgraduate Chemistry Education"
15:05 – 15:20	**Oral 19:** Heather Myler, Beyond Labz. "How to Teach Scientific Inquiry with Beyond Labz"
15:20 – 15:50	Tea/Coffee, Networking and Poster Viewing
15:50 – 16:30	Presentation of Awards to Oral and Poster winners
16:30 – 17:00	Close of CASi 2025 (Conference Chair: Prof. Eric Moore, UCC)

CASi 2025 Awards

- Agilent Presentation Gold Award
- Eli Lilly Presentation Gold Award
- Johnson and Johnson Presentation Gold Award
- RSC Separation Science Group Presentation Award
- Merck Sharp and Dohme Poster Silver Award
- Particular Sciences Poster Silver Award
- Pfizer Poster Silver Award
- RSC Separation Science Group Poster Award
- Eurachem Ireland Poster Award
- Eurachem Ireland Poster Award
- Analytical Methods Poster Award
- Analyst Poster Award

Analyst 150 YEARS ANNIVERSARY

Pfizer

Particular Sciences

Eurachem Ireland

Agilent

MSD

Analytical Methods

Johnson&Johnson

Lilly

RSC INTEREST GROUP SEPARATION SCIENCE

Sustainable Analytical Science: Future-Proofing Methods From Bench to Field

Dr Ruth Godfrey

Swansea University Medical School, Swansea University, Singleton Park, Swansea, UK, SA2 8PP

Abstract:

As the pressures of climate change and resource scarcity intensify, the demand for efficient, sustainable, and greener analytical approaches becomes increasingly urgent. These methods are essential for ensuring long-term resilience and adaptability across a range of sectors, including pharmaceuticals, smart materials manufacturing, healthcare, and environmental monitoring.

This session will explore the concept of *sustainable-by-design* analytical science—approaches that are not only environmentally conscious but also automated, portable, miniaturised, and robust across diverse operational settings. We will highlight how to assess methods, with innovations that reduce energy consumption, minimise waste, and streamline instrumentation through compact, integrated systems. Particular emphasis will be placed on reducing reliance on multi-method and multi-instrument workflows, advancing field-deployable, low-power platforms and modular technologies designed for scalability, accessibility, and long-term impact.

Optimizing parameters for solar electrolysis of water to yield green H_2 using Broadband Acoustic Resonance Dissolution Spectroscopy

Mr. Christopher Kent[1,2], Mr. Alex Knowles.[1], Mr. Ailbhe Ó Manacháin.[1,2,3], Prof. Colm O'Dwyer.[1,3], Dr Dara Fitzpatrick.[1,2]

[1]School of Chemistry, The Kane building, University College Cork, Cork City, Ireland, [2]Analytical and Biological Chemistry Research Facility, University College Cork, Cork City, Ireland, [3]Enviromental Research Institute, Ellen Hutchins Building, Lee Road, University College Cork, Cork City, Ireland, [4]Tyndall National Institute, Lee Maltings Complex, Dyke Parade, University College Cork, Cork city , Ireland

Abstract:

The use of abundant earth materials for novel electrodes for solar driven electrolysis will play a significant role in the future production of hydrogen as a green energy source. The choice of electrolyte will play a major role in how efficient and stable future photoelectrochemical cells (PEC) operate. A new approach to determining PEC efficiency using Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS) is investigated to analyze the real-time production of hydrogen and oxygen at platinum electrodes in different electrolyte solutions. The parameters investigated include concentration of electrolyte, surface area of the electrode and the potential applied to the cell. Here, we show the suitability of neutral buffer as an electrolyte on a par with either acid or basic electrolytes. This finding allows for the potential design of solar to hydrogen electrolysers which can operate under mild, neutral and stable conditions using earth abundant materials for hydrogen production. It is also shown how BARDS can readily visualize and track gas evolution in real-time and in-situ in an open system without the need for gas collection. We anticipate that the technique can be utilized in the future evaluation of newly developed electrode materials in terms of efficiency, stability and life span.

Acknowledgements

This project has received funding from the European Union under grant agreement No 101084261 (FreeHydroCells). Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or CINEA. We also acknowledge support from the Irish Research Council under an Advanced Laureate Award (IRCLA/19/118). This work is partly supported by an Enterprise Ireland Commercialisation Fund as part of the European Regional Development Fund under contract no. CF-2018-0839-P.

Keywords

Electrochemistry, spectroscopy, water splitting

Graphitic Carbon Nitride-ZnO Nanocomposites as Efficient Cold Field Emission in Green Energy Applications

Mr. Pankaj Kumar[1], Dr Diptonil Banerjee[2]
[1]Teerthanker Mahaveer University, Moradabad, INDIA, [2]Teerthanker Mahaveer University, Moradabad, INDIA

Abstract:

Zinc oxide (ZnO) has emerged as a promising material for cold field emission (CFE) applications due to its unique electronic properties, high aspect ratio nanostructures, and excellent chemical stability. However, the performance of pure ZnO in field emission devices remains limited by its moderate electrical conductivity and electron mobility. In this work, we explore the enhancement of CFE characteristics by synthesizing graphitic carbon nitride (g-CN)-ZnO nanocomposites, aiming to optimize their performance for use in electron guns and contribute to the advancement of green energy technologies.

ZnO and g-CN-ZnO nanostructures were synthesized via a hydrothermal process and characterized using X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDX), and contact angle (CA) measurements. XRD revealed the nanostructure's crystalline quality and confirmed the successful integration of g-CN into the ZnO lattice. The FESEM images showed uniform, rod-like structures, with g-CN incorporation leading to the formation of surface wrinkles, which enhanced the density of emission sites. The surface energy was calculated from the water contact angle data.

The current density-field (J-E) measurements indicate superior field emission characteristics, including a lower turn-on field and higher emission current density for the g-CN-ZnO composite. These improvements suggest that the g-CN-ZnO nanostructures significantly enhance the efficiency of cold field emission. The enhanced CFE properties, combined with the potential for low-energy consumption and high efficiency, make this nanocomposite a promising candidate for green energy applications. Specifically, the optimized electron emission can contribute to the development of more efficient vacuum electronics, such as electron guns in green energy devices, where low power consumption and sustainability are crucial. The findings present a viable pathway toward efficient hydrophobic electron gun technology in vacuum electronics, supporting the transition to greener and more sustainable energy solutions.

Acknowledgements

Teerthanker Mahaveer University

Keywords

ZnO, g-CN, CFE, Green Applications

Advancing Quantification Standards: Coulometric Titration Validation for Potassium Hydrogen Phthalate

Mrs. Jessica Smith Osorio[1,2], Professor Andrea P Sandoval-Rojas[2], Henry Torres Quezada[2], Professor Jesús A. Ágreda Bastidas[2]

[1]University of Limerick, Limerick, Ireland, [2]Universidad Nacional de Colombia, Bogotá D.C, Colombia

Abstract:

Certified reference materials (CRMs) play a critical role in both industry and scientific research.[1] Their quantification requires highly specialized techniques known as "primary method".[2] Potassium hydrogen phthalate (KHP) is widely used as standard in acid-base titrations and pH buffers preparation.[1] Therefore, National Metrology Institutes (NMIs) around the world are responsible for implementing primary methods such as coulometry for its certification.[2] Coulometry enables the direct quantification of a substance by relating it to the charge required to complete a chemical reaction.
In the coulometric titration of KHP, three steps are typically involved: i) an initial titration to quantify the initial acidic impurities present in the sample, ii) The main titration accounting for approximately 99.8% of the sample, and iii) a final titration. Traditionally, nonlinear regression using an exponential W-function has been employed to determine the amount of substance.[2,3]

In this work, we propose a novel approach based on a mathematical model derived from the theoretical titration curve (TC) of KHP. This method offers a key advantage: it corrects the effect of carbon dioxide as its main impurity and the direct estimation of the KHP concentration. The TC approach yielded a significantly lower relative uncertainty (0.102%) compared to the traditional method eWf (0.247%).[4] Furthermore, two factorial experimental design was implemented to evaluate the effects of coulometric cell geometry (vertical vs. horizontal), and the convection mode (magnetic stirring vs ultrasound), on the accuracy of the titration. While no statistical difference was found between cell geometries, magnetic stirring produced the most accurate results. The optimization and validation of this coulometric method contributed to a substantial reduction in the overall uncertainty associated with the certification of KHP at the National Metrology Institute of Colombia.

References

(1) Máriássy, M.; Pratt, K. W.; Spitzer, P. Major Applications of Electrochemical Techniques at National Metrology Institutes. Metrologia 2009, 46, 199–213. https://doi.org/10.1088/0026-1394/46/3/007.
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(4) Smith-Osorio, J. L.; Torres-Quezada, H.; Sandoval-Rojas, A. P.; Ágreda, J. A. Implementation of the Theoretical Coulometric Titration Curve in the Determination of the Amount of Substance of Potassium Hydrogen Phthalate: The Search for a Better Metrological Approach. ACS Omega 2022, 7 (51), 47851–47860. https://doi.org/https://doi.org/10.1021/acsomega.2c05642.

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Rapid determination of the active pharmaceutical Ingredient (API) content of suspension formulations using Broadband acoustic resonance dissolution spectroscopy (BARDS)

Dr Niamh O'Mahoney[1,2], Dr Dara Fitzpatrick[1,2]
[1]School of Chemistry, The Kane building, University College Cork, Cork City, Ireland, [2]Analytical and Biological Chemistry Research Facility, University College Cork, Cork City, Ireland

Abstract:

Oral suspension formulations are advantageous over other drug dosage methods due to ease of administration, swallowability and taste masking. A large market exists for this particular form of drug introduction, particularly among paediatric and geriatric patients. This paper highlights a proof of concept approach to an alternative quality control test for oral suspension formulations using Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS). BARDS measurements are based on reproducible changes in the compressibility of a solvent during the dispersion of a formulation, which is monitored acoustically via associated changes in the frequency of induced acoustic resonances. This study offers a new approach to tracking the loading of oral suspension formulations. Suspension formulations containing various Active Pharmaceutical Ingredients (APIs) and excipients were investigated to examine the effect of API dosage and formulation on their overall dissolution. The data shows oral suspension formulations have an intrinsic acoustic signature specific to their manufacturing and formulation composition. It was also found that the level of API present determines the acoustic response. BARDS represents a possible future surrogate for In-Process Control (IPC) testing as a Process Analytical Technology (PAT) method. It also offers an alternative approach to assessing patient compliance and for determining drug precipitation. This study represents a greener, cost-effective, and time-efficient product testing method with no requirement for organic solvents or high-end instrumentation.

Acknowledgements

We wish to thank the National University of Ireland (NUI) Awards for Niamh O'Mahoney's PhD funding.

Keywords

ANALYSIS, Spectroscopy, Oral FORMULATION, Precipitation

An Overview of Host Cell Proteins in Manufacturing and Analytical Processes

Dr Marion Kennefick

Johnson and Johnson, Ringaskiddy, Co. Cork, Ireland

Abstract:

Host cell proteins (HCPs) are considered process impurities in the manufacturing of biopharmaceutical antibodies, posing considerable analytical challenges for precise detection and quantification due to their inherent variability in upstream pharmaceutical processes. This presentation will provide a comprehensive overview of HCPs throughout both upstream and downstream development phases, the advancement of analytical methodologies, and the regulatory expectations set forth by health authorities.

Accessible Hepatitis C Virus (HCV) Diagnostics via Unamplified Nucleic Acid Detection

Dr Mohamed Sharafeldin

School of Chemistry, University College Cork, Cork, Ireland

Abstract:

Hepatitis C Virus (HCV) remains a significant public health burden in Egypt, and other areas with limited resources, where access to affordable and rapid diagnostic tools is essential for effective disease management. Current gold-standard methods, such as PCR and isothermal amplification, though accurate, are costly, labor-intensive, and time-consuming, posing major barriers to widespread application. In this work, we present an accessible and cost-effective diagnostic platform for the direct detection of HCV RNA without the need for amplification. The approach employs the crosslinked Enhanced Emission (CEE) effect triggered by the interaction between fluorescent amino-functionalized, silica-coated nitrogen-doped carbon dots (N-CDs/SiO_2/NH_2) and magnetically extracted HCV RNA from patient samples. This interaction results in a rapid and significant fluorescence enhancement, allowing direct detection of unamplified viral RNA. The method was applied both in a conventional 96-well plate format and a portable, semi-automated, 3D-printed microfluidic chip. The chip-based assay achieved a detection limit of 500 IU/mL and a turnaround time of less than 20 minutes, while the well-plate format showed comparable performance with a 1000 IU/mL detection limit. Evaluation of 141 clinical samples demonstrated high diagnostic accuracy, with 96.47% sensitivity and 98.79% specificity.

Enabling early detection of ovarian cancer using a novel electrochemical sensing platform

Ms. Atieh Mousavi[1,2], Professor Michael Thompson[3], Dr Paul Galvin[1], Dr Sofia Rodrigues Teixeira[1]

[1]Tyndall National Institute, University College Cork, Cork, Ireland, [2]School of Biochemistry & Cell Biology, Cork, Ireland, [3]Department of Chemistry, University of Toronto, Toronto, Canada

Abstract:

Ovarian cancer (OC) is the deadliest gynecological cancer, affecting 300,000 women annually. CA125, the current screening marker, lacks reliability for early detection, missing 20% of cases, and is also known to result in both positive and negative assays. Despite a 90% chance of survival within five years if detected at stage I, only 25% of cases are detected due to inadequate screening methods and initials symptoms. Our research involves the development of a disruptive multiplexed near-patient diagnostic solution, to enable early detection of Stage I and II OC using three different biomarkers.

Gold flexile electrodes were modified with a polymer layer and the antibodies of interest, anti-HE4 and anti-CA125, were immobilized on the surface of electrodes. Preliminary results show that the sensor has a linear range of 0.1 fg/ml to 10 pg/ml and 10 fg/ml to 1 ng/ml for HE4 and CA125 respectively. The sensitivity of 0.31 and 0.53 KΩ.mm2/ml were calculated for HE4 and CA125 in sequence.

This diagnostic device shows a novel high sensitivity electrochemical sensor platform, in which the combination of multiple biomarkers facilitates a high level of accuracy.

Acknowledgements

This research was funded in part from the Insight Research Ireland Centre for Data Analytics (grant number 12/RC/2289-P2

Keywords

Immunosensor, Ovarian cancer, CA125, HE4

A sensitive non-enzymatic lactate sensor based on pulse electrodeposited nickel oxide on carbon electrode

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[1]Insight Research Ireland Centre for Data Analytics, School of Chemical Sciences, Dublin City University, Dublin 9, Ireland

Abstract:

Lactate serves as an analytical biomarker with significant implications in continuous monitoring for sports medicine and clinical diagnostics. Elevated lactate levels are frequently associated with pathological conditions such as hypoxia, seizures, and trauma or shock, thereby underscoring the need for accurate and real-time detection in physiological fluids. In this study, we report the development of a highly sensitive, non-enzymatic lactate sensor fabricated via pulse electrodeposition of nickel oxide (NiO) onto a glassy carbon electrode (GCE). Electrochemical characterization of the sensor was performed using cyclic voltammetric and amperometric measurements within a conventional three-electrode system. The sensor demonstrated a detection limit of 0.17 µM, which is significantly better than recent reports. This suggests its potential utility in developing robust analytical methodologies for quantifying lactate in serum and other biological samples.

Acknowledgements

This work has emanated from research supported under the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101034252

Keywords

Lactate, seizure, electrodeposition, electrochemical sensor

A pilot study evaluating the performance of a prototype impedance sensor integrated on a biopsy needle for breast cancer detection

Dr Justina Ugwah[1,5], Darren Dahly[6], Edel Whelton[1,5], Dr Yineng Wang[1,5], Ann-Marie O'Donovan[3], Brian D.O. Donnell[4], Prof. Martin J.O'Sullivan[2], Prof. Eric J. Moore[1,5].

[1]Science & Separation group, School of Chemistry, University College Cork

[2]Department of Surgery, Cork University Hospital, Cork

[3]Department of Pathology, Cork university Hospital, Cork

[4]Department of Anaesthesia, Cork University Hospital, Cork

[5]Life Sciences Interface, Tyndall National Institute, University College Cork, Ireland

[6]HRB Clinical Research Facility Cork, School of Public Health, University College Cork

Abstract:

Breast cancer ranks as the second most prevalent malignancy among women worldwide. While diagnostic imaging has advanced significantly, an unmet clinical need exists for real-time, intraoperative tissue characterization during breast biopsy procedures. We investigated a novel bioimpedance needle sensor that provides quantitative measurements of tissue electrical properties, aiming to evaluate its potential as a risk stratification tool and inform the design of future large-scale clinical validation studies.

In this prospective pilot study, we evaluated a bioimpedance needle sensor using paired tissue samples (healthy tissue and mass of concern) obtained from 55 patients undergoing excisional breast biopsy at Cork University Hospital. Bioimpedance measurements were analyzed against corresponding histopathological findings to assess diagnostic performance.

Analysis revealed significantly distinct impedance signatures between malignant and healthy breast tissues, characterized by differential spectral patterns. The diagnostic model achieved robust discriminative performance (C-statistic >0.80), with clinically relevant sensitivity and specificity values suitable for preliminary validation.

The bioimpedance needle sensor demonstrated potential as a real-time detection tool during breast biopsy procedures. This technology may reduce sampling redundancy and enhance diagnostic precision in clinical practice. While these initial results are promising, in-vivo validation studies are necessary to confirm these findings and establish clinical utility.

Acknowledgements:

We would like to thank Enterprise Ireland for funding through the Enterprise Ireland Commercialisation Fund.

Keywords:

Breast Cancer, Bioimpedance, Real-Time Detection, Ex-Vivo Study

Next Generation Forensic Screening using Accurate Mass High Resolution Mass Spectrometry

Johnathan Spencer

Agilent Technologies

Abstract:

Forensic screening by liquid chromatography coupled with mass spectrometry (LC/MS) has largely been dominated by triple quadrupole (TQ) instrumentation. LC/TQ conveniently meets the requisite sensitivity, selectivity and dynamic range while offering practical benefits such as ruggedness and simplicity of data handling. Compared to TQ instruments, high resolution accurate mass spectrometry such as quadrupole time-of-flight (QTOF) instruments offer significantly more versatility: QTOFs are typically operated in non-targeted acquisition modes, offering the possibility to perform targeted quantitation and screen for evidence of thousands of suspect analytes in a single method, perform retrospective analysis for emerging analytes of interest in historic data, and even ton attempt to identify unknown components in samples. Because QTOF data is more complex than TQ data, following an appropriate data analysis workflow to streamline and simplify QTOF screening is key for any routine testing lab. This talk will explore how the MassHunter Quantitative Analysis software can be utilised to make QTOF screening as easy and accessible as possible and will also cover some of the key tools that are available to QTOF screening analysts, like the MassHunter Screener Tool and retention time prediction.

Applications of THz-Raman Spectroscopy

Dr Anjan Roy

Coherent Corp

Abstract:

THz-Raman spectroscopy extends traditional Raman spectroscopy into the low-frequency or "Terahertz regime," capturing both chemical and structural spectral signatures. This technique enhances sensitivity and improves identification and analysis of a wide variety of materials, including pharmaceuticals, explosives, and biologicals, offering a unique solution for comprehensive material characterization. Ease of sampling and the fact that low frequency Raman modes are often an order of magnitude larger in intensity makes THz-Raman a powerful technique.

Development of a mobile CE workstation with a C4D detector for rapid detection of Organophosphates under CBRN field conditions.

Dr Yineng Wang[1,2], Dr Xi Cao[1,2], Dr Walter Messina[1,2], Ed van Zalen[3] and Prof. Eric Moore[1,2]

[1]Science & Separation group, School of Chemistry, University College Cork

[2]Life Science Interface, Tyndall National Institute, Cork, Ireland

[3]Netherlands Forensic Institute, The Hague, Netherlands

Abstract:

The objective of this research is to develop a comprehensive solution for accurately and rapidly analysing suspected chemical agents at forensic sites. To reduce the time required to send samples to a forensic laboratory, this study aims to enable real-time data collection for mobile forensic analysis. The proposed system is designed to be portable and capable of operating directly at the crime scene.

This research explores the compatibility of Capillary Electrophoresis (CE) with Capacitively-Coupled Contactless Conductivity Detection (C4D) technology on a miniaturised microfluidic chip device. It compares the practicality of using high-cost, sophisticated micro/nanofabricated silicon chips with that of low-cost, disposable polymer microchips.

The outcome of the project is an integrated chemical analysis workstation tailored for mobile, on-site forensic tasks. This research forms part of a sub-work package within the EU FP7 GIFT (Generic Integrated Forensic Toolbox) programme.

Using a portable Near-Infrared Spectroscopy (NIRS) instrument with chemometrics for rapid drugs analysis: A recent evaluation at Forensic Science Ireland

John Moran

Forensic Science Ireland, Dublin, Ireland

Abstract:

As drug trends continue to evolve across Europe, with increasing analytical complexity, forensic laboratories are dealing with an ever increasing volume of exhibits which has resulted in capacity issues. Recently, a handheld near-infrared (NIR) spectrometer combined with chemometric modelling, has been trialled at Forensic Science Ireland (FSI) for the rapid analysis of plant material, powders, and tablets.

FSI have evaluated the NIRLAB system, which uses a portable spectrometer. The system connects to a smart phone via Bluetooth and uses the NIRLAB app on a phone or tablet. A variety of routine casework samples analysed with the NIRLAB system were benchmarked to the well-established forensics techniques such as gas chromatography–mass spectrometry (GC-MS) and thin-layer chromatography (TLC).

True positive and false positive analysis was performed across a range of controlled and non-controlled substances. The findings show that the instrument combined with a chemometrics approach, offers a rapid, non-destructive, and chemical-free method for preliminary drug screening, and it can also offer quantification results for a range of controlled substances. The trial has highlighted many potential uses of the analytical tool in the workflow of a forensics drugs laboratory and for early-stage triage. Additionally, the portability of the instrument means it can be utilised at crime scenes and give quick results for large off-site drugs seizures.

Veterinary Toxicology and Geochemical Risk

John Moriarty

Biochemistry/Toxicology Section, Pathology Division, Department of Agriculture, Food & Marine Laboratories, Backweston.

Abstract:

The Veterinary Biochemistry & Toxicology section of the Department of Agriculture, Food & Marine (DAFM) Laboratories provides diagnostic support for animal health investigations, interagency investigations and surveillance. It also carries out special studies and risk assessments on toxicants for DAFM when required.

Lead is a common cause of poisoning in animals and sources include access to car batteries or natural consumption of geochemically enriched soils while grazing. Though outbreaks have reduced in number over the last few years, they still present an animal welfare and food safety concern, therefore outbreaks are actively managed to secure the food chain.

A predictive model for lead depletion in tissues of sheep was developed from studies on sheep grazing on geochemically enriched soils and after moving to clean pastures. Extended depletion times, to the maximum limit (ML) allowable for consumption, of up to 486 days was identified in liver and kidney of lambs. Muscle was found to be safe. These findings support the risk management strategies applied to some farming areas containing high lead soil where offal discard is applied to these animals at slaughter.

Taking Chromatographs out into the Field – Quite Literally

Ibraam Mikhail[1,2], Shing Chung Lam[3], Andrew Gooley[2,3], Kurt Debruille[1], Yonglin Mai[1], Eoin Murray[4] and Prof. Brett Paull[1,2]

[1]Australian Centre for Research on Separation Science (ACROSS), School of Natural Sciences, University of Tasmania, Private Bag 75, Hobart 7001, Australia

[2]ARC Training Centre for Hyphenated Analytical Separation Technologies (HyTECH), School of Natural Sciences, University of Tasmania, Private Bag 75, Hobart 7001, Australia

[3]Trajan Scientific and Medical, 7 Argent Place, Ringwood, Victoria 3134, Australia

[4]Research & Development, Aquamonitrix Ltd, Tullow, Carlow, Ireland (formerly)

Abstract:

Taking chromatography out of the analytical laboratory and out into the environment is not a new ambition, indeed examples of isolated studies using small and mobile devices go back many decades. However, having said this, it would be fair to say that those working with gas chromatography have seen greater progression in terms of instrument portability over this period, than those working with modes of liquid chromatography. The reasons for this are multiple, but recently (over the past decade in particular) there has been increased interest in liquid chromatographs which can be used outside of the traditional laboratory, such that several commercial instruments, which can be classified as truly 'portable' high-performance liquid chromatographs, are now available. Of course, liquid chromatographs come in many different modes and configurations, but for all potential applications a very significant consideration is always going to be detection. For most field applications of current interest, this presents a challenge, and solutions can range anywhere from low-cost 3D-printed absorbance detectors to small-footprint mass spectrometers. Over these past 10 years or so, we have been working on developing both instruments and methods which are field compatible, portable, deployable and mobile, and combinations thereof. Such definitions are subject to debate, but our ambitions have been to develop "application-specific" or "fit for purpose" instruments, which solve problems. Our design focus has been to ensure they are easy to use by non-chromatographers, and importantly provide data on-site to enable real-time actionable decisions. We have been tackling environmental issues of current concern from excess nutrients in waterways to PFAS contaminated soils, sediments and river catchments, and quite literally taking our chromatographs out into the fields!

Unravelling Sterol Biosynthesis in Fungi: Where Analytical Chemistry Meets Medical Mycology

Marjorie Albassiera, Ianca Albuquerquea, José Rivaldo de Limaa, Rose-Anne Lavergneа, Florent Morioa, Fabrice Pagnieza and Dr Isabelle Ourliac-Garniera*

Nantes Université, CHU Nantes, Cibles et médicaments des infections et de l'immunité, IICiMed, UR 1155, F-44000 Nantes, France *email : isabelle.ourliac@univ-nantes.fr

Abstract:

Sterols are key structural and functional components of fungal cell membranes, critical for maintaining the integrity, rigidity and fluidity of the plasma membrane[1]. While ergosterol has historically been considered the defining fungal sterol, advances in research have revealed a more complex sterol landscape. Multiple biosynthetic pathways, which are species-dependent, can lead to ergosterol or alternative sterols end products, which often co-exist as mixtures with one dominant form[2].

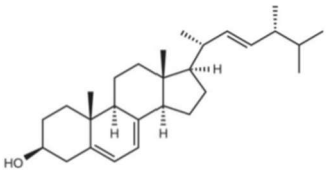

Figure 1. Structure of ergosterol

In pathogenic fungi such as Candida spp. and Aspergillus spp., sterols are indispensable for growth and survival, making them prime targets for antifungal therapy. Azoles, the most widely used class of antifungals, inhibit ergosterol biosynthesis. However, resistance is increasingly reported and typically involves mutations or overexpression of ERG11, efflux pump activation, metabolic adaptation, or biofilm formation[3]—many of which ultimately alter membrane sterol profiles[4,5].

We have developed a method based on GC-MS that enables us to identify and quantify all the sterols present in fungal membranes[6]. The development of this method meets two main research objectives: (1) characterization of sterol composition in various fungal species under basal and azole-treated conditions, aiding in species identification and resistance mechanism elucidation and (2) investigation of the mechanism of action of novel azole derivatives synthesized in-house or by collaborators

Case studies will highlight the importance of sterol profiling as a tool for understanding antifungal resistance and supporting the development of next-generation antifungal agents.

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Electrosynthesis of Free-Standing Conducting Polymer Thin Films at a Polarized Liquid|Liquid Interface for Electroanalytical Applications

Prof. Micheál D. Scanlon[1], Dr Nicolás Rojas-Sanabria[1], Dr Andrés F. Quintero Jaime[1], Dr Sara N. Moya Betancourt[1], Dr Alonso Gamero-Quijano[2]
[1]Department of Chemical Sciences and Bernal Institute, University of Limerick (UL), Limerick, Ireland, [2]Instituto de Catálisis y Petroleoquímica − Consejo Superior de Investigaciones Científicas (ICP − CSIC), Calle de Marie Curie 2, Spain

Abstract:

The broken symmetry of a liquid|liquid interface is ideal for the electrosynthesis of dimensionally confined nanomaterials, i.e., thin films. Certain liquid|liquid interfaces are electrochemically active [1, 2]. Tuning the electric field provides a powerful external stimulus to overcome kinetic barriers to interfacial electrosynthesis. The rate of thin film formation can be controlled by electric field driven motion of molecules (such as the oxidant) to the interface. Subsequently, free-floating thin films can be transferred to any solid conductive electrode surface for ex situ electroanalytical applications or even used in situ at the polarized liquid|liquid interface for sensing applications.

In this presentation, recent breakthroughs in the electrosynthesis of commercially vital conducting polymers, such as biocompatible poly(3,4-ethylenedioxythiophene (PEDOT) [3, 4], as well as metallic nanoparticle/PEDOT nanocomposites, as thin films in a single-step at a polarized liquid|liquid interface will be discussed. The electrosynthesis can be controlled externally using a 4-electrode electrochemical cell in conjunction with a potential or initiated chemically using an electrodeless approach. The latter allows ease of scale-up and transfer of the conducting polymer thin films to solid electrode surfaces.

The electroanalytical performance of gold nanoparticle/PEDOT films on glassy carbon (GC) electrodes using dopamine (DA) as a redox probe was studied. The nanocomposite thin films show enhanced kinetics of the DA redox reaction compared to a bare GC electrode, with an improvement of the heterogeneous electron transfer rate constant up to 4 orders of magnitude.

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Keywords

Liquid|liquid interfaces
Conducting polymers

Chemical analysis of the atmosphere — Towards sensitive, fast, and lower cost spectroscopic sensors

Dr Dean Venables[1]
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Abstract:

Absorption spectroscopy is a major tool for characterising the chemical composition of the atmosphere. However, mixing ratios of important atmospheric species range from ppb to sub-ppt levels. To reach atmospherically-relevant sensitivities, long optical pathlengths are needed. Such pathlengths may be achieved with long physical pathlengths through the atmosphere (as in satellite and other remote sensing techniques), or through optical cavities that can produce optical pathlengths of kilometers in a sample cell of tens of centimetres. At the same time, low-cost sensors have shown the value of expanding the spatial coverage and extent of monitoring in air quality networks.

Here, I present established and evolving strategies for sensitive detection of major trace gas species based on their absorption in the visible and ultraviolet spectral regions. Focusing on measurement of nitrogen dioxide (NO_2), a priority air pollutant associated with vehicular emissions, I describe progress towards developing novel spectroscopic sensors that achieve a sensitivity of 1 ppb in less than 5 s and cost less than €1,000. Application to mapping of transport pollution in Cork city is shown.

This presentation is in memory of my colleague Professor Jeremy Glennon.

Acknowledgements

We acknowledge funding from Research Ireland through grant 21/FFP-P/10220.

Keywords

atmosphere
absorption
spectroscopy
nitrogen dioxide

Pills, Pressure, and Parting Ways: Innovative Separations in Modern BioPharma

Prof. Melissa Hanna-Brown

Chair Analytical Chemistry, School of Chemistry, University College Cork, Cork, Ireland

Abstract:

Compressed timelines, the 'need for speed' and capacity pressures are common parlance in the BioPharmaceutical industry in modern times. Add to this the societal challenge to reduce environmental impact and you have an analytical R & D pressure vessel. This talk will examine the areas where separation science continues to contribute to increasing capacity and accelerating timelines and will take a glimpse into the exciting changes being realised that just might catalyse new ways of working.

Eiroshell™-Enabled Extension to LC Method Development Screening Platforms

Dr John Lough

School of Pharmacy and Pharmaceutical Sciences, University of Sunderland, UK.

Abstract:

In revisiting the classical p-acid stationary phases prepared for normal-phase operation during the early years of high-performance liquid chromatography (HPLC), it was discovered that a very simple prototype phase based on a 3,5-dinitrobanzamido- moiety possessed all of the characteristics, in particular orthogonal selectivity tin reversed-phase operation to the commonly used C18 stationary phases, required for it to play a significant role in modern LC practices such as LC method development screening platforms, 2D-LC and all formats of mixed-mode LC . For this potential to be realized it was first necessary to prepare a version of the DNBA- material based on up-to-date, efficient particle technology. This was achieved by using 2.6 mm superficially porous (silica) particles (spp) manufactured by Glantreo Innovative Science Solutions, Ireland. This new version of the DNBA material silica exhibited the anticipated higher efficiency and better mass transfer at high flow rates while still maintaining the same selectivity, durability and robustness. Importantly, its suitability for being an important contributor to LC method development screening platforms was illustrated by its use to give improved related substances separations of baclofen, dothiepin, paroxetine, fluoxetine that had previously proved challenging on other stationary phases. An additional bonus was that for p-basic analytes it could be used to bring all such compounds in a mixture in a short separation window (amitriptyline metabolites) and/or pull them well clear of potentially interfering matrix components (propranolol in propranolol oral solution). Such reversed-phase application work is continuing. Further, there is a clear indication the sphere of influence of DNBA- can be extended to use in mixed-mode LC, 2D-LC and super-critical fluid chromatography (SFC), revitalising normal-phase LC, facilitating sustainable LC and modification for use in solid-phase extraction (SPE).

An Approach to Method Development in SFC Leveraging Machine Learning for the Development of a Late-Stage Oncology Drug Candidate

Ryan Osborne

Pfizer, Ringaskiddy, Co. Cork, Ireland

Abstract:

During drug development, chromatography is frequently used for purity and stability testing of both drug substance and drug product. Reversed phase liquid chromatography (RPLC) is one of the most widely used methodologies due to its wide scope of application. In the later stages of drug development, the specified impurities and degradation products that define the critical quality attribute of the final API, also known as *Key Predictive Sample Set* (KPSS), are usually well defined and controlled. At this point, a method review enables selecting the most appropriate technique which should be the one providing optimal robustness (ICH-Q14[1]), with the support of Quality by Design (QbD) approaches. Supercritical Fluid Chromatography (SFC) is a preferred technique for its proven diversity in selectivity. The adoption of a technique which presents the most favourable environmental impact, such as, but not limited to, SFC, is also becoming increasingly important as laboratories strive to reduce carbon footprint. *Re*-developing a method requires high resource-demands in terms of staff, materials, and time. Any step of the process that can be automated can facilitate this approach, speeding up the delivery of the method whilst preserving robustness.

In this talk we describe how an SFC method was developed for the purity profiling of a late-stage oncology candidate, taking advantage of the superior selectivity of SFC towards structurally similar analytes, owed to the high orthogonality with R^2 as low as 0.014 towards the KPSS. An optimization via a Bayesian algorithm, which was completed in one night, highlighting the potential and limitations, with an insight into the robustness. This method achieved baseline separation with near total automation embedded into the process and a large reduction of the resource demands when compared to traditional optimisation methods.

Biomimetic Chromatography-Based Investigation of Environmental Contaminant Toxicity and Biological Barrier Permeation

Dr Ilaria Neri [1], Giacomo Russo [2], Lucia Grumetto[1]

[1.] Department of Pharmacy, University of Naples Federico II, Naples, Italy

[2.] School of Applied Sciences, Edinburgh Napier University, Edinburgh, UK

Abstract:

The skin is a complex and highly selective biological barrier, whose structure—comprising epidermis, dermis, and hypodermis—modulates the diffusion of xenobiotics. Understanding how environmental contaminants interact with and cross this barrier is crucial to assess their toxicological impact on human health. Traditional methods for studying dermal absorption often rely on animal models, which are ethically problematic, variable in performance, and low to medium throughput. To overcome these limitations, this research integrates biomimetic chromatography, in vitro permeability assays, and computational predictions to establish alternative and reproducible approaches for investigating the cutaneous absorption and toxicity of environmental contaminants.

A key component of this investigation is the development of **ChromaSkin**, an innovative analytical platform based on **comprehensive two-dimensional liquid chromatography (2D-LC)**. This system employs a **ceramide-like stationary phase** in the first dimension to mimic the lipid-rich epidermis, and an **immobilized artificial membrane (IAM) phase** in the second dimension to represent the dermis. To validate the platform, we analysed 50 pharmaceutical and cosmetic compounds with known skin permeability (log Kp), investigating meaningful correlations between chromatographic behaviour and dermal penetration.

To further validate the approach, **Permeapad® 96-well plates**, which simulate phospholipid-based membranes, were used to conduct high-throughput transdermal permeability studies. These were coupled with miniaturised column chromatography and mass spectrometry. Additionally, log Kp values were calculated and compared with literature data and chromatographic retention metrics, enabling multivariate analysis of permeability and toxicity potential.

Finally, this research is embedded in a broader effort to identify safer alternatives to conventional preservatives using green chemistry, and to replace animal testing with modern, ethical tools. The combination of biomimetic chromatographic techniques with computational modelling and in vitro methods offers a powerful, sustainable, and high-throughput strategy for evaluating the dermal toxicity of emerging contaminants, aligning with the goals of regulatory innovation, environmental protection, and ethical responsibility.

Keywords*:* multiple approach, toxicity, transdermal passage

The Mystery of the Disappearing Excipient: An Analytical Case Study, Investigating a Reduction in Polysorbate Content in a Monoclonal Antibody Drug Substance

Dr Mark Milford

Eli Lilly, Dunderrow, Co. Cork, Ireland

Abstract:

Pharmaceutical excipients can play a wide range roles within the formulation of a drugs substance or drug product, including buffering, stabilising or otherwise preserving the active pharmaceutical ingredient (API) within the formulation. Polysorbates are commonly used as excipients within protein-based biopharmaceuticals, acting as both cryoprotectants for frozen formulations and preventing protein aggregation in liquid settings. In this presentation, a case study is presented where the measured excipient content of a formulated drug substance was unexpectedly low. Multiple orthogonal analytical techniques (including ELSD, Mass Spectrometry and HCP profiling) were utilised an investigative mode, to determine the degradation pathway responsible for the observed loss of polysorbate, along with the underlying causes of the polysorbate degradation within the purified drug substance. The study illustrates that an in-depth understanding of the differences in data generated from orthogonal techniques can elucidate pathways that cannot be determined by any one individual technique.

Hydrogel Lollipops for Early Detection of Cancer

Dr Ruchi Gupta[1], Mr. Khalid Haliru, Dr Nicholas Goddard
[1]University of Birmingham, UK

Abstract:

Oral cancer is the 6th most common cancer worldwide with 650,000 new cases annually. 62% of cases are diagnosed in stages 3 and 4, contributing to low 5-year survival, and has not improved over the last few decades.

Liquid biopsy can disrupt cancer care by non-invasive early detection. For oral cancer detection, saliva biopsy can offer improved specificity over systemic body fluids such as blood. Furthermore, protein biomarkers are advantageous over DNA. However, protein biomarkers are present at much lower levels in saliva than in blood. To overcome this challenge, we have developed a hydrogel that can concentrate and fluorescently label proteins in a single step. Proteins are concentrated in our hydrogel while ensuring abundant interferent proteins such as mucins are removed. The proteins can then be released from the hydrogel by illumination with UV-A light, selectively captured using primary antibodies, and quantified by measuring fluorescence intensity using standard instruments. We have selected two potential salivary biomarkers, IL6 and IL8, which have been consistently shown to be present at higher levels in oral cancer patients than healthy controls.

Our hydrogel is made of derivatives of polyethylene glycols, which are known to be biocompatible. We have shown that our hydrogels can concentrate proteins by a factor of ~300 and proteins can be quantified with a limit of detection of ~ ng/mL. Our hydrogel concentrates total proteins below a molecular weight cutoff for evaluating multiple biomarkers in a single sample. Furthermore, we have shown that target proteins can be measured in the presence of ~50 mg/mL of interferents such as mucins in saliva and albumin in serum. This contrasts with the state-of-the-art method, enzyme-linked immunosorbent assay (ELISA), which typically requires dilution of body fluids by a factor of 100 or more to reduce non-specific adsorption to acceptable levels. Unlike ELISA, proteins released from our hydrogels can be detected using primary antibodies alone.

Our hydrogel can be adapted to measure any protein biomarkers in diverse body fluids for early detection of different types of cancers and for extending its use to measure new protein biomarkers. Nevertheless, our key goal is to deliver hydrogels as lollipops for early detection of oral cancer using a much kinder approach than is currently possible.

Acknowledgements

We acknowledge funding from CRUK.

Keywords

Proteins; interferents; preconcentration; labelling; hydrogels

Chemoenzymatic Glycoengineering of Monoclonal Antibodies

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Abstract:

Current approaches for generating single glycoform monoclonal antibodies (mAbs) include genetic manipulation, cell culture modification, and chemoenzymatic methods. While genetic approaches offer precision when target glycan modifications are predetermined, they are costly and time intensive. Metabolic approaches provide financial advantages but rarely achieve homogeneity. Chemoenzymatic methods, though expensive, can be retrospectively applied to various therapeutics [1].

Recent chemoenzymatic glycoengineering strategies have utilized glycosyl transferases and hydrolases on solid support membranes or employed endo-β-N-acetylglucosaminidase ENGases) with monosaccharyl transferase mutants [2][3]. Our proposed methodology advances beyond these approaches in two significant ways: 1) implementation in solution phase, offering cost advantages and avoiding glycan-site accessibility limitations on intact proteins, often associated with solid support coupling, and 2) utilization of a unique combination of glycosyl transferases and endoglycosidases to generate novel mAb glycoforms.

We will demonstrate an in-vitro glycoengineering technology enabling solution-phase creation of single glycoform mAbs with enhanced safety, efficacy, and effector functions compared to their heterogeneous counterparts. We will showcase the formation of these mAbs using a polyclonal IgG and an IgG2a mAb developed against the Aspergillus fumigatus siderophore TAFC [4][5]. Characterisation of the mAbs will be demonstrated using our established HILIC UPLC methodology [6]. We will demonstrate the altered biological properties of these functionalised mAbs using effector assays and Fc binding studies.

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6. (Millan-Martin, 2023, PMID: 37929772)

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PhD candidate Andreea Cislaru
P.I. Dr Róisín O'Flaherty
Department of Chemistry, NUIM
John and Pat Hume scholarship

Keywords

Chemoenzymatic Glycoengineering single-glycoform UPLC characterization

Polarized Excitation Emission Matrix (pEEM) spectroscopy for the rapid, non-destructive analysis of proteins.

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Abstract:

Expanding excitation-emission matrix (EEM) fluorescence spectroscopy by the addition of polarization information offers some significant advantages for the analysis of macromolecules in a range of different environments. Polarized excitation-emission matrix (pEEM) measurements when implemented in standard benchtop spectrometers using deep UV transparent wire grid polarizers enables the measurement of intrinsic protein emission and thus provides a new suite of label free analysis/measurement methods for biopharmaceutical manufacturing.

Polarization provides two distinct benefits, first using polarizers enables one to selectively enhance the spectra to be more or less sensitive to the presence of particles in samples of varying turbidity. Parallel polarised EEM∥ measurements have obvious benefits for the analysis of samples where one needs to identify the presence of particles or aggregation via analysis of the Rayleigh scattered light signal. Perpendicularly polarised, EEM⊥ measurements are useful in turbid samples where light scatter effects can be minimised producing clearer, truer fluorescence emission signals.

The second benefit is that the pEEM data can provide anisotropy information enabling the extraction of information about protein mobility and local viscosity, which can be used for quality control analysis of proteins in relatively clean sample matrices, such as that found in downstream purification operations. Here we describe a variety of case studies where we have used pEEM for monitoring protein conjugation reactions, quantifying proteins in complex environments, and the interaction of proteins with nanoparticles.

Acknowledgements

The work described in this presentation has been funded via multiple sources including the Irish Research Council, Science Foundation Ireland (Grant no: 14/IA/2282, Advanced Analytics for Biological Therapeutic Manufacture (AA-BTM)) and Research Ireland (Grant no: 22/FFP-A/10271, Downstream Protein Analysis - Polarized Emission Spectroscopy (DPA-PES))

Keywords

Fluorescence
Spectroscopy
Biopharmaceutical
Aggregation
Protein

Optical Evaluation of the Impact of Filtration on Diagnostic Salivary Components

Ms. Somali Dhal[1], Ms. An Hoang Luu[2], Dr Sanathana Konugolu Venkata Sekar[1,2], Dr Katarzyna Komolibus[1], Prof. Stefan Andersson-Engels[1,2], Dr Nilushni Sivapragasam[2], Dr Rekha Gautam[1]

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Abstract:

Human saliva is a readily available biofluid that represents an individual's physiological and pathological conditions. It encompasses a diverse array of biomolecules, including proteins, enzymes, immunoglobulins, glycoproteins, and metabolites such as amino acids, acylcarnitines, biogenic amines, glycerophospholipids, and sphingolipids. These constituents hold significant promise for point-of-care clinical diagnostics, particularly in diseases like inflammatory bowel disease (IBD), oral cancer (OC), and other systemic disorders [1]. Nevertheless, saliva composition can be influenced by numerous factors, including physiological variations, circadian rhythms, personal health status, and external conditions.

Recently, researchers have been focusing on deriving the impact of these factors on saliva, particularly through Raman Spectroscopy (RS), which enables non-destructive measurements with high specificity towards biochemical variations in molecular composition biofluids (e.g. plasma, saliva) and tissues. RS is particularly advantageous in this context, as it can analyse larger salivary proteins, which are crucial for oral cancer diagnosis, unlike mass spectrometry, which is limited to detecting proteins below 50 kDa. As a result, RS can provide a more comprehensive analysis of saliva enabling non-invasive, rapid screening and aiding the clinicians to streamline decision-making process. Additionally, this approach will reduce healthcare costs and minimize patient discomfort, making screenings more accessible and routine. However, reproducibility and background fluorescence signals from contaminants pose significant challenges.

Filtration plays a critical role in saliva processing, helping to eliminate large proteins (e.g., mucins) and food debris that could obscure signals from smaller, diagnostically relevant biomolecules such as cytokines, glycoproteins, and metabolites. However, the lack of consensus in filtration protocols introduces significant variability: pore sizes ranging from 30 kDa to 0.45 μm yield irreproducible spectral profiles, as smaller pores exclude mid-sized proteins (e.g., α-amylase, 54 kDa) while larger pores fail to remove mucins (>1 MDa). This inconsistency complicates cross-study comparisons and undermines the clinical translation of spectroscopic techniques. Furthermore, hydrophobic interactions between salivary proteins and filter membranes can induce nonspecific aggregation, creating artificial clusters that might restrict the passage of certain proteins like IL-8 (8 kDa) or histatin-3 (3 kDa). Compounding these challenges, circadian rhythms and dietary intake modulate salivary composition—for instance, postprandial samples may contain lipid residues or food-derived metabolites that alter spectral baselines. To address this, our study combines (1) standardized morning (fasted) and afternoon (postprandial) saliva collections to assess circadian/dietary impacts, and (2) systematic filtration (30 kDa, 300 kDa, 0.45 μm) to evaluate pore-size effects on protein/carbohydrate partitioning. Raman signatures of filtered/unfiltered fractions will be correlated with Lowry protein and phenol-sulfuric acid assays, establishing objective pre-analytical criteria. The optimized protocol will guide filter selection, advancing robust point-of-care platforms for early salivary molecular detection and quantitative diagnostics.

Healthy male and female volunteers with no known medical conditions were recruited under ethical approval from the UCC Clinical Research Ethical Committee, with informed consent obtained prior to participation. Participants fasted overnight before providing saliva samples in the morning (9:00–10:00 AM), followed by a second collection in the afternoon (2:00–3:00 PM), one hour postprandially. To minimize contamination, individuals rinsed their mouths thoroughly with water for 1–2 minutes, discarding the rinse prior to unstimulated saliva collection via drooling/spitting into sterile tubes (Saliva Sample Collection Kits, Suntrine). Immediately after collection, whole saliva was aliquoted into 2 mL centrifuge tubes and centrifuged at 10,000 rpm for 10 minutes to pellet cellular debris and food particles; the clarified supernatant was transferred to fresh tubes, labeled, and stored at −80°C for further analysis.

For downstream processing, frozen aliquots were gradually thawed (−80°C → 4°C → room temperature) to preserve biomolecular integrity. Thawed samples (500 µL) were filtered using centrifugal devices with 30 kDa, 300 kDa, and 0.45 µm non-reactive membranes (10,000 rpm, 20 minutes), generating paired filtrate (FL) and retentate (RT) fractions.

A customized Raman microspectrometer equipped with a 785 nm diode laser and high-sensitivity CCD detector was used for recording the Raman spectra. The optical setup included collimated laser light focused via a microscope objective, with Raman-scattered photons isolated using dichroic and long-pass filters before detection. RS analysis was performed on unfiltered (UNF), FL, and RT samples using the laser (20 mW power, 30-second integration time) coupled to a 50× objective. For spectral acquisition, 20 µL aliquots were air-dried on aluminum foil-wrapped glass slides, forming coffee-ring patterns. Spatial consistency was ensured by collecting spectra from different peripheral regions along the coffee ring. All spectral data were acquired using LightField software. Further, biochemical validation will be conducted via the Lowry protein assay and phenol-sulfuric acid assay to correlate optical signatures with absolute biomolecular concentrations.

Spectral analysis of UNF, RT, and FL revealed reduced intensity in protein-associated bands (1003 cm^{-1} phenylalanine; 1655 cm^{-1} amide I) in FL samples, indicating a decrease in the proteins after filtration. Concurrently, carbohydrate-dominated spectral features emerged, characterized by shifts from 1450 cm^{-1} to 1460 cm^{-1} and intensified signals at 855 cm^{-1} (C–C stretching) and 1125 cm^{-1} (glycosidic bonds). Lowry protein and phenol-sulfuric acid assays further quantitatively confirmed a higher carbohydrate-to-protein ratio in filtrates. However, to validate the statistical significance of the results, the study will be conducted on a larger cohort of volunteers.

Acknowledgements

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Keywords

Biofluid, Raman Spectroscopy, Saliva

Future Proofing Learning and Teaching through Gamification and VR Laboratories

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Abstract:

From early childhood we learn from playing games, we are encouraged to develop our problem solving and trouble shooting skills and to do this in a fun and enjoyable way. Gaming is an engaging activity that immerses the student into the experience. As part of a new postgraduate course in Bioanalytical Chemistry at University College Cork we have developed in partnership with industry, highly innovative scenario-based games and virtual reality (VR) labs. With the first of these innovative tools the scenario-based games present our students with bespoke challenges that are based on real or potential situations that have or could occur in an industry setting. This is a novel approach that puts into practice the student's ability to apply their knowledge base from the curriculum and to assess their decision making and problem-solving capabilities. We can through these games, challenge students to deal with real potential problems and situations that present in real world scenarios.

The second of our gamification strategy focuses on developing bespoke VR labs in partnership with another company (Fourth Reality). Here we have challenged the status quo and brought students into an immersive environment where they can perform virtual labs through VR. These VR labs are based directly on the in-person labs and contain all of the elements and procedures that are required to do these labs in reality.

In both situations, students through playing, they can make mistakes in a safe environment, repeat the games as often as they like, learn from their choices and ultimately learn to make better informed decisions. Gamification allows us to go deeper with our assessment by linking consequences to decisions, it immerses the student in the real-life scenario and greatly enhances their student experience. It also prepares them to tackle real scenarios such as laboratory sessions and give them additional confidence to perform without the limitations of once of laboratory sessions.

What If Your Toughest STEM Courses Became Your Students' Success Stories?

Charlotte Hamblet

Labster

Abstract:

They can, even in those critical science courses where students begin their careers at University. Join us to discover how virtual labs are boosting learning outcomes, lab skills, and confidence, whilst eliminating traditional gaps in achievement. Through examination of learning analytics and student performance data, we present evidence of how virtual labs bridge the gap between theoretical knowledge and practical application, particularly in courses that traditionally serve as requirements for STEM career pathways.

Development of a Virtual Reality Capillary Electrophoresis Experiment for Postgraduate Chemistry Education

Ms. Janine Boertjes[1,2], Mr. Gary Pearson[3], Dr Niamh O'Mahoney[1], Dr Elizabeth Gilchrist[2] and Prof. Eric Moore[1]
[1]Sensing and Separation Group, School of Chemistry, University College Cork, Ireland, [2]School of Chemistry, University College Cork, Cork, Ireland, [3]Fourth Reality, Annamoe, Ireland

Abstract:

Virtual Reality (VR) is a promising tool to enhance the student learning experience in chemistry education. For analytical chemistry labs, the cost of instrumentation, chemicals and consumables can be prohibitive, and students tend to get limited hands-on experience with delicate instrumentation. VR chemistry experiments performed pre- or post-lab allow students to get additional experience to strengthen their understanding of the experiment and the technique. This is in line with green chemistry principles, as it does not create additional waste from single use consumables and chemicals.

In collaboration with Fourth Reality, a virtual reality capillary electrophoresis (CE) experiment was developed. This was based on the real-life experiment completed by MSc Analytical Chemistry students in UCC, where the effects of voltage and buffer concentration on the separation of amino acids is investigated. The four modules cover instrument set-up, preparation of solutions, analysis on CE and troubleshooting. The students work independently through the modules, following instructions on a tablet, which also prompts them with multiple choice questions to enhance their understanding. In multiplayer mode, up to 8 students are brought into the virtual Science Studio, each with their own lab station and tablet, and complete the experiment under the guidance of a demonstrator.

MSc Analytical Chemistry students who had previously completed the real-life experiment were invited to test the VR experiment and their feedback was captured in a survey as well as through observations made by the demonstrators. The vast majority of participants indicated that after completing the VR experiment, they knew the main steps to set-up the CE instrument and knew the basic operation of the instrument and data analysis in ChemStation software. The feedback was used to improve the VR experiment further to ensure that all desired learning outcomes were achieved and it is an enjoyable experience for the students.

Acknowledgements

This work is supported by the Virtual Labs HCI P3 Initiative.

Keywords

Virtual Reality
Capillary Electrophoresis
Education

How to Teach Scientific Inquiry with Beyond Labz

Heather Myler

Head of Instructional Design, Beyond Labz

Abstract:

Virtual labs allow students to engage in scientific learning in a safe, low stress but highly realistic environment. This allows students to investigate their questions, generate real data and analyse the results to draw conclusions. Since the supplies cost is gone, there is freedom to explore and make mistakes without the physical constraints that would normally limit the independence a student can have. We have programmed the chemistry labs to give unique results for every student, every day, so it is as realistic an environment as possible to truly allow students to independently engage in scientific inquiry in a lab. By removing the physical constraints of a wet lab, they can learn science by actually "doing science", rather than having to just follow lab instructions like a cookbook because of being worried of wasting materials or time by deviating off of the planned course.

Poster Abstracts

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2	Robyn O'Sullivan	Computational Analysis of Metal Organic Frameworks…
3	Artem Zharikov	Identification of polar metabolites in coffee plants and…
4	Edel Whelton	Characterisation of benign, healthy and cancerous…
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19	Conor William Dorney	Development of a portable two channel spectrometer…
20	Ilaria Neri	Transforming Predictive Chromatographic Method…
21	Ciara Howard	Method Development and Validation for the…
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23	Devansh Shah	Development and Evaluation of a Non-Porous…
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30	Rétif Julie	Distribution of Rare Earth Elements in the Food Web of…
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32	Justina Ugwah	SMARTBioP: Advancing Biopsy Precision with a Novel…
33	Jack Daly	The Analysis of Cu(II) N,N-disubstituted-N'…

Preparation and characterization of ionic liquid-based nanoemulsions for effective delivery of pesticide

Miss. Aashima Anand[1], Dr Juhi Saraswat[1], Dr Rajan Patel[1]
[1]Jamia Millia Islamia, New Delhi, India, New Delhi, India

Abstract:

Effective pesticide utilization is a prevalent subject of immense relevance but is often neglected owing to the poor solubility or inadequate wettability of the pesticide spray solution. In the present study, a water-insoluble insecticide lambda-cyhalothrin (LCT) was chosen to be loaded into two different nanoemulsions (NE), fabricated out of a surfactant Tween 20 and two ionic liquids (ILs), 1-octyl-1-methylpyrrolidinium bromide [PyrC_8] Br^- and 1-dodecyl-1-methylpyrrolidinium bromide [PyrC_12] Br^-, in an aqueous medium, prepared via sonication method. Numerous ratios of Tween 20 and ILs were examined along with varying the time of magnetic stirring and sonication processes and on achieving optimization, two sets of NEs were obtained. The effect of the chain length of the ILs was also determined. The characterization of these NEs and the NEs loaded with a minimum amount of LCT was carried out utilizing the techniques of UV-visible absorption, fluorescence spectroscopy and dynamic light scattering (DLS). It was determined that near the critical micellar concentration (cmc) of the ILs, the formation of the NEs took place. The confirmation of the sizes and morphology was carried out with DLS, scanning electron microscopy (SEM) and atomic force microscopy (AFM) and the size of each NE was found to be below 200nm. Further, static contact angle analysis was performed for the prepared NEs (loaded and unloaded with LCT) on the leaves of chili and lemon crops. The NEs were found to enhance the wettability of the insecticide solution. Superior performance was obtained for the long chain IL [PyrC_12] Br^-. Moreover, the stability of these NEs was also evaluated with DLS for up to 30 days. The stability and reactivity of the interaction of LCT with both the ILs was established computationally through density functional theory (DFT). Hence, the prepared NEs were found to enhance the solubility and wettability of the pesticide solution drastically along with reducing the amount required for its application.

Acknowledgements

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Keywords

Nanoemulsion, ionic liquid, contact angle

Computational Analysis of Metal Organic Frameworks for use in HPLC

Ms. Robyn O'Sullivan[1], Prof. Melissa Hanna-Brown[1], Dr Davide Tiana[1]
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Abstract:

Metal-organic frameworks (MOFs) have arisen as a promising class of porous crystalline materials with extraordinary structural diversity. This diversity makes MOFs highly attractive for a range of applications, including gas storage, catalysis and increasingly, separation science. In the context of high-performance liquid chromatography (HPLC), the use of MOFs as stationary phases presents an innovative area of research. Traditional silica-based columns often lack flexibility and specificity required for the separation of complex analytes. MOFs, by contrast, offer potential for enhanced selectivity, owing to their customisable pore environments and adaptable framework structures. This project is dedicated to modelling and simulating the interactions between MOFs and analytes to better understand their behaviour as stationary phases in HPLC. By leveraging computational tools this study aims to identify and evaluate the key structural and chemical characteristics of MOFs that govern their separation capabilities. The intended purpose of this study is to provide insights that will inform the rational design of MOF-based chromatographic materials with improved efficiency, selectivity and chemical stability.

MOFs present a promising alternative to traditional silica-based chromatography; these materials offer precise control over pore size, shape and surface chemistry which is fit for applications such as chiral separations or separations of structurally similar compounds. These materials also notably have much higher surface areas than those of typical silica materials, which in turn means more active sites for analyte interaction, potentially leading to better separation efficiency and capacity. MOFs can also be functionalised post-synthetically or during synthesis to tailor the chemical environment, enhancing specific interactions, making them highly versatile. The stability of MOFs under varied conditions has potential to open applications in aqueous chromatography or extreme pH separations, where silica may dissolve or degrade. These materials provide novel selectivity profiles, making them especially useful for hard to separate analytes or emerging analytical challenges such as complex biological molecules, enantiomers or trace-level contaminants.

Understanding of molecular level interactions within MOF-packed HPLC columns is crucial for optimising performance for analytes that may require tailored chromatographic separation. Molecular dynamics simulations are employed to investigate solute-MOF interactions to predict retention time. Comparison of these MOF-packed columns with that of the conventional silica packed columns lends an insight into the efficacy of these systems. A series of computational runs using GROMACS, a molecular dynamics software, were performed to simulate MOF surfaces and their interactions with analytes and solutes under operational conditions. In gaining a deeper understanding of these interactions, this study aims to provide valuable insights that will guide the selection and design of MOFs tailored for enhanced performance in liquid chromatographic applications, ultimately contributing to advancements in separation science and analytical chemistry.

Acknowledgements

I would like to thank Glantreo for their support and collaboration throughout this research. I would also like to acknowledge the use of the GROMACS molecular dynamics software package for conducting simulations in this work.

Keywords

Molecular-Dynamics, Metal-Organic-Frameworks, Predictive-Chromatography

Identification of polar metabolites in coffee plants and associated microbiome using SPE HILIC with subsequent analysis on LC/MS Q TOF

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[1] Plant Systems Biology Lab, School of Biological & Chemical Sciences, MaREI Centre for Marine, Climate and Energy, Ryan Institute, University of Galway, H91 TK33 Galway, Ireland

Abstract:

The identification of polar metabolites is essential for understanding plant-microbiome interactions at metabolic level. This study presents a systematic approach for the extraction and analysis of polar metabolites from root exudates, leaves, stems, roots and microbiome soil using Solid-Phase Extraction (SPE) with Hydrophilic Interaction Liquid Chromatography (HILIC) and subsequent analysis on an LC/MS Q-TOF system.

Sampling was carried out using the protocol described in (Venkatachalam Lakshmana et.al.,2017) with some modifications. Sample preparation consisted of solid-phase purification on a HILIC sorbent to remove interfering impurities and concentration of the extract, followed by qualitative analysis using HRMS. The mass spectrum was recorded in the full scan mode on LC MS Q TOF 6530.

Data processing was carried out using Mass Hunter, MZmine, GNPS2, and MSDIAL when searching for compounds against mass spectrometry databases and in the end, we managed to identify 32,27,27,12 and 18 unique compounds in leaf, stem, roots, root exudates, and microbiome soil, respectively, in positive ion mode. Detected features were matched against available mass spectrometry databases GNPS, MSDIAL, MetaboKit with cosine similarity over 0.7. In the future, it will be necessary to improve the performance of non-targeted analysis by developing new databases to make the HR-MS approach a tool for monitoring the qualitative identification of polar metabolites in plant samples.

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Keywords

mass spectrometry, microbiome, HILIC, LC/MS

Characterisation of benign, healthy and cancerous tissue in breast disease via bioimpedance sensing on a two-electrode system

Edel Whelton[1,2,] Eva Flynn[1,2], Dr Yineng Wang[1,2] Dr Justina Ugwah[1,2], Martin O'Sullivan[3], Brian O'Donnell[3], AnnMarie O'Donovan[3], Denise Domeney[3], Emma Hoey[3,] Joan Scanlon[3] Ray Burke[4] and Prof. Eric Moore[1,2]

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[2] Life Science Interface Group Tyndall National Institute, Cork, Ireland,

[3] Cork University Hospital, Cork, Ireland

[4] Biophotonics Group, Tyndall National Institute, Cork, Ireland

Abstract:

The method of the SMARTBioP in differentiation of cancerous tissue from non-cancerous tissue in breast cancer was a proven hypothesis in preliminary research studies. The development of a data bank of benign, cancerous and healthy tissue will help aid biopsy procedures and further fast tracking the investigation of cancerous or suspicious lesions, reducing patient discomfort and anxiety and generally improving and speeding up the diagnostic pathway. Postulating that bioimpedance may play a role to improve accuracy of the biopsy samples obtained during breast cancer screening. Bioimpedance is the opposition to flow of an applied electrical current through biological tissue.

Polarized Liquid|Liquid Interfaces as a Platform for Analytical Probing of Nanoparticle Solutions

Dr Sara Natalia Moya Betancourt[1], Dr Nicolás Rojas-Sanabria[1], Dr Alonso Gamero-Quijano[2], Prof. Micheál D. Scanlon[1]

[1]University of Limerick, Limerick, Limerick, [2]Instituto de Catálisis y Petroleoquímica − Consejo Superior de Investigaciones Científicas (ICP − CSIC), , Madrid

Abstract:

Metal nanoparticles have garnered significant attention across various fields due to their unique properties, including their small size, large surface-to-volume ratio, and photocatalytic activity [1]. These characteristics enable a wide range of applications in fields such as electronic storage, electrochemistry, and catalysis—areas that are pivotal in modern technology and society [2]. Given their versatility and relevance, developing efficient platforms to rapidly assess and characterize the physicochemical properties of metal nanoparticles is increasingly crucial. All of this creates the necessity of an analytical detection of nanoparticles in the environment, as they are being so widely used but could have negative impacts on health if they are present in too high quantities. This study introduces a novel approach using polarized liquid|liquid (L|L) interfaces as a platform to characterize the physical and chemical properties of metal nanoparticles.

In this work, the concept explored is the generation of currents during the nano-impacts of gold nanoparticles (AuNPs) at a polarized L|L interface functionalized with a film of the conducting polymer poly(ethylenedioxythiophene) (known as PEDOT). The currents arise under potentiostatic conditions due to the catalysis of interfacial electron transfer (IET) between an aqueous soluble redox species and an organic soluble redox species by the AuNPs upon impact at the L|L interface. The electrochemical experiments at the polarized L|L interface was performed in a specialized four-electrode electrochemical cell.

The synthesis of AuNPs was carried out using ethylenedioxythiophene (EDOT) and PEDOT/poly(styrenesulfonate) (PSS) as both reducing and stabilizing agents, resulting in Au-PEDOT and Au-PEDOT/PSS nanoparticles with average sizes of 5 ± 2 nm and 8 ± 1 nm, respectively. Prior to the injection of AuNPs to the aqueous phase, a PEDOT film was electrosynthesized at a polarized aqueous|α,α,α-trifluorotoluene (TFT) interface. The electrosynthesis of PEDOT films was performed using an aqueous oxidant (Ce4+) and a monomer soluble in the organic phase (EDOT), as described by our group previously [3,4]. Repetitive cyclic voltammetry (CV) cycling was employed to tune the PEDOT film thickness, i.e., more cycles lead to a thicker film.

Real-time detection of AuNP impacts was recorded using chronoamperometry at ~0.46 V on the Galvani scale, a potential known to drive IET between Ce4+ and the EDOT monomer during PEDOT growth [3, 4]. The resulting current spikes provided valuable statistical analytical information about the size, as well as their catalytic properties of the nanoparticles. Under these conditions, transient current spikes were successfully observed, with both spike current and frequency increasing when thinner films were used, demonstrating higher sensitivity during the initial stages of film formation. These current spikes were attributed to the catalytic effect of the AuNPs on the IET process between Ce4+ and EDOT.

Acknowledgements

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Keywords

Polarized Liquid|Liquid Interfaces, nanoimpacts, nanoparticles

Optimizing Differential Pulse Voltammetry for the Quantification of Paracetamol in Over-The-Counter Medicines

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Abstract:

The increasing interest for fast, reliable, and cost-effective methods to evaluate the quality and content of pharmaceuticals has placed electrochemical sensing at the forefront of modern analytical chemistry. Paracetamol, or N-acetyl-p-aminophenol, is the most widely used Active Pharmaceutical Ingredient (API) in multiple over-the-counter drugs for pain relief. The oxidation of Paracetamol to N-Acetyl-p-benzoquinone imine (NAPQI) in acid media can be sensed by voltammetry [1]. Although, pulse voltammetry techniques have been widely applied to quantify redox pharmaceutical compounds, its implementation is not usually accompanied by the optimization of the pulse parameters for the sensor-analyte system [2, 3]. The aim of this work is to show how to optimize peak intensity and sharpness for the electrochemical quantification of paracetamol by Differential Pulse Voltammetry (DPV), by means of one factor at a time and design of experiments approaches [4], assessing the effect of modulation amplitude, modulation time and interval time. After obtaining the tailored pulse parameters, the method was validated using peak current and charge as analytical signals by external standard calibration. Finally, paracetamol content was tested in commercial formulations, such as sachets and tablets, for which the sample recovery was 100 ± 4%. The linear range was stablished between 1 – 70 mg/L, with competitive limits of detection and quantification equal to 1.14 mg/L and 3.45 mg/L for peak current, and 1.44 mg/L and 4.36 mg/L for peak charge.

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Keywords

Acetaminophen, Glassy Carbon, Multilinear Regression.

In situ UV-Vis Spectroscopic Detection of Hydrogen Peroxide Formation by Photoexcited P3HT/PT3 Films at the Liquid|Liquid Interfaces

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Abstract:

The electrochemical properties of conducting polymers (CPs) make these materials promising for applications in biosensing, solar and storage devices, and driving the development of new synthesis techniques.[1,2] Among these, our research group has pioneered the electrosynthesis of free-standing CP thin films at the interface between two immiscible electrolyte solutions (ITIES), including PEDOT (poly(3-4-ethylenedioxythiophene),[3,4] and the copolymer P3HT/PT3 (poly(3-hexylthiophene)/poly(2,2':5'5''-therthiophene)). This novel methodology of polymerization involves the interfacial electron transfer between an aqueous soluble oxidant agent, Ce^{4}+, and the monomers present in the organic phase.[3]

The copolymer P3HT/PT_3 thin films can catalyze the oxygen reduction reaction (ORR) under aerobic conditions in the presence of an organic soluble electron donor species, giving rise to the generation of photocurrents.[5] To demonstrate that the ORR is catalyzed by the film, we developed an in-situ detection methodology to the formation of hydrogen peroxide (H_2O_2) as photoproduct. Using a four-electrode electrochemical cell, the interface was polarized at 0.419 V at the Galvani scale and the film was illuminated under blue light LED, with lithium iodide (LiI) as the aqueous supporting electrolyte. A parallel UV-Vis beam crossed the aqueous phase close to the interface and the spectra were recorded to monitor the formation of triiodide ion (I_3-), produced via reaction with H_2O_2, thereby confirming its generation.

Additionally, we further investigated the influence of pH (acidic and near-neutral conditions) and electron donor strength on the ORR kinetics at the interfacial P3HT/PT_3 film. Our results revealed that under acidic conditions, the kinetics of H_2O_2 production is significantly enhanced, particularly with decamethylferrocene acting as a strong electron donor. In contrast, slower reaction rates were observed with near-neutral conditions and weaker electron donors such as hexadecylferrocene. These findings indicate that the hydronium ions availability and electron donor strength facilitate the interfacial electron transfer across the film. Understanding the mechanism for the generation of photocurrents in the P3HT/PT_3 copolymer at the ITIES contributes to the optimization of this material for solar energy conversion and its potential integration into a novel biphasic solar cell architecture.

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Keywords

Conducting-polymers, H_2O_2-detection, liquid-liquid-interfaces, oxygen-reduction-reaction

Loop-Mediated Isothermal Amplification (LAMP) -Based Electrochemical Detection of Escherichia Coli in Reclaimed Water

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Abstract:
In 2020, the European Union published the EU water reuse Regulation (EU) 2020/741, which sets the quality requirements for reclaimed water for agricultural irrigation.[1] These quality standards focus primarily on Escherichia Coli (E. Coli) as it is an indicator of faecal contamination. Reclaimed or treated municipal water is tested weekly for E. coli according to the EU water reuse regulation 2020/741 using a method for the enumeration of E. Coli and coliform bacteria involving culture growth (ISO 9308-2:2012).[2] This detection method, though effective, is time-consuming and can take over 24 hours between resuscitation and incubation periods. An effective and well-developed alternative E. Coli detection method is Loop-Mediated Isothermal Amplification (LAMP). It is a rapid, low-cost, and highly specific method that is ideal for point-of-care (POC) testing. Unlike other DNA amplification methods, like Polymerase Chain Reaction (PCR), LAMP operates under constant temperature, eliminating the need for expensive thermal cyclers.[3] While common detection methods like fluorescence and gel electrophoresis are effective, they are costly and difficult to miniaturize for POC applications. Electrochemical detection offers a promising alternative—it is scalable to microscale, cost-effective, and compatible with LAMP. This combination enables fast (<1 hour), sensitive (< 0.1 CFU/mL), and on-site detection of E. coli DNA. The main focuses of this research will be to target conserved regions of the E. Coli DNA and amplify these regions using specific complex primers under isothermal conditions. Using a redox reporter that associates with the DNA via intercalation and electrostatic interaction[4], confirmation of the DNA amplification and the degree to which it has occurred can be detected electrochemically.

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Keywords

LAMP, E. Coli, Electrochemistry, Water

Iron nickel boride bifunctional electrocatalysts for water splitting at porous electrodes

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Abstract:

Here we present new sustainable, low cost electrocatalytic materials for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Transition metal borides (NixB and Fe-NixB) were synthesised via a facile wet-chemical approach, with optimised iron-nickel ratio. Initial HER and OER experiments were performed at a glassy carbon electrode (GCE) and extended to 3D and 2D nickel foam porous substrates (in the case of OER) and carbon cloth (in the case of HER). These substrates provided a high surface to volume ratio for catalyst immobilisation. Materials were tested under alkaline conditions, and their stability examined by monitoring the current over time. The optimised Fe-NixB material exhibited promising catalytic activity for HER and OER under chronoamperometric conditions. In the case of HER activity, Eonset values of -0.0292 V vs RHE, decreased to -0.0753 V post stabilisation, reaching -0.0616 V and -0.0902 V (j = 10 mA) pre and post stability respectively.

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Keywords

Hydrogen, Transition metal Borides, Electrolysis

Viral Inactivation (VIN) Process Monitoring by Polarized Fluorescence Spectroscopy

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Abstract:

Monoclonal antibody (mAb) therapeutics are highly specialized molecules offering important advantages in the treatment of cancers, autoimmune diseases, and infections compared to traditional therapies. Downstream processing of mAbs is a highly complex and specialized set of processes which rely on different analytical methods such as size exclusion chromatography (SEC), dynamic light scattering (DLS), and UV-Vis spectroscopy. These methods require extensive equipment, training, and time for quantification. Thus, a rapid, single-measurement tool is needed for on-line monitoring of protein aggregation during VIN.

Here we explore the use of a multichannel spectrofluorometer (Aqualog, Horiba) capable of rapid (<1 min.) polarized Excitation Emission Matrix (pEEM) measurements as a robust tool for on-line monitoring of protein concentration, stability, and aggregation during VIN. pEEM provides several sources of information: Rayleigh scatter for identifying aggregate/particle formation, fluorescence emission to assess chemical and structural stability, and absorbance of UV light to measure protein concentration. Here we use a Bovine IgG aggregation model in a simulated low pH incubated post-Protein A buffer solution over an 8-24 hour period. Bovine IgG (concentration of 1mg/mL) was incubated at various pH levels (3.2, 3.6, 3.8) at 20°C with continuous stirring. pEEM, DLS, SEC, and UV-Vis measurements were made hourly and then compared.

The fluorometer operating in vertical-vertical (VV) polarization mode was more sensitive to early-stage protein aggregation than traditional UV-Vis spectroscopy. The ratio of the Rayleigh to fluorescence signals (IR/IF) from EEMVV spectra increases (0.65 to 2.13) with the degree of aggregation and this correlates with the degree of polydispersity (PdI width increases from 52 to 990 nm). Specifically, IR/IF values increase exponentially (R2 = 0.96) at pH 3.2 where there was protein instability and rapid aggregation, whereas at pH 3.6 IR/IF values increase linearly (R2 = 0.97). Simultaneously the absorbance measurements show significant increases due to scattered light and as a consequence the aggregation index (A350/(A280-A350)×100) values range from -1.8 to 26.6%. Extracting the correct soluble protein concentration required multi-variate data analysis of the absorbance spectra to separate out the scattering and emission components.

Acknowledgements

This research was supported by a Research Ireland Grant to AR: Downstream Protein Analysis - Polarized Emission Spectroscopy (DPA-PES). 22/FFP-A/10271

Keywords

mAb, Polarized, EEM, Fluorescence, Spectroscopy

Biothiol and peroxide electroanalysis at nanoporous gold modified poly(3,4-ethylenedioxythiophene) electrodes

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Abstract:

The dysregulation of iron metabolism and the accumulation of reactive oxygen species (ROS) is implicated in iron-dependant programmed cell death or ferroptosis. The accumulation of iron in the cytoplasm plays an important role that drives the Fenton reaction which in turn leads to the production of hydroxyl radicals from hydrogen peroxide [1]. To combat this, the body is equipped with antioxidants such as glutathione (GSH) [2]. This three-amino acid tripeptide has a -SH group that donates electrons and protons to the unstable ROS that leads to their neutralisation. Glutathione exists in the body in the reduced (GSH) and oxidised (GSSG) forms (normal ratio of 500:1). An alteration in the levels of GSH and hydrogen peroxide plays a role in neurodegenerative disease and these small molecule biomarkers are the target analytes in the chemosensor design presented in this work. Electrodeposition of the conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) on glassy carbon electrodes (GCE) involved application of Eapp = 1.5 V for 10 s, forming an underlying nanoporous semiconducting support (Figure 1.) for subsequent metal (Au, Cu) nanoparticle electrosynthesis. GSH anodic responses were observed at GCE/PEDOT surfaces over the range 100 to 1000 µM at Ep = 0.5 V and 0.8 V in 0.1 M sodium acetate buffer (pH 4.45) and 0.1 M phosphate buffer (pH 7.4) respectively. Pulse and constant potential electrochemical techniques were subsequently employed for quantitative studies with a limit of detection of 0.2 mM at pH 4.45. In relation to hydrogen peroxide sensing, pulsed electrodeposition of nanogold particles (GCE/PEDOT/Au) from 5 mM HAuCl4, (optimised for nucleation and growth parameters) resulted in hydrogen peroxide anodic response at 0.721 V with current increase over the range 300 to 5000 µM, under physiological pH conditions.

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Keywords

Biothiol
Oxidative stress
Sensor
Voltammetry

Electrochemical investigations into 1,10-Phenanthroline-5,6-dione as a redox mediator for glucose sensing at glassy carbon and carbon cloth electrodes

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Abstract:

Preparation of a biocompatible graphite ink formulation is reported for glucose biosensing at both conventional (glassy carbon) and flexible carbon cloth porous substrates with a view to design wearable transducers for diabetic monitoring. The bioink was characterised via reflectance microscopy, thermal (differential scanning calorimetry) and electrochemical approaches (electrochemical impedance spectroscopy). It was then deployed as an underlying layer for encapsulation of the heterocyclic quinoid species, 1,10-phenanthroline 5,6 dione (PD) redox mediator via electrodeposition (potentiodynamic) both with and without the aid of an enzymatically driven approach. The immobilised mediator acted as a proton and electron acceptor for $FADH_2$ cofactor regeneration (glucose oxidase). Scanning electron microscopy revealed interesting microstructures of insoluble pPD on both substrates while film studies established surface confined behaviour and the expected proton coupled electron transfer process. A layer-by-layer approach was employed for glucose oxidase entrapment using chitosan (biopolymer) and crosslinker (poly(ethylene glycol) diglycidyl ether). Following an enzyme loading study, translation of the optimum method onto carbon cloth resulted in successful glucose biosensing using cyclic voltammetry, differential pulse voltammetry and coulometric approaches over 1-10 mM glucose in phosphate buffer (pH 7.4) with apparent Michaelis Menton constant (Km') of 0.72 mM. The work paves the way forward for a wearable "smart patch" device for non-invasive sample acquisition (perspiration/interstitial fluid) and diabetic biomarker quantitation.

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Keywords

Glucose biosensing

Sensing Sialic Acids with Multi-Functional Electrochemical Probes

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Abstract:

Sialic acids (Sias) are carbohydrates found on the surface of cells or in bodily fluids. They play important roles in the human nervous/immune system, and altered levels can reflect multiple disorders. Therefore, the design of new analytical methodologies for this family of monosaccharides may be useful for disease treatment and diagnosis [1]. Boronic acids are well-known carbohydrate receptors which form pH-dependent covalent interactions with diol-containing target molecules, leading to boronate ester species; at acidic pH values, they bind α-hydroxy acids, which are present in Sias. Electrochemical sensing of Sias using commercially available electroactive boronic acids is limited by their structural simplicity and can result in lactic acid interference, but it can be easily implemented compared to other methods and may avoid interference from neutral saccharides [2].

In this work, a series of novel electroactive ferrocene phenylboronic acids were synthesised and characterised; their ability to bind with the model sialic acid N-acetyl-D-neuraminic acid (Neu5Ac) was examined. Neu5Ac is the most common Sia naturally found in healthy humans, and it may be found free in solutions such as the cerebrospinal fluid of people with pyogenic meningitis [1]. The presence of an α-hydroxy acid group, carbohydrate structure and the anionic nature of Neu5Ac (pKa = 2.6) [1] was exploited for selectivity purposes, providing rationale for probe design and binding conditions employed. For example, a phenyl ring may allow for CH-π interactions [3]. The redox properties of the synthetic probes were established (cyclic voltammetry and differential pulse voltammetry), which led to the most promising compound for Neu5Ac recognition. Qualitative and quantitative Neu5Ac interactions were examined by monitoring the altered redox properties of this chemoreceptor (Fc-LC) both in solution and via confinement within a carbon paste matrix. Neu5Ac binding vs. competing interferents (lactic acid and co-existing biological mono/disaccharides) establishes the potential of this methodology as a portable, rapid and selective biodiagnostic tool. Fc-LC apparently recognises Sialic acid with reduced interference from lactic acid.

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Keywords

Sialic acid; Voltammetry; Carbon paste

The Use of 31P NMR Chiral Sensors for Enantiopurity Measurement in Chiral Organophosphorus Compounds

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Abstract:

The enantiopurity of chiral organophosphorus compounds is of critical importance in pharmaceutical development, where differences in enantiomeric composition can lead to profound variations in biological activity. Conventional enantiopurity analysis often relies on chromatographic techniques using chiral stationary phases; while effective, these methods are time- and resource-intensive. In contrast, Nuclear Magnetic Resonance (NMR) spectroscopy offers a rapid, non-destructive alternative, yet its application to enantiopurity analysis remains limited, particularly in the context of 31P NMR spectroscopy.

This project investigates the use of 31P NMR spectroscopy, in conjunction with a chiral phosphorus-based sensor molecule, for the direct enantiorecognition of stereogenic phosphorus-containing analytes. The method exploits the formation of diastereomeric sensor–guest complexes, which generate distinct 31P chemical shifts (ΔδP) for each enantiomer.

Initial screening experiments qualitatively confirmed host-guest complex formation, while quantitative analysis revealed that chiral discrimination is influenced by multiple non-covalent interactions, including electrostatic attraction, π–π stacking, and hydrogen bonding. Structural features of both sensors and guests — such as rigidity, electronic properties, and conformational flexibility — were found to significantly affect resolution efficiency.

Ongoing work focuses on evaluating experimental parameters (e.g., solvent choice, concentration, sensor:guest stoichiometry, temperature, and magnetic field strength) to optimise the method's sensitivity and robustness. Results are benchmarked against chiral HPLC for validation. This approach represents a promising step towards a generalisable, NMR-based platform for fast and accurate enantiopurity determination in chiral phosphorus chemistry.

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Keywords

Chiral organophosphorus
31P-NMR spectroscopy
Enantiorecognition

Using polarized intrinsic emission (PIE) to measure the kinetics of protein-liposome interactions on a second timescale: Exploring the Role of Ionic Strength

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(A.G.R) Grant number: China Scholarship Council (CSC), No. 202308310150 to HW

Abstract:

Liposomes are widely used as drug delivery systems due to their ability to encapsulate therapeutic agents and interact with biological environments. Upon intravenous administration, liposomes are immediately exposed to plasma proteins, leading to the formation of a dynamic "protein corona" that governs their biological fate, stability, and clearance1. One of key factors affecting protein-liposome interactions is ionic strength, which influences protein binding, aggregation, and membrane penetration2. To properly understand these interactions and effects, one needs fast measurements (<1 sec) which can accurately monitor the early-stages of protein-liposome interactions in these turbid samples. Here we developed a novel analytical method based on polarized intrinsic emission (PIE) spectroscopy, combined with a rapid mixing accessory, to monitor the real-time kinetics of human serum albumin (HSA) interactions with DMPC liposomes by measuring the intrinsic emission of HSA at second-time scales.

HSA and DMPC liposomes in ABC (ammonium bicarbonate) buffer solutions(pH~8.0), with ionic strengths (25, 50, 100, and 150 mM) were prepared. Liposomes were formed via thin-film hydration and extrusion. Real-time measurements were performed using a Horiba Aqualog fluorometer with wire grid polarizers. PIE spectra (VV and VH polarizations) were recorded at 1-second intervals with fixed 280 nm excitation and a 200–800 nm emission range. Dynamic Light Scattering (DLS) provided reference particle size, polydispersity, and diffusion data.

This was the first use of PIE for real time monitoring of HSA-liposome interactions and the effect of ionic strength on the interaction process. Using the ratio of the Emission to Rayleigh scatter from PIE spectra which can be correlated with particle size provides a faster, and more accurate, in-situ, picture of the process compared to DLS (which takes 10× time longer). The protein-liposome interaction process was observed (via parameters like wavelength shifts, intensity changes and fluorescence to Rayleigh ratios) to consist of four phases: a chaotic initial mixing phase up to ~100 seconds after mixing, an penetration and rearrangement phase (up to 30 minutes), a stable phase (30-60 mins), followed by slow aggregation (1-3 hours after mixing).

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China Scholarship Council (CSC)

Keywords

PIE protein-liposome interactions Ionic Strength

Exploring Sorbent Materials for Wearable Human Skin VOC Collection

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Abstract:

Human skin emitted volatile organic compounds (VOCs) have been garnering interest from the research community as a matrix containing information on physiological health status, disease and environmental exposure biomarkers. Currently, headspace solid-phase microextraction (HS-SPME) is the approach used in our research group for skin VOC capture, coupled with gas chromatography (GC-MS) analysis. SPME is based on equilibrium partitioning of VOCs between the skin and a coated SPME fibre (triple phase) and hence quantitation of VOCs is challenging, particularly as the skin VOC profile is reasonably complex. In turn, this work investigates a move from SPME towards flexible, wearable planar sorbent films for collecting skin VOCs.

These sorbent films can be applied to skin within a plaster or dressing and worn comfortably on the skin for long sampling durations. Sorbents selected for this work include Tenax®-TA (polydiphenylphenylene oxide), Tenax®-TA/divinylbenzene, and polydimethylsiloxane. Exploring these non-polar materials in planar film format is crucial towards wider scale skin VOC sampling – enhancing study participant cohort sizes.

Thus, this research investigated films comprising these different sorbents as passive samplers for skin VOCs. The initial work involved testing the uptake of VOCs from a skin VOC standard in a closed HS. Following incubation of the different materials in this HS for different periods of time, film-adsorbed VOCs were solvent-extracted and analysed via GC-MS and the uptake efficiencies and kinetics for the different film chemistries compared. Finally, we were interested in translating these findings to develop an effective sorbent film optimised for skin VOC collection and hence these candidate materials were integrated into a wearable adhesive layer and tested in-vivo for skin VOC uptake.

Acknowledgements

Insight Research Ireland Centre for Data Analytics
School of Chemical Sciences, Dublin City University

Keywords

Human Skin VOCs, Sorbents, GC-MS

Electrical Impedance-Based Transduction of Responsive Hydrogels Swelling for Epidermal Sensing of Ions

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Abstract:

Responsive hydrogels have emerged as promising candidates for epidermal sensing platforms due to their intrinsic hydrophilicity, biocompatibility, and mechanical softness, which closely match the properties of biological tissues. Additionally, their tunable chemical functionalities allow them to respond selectively to various biochemical and physical stimuli. However, while the swelling behavior of hydrogels in response to environmental changes is well understood, translating this behavior into practical, real-time sensing mechanisms for wearable devices remains a key challenge, particularly in achieving transduction methods that are both sensitive and amenable to miniaturization.

In this work, we investigate a crosslinked poly(acrylic acid-co-N,N'-methylene-bis-acrylamide) (PAAc-co-MBA) hydrogel as a model stimuli-responsive material for epidermal sensing applications. The hydrogel's capacity to undergo volumetric changes upon solute uptake was exploited as the sensing mechanism, with electrical impedance spectroscopy (EIS) employed to transduce these changes into measurable electrical signals. Specifically, we extracted a hydrogel resistance parameter (ΔRgel) from the modeled impedance spectra, which was quantitatively correlated with the hydrogel's equilibrium swelling behavior, represented by the change in mass (ΔSgel) upon solute absorption.

A series of experiments were conducted to characterize the swelling and electrical response of the hydrogel under different conditions, including variations in solute type, concentration, and hydrogel crosslinking density. These studies revealed relationships between hydrogel composition, swelling kinetics, and impedance response, providing insights into the optimization of sensing performance for different analyte profiles. Furthermore, the physical properties of the hydrogel films, such as conformability, adhesiveness to skin-mimicking substrates, and mechanical stability, were assessed to ensure suitability for integration into epidermal devices. To demonstrate real-world applicability, the hydrogel films were applied to the surface of kiwi fruit tissue as a biological analog to human skin. In this proof-of-concept experiment, the system successfully monitored real-time changes in tissue pH, showcasing the hydrogel's potential for non-invasive monitoring of small hydrophilic biomarkers at the skin surface. These findings establish a foundational approach for designing simple, scalable, and wearable hydrogel-based sensing systems. By leveraging the swelling-induced changes in impedance, this platform opens new avenues for epidermal biosensors that are both highly responsive and readily integrable into flexible electronics for continuous health monitoring.

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Keywords

Responsive hydrogels, electrical impedance spectroscopy

A low-cost nitrogen dioxide instrument using cavity-enhanced absorption spectroscopy

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Abstract:

A low-cost (<$1,500) nitrogen dioxide (NO_2) measurement instrument was developed using incoherent broadband cavity-enhanced absorption spectroscopy (IBBCEAS). Light from an LED centered at 410 nm was coupled into an optical cavity consisting of two high-reflectivity mirrors (R > 0.9998), yielding an effective optical path length of 1.1 km over a physical length of 22 cm. A 1σ measurement precision of 1 ppb was achieved with an integration time of 1 second. Comparative NO_2 measurements conducted in chamber showed good agreement with the chemiluminescence method, yielding a correlation coefficient of 0.999. The instrument was installed in an electric vehicle and carried out for mobile monitoring in Cork city. The measured data showed that the concentrations of NO_2 exceeding 20 ppb were observed in the city center, train station and in traffic jams.

Acknowledgements

This work was supported by the Science Foundation Ireland (21/FFP-P/10220).

Keywords

low-cost, NO2, spectroscopy, mobile monitoring

Development of a portable two channel spectrometer for fast, inexpensive measurements of nitrogen dioxide in urban environments

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Abstract:

Nitrogen dioxide (NO_2) is a major air pollutant and strongly associated with vehicle emissions. At present, there are no fast and low-cost instruments suited to mobile measurements or measurements at stationary roadside sites. Here we describe the development of a low-cost, two-channel Cavity-Enhanced Absorption Spectrometer (2-CEAS) system for in-situ measurements of NO_2 in urban environments. A blue LED centered at 440 nm was used as a light source with a 16 cm optical cavity to enhance the absorption sensitivity. Transmitted light at two wavelengths (438 nm and 439 nm) was detected with silicon photomultipliers. The instrument time resolution was 20 s with a low ppb level of sensitivity to NO_2. We report system characteristics and performance and discuss the outlook for using the approach in city-wide NO_2 mapping.

Acknowledgements

Thanks to research Ireland for funding this project,
21/FFP-P/10220

Keywords

NO_2, spectroscopy, low-cost, absorption

Transforming Predictive Chromatographic Method Development

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Abstract:

Chromatography is a cornerstone technique in chemical analysis and purification across industries ranging from pharmaceuticals to environmental science. Traditional method development in chromatography, however, remains highly empirical, time-consuming, and resource-intensive. Our project addresses this challenge by developing a predictive chromatography framework that leverages experimental data and machine learning models to forecast chromatographic behaviour and optimize separation parameters[1].

While recent advances in cheminformatics and computational power have improved model accuracy, significant challenges remain in achieving broad applicability and robust extrapolation. 1) Dataset selection: a critical balance must be achieved between dataset size and chemical relevance. Large datasets provide statistical power, but unless they include sufficient structural similarity among compounds, the model may fail to generalize meaningfully within a given chemical space. Conversely, narrow datasets limit the model's applicability. This tradeoff poses a significant barrier to developing universal models and necessitates better strategies for chemical space coverage and dataset curation[2]. 2) Inadequate molecular descriptors: current models rely on standard molecular descriptors (e.g., topological, physicochemical, or 3D descriptors) that inadequately capture the complex physicochemical interactions governing retention — particularly those involving mobile and stationary phase chemistry. This shortfall limits the interpretability and transferability of models across chromatographic systems. 3) Limited generalizability: most existing models accurately predict retention only under the exact experimental parameters used to generate the training data. This confines their utility, especially when greener or more sustainable chromatographic methods are desired.

Our work aims to develop a new dataset, comprising a selection of structurally varied compounds, balancing a good spread of physicochemical/structural diversity while simultaneously having enough structural similarity across the compound library, in order to effectively test and train predictive models. The compounds included in the dataset will be analysed under both reversed-phase liquid chromatography (RPLC) and supercritical fluid chromatography (SFC) conditions, enabling the development of models applicable to a broad range of separation techniques. The main objective is to reduce trial-and-error in method development by constructing robust, generalizable models capable of predicting retention times across various compound classes. The long-term goal is to explore custom descriptors that better represent solute-solvent-stationary phase interactions, aiming to bridge the critical gap mentioned above. Finally, by integrating high-quality experimental data with molecular descriptors and operational parameters (e.g., solvent gradients, flow rate, temperature), algorithms will be trained to predict more environmentally friendly conditions.

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Acknowledgements
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Keywords
predictive chromatography, machine learning

Method Development and Validation for the Determination of Nine Volatile N-Nitrosamines in Processed Meat Products using Liquid Chromatography-Tandem Mass Spectrometry

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Abstract:

N-Nitrosamines (NAs) are a class of compounds identified by the European Food Safety Authority (EFSA) as potential carcinogens. Ten NAs, including N-nitrosodimethylamine (NDMA) and N-nitrosodiethylamine (NDEA) have been highlighted as substances of concern in food. These compounds can form during food processing through reactions between nitrosating agents (nitrite, nitrogen oxides) and secondary amines. NAs have been detected in a variety of foodstuffs, including cured meats, processed fish, beer, cheese, soy sauce, oils and human milk. Although no European Union (EU) legislation currently sets maximum limits for NAs in food, a threshold of 10 µg/kg is often applied for risk management purposes.

This study aimed to develop and validate a sensitive and robust analytical method for the determination of nine volatile N-nitrosamines (VNA) in cured meat products using liquid chromatography coupled with atmospheric pressure chemical ionisation and tandem mass spectrometry (LC-APCI-MS/MS). The target analytes included NDMA, NDEA, NMEA, NDPA, NDBA, NMOR, NPIP, NPYR and NDPhA. Sample extraction employed a modified QuEChERS procedure using acetonitrile and heptane. Validation was conducted using a spiked pork meat matrix at three concentration levels: 1, 10 and 60 µg/kg. Limits of detection (LOD) were ≤ 1 µg/kg for all compounds except NDBA and NDPhA. Limits of quantitation (LOQ) ranged from 0.9 to 1.6 µg/kg for NDEA, NDPA, NDMA, NMEA and NPYR and from 2.4 to 4.0 µg/kg for NMOR, NPIP and NDBA. Excellent linearity was observed over the range 0.5 - 70 µg/kg, with correlation coefficients (R^2) exceeding 0.999 for all analytes.

At the 1 µg/kg spiked level, recoveries were satisfactory for NDMA, NDEA, NMEA and NDPA (73-106%). NMOR and NPIP exhibited elevated recoveries (≥ 130%) but good precision (RSD ≤ 10%). NDBA and NDPhA showed poor recoveries (48.5% and 25.3% respectively). Similar trends were observed at 10 and 60 µg/kg levels. Precision was excellent for most analytes, with RSD values ranging from 1.2 to 10.8% (n= 8 independent replicates per level).

Experimental runs using different types of processed meat spiked at 1 and 10 µg/kg supported these findings. At the lower level, recoveries were generally acceptable, though precision was poor for most analytes (RSD 22-39%), with only NDMA showing acceptable variability (RSD 16%). NDPhA was largely undetectable. At 10 µg/kg, recoveries ranged from 825 to 135%, with excellent precision for all analytes (RSD ≤15%) except NDBA and NDPhA. LC-APCI-MS/MS proved effective for quantifying eight of the nine target VNAs. However, NDPhA exhibited poor ionisation efficiency and was deemed unsuitable for detection using APCI.

Acknowledgements

The author would like to thank the industry project supervisor for their guidance and support and the Public Analyst's Laboratory, Cork, for the provision of instrumentation and materials.

Keywords

Volatile N-Nitrosamines, LC-MS/MS, APCI, QuEChERS

Developing a Standardised Method for Skin VOC Sampling using Solid Phase Microextraction

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Abstract:

In recent years, there has been a growing interest in the development of non-invasive methods for human health monitoring and improved diagnostics. Consequently, there has also been an increased interest in volatile organic compounds (VOCs) which are generated via metabolic pathways in the body, and subsequently released via breath, urine as well as through skin.

Our study focuses on the VOCs that are emitted from the skin surface. We use a headspace-solid phase microextraction (SPME) method for sampling and gas chromatography- mass spectrometry (GC-MS) for their recovery and identification, where it is important to note that SPME is a partition-coefficient-based extraction technique. Although this workflow has been widely used in areas such as environmental and food/flavour VOC analysis, it's use in skin VOC profiling is less prevalent.

In this work, we investigate the impact of HS-SPME sampling time on the profile of skin VOCs recovered as a function of body site (and hence gland type and distribution). Preliminary data shows us that the profiles we recover are dependent on sampling time and thus by recovering samples collected over a range of sampling times (5-45 min), a richer, more diverse skin VOC profile may be observed, compared with sampling at only at a single fixed timepoint.

A significant challenge for SPME sampling is the quantification of VOCs of interest, as their adsorption is a dynamic process and also depends on various factors such as the materials used for sampling. Therefore, standardisation and calibration methods are being explored so that emission fluxes of the different VOCs being emitted from the skin can be estimated.

The findings of this work will influence how sampling is carried out for future participant studies looking at the identification of skin volatile biomarkers that can be used for non-invasive, continuous health monitoring.

Acknowledgements

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Keywords

SPME, GC-MS, Skin Volatiles

Development and Evaluation of a Non-Porous Protein-A Silica Column for Monoclonal Antibody Analysis by High-Performance Affinity Chromatography

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Abstract:

Accurate quantification of monoclonal antibodies (mAbs) is critical at all stages of biopharmaceutical development, particularly for monitoring cell culture harvest samples during upstream processing. High-Performance Affinity Chromatography (HPAC) using immobilised Protein-A ligands offers several advantages over traditional immunoassays such as enzyme-linked immunosorbent assay (ELISA), including improved speed, robustness, and reproducibility. Non-porous silica was chosen for its low surface area and absence of internal pore structures, which minimise diffusion limitations and enable faster mass transfer. Compared to porous silica and polymeric resins, non-porous silica offers sharper peak profiles, reduced risk of fouling when working with complex samples such as cell culture supernatant, and better mechanical stability for long-term usage.

In this study, non-porous silica particles were successfully functionalised with recombinant Protein-A ligand and characterised using multiple techniques. Scanning Electron Microscopy (SEM) confirmed particle uniformity, and bicinchoninic acid (BCA) assay was used to estimate the immobilised Protein-A content.

The functionalised resin was packed into a PEEK column and evaluated using HPAC. Initial column evaluation with Rabbit Immunoglubilin G (IgG) standard demonstrated excellent chromatographic efficiency. Further evaluation with a monoclonal antibody feedstock sample confirmed effective separation of IgG from cell culture components, achieving a resolution of over 31 and maintaining high efficiency.

These findings highlight the potential of the non-porous Protein-A silica column as a robust and high-resolution tool for rapid mAb titre analysis. Ongoing work will explore to broaden the platform's applicability to a wider range of antibody formats, through the immobilisation of alternative ligands, such as Protein-G and Protein-L.

Acknowledgements

Dr. John Hanrahan, Glantreo Limited
Prof. Eric Moore, University College Cork

Keywords

Protein-A chromatography, non-porous silica, HPAC

Noninvasive In-vivo Bone Characterisation Using Dual Wavelength Inverse Spatially Offset Raman Spectroscopy

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Abstract:

Bone-related disorders such as osteoporosis are characterised by reduced bone mineral density (BMD) and alterations in bone microarchitecture, which together increase the risk of fractures and result in a significant socioeconomic burden. While dual-energy X-ray absorptiometry (DXA) is the current gold standard for assessing BMD, it fails to provide insight into the organic matrix and microstructural integrity of bone, thereby limiting its predictive capability for fracture risk. Raman spectroscopy presents a promising alternative as it enables biochemical characterisation of bone tissue by probing both fingerprint and high-wavenumber spectral regions. However, most existing Raman systems using dual wavelengths are constrained to surface-level measurements and lack the capacity to interrogate subsurface bone composition effectively.

In this study, we present a dual-wavelength inverse spatially offset Raman spectroscopy (DW-iSORS) system that enables the acquisition of Raman signals from deeper tissue layers. By employing ring-shaped illumination and central collection geometry, the system enhances the detection of subsurface signals while minimising the power density on the sample surface. An optimal spatial offset, which balances penetration depth and signal-to-noise ratio, was determined through Monte Carlo simulations and validated experimentally. This optimised offset configuration was employed in both phantom studies and in-vivo measurements, demonstrating the feasibility of using DW-iSORS for non-invasive, comprehensive assessment of bone quality.

Phantom models were designed to mimic layered tissue structures. The bottom layer bone phantom was fabricated by mixing equal parts of hydroxyapatite (HA) granules and ammonium chloride, which were ground, homogenised, and pressed into a petri dish, then covered with a calcium fluoride window. A silicone-based phantom with well-defined optical properties (absorption coefficient of 0.1 cm^{-1} and reduced scattering coefficient of 10 cm^{-1}) was used as the top tissue-mimicking layer. Additional hydration phantoms with water contents of 89.1% and 81.7%, and HA phantoms with 4% and 7% concentrations, were prepared to evaluate the system's sensitivity to compositional changes.

The experimental setup consisted of a dual-wavelength laser source providing 730 nm and 830 nm excitation. The laser beam was collimated, filtered, and directed through an axicon lens to generate an adjustable ring-shaped illumination pattern. The ring size was varied to create different spatial offsets. The backscattered Raman signal was collected centrally, filtered to remove elastic scattering, and coupled into a spectrometer equipped with a deep depletion CCD detector. The spectral detection range covered both fingerprint (382–2191 cm^{-1}) and high-wavenumber (2034–3840 cm^{-1}) regions, depending on the excitation wavelength.

The system was calibrated using a neon-argon lamp and a silicon standard (520.5 cm^{-1} peak). Raman spectra were recorded under dark conditions with integration times adjusted to remain below the maximum permissible exposure for laser illumination. Various ring sizes, ranging from 3 mm to 11 mm in radius, were tested to evaluate the impact of offset on penetration depth. For each configuration, five spectra were recorded. The data was pre-processed by subtracting fluorescence background using the Asymmetric Least Squares method.

A quantitative metric, termed the enhancement-to-noise ratio (ENR), was developed to identify the optimal offset. ENR was defined as the ratio of the bottom-layer Raman signal to the product of the top-layer signal and the coefficient of variation (CV) of the bottom-layer signal. The CV was

calculated as the standard deviation over the mean of the signal at each configuration. Monte Carlo simulations were performed using MCX to model photon transport in a two-layer geometry, where a cubic bottom layer was overlaid by top layers of varying thickness (1–10 mm). Fluence maps were generated for both excitation and detection positions, and their product yielded the photon path distribution between source and detector. The total signal was calculated as the integrated fluence in each layer, and noise was estimated as the square root of the signal.

The simulation results showed a parabolic relationship between ENR and spatial offset for each top-layer thickness, with the peak ENR corresponding to the optimal offset. Experimental validation using phantoms confirmed these findings. For a 5 mm thick top layer, the optimal ring radius was found to be 6 mm. As the offset increased, the Raman contribution from the superficial layer decreased while that from the deeper layer increased, albeit with higher associated noise. This trade-off was captured effectively by the ENR metric, which enabled the identification of an ideal configuration.

To test the sensitivity of the system to changes in bone quality, Raman spectra were collected from phantoms containing different HA concentrations and hydration levels, both with and without a 6 mm thick overlying tissue phantom. In the fingerprint region, a distinct peak at 960 cm^{-1} corresponding to phosphate vibrations was observed, with greater intensity in the 7% HA phantom compared to the 4% one. In the high-wavenumber region, the broad O-H stretching band from water decreased in intensity as hydration was reduced from 89.1% to 81.7%. These differences were clearly detectable through the 5 mm top layer when measured using the optimised 6 mm offset.

Finally, to demonstrate the system's translational potential, preliminary in-vivo measurements were performed on healthy human volunteers. Raman spectra were acquired from the tibia, a superficial bone site, using the optimised DW-iSORS configuration. The measurements were conducted under ethically approved protocols, with laser power and exposure time set within safety limits. The in-vivo spectra showed characteristic bone peaks and confirmed the feasibility of subsurface bone analysis in a clinical context.

In conclusion, this study presents the design, optimisation, and validation of a dual-wavelength inverse spatially offset Raman spectroscopy system for subsurface bone characterisation. The novel ENR-based metric provides a practical and effective approach for selecting spatial offsets that maximise signal quality from deeper layers. The system was successfully applied to layered phantoms and in-vivo bone measurements, demonstrating its sensitivity to subtle compositional changes, such as 3% variations in HA content and 7% changes in hydration. These findings support the system's potential use in non-invasive diagnostics and monitoring of bone-related diseases, offering a portable, label-free tool for assessing bone quality beyond conventional surface-limited techniques.

Acknowledgements

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Keywords

bone, characterisation, in-vivo, non-invasive, Raman

Laser Induced Graphene: A Sustainable Platform for Monitoring Health and Wellbeing

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Abstract:

Accurate detection and continuous monitoring of biochemical markers are critical for advancing personalized healthcare and enhancing overall wellbeing, particularly through non-invasive, point-of-care diagnostic technologies. Among such biomarkers, pH and uric acid are especially important: pH reflects key physiological and metabolic conditions, including acid-base balance and kidney function, while abnormal uric acid levels are associated with disorders such as gout, kidney disease, and metabolic syndrome. Early and reliable detection of these parameters can significantly aid in the timely diagnosis and management of chronic diseases. In this work, we present a sustainable, laser-induced graphene (LIG) based sensing platform for the selective detection of pH and uric acid. The platform is developed using a rapid, chemical-free laser scribing technique on flexible polyimide film, utilizing a cost-effective 450 nm hobbyist laser. LIG, with its high surface area, tunable surface chemistry, and excellent electrical conductivity, provides an ideal foundation for sensitive electrochemical biosensing. The pH sensor, functionalized with polyaniline (PANI) nanowires, demonstrated a sensitivity of 56.73 mV/pH across a broad range (pH 4–10), with low hysteresis (2.29 mV) and minimal potential drift, indicating high stability and reproducibility. The non-enzymatic uric acid sensor exhibited a sensitivity of 707.1 nA/μM/cm² and a limit of detection (LOD) of 2.83 μM, effectively covering the physiological range (10–80 μM). Both sensors maintained reliable performance in artificial urine, confirming their potential for integration into wearable or portable diagnostic devices. This work highlights the potential of LIG as a sustainable, low-cost, and eco-friendly material for next-generation health monitoring technologies, supporting early disease detection and improved wellbeing through accessible and real-time biosensing.

Acknowledgements

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Keywords

Electrochemical Sensors, Health and Wellbeing

The Use of Citizen Science Tools for Pesticide and Contaminant Detection in Freshwater Bodies

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Abstract:

Citizen Science (CS) refers to the active involvement of non-professional scientists in scientific research, particularly in the collection, analysis, and interpretation of data. It represents a powerful model for public engagement, fostering collaboration between scientists and communities to enhance scientific knowledge and empower individuals to contribute meaningfully to data-driven environmental initiatives. Through citizen science, members of the public participate directly in monitoring and research, helping to address complex environmental challenges with broader spatial and temporal coverage than traditional scientific methods alone can achieve. The European Union recognises citizen science as a valuable and cost-effective approach to environmental data collection. It enables the generation of complementary datasets that support official environmental monitoring programmes. Importantly, citizen science has been identified as a tool not only for augmenting data used in the implementation of EU environmental policy but also as a potential mechanism for providing early warnings about emerging environmental trends and specific localised issues.

The monitoring of water quality, especially in the context of hydrological and hydroclimatic events, is an area where citizen science can play a pivotal role. These events—such as intense rainfall, flooding, or storm surges—can lead to the sudden introduction of a variety of contaminants into aquatic ecosystems. Rapid and widespread data collection becomes essential in the immediate aftermath to assess environmental impact and safeguard public health and biodiversity. Citizen science networks, when activated in these critical windows, can provide valuable real-time data from multiple locations.

Among the most concerning pollutants mobilised during such events are pesticides, which are known to pose serious risks to freshwater ecosystems. Due to their widespread use in agriculture and their propensity to be transported via surface runoff, especially after heavy precipitation or flooding, pesticides can enter water bodies in concentrations that threaten aquatic life and water quality. Monitoring for pesticide residues in freshwater systems, particularly following hydrodynamic events, is therefore essential. Citizen science initiatives, equipped with appropriate protocols and tools, can significantly enhance the spatial resolution and responsiveness of pesticide monitoring, supporting more effective water resource management and environmental protection.

This research describes the development of a simple-to-use citizen science tool using the concept of solid phase extraction (SPE) to collect samples from water bodies in a 3-step process. The steps include sample filtering and transfer of the water into 500 mg SPE cartridges. These samples are then transported to DCU for lab analysis using LC-MS. The innovation lies in the sample collection tool that enables CS to gather data on less well monitored locations.

The samples collected by the CS volunteers across Ireland are analysed for targeted pesticides to help address the question of impact of hydro-climatic events on water quality. The data presented will show the development, trial, testing and demonstration of the novel CShydro tool and will identify the potential for engaging citizens in water quality monitoring given high quality devices with training and feedback as part of the DCU CS Framework.

Acknowledgements

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Keywords

Citizen Science Pesticides Freshwater LCMS

DNA repair, sound faults, and the echo of unresolved harm

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Abstract:

This presentation explores a frontier perspective at the intersection of analytical science, DNA repair, and the unresolved harm embedded in the collective biology of humanity. Drawing on clinical and field research, I propose that unhealed trauma—whether through famine, conflict, environmental exposure, or systemic neglect—leaves a detectable imprint not only on the individual but on the global biosphere. Unresolved shadow held in cellular memory causes structural misalignment sound and motion distortion. Across multiple nations, populations have suffered as collateral in historic and modern upheavals, from forced starvation to radiation testing.

While this talk does not assign blame, it seeks to open inquiry into how such events leave a resonance—an acoustic fault line—a sound fracture within the collective atmosphere. This 'shadow,' is held in cellular function and is detectible through subtle anomalies, behavioural disorders, and degenerative biological signatures. Using a multidisciplinary approach, I will outline how unresolved toxic harm creates disturbances in mechanisms and can be identified in the body and the wider environment.

I will also touch on the action required to support biological and energetic repair, including treatment of violence protocols, international research collaboration, and policy reorientation towards repair. I will provide videos to clarify. This presentation invites analytical science to a collaborative dialogue: one that examines force in the living mechanism not only as a measurable reaction but as a transmissible legacy. We will investigate realignment of the structure that governs the function symmetry motion and chemistry of the living mechanism in interdependent collaboration with organic natural Law authority.
*UK government research commissioned by director of operations report on the prison integrated medicine regime development led and implemented by Marian Mulligan. Marian worked in UK prisons over a period of 14 years with a team of 200 naturopaths. Attached
Link https://sphenoidireland.ie/category/articles
Research article Number 46 https://cdn.researchfeatures.com/3d_issues/RF156/index.html

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Professor Dr. Surya Bahadur Karki Coordinator International relationships Nepal. Dr. Dharma Raj Karki Director of research training and natural health services. Invited Member of executive South Asia initial yoga Olympic committee.
Short listed for award in integrated medicine, then Prince Charles, Foundation of integrated medicine.

Keywords

UK government research
Research article

Development of SPE-CZE-UV methods for the detection of APIs in wastewater effluents and their comparison to implemented HPLC-UV methods

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Abstract:

In this research, Capillary Zone Electrophoresis (CZE) methods were developed to determine the presence of Active Pharmaceutical Ingredients (APIs) in a pharmaceutical manufacturing company's wastewater effluent. Wastewater effluents are a significant contributor to pharmaceutical pollution, which can cause irreversible effects to the aquatic environment and has the potential to affect human health. The target analytes chosen for this research include an antibiotic API known as NB23 and an anti-parasitic known as ZB23. To determine the optimum CZE method, acetate/citrate, phosphate and borate buffers were analysed over a wide pH range of 3 – 10.5 and a concentration range of 10 – 25 mM. With the APIs' solubility issues, the addition of an organic modifier was analysed using methanol (MeOH), acetonitrile (ACN) and acetone. To keep the method environmentally friendly, the organic modifiers were kept within a 5 – 15 % v/v range. A voltage range of 5 – 20 kV and an injection pressure range of 10 – 75 mbar for 5 seconds were also analysed.
The developed CZE methods were validated and then compared to the company's internal HPLC method, which determined that the developed CZE method required less preconditioning and shorter run times. When compared to the HPLC method, the developed CZE method was significantly more environmentally friendly with its water-based buffers and the reduction of organic solvents, with the CZE methods requiring 3.75 mL when compared to the 2 L required for the HPLC. It was determined that the HPLC method for NB26 had a lower limit of detection (LOD) than the developed CZE, and, therefore, solid-phase extraction (SPE) methods were developed and compared using two different sorbent types: natural (silica) and synthetic (styrene-divinylbenzene (SDVB) polymer). From the analysis of these two sorbents, it was determined that the synthetic sorbent lowered NB26's CZE LOD.

Leveraging AFFFs to support suspect screening of PFAS in marine biota of low trophic level

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Abstract:

Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals known for their unique properties, which have led to widespread environmental contamination, particularly in marine ecosystems. While some legacy PFAS have been regulated, emerging alternatives complicate contamination profiles. High-resolution mass spectrometry (HRMS), coupled with non-target and suspect screening, provides a broader perspective on PFAS contamination. However, these methods have primarily been applied to heavily contaminated sites and top predators, with limited use in lower trophic organisms. Yet, such studies are essential for detecting PFAS precursors that may undergo biotransformation at higher trophic levels. This study explores the use of aqueous film-forming foams (AFFF) formulations as qualitative reference materials to support suspect screening of PFAS in marine bivalves, offering a practical approach to broaden PFAS detection in environmental samples. Mussels and oysters were collected in 2021 from 23 sampling sites along the French coast and analysed by liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS). Suspect screening was performed using El-MAVEN software and an in-house suspect list of 866 PFAS. To support detection and identification, electrochemical fluorination (ECF)-based and telomerization (FT)-based aqueous film-forming foams (AFFFs) were analysed and used as reference materials. A total of 79 PFAS from 29 classes were detected, including non-biotransformed precursors, some of which were identified for the first time in marine organisms (e.g., X:2 FTSAm). Several compounds, such as 6:2 FTAB and FHxSA were consistently found across all sampling sites, raising concerns about their widespread occurrence. Most of the compounds detected in the bivalves were also detected in AFFFs. The PFAS identified as perfluoroalkyl compounds were mainly detected in ECF-AFFFs while the ones identified as polyfluoralkyl compounds were mainly detected in FT-AFFFs, consistently with known formulation compositions. This work demonstrates the effectiveness of using AFFF formulations as reference tools in PFAS suspect screening workflows. Applied to low trophic level species such as mussels and oysters, this approach enhances the detection of precursor compounds that might be otherwise biotransformed or undetectable in higher trophic levels. The methodology presented here offers a practical and informative strategy for expanding PFAS monitoring efforts in marine environments.

Distribution of Rare Earth Elements in the Food Web of Two French Estuaries

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Abstract:

Rare earth elements (REEs) regroup 17 metallic elements including the 15 lanthanoids (from lanthanum to lutetium), yttrium and scandium. Their increasing use in many industrial sectors causes an increase of discharges into the environment and particularly in estuarine areas subject to strong anthropogenic pressures. This study focused on assessing the distribution of REEs along the food web of two French estuaries: the Loire and the Seine estuaries, subject to different anthropogenic pressures. Several species representative of different levels of the estuaries food webs were sampled: *T. luscus, O. eperlanus, P. flesus, D. labrax, C. ramada, S. Solea, A. anguilla, S. sprattus, C. crangon, P. logirostris, C. volutator, S. plana, L. balthica, N. hombergii, N. diversicolor, H. filiformis, F. vesiculosus, F. spiralis, U. lactuca, U. intestinalis* for the Loire estuary and *L. limanda, P. flesus, P. platessa, E. vipera, C. fornicata, S. plana, L. balthica, N. diversicolor, U. intestinalis, C. rupestris, Ulothrix spp.* for the Seine estuary. The REE concentrations were measured in organisms by ICP-MS and trophic relations were estimated by stable isotope analysis (C and N). For fish, REE concentrations were also determined in muscles and gonads. Intra-species differences have been highlighted withgreater concentrations of light REEs than medium and heavy ones for all species of the two estuaries. In addition, a higher REE accumulation was observed in lower trophic level species (algae, annelids, crustaceans and molluscs) compared to fish, belonging to higher trophic levels. These inter-species variations demonstrate a phenomenon of trophic dilution. For both estuaries, total mean REE concentrations values were the highest for *U. intestinalis* (34 and 166 µg/g dw) whereas the lowest was for *T. luscus* (0.1 µg/g dw) in the Loire estuary and for *P. platessa* (0.03 µg/g dw) in the Seine estuary. Inter-phylum disparities were also noticeable. For example, in the Loire estuary, *H. filiformis* showed much higher concentrations than the two other annelid species and among the vertebrates, *C. ramada* presented twenty times higher concentrations than *T. luscus*. Globally, REE concentrations in fish were lower in muscles and gonads than in the total organisms. Post Archean Australian Shale normalization allowed to highlight gadolinium positive anomalies in the REE patterns of most studied species, especially visible in fish of the Loire estuary and in aglae of the Seine estuary.

The Computational Chemistry world applied to the Analytical chemistry. How can we help?

Dr Davide Tiana
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Abstract:

At the Cork Computational Chemistry and Programming (CCCP) group we avail of computational chemistry techniques to investigate and solve complex chemical problems. Through advanced simulations we explain chemical properties at atomic level, enabling the prediction and understanding of physico-chemical behaviours.

When applied to analytical chemistry computational methods such as 1st principle calculations, molecular dynamics, Monte Carlo, etc complement experimental techniques by providing theoretical insights into chemical phenomena.

For instance, simulations can be used to calculate spectroscopic data such as UV-vis, IR and Raman, Mass spect, etc... Additionally, we can predict the kinetics and thermodynamics of chemical reactions providing reaction pathways of the evolution of pollutants. Our models can also be used to describe and quantify the interactions between analytes and the stationary phase allowing the optimisation of the separation conditions, the testing different solvents or the design new materials. Finally, our simulations can be used to build a dataset of specific in-silicon chemical descriptors to feed and construct successful artificial intelligence machines.

SMARTBioP: Advancing Biopsy Precision with a Novel Needle-Integrated Bioimpedance Sensor for Real-time Tissue Differentiation

Dr Justina Ugwah[1,4], Darren Dahly[5], Edel Whelton[1,4], Dr Yineng Wang[1,4], Brian D.O. Donnell[3], Prof. Martin J.O'Sullivan[2], Prof. Eric J. Moore[1,4].

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Abstract:

Traditional biopsy procedures suffer from blind sampling, high miss rates (15-30%), and inconsistent procedures. We developed SMARTBioP, a biopsy system with a novel needle-integrated bioimpedance sensor for real-time tissue differentiation.

The system combines bioimpedance sensing technology with machine learning algorithms to characterize tissue types during biopsy procedures. A needle-integrated sensor provides real-time electrical impedance measurements, while the innovative software analyses bioimpedance signatures for immediate tissue identification.

Preliminary validation demonstrates successful discrimination between tissue types based on bioimpedance measurements. The integrated platform provides immediate analytical feedback during procedures, with the potential to reduce miss rates and improve sampling accuracy.

SMARTBioP represents a significant advancement in analytical instrumentation for medical diagnostics, offering real-time tissue characterization capabilities that could transform biopsy procedures. Future work includes device validation, first-in-human studies, and regulatory compliance.

Acknowledgements:
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Keywords:
Bioimpedance, real-time tissue analysis, biopsy guidance, medical diagnostics, AI-assisted healthcare, analytical instrumentation

The Analysis of Cu(II) N,N-disubstituted-N'-acylthiourea Complexes- "It's Complex"

Jack Daly, Davide Tiana and David Otway
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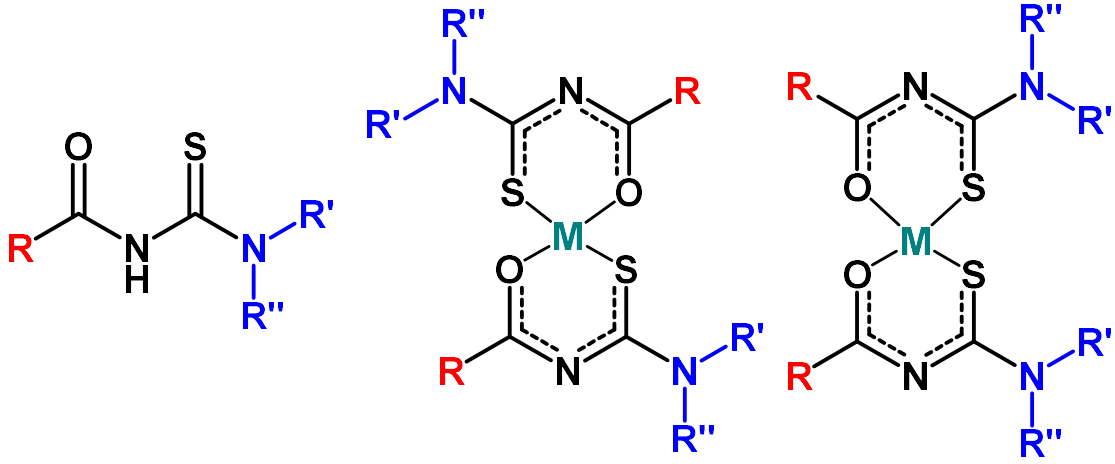
Abstract:

Antifungal resistance is an escalating global health concern, underscoring the urgent need for novel antifungal agents. This study investigates *N,N*-disubstituted-*N'*-acylthiourea copper(II) complexes as promising potential antifungal candidates. Acylthiourea ligands, known for their bioavailability and tuneable structure, offer unique chelating properties that enable modulation of biological activity through modifications to both the acyl group and terminal amine substituents.

The primary focus of this work is on the synthesis and characterisation of Cu(II) complexes, with particular attention to the significant analytical challenges posed by Cu(II)'s paramagnetic nature, variable coordination geometries, and tendency to form mixtures of species in solution. These characteristics complicate the determination of both structure and purity—factors that are essential for ensuring reliable and reproducible biological testing. Impurities or uncharacterised by-products can obscure biological activity profiles or lead to misleading conclusions.

To address these difficulties, a multi-technique approach was employed, combining spectroscopic, thermal and structural methods to achieve confident characterisation of the target complexes. Care must be taken to confirm the purity and identity of each complex, as even small inconsistencies could compromise the interpretation of antifungal screening results. This rigorous analytical foundation is crucial not only for validating biological activity, but also for enabling meaningful structure–activity relationship studies that can guide future antifungal drug design.



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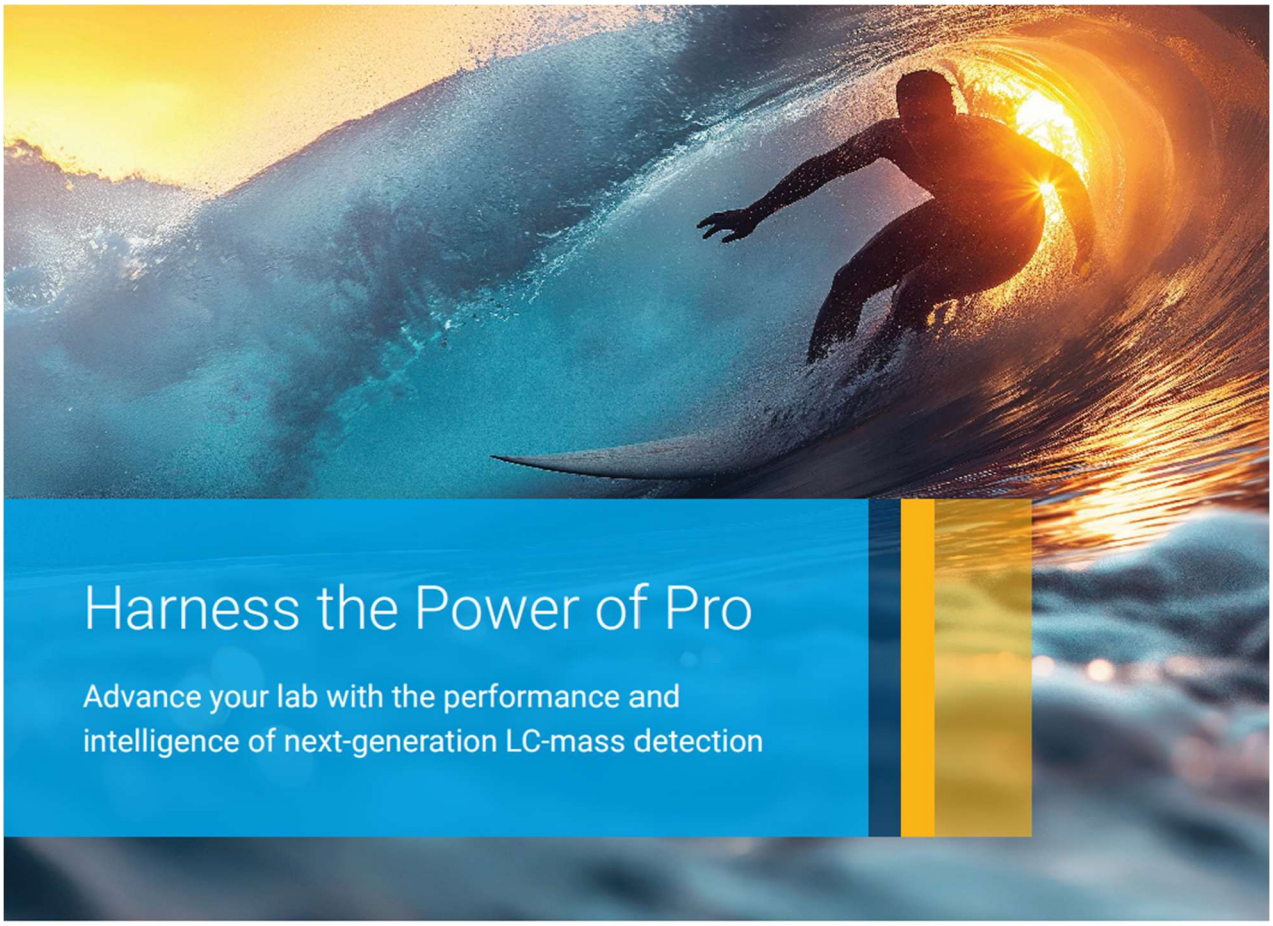

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