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ABSTRACT BOOK

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October 17-18, 2022 | Virtual

Meeting Time Zone:
(GMT-4:00) Eastern Time

Day 01 | October 18, 2022

PLENARY PRESENTATIONS

MA'AT Analysis: Applications to Determine Conformational Equilibria and Dynamics of Molecules in Solution

Anthony S. Serianni[1*]
Ian Carmichael[2]
Robert J. Woods[3]

[1]Department of Chemistry and Biochemistry
[2]Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556-5670 USA
[3]Complex Carbohydrate Research Center, University of Georgia, Athens, GA 30602 USA

Abstract:

This laboratory has been investigating MA'AT analysis [Meredith et al., J. Chem. Inf. Model. 2022, 62, 3135–3141] to determine conformational equilibria and dynamics of saccharides in solution. The work is motivated by the fact that, historically, it has been difficult to validate similar information obtained from molecular dynamics simulations and related computational methods which are relied upon to interpret experimental NMR data such as residual dipolar couplings and nuclear spin relaxation. We have been trying to provide this validation using a new method that depends on multiple redundant NMR spin-coupling constants as experimental structure constraints, density functional theory to derive quantitative relationships between these Jcouplings and molecular torsion angles, and circular statistics (MA'AT analysis) to obtain probability distributions of molecular torsion angles from which conformational models are constructed. This talk will focus mainly on applications of the MA'AT method to saccharides but will also describe recent applications to peptides and to the furanose rings of RNA and DNA. The strengths and limitations of MA'AT analysis will also be discussed. [Supported by NSF CHE 1707660 and CHE 2002625]

Biography:

Anthony Serianni is Professor of Chemistry and Biochemistry at the University of Notre Dame. His research interests include (a) methods development for site-specific stable isotopic labeling of carbohydrates and their derivatives, (b) synthesis and conformational studies of simple and complex carbohydrates related to the N-glycans of human glycoproteins by nuclear magnetic resonance (NMR) spectroscopy, x-ray crystallography and other biophysical techniques, (c) applications of density functional theory and molecular dynamics to aid in the interpretation of NMR parameters in saccharides, (d) structure-function studies of non-enzymatic protein glycation, and (e) chemical evolution.

KEYNOTE PRESENTATIONS

Analysis of Drug Interactions with Humic Acid using Entrapment-Based Microcolumns and High-Performance Affinity Chromatography

David S. Hage[1*]
Sazia Iftekhar[1]
Saumen Poddar[1]
Madeline Rauhauser[1,2]
Daniel D. Snow[2]

[1]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, USA
[2]Water Science Laboratory, University of Nebraska-Lincoln, Lincoln, NE, USA

Abstract::

Reversible interactions between drugs and humic acid in water can be an important in determining the bioavailability and effects of these pharmaceuticals as micropollutants in the environment. In this study, high-performance affinity microcolumns containing entrapped humic acid were used in liquid chromatography to examine the binding of this agent with the drugs tetracycline, carbamazepine, ciprofloxacin, and norfloxacin. Parameters that were varied to optimize the entrapment of humic acid within HPLC-grade porous silica included the starting concentration of humic acid, the mass ratio of humic acid vs silica, and the method of mixing the reagents with the support for the entrapment process. The binding constants measured for the given drugs with microcolumns containing entrapped Aldrich humic acid, which was used as a model in this study, gave good agreement with values reported in the literature under similar pH and temperature conditions for this and other forms of humic acid. Besides providing valuable data on the binding strength of various drugs with humic acid, this work illustrates how high-performance affinity microcolumns may be used in liquid chromatography for screening and characterizing the interactions of drugs and man-made contaminants with humic acid or related binding agents in water and the environment.

Biography::

David S. Hage is the James Hewett University Professor in the Department of Chemistry at the University of Nebraska-Lincoln. His research group is interested in theory, development, and use of affinity-based separations in HPLC and capillary electrophoresis. He has over 310 papers, book chapters, and books in this field, along with seven U.S. patents. He has several awards for his work in these areas, including the 2021 American Chemical Society Award in Chromatography and the 2017 Pierce Award in Affinity Technology. He is current Editor-in-Chief for the Journal of Chromatography B, and the editor of the Handbook of Affinity Chromatography.

Post-Deconvolution MS/MS Spectra Extraction with Data-Independent Acquisition for Comprehensive Profiling of Urinary Conjugated Metabolome

Yuan-Chih Chen
Hsin-Yi Wu
Chih-Wei Chang
Pao-Chi Liao*

Department of Environmental and Occupational Health, College of Medicine, National Cheng Kung University, Tainan 701, Taiwan

Abstract:

Conjugation reactions are of critical significance in human metabolism. Identification of these conjugated metabolites is still challenging. Here, we propose a strategy, post-deconvolution MS/MS spectra extraction with data-independent acquisition (PDMS2E-DIA), to comprehensively profile the glucuronide conjugated metabolome. PDMS2E-DIA enables the identification of conjugated and unconjugated metabolite pairs through neutral loss filtering combined with a significant change in abundance after the deconjugation reaction. Purified DIA MS/MS spectra were constructed by extracting MS/MS fragments shared between spectra derived from conjugated and unconjugated metabolites. The feasibility of this approach was first demonstrated by the identification of two glucuronide-conjugated metabolite standards spiked in urine samples. For human urine samples, 479 features were structurally annotated as potential glucuronide-conjugated metabolites, resulting in the identification of 211 metabolites. Fragment peaks derived from interferents were found to be removed by PDMS2E-DIA, which increased about 6 times the number of identified urine metabolites compared with those calculated from raw DIA deconvoluted MS/MS spectra. This approach was found to have great potential for identifying glucuronide-conjugated metabolites, as well as other kinds of chemical conjugations.

Biography:

Pao-Chi Liao completed his Ph.D. in Analytical Chemistry from Michigan State University (MSU) in 1995 before doing postdoctoral research in the Department of Biochemistry at MSU. Dr. Liao joined the faculty at Department of Environmental and Occupational Health, National Cheng-Kung University, Taiwan in 1997, where he was promoted to full professor in 2006, and named Distinguished Professor in 2011. Dr. Liao's research interests and fields of specialty include analytical chemistry, mass spectrometry, proteomics, biomarker discovery, cancer biomarkers, lung cancer metastasis, and environmental and occupational health.

Analysing the Physicochemical Properties of Ultra-Sonicated Tapioca Starch to use as a Potential Pharmaceutical Binder

Mohamed Rasmi Pathuma Chasna[1*]
Chathuni Jayathilake[1]
Tharaka Gunawardhana[2]

[1]University of Sri Jayewardenepura, Sri Lanka
[2]Industrial Technology Institute, Sri Lanka

Abstract:

Tapioca starch is one of the pharmaceutical grade starches used as an excipient in solid dosage formulations. As the physicochemical properties of native starch unfavorably affect the pharmaceutico-technical properties of the dosage, modification experiments have been carried out to enhance desirable characteristics. Ultra sonication is an emerging concept of Greentech and it not only modified starch but also sterilized it. This study was designed to explore the potential binder properties of ultra-sonicated tapioca starch by analyzing its physicochemical properties. Starch was extracted by wet milling and ultra-sonicated using an ultrasonic processor at a power of 100 W. The physicochemical characteristics of native and ultra-sonicated starch were analyzed, including color, morphology, pH, solubility, and swelling index. The L* value indicated that ultra-sonicated starch was significantly ($p<0.05$) whiter than that of native starch, and it had a slightly acidic pH which was 6.17. Ultra-sonicated starch granules were similar to those of native starch, round in shape with concave pits in a size range of 10–15 µm. However, an aggregated structure was observed in ultra-sonicated starch, resulting in a greater degree of association, which in turn significantly lowered the swelling. And there was no significant difference observed in solubility. Based on the results, it was evident that the physicochemical properties of ultra-sonicated starch were consistent with the required characteristics of starch used as a pharmaceutical binder, thus ultra-sonicated starch could be explored for its potential use as a binder in solid dosage formulations.

Biography:

Mohamed Rasmi Pathuma Chasna is a Food Science graduand at the University of Sri Jayewardenepura, Sri Lanka. She is expecting to receive the bachelor's honors degree in Food Science and Technology, and the certificate of efficiency in pharmacy from Sri Lanka Medical Council. She is looking for a PhD opportunity and interested in quantitative analysis, qualitative analysis, food & beverage analysis and pharmaceutical analysis.

Analytical approaches for Chemo/ Bio-Sensing: Surface and Electrochemistry Perspective

Parthasarathy Srinivasan[*]

Department of Electronics and Communication Engineering, Amrita School of Engineering, Chennai, Amrita Vishwa Vidyapeetham, India

Abstract:

In the modern era, analytical methods play an important role in the sensing/ probing

of various chemical/bio species. The analytical approaches which we implement for different applications including healthcare, environmental, and food quality assessment with the key insights have been addressed. In the first part of this talk, the key results and observation of the analytical methods which we have employed for the detection of quorum sensing signals have been emphasized. The probing of quorum sensing signals using the photo-luminescence principle for the early diagnosis of the Urinary Tract Infection (UTI) is highlighted. These biosensing measurements based on PL intensity variations corresponding to the acceptor defect level of metal oxides (ZnO and TiO2) with reference to the cysteamine functionalized metal oxides have been considered. In the second part of the talk, the electrochemical analysis involved in the detection of hydrogen peroxide in river water with a novel mechanism is emphasized. The third part of this talk covers a novel electrochemical comparator-based analytical system for the detection of formalin levels in fishes. In the final phase of this talk, the chemosensors developed for analyzing the human exhaled breath have been focused.

Biography:

Parthasarathy Srinivasan is currently serving as an Assistant Professor in the Department of Electronics and Communication Engineering, Amrita School of Engineering, Amrita Vishwa Vidyapeetham, Thiruvallur, Chennai. His current research work includes the development of chemosensors, electrochemical, and photoluminescence biosensors towards food quality, environmental, and health care applications using different nanostructures of metal oxides and 2-D materials. In addition, he has been working on the development of a chemo-sensors array (electronic nose) for the quality assessment of food items.

Development and Application of Electrochemical Sensors for the Detection of the SARS-CoV-2 Antigen and Antibody Proteins

Lokman Liv

Electrochemistry Laboratory, Chemistry Group, The Scientific and Technological Research Council of Turkey, National Metrology Institute, (TUBITAK UME), 41470, Gebze, Kocaeli, Turkey.

Abstract:

The unparagoned coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome-Coronavirus-2 (SARS-CoV-2), has heavily ruined public health systems and economies worldwide. The disease progresses with stages of dry cough, fever and finally difficulty in breathing. Although there are many different techniques for the determination of viruses, electrochemical biosensing methods stand out in terms of cheapness, simplicity, rapidity, sensitivity and selectivity [1–3].

In view of those drawbacks, it is aimed to develop electrochemical methods for determining the SARS-CoV-2 antigen or antibody proteins in synthetic and/or real samples. As a result, three different biosensing platforms including SARS-CoV-2 spike antibody modified functionalised graphene oxide [1], SARS-CoV-2 spike antigen, glutaraldehyde, cysteamine and gold-clusters modified electrode [2] and SARS-CoV-2 spike antigen, mercaptoethanol and gold-clusters modified electrode [3] were produced to diagnose COVID-19 in synthetic and/or real samples.

Biography:

Lokman Liv received his bachelor's degree from Balıkesir University, Turkey, in 2010 and received his Ph.D. degree in Analytical Chemistry from the same university in July 2017. He is a chief researcher and the head of Electrochemistry Laboratory at The Scientific and Technological Research Council of Turkey, National Metrology Institute, (TUBITAK UME). His research interest includes production of chemically modified electrodes and sensors, development of voltammetric methods for determining inorganic, organic and biological materials.

Magnetic Levitation-Based Cell Response Analysis

Seren Keçili[1*]
Sümeyra Vural-Kaymaz[2,3]
Meltem Elitaş[4]
H. Cumhur Tekin[1,5]

[1]Izmir Institute of Technology, Turkey
[2]Sabanci University, Turkey
[3]Sabanci University Nanotechnology Research and Application Center (SUNUM), Turkey
[4]Faculty of Engineering and Natural Sciences, Sabanci University, Turkey
[5]METU MEMS Research and Application Center, Turkey

Abstract:

The properties of cells, such as density, deformation, and area, may be used to identify cellular responses to different conditions. These changes may be used as biomarkers to analyze the efficacy of different drugs. Magnetic levitation (MagLev) method allows measurement of cell densities down to a single-cell level and could simplify single-cell analysis without a labeling. Here, single-cell densities, and also cell deformability and area were measured in a MagLev setup at the same time. The MagLev setup is composed of two opposing N52-grade neodymium magnets, a capillary channel to observe the cells in a paramagnetic medium, and two mirrors to observe the cells in the channel under an inverted bright field microscope. Levitation heights and densities of cells were determined in the platform, and the cell deformation index and area were also identified on cell images. In our platform, we observe the response of U937 monocyte cells exposed to different mediums, i.e., Rosewell Park Memorial Institute medium (RPMI) and phosphate buffer saline (PBS). We observed that levitation heights were 829.67±24.11 and 787.44±64.52 in RPMI and PBS, respectively. Furthermore, PBS changes osmotic pressure of cells and it resulted in difference of densities, area and deformation indices of cells. The densities and deformation indices of cells were increased by 11.9% and 26.6%, respectively, and areas of cells were decreased by 22.25% in PBS compared to cells in RPMI. Hence, our platform could allow us to monitor cell responses in real time in a label-free manner.

Biography:

Seren Kecili received her BSc and MSc degrees in Biology Department from Istanbul University, Turkey in 2015, and Biotechnology Program from Izmir Institute of Technology (IZTECH), Turkey in 2019, respectively. She is a PhD candidate in Bioengineering Department of IZTECH, and she works in Laboratory of Biomedical Micro and

Nanosystems established by Dr. H. Cumhur Tekin. Her fields of interest are microfluidics, microfabrication, 3D printing technology, magnetic levitation, protein detection and tissue engineering.

A Paper-Based Chemiluminescent Immunoassay on Magnetic Microbeads Format for Food Allergen Traces Detection

Donato Calabria*
Ilaria Trozzi
Martina Zangheri
Andrea Pace
Elisa Lazzarini
Massimo Guardigli
Mara Mirasoli

Department of Chemistry "Giacomo Ciamician", University of Bologna, Bologna, Italy

Abstract:

In developed countries, the global perception of "food allergy" in the population is around 20%, while according to recent epidemiological data food allergies affect the population by more than 1-2% and less than 10%. Ingestion of a food allergen by an allergic person can induce severe clinical responses, up to fatal anaphylaxis. Since cross-contaminations inevitably occur in the food production chain, cheap, rapid, and field-deployable biosensors are required for monitoring the presence of allergens. Herein, we present a point-of-use biosensor for the detection of ovalbumin allergen in food exploiting chemiluminescence (CL) detection. A competitive CL immunoassay was developed employing magnetic microbeads as a solid phase and CL detection in a paper-based format using a portable CCD-based detector. An origami architecture has been designed, in which each paper level has a specific role in the analytical procedure and correct folding of the sheets ensures quantification of the target. The advantage of this format is to exploit the separation and purification of the analyte from the sample matrix on magnetic microbeads, which can be easily recovered from their suspensions by applying a magnetic field. This soft sample isolation approach simplifies and speeds up the incubation and washing steps of ELISA tests, thus facilitating the transfer of such methods into miniaturized formats, such as in paper-based or microfluidic devices. In addition, it facilitates the transport, immobilization, and concentration of the analyte in the biosensor's areas of interest. Calibration curves for ovalbumin provided a limit of detection of 0,5 ng/mL.

Biography:

I am a junior professor assistant at Department of Chemistry "Giacomo Ciamician", University of Bologna, 40126 Bologna, Italy. The interests of my research activity are the development of optical biosensors; chemiluminescence biosensors; chemosensors; paper-based devices for point of use and point of care application in nutraceutics, environmental and health care analysis.

Application of Metallomics and Metabolomics to Environmental Metal Toxicity Assessment

J.L. Gómez-Ariza[1,2*]
T. García-Barrera[1,2]
Alejandro Regaña Establier[1,2]

[1]Department of Chemistry, Faculty of Experimental Science, University of Huelva, Spain.
[2]Research Centre of Natural Resources, Health and the Environment, University of Huelva, Spain.

Abstract:

Neurodegenerative diseases constitute one of the most important social, human, family and economic problems of the 21st century. On the one hand, because its etiology, pathology, symptoms and evolution are not yet well known, so that new analytical methodologies based on massive information and other frontier approaches are necessary. One important point is that people living in cities are exposed to high levels of air and noise pollution, and a lack of natural outdoor environments, which has been associated with premature mortality and other detrimental health effects, including premature aging, mental health and neurodegenerative diseases, particularly Alzheimer's disease. Neurotoxic metals such as lead, mercury, aluminum, cadmium, and arsenic, as well as some pesticides and metal nanoparticles, have been implicated in AD due to their ability to increase beta-amyloid peptide (Aβ) and phosphorylation of Tau protein (P-Tau). For this purpose, suitable a number of methodological tools based on elemental and molecular mass spectrometry have been proposed: 1.- Analysis of traces and ultra-traces of metals and metalloids, of an essential nature (Ca, P, S, K, Na, Cl, Mg, Fe, Zn, Mn, Cu, I, Cr, Mo, Se, Co), toxic (Cd, Pb, Al), or neurotoxic (Hg, As), in tissues and biological fluids; 2.- Analysis of traces of chemical species of toxic or essential elements (speciation): As, Hg, Se; 3.- Methodologies for the identification and analysis of metallo-biomolecules (Metallomics); 4.- Methodologies for the massive characterization of metabolites altered by pathological processes (Metabolomics); 5.- Methodologies for the massive characterization of proteins altered by pathological processes (Proteomics).

Biography:

Jose Luis Gómez-Ariza is full professor of Analytical Chemistry of the University of Huelva (Spain). Member of the Spanish Society for Analytical Chemistry (SEQA). In 2003 received the Andalusia Research Award and the Huelva Industry Award. Actual topics of interest are the development and application of omic methodologies for the study of pollution on aging and related neurodegenerative pathologies. Over 300 scientific publications, 20 book chapters and 600 conferences contributions. He belongs to the advisory board of Metallomics journal and is co-editor of Current Alzheimer Disease.

Simple and Cheap Potentiometric Sensor for Chloride Monitoring in Water Samples

Cecylia Wardak[1*]
Karolina Pietrzak[1]
Szymon Malinowski[2]

[1]Maria Curie-Sklodowska University in Lublin, Poland
[2]Lublin University of Technology, Poland

Abstract:

Potentiometry with ion-selective electrodes (ISEs) allows to directly determine free ion concentration in aqueous samples. The main advantages of this technique are low costs, speed which samples can be analyzed with, device portability, no sample destruction and the requirement of minimum sample preparation. Among the various types of ISEs, those with solid contact (SCISEs) are becoming increasingly popular. To obtain solid contact ISEs with stable and reproducible potential various conductive and electroactive materials have been used.

In this work the construction, properties and analytical application of chloride ion-selective electrode with solid contact will be presented. Various types of nanomaterials including polyaniline nanofibers dopped with chloride ions, multiwalled carbon nanotubes and the nanocomposite of chloride-doped polyaniline nanofibers and multiwalled carbon nanotubes were used for the electrode construction. Many types of electrodes were tested, differing in the composition of the solid contact material and the thickness of its layer placed between the electrode material and the ion-selective membrane. An extensive analysis of the electrical parameters of the sensors was carried out and their analytical parameters were compared. The best analytical parameters showed electrode with solid contact based on nanocomposite material. It had a theoretical slope of the electrode characteristic curve in a wide measuring range and good potential stability. Moreover proposed electrode was resistant to changing measurement conditions (redox potential, light, presence of gases). The chloride content in the river and tap water samples was successfully determined with the use of such electrode.

Biography:

Cecylia Wardak received her Ph.D. degree in analytical chemistry in 2004 and her DSc degree in analytical chemistry and electrochemistry in 2015 from Maria Curie Sklodowska University (MCSU), Lublin, Poland. Since then, she has been working as associate professor in the Department of Analytical Chemistry of Maria Curie-Sklodowska University. She is an active COST member. Her main scientific interests are research, development, and analytical applications of electrochemical sensors and biosensors. Her latest research focused on the use of nanomaterials and composite materials in the construction of ion-selective electrodes. She has published over 70 peer-reviewed papers

Voltammetric Analysis of Δ9-Tetrahydrocannabinol and Cannabidiol in Seized Samples using Disposable Electrodes Chemically Modified with Graphene Oxide

Marcelo Firmino de Oliveira*
Juliene Morais de Faria

Departamento de Química – Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto – Universidade de São Paulo, Brasil.

Abstract:

The Δ9-tetrahydrocannabinol (Δ9-THC) and the Cannabidiol (CBD) are the main

cannabinoids present in the plant Cannabis sativa L. Hemp plant has been used by humanity for centuries for various purposes such as food, religious rituals, medicinal practices and, mainly, recreational use. The most well-known drug from C. sativa is marijuana, a hallucinogenic drug. The initial confirmation of the presence of cannabinoids in samples seized by police forces is currently done by colorimetric testing using the reagent Fast Blue B salt and by thin layer chromatography. In order to optimize existing methodologies, some studies involving the voltammetry technique for cannabinoid detection are being carried out as it is a precise and selective technique. In this work, the authors developed a voltammetric method employing disposable screen-printed electrodes chemically modified with graphene oxide (GO-SPE) for detection of Δ9-THC and CBD in seized samples. These SPEs presented 5 cm long, 1 cm wide and 1 mm thick in a inert polymeric surface and the three electrodes (working, auxiliary and reference) were printed using a conductive polymer. The working electrodes received a layer of graphene oxide ink, and the reference electrode was painted with Ag/AgCl ink. The voltammetric techniques were employed using the GO-SPEs and carried out using an Autolab potentiostat. Standard solutions of Δ9-THC and CBD were employed in this study. Samples seized by the Scientific Police of the Ribeirão Preto city were evaluated. This methodology enabled the detection of cannabinoids in marijuana samples quickly and selectively.

Biography:

Marcelo Firmino de Oliveira has completed his PhD in analytical chemistry at the age of 30 years from Universidade Estadual Paulista – Instituto de Química, Brazil. He is a Professor of Forensic Chemistry at Universidade de São Paulo – Departamento de Química - FFCLRP, Brazil. He has published 80 papers in reputed journals. His research group – GEEQFOr – works with electrochemical analysis and the development of new sensors for crime scene analysis.

Mapping Differential Intracellular Trafficking of Quantum Dot Cargo with Machine Learning

Oleg Kovtun[1,2*]
Sandra J. Rosenthal[1,2]

[1]Department of Chemistry, Vanderbilt University, Nashville TN 37235, USA
[2]Vanderbilt Institute for Nanoscale Science and Engineering, Vanderbilt University, Nashville TN 37235, USA

Abstract:

Detection of intracellular cargo transport with high spatiotemporal resolution holds great promise for unlocking the molecular mechanisms of viral infection, drug delivery, and sustained signaling from intracellular compartments. High photon budget, excellent colloidal stability in complex environments, and diversity of functionalization approaches make quantum dots (QDs) uniquely suitable for analyzing the distribution, intracellular state, and diffusion dynamics of internalized cargo. Despite recent advances, critical knowledge gaps remain regarding the ability of QDs to distinguish between intracellular trafficking of targeted and non-targeted cargo or diffusion dynamics of specifically targeted cargo under stimulated conditions versus constitutive endocytosis. Here,

we investigated postendocytic transport of single QD cargo in living cells under these biological scenarios using a combination of dynamic fluorescence microscopy, single particle tracking methodology, and machine learning techniques. We found significant differences in intracellular transport of QDs specifically targeted to a membrane protein versus untargeted QDs as well as strong dependence of intracellular trafficking on the cell type. Further, we deployed dimensionality reduction and hierarchical clustering techniques to the trajectory data sets and mapped diffusion dynamics at the single-cell level based on a unique set of 16 diffusion features per cell. Next, we deployed a Random Forest classifier to identify distinct motion types within each trajectory pool with 87% accuracy. These results provide important clues about the cargo- and cell type-dependent intracellular trafficking. Our experimental framework can be extended to various imaging modalities and biological scenarios to develop effective drug delivery techniques and capture intracellular transport of pathogenic agents.

Biography:

My long-term research interests center on the development of a comprehensive understanding of molecular mechanisms underlying integral membrane protein (IMP) function and how disruptions in neuronal IMP trafficking contribute to the etiology and pathophysiology of neuropsychiatric disorders. I am currently a Research Assistant Professor in the Department of Chemistry at Vanderbilt University. In my recent studies, I continue to harness the unique photophysical properties of semiconductor nanocrystals and pursue quantitative characterization of the role of nanoscopic IMP organization in neuronal signaling using a state-of-the-art combination of single particle tracking, super-resolution microscopy, and electron microscopy.

Challenges in Bioanalysis of INCB000928 in Human Saliva and Dialysate: Non-Specific Binding, Inhomogeneous Concentration, and Surrogate Matrices

Zhiyin Xun*
Brad Yuska
Ryan McGee
Phillip Wang
Swamy Yeleswaram

Drug Metabolism and Pharmacokinetics and Clinical Pharmacology, Incyte Research Institute, 1801 Augustine Cut-off, Wilmington, DE 19803, USA

Abstract:

INCB000928 is a novel and potent oral inhibitor of wild-type and mutant (R206H) activin receptor-like kinase-2 and represents a potential therapeutic strategy for hepcidin-induced anemia and fibrodysplasia ossificans progressiva (FOP). Abnormal bone formation is a hallmark of FOP and may be exacerbated by trauma from invasive blood draws. Saliva is a noninvasive alternative and is viable if concordance with plasma pharmacokinetics can be established. Pharmacokinetics of drugs used in end-stage renal disease patients undergoing regular hemodialysis may be altered and result in increased safety risks. A bioanalytical method for the quantification of INCB000928 in human saliva and dialysate is warranted to support initial investigation of the correlation between saliva and plasma pharmacokinetics in healthy adult volunteers and to provide

specific dose recommendations for use in patients with chronic kidney disease. Challenges encountered in bioanalysis of INCB000928 in human saliva and dialysate involved mild to moderate non-specific binding in saliva and severe non-specific binding in dialysate, inhomogeneous concentration across saliva sample tube depths which led to initial incurred sample reanalysis failure in a healthy volunteer study, and high cost plus difficulty to source commercially available dialysate matrix. Strategies to overcome the challenges, approaches to solve the issues, and validations of the bioanalytical methods according to the US Food and Drug Administration and European Medicines Agency guidelines will be presented.

Biography:

Zhiyin Xun received her Ph.D. in Analytical Chemistry from Indiana University, Bloomington, and conducted postdoctoral research at the University of California, Davis and Lawrence Berkeley National Laboratory in California. Zhiyin began her career in Industry at Pfizer and is currently a Principal Investigator in the Department of Drug Metabolism & Pharmacokinetics & Clinical Pharmacology at the Incyte Research Institute in Delaware. At Incyte, Zhiyin leads critical method development and validation activities evaluating novel investigational drug candidates within a regulated bioanalytical group in support of both pre-clinical and clinical studies.

Portable and Laboratory Analytical Photometric and Fluorometric Systems Based on the use of 3d Printed Devices

Víctor Cerdà[1*]
Kaewta Danchana[1]
Piyawan Phansi[2]
M.A. Vargas-Muñoz[3]
Diego Barzallo[3]
Edwin Palacio[3]

[1]Sciware Systems. 07193 Bunyola. Spain
[2]Department of Chemistry, Faculty of Science and Technology, Thepsatri Rajabhat University, Lopburi 15000, Thailand
[3]Department of Chemistry, University of the Balearic Islands, 07122 Palma de Mallorca, Spain

Abstract:

The design of several 3D printed devices and some electronic boards, combined with the use of digital imaging detectors, has allowed to build different kinds of portable and cheap photometric systems. 3D printed devices are used to hold the detectors, usual and flow cells, and the light source. Detectors and light sources are powered through two USB of a notebook, avoiding the need of extra power sources. Several kind of image detectors have been tested: webcam, digital microscope, and CCDs. They have been used for colorimetric, spectrophotometric and fluorimetric determinations of different kind of samples. Data treatment are manually managed with different software packages, like YouCam, ImageJ, Chemostat, and automatically using AutoAnalysis.

Biography:

Víctor Cerdà was graduated and PhD in Chemistry by the University of Barcelona. Has been Lecturer and Professor at several universities: Barcelona, Tarragona, and Valladolid. Since 1982 was Full Professor of Analytical Chemistry at the University of the Balearic Islands (UIB). Since 2021 is Professor in the UIB. Has conducted 46 Ph.D. Thesis, written 14 books, and collaborated with 16 chapters. Has published more than 600 papers and presented 826 contributions on analytical chemistry in national and international conferences. Has been Vice-President of the Spanish Society of Analytical Chemistry, Vice-Chancellor of Scientific Policy and Innovation of the UIB. Currently is President of Sciware Systems, and of the Association of Environmental Sciences and Techniques.

Qualitative and Quantitative Analysis of Organic Matter and Dissolved Organic Matter in Agricultural Soils Amended with Biochar

Alessandro Girolamo Rombolà[1*]
Cristian Torri[1]
Ivano Vassura[3]
D. Fabbri[1]

[1]Department of Chemistry "Giacomo Ciamician", University of Bologna, Italy
[2]Department of Industrial Chemistry "Toso-Montanari", University of Bologna, Italy

Abstract:

Biochar soil amendment continues to receive worldwide interest for integrated agricultural/environmental strategies to build soil, enhance water quality, and increase agricultural productivity, while sequestering C and thus mitigating global climate change. However, little is known about how biochar addition affects soil organic matter (SOM) composition, especially dissolved organic matter (DOM). Biochar amendment to soil could change SOM and DOM contents and composition, which in turn will influence overall carbon dynamics and microbial communities in soil. The effect of biochar addition on the content and composition of SOM and DOM in agricultural soil was investigated by combining analytical pyrolysis and optical techniques. A method was developed to quantify biochar levels by thermogravimetric analysis that enabled to identify deviations from the amendment rate. Biochar addition to soils induced changes in SOM and DOM contents and composition depending on soil type and biochar amendment rate. The water-soluble organic carbon concentrations in the amended soils were significantly lower than those in the control soils, indicating that biochar decreased the leaching of DOM. The findings revealed that biochar application increased the proportion of aromatic compounds in SOM and DOM. Moreover, a relatively high abundance of compounds with N was observed in pyrolysates of treated soils, suggesting that biochar increased the proportion of microbial DOM. The results from thermal and spectroscopy techniques are consistent in highlighting significant changes in DOM levels and composition due to biochar application with important effects on soil carbon storage and cycling.

Biography:

Alessandro Girolamo Rombolà received his master's degree in Environmental Science in 2011 and was awarded the title of Ph.D. in Environmental Science in 2015 from the

University of Bologna. He was a post-doc fellow at Centro Interdipartimentale di Ricerca Industriale Energia Ambiente (2015-2017) and at the Dipartimento di Chimica "Giacomo Ciamician" (2017-2022) of the Università di Bologna. He has over 20 publications in high-ranking international peer-reviewed journals. He presented papers in more than 20 national and international conferences. He was involved in international, national and regional research projects on the valorization of low-cost agricultural and industrial residues into valuable compounds.

Predictive In Vitro Sensing Tools Exploiting 3d Spherical Bioluminescence Microtissues

Maria Maddalena Calabretta*
Denise Gregucci
Elisa Michelini

Department of Chemistry, Alma Mater University of Bologna, Bologna, Italy

Abstract:

In recent years, there has been an increasing demand for predictive and sensitive in vitro tools for drug discovery. Living cells used as sensing systems have proved to be valuable tools for prediction of the physiological response to drugs, chemicals, and samples in complex matrices, which toxic effects and specific biological activities can be evaluated in an easy and straightforward manner. Thanks to their superior predictivity, 3D cell models (i.e. spheroids, organoids and microtissues) are increasingly replacing conventional 2D cell cultures, enabling to recapitulate the extracellular matrix and cell-cell interactions and creating an architecture that faithfully reflects the native morphology of organs and tumors. Bioluminescent (BL) reporter assays represent the gold standard for several high throughput screening assays employed in drug discovery and in effect-based analysis and BL proteins showed a formidable tool for unravelling molecular pathways involved in the etiopathogenesis of several diseases. Moreover, ligand-induced complementation of split luciferases is emerging as a suitable approach for monitoring protein-protein interactions. Here we report the development of predictive in vitro sensing tools suitable for analyzing molecules with androgenic activity, including new drugs or endocrine disrupting molecules, for providing rapid information about different bioactivities (antioxidant and anti- inflammatory activities) of environmental sample and for understanding their mechanisms of action on different molecular pathways. New strategies have been explored to obtain straightforward assays with BL 3D spherical microtissues that do not require advanced equipment, can be easily implemented in other laboratories, simply equipped with basic cell culture facilities and luminometer.

Biography:

Maria Maddalena Calabretta is Junior assistant professor in Analytical Chemistry at the Department of Chemistry (University of Bologna). Her scientific activity involves the development of analytical methods with bio-chemiluminescence detection applied to biomedical and pharmaceutical screening, environmental and food. She is coauthor of papers on high-impact scientific journal of Analytical Chemistry (h-index 15, 798 citations) and she participated to several projects funded by PRIMA Partnership, NATO-SPS, EU, Bill and Melinda Gates Foundation, MIUR. She received several awards including the Lions

Prize “Claudio Bonivento” SCIENTIFIC RESEARCH AND TECHNOLOGICAL INNOVATION and “Premio Spada” (2018) for the best PhD thesis in Analytical Chemistry.

Influence of Ionic Liquids as Mobile Phase Additives on the Behavior of Selected Cytostatic Drugs on Alkyl and Phenyl Based Stationary Phases in Reversed-Phase Liquid Chromatography

Alina Plenis[*1]
Natalia Treder[1]
Ilona Olędzka[2]
Anna Roszkowska[2]
Piotr Kowalski[2]
Tomasz Bączek[2]

[1]Department of Analytical Chemistry, Medical University of Gdańsk, Hallera 107, 80-416 Gdańsk, Poland
[2]Department of Pharmaceutical Chemistry, Medical University of Gdańsk, Hallera 107, 80-416 Gdańsk, Poland

Abstract:

The application of ionic liquids (ILs) as additives to the mobile phase in reversed-phase liquid chromatography (RP-LC) can influence the dynamic coating of the stationary phases and provide to change their chromatographic properties [1,2]. In this work, the interaction between different ILs added to 0.1% formic acid used as an aquatic mobile phase and the functional groups on alkyl and phenyl based stationary phases was investigated during RP-LC separation of four cytostatic drugs (athracycline antibiotics). Changes in behaviors of the studied analytes during RP-LC analysis were established based on retention factor (k), peak area (A), number of theoretical plates (NA) and tailing factor (Tf). Moreover, cluster analysis was performed for visualization relationships in chromatographic parameters of the studied cytostatics calculated on each stationary phase. The results confirmed that π-π type interactions occurring on the phenyl based columns gave more pronounced effects from the ILs compared to those observed on the alkyl column [3]. CA results indicated that the studied cytostatic drugs were classified consistent with their chemical structures on each tested column, when different subclusters of the k, A, NA and Tf parameters were found. It confirms that the addition of ILs leads to various changes in the chromatographic parameters of the studied analytes. Independent to the type of used stationary phase, it was possible to reduce the analysis time, improve the peak shape as well as the column efficiency as the result of adding appropriate IL to the mobile phase.

Biography:

1. N. Treder, T. Baczek, K. Wychodnik, J. Rogowska, L. Wolska, A. Plenis, The influence of ionic liquids on the effectiveness of analytical methods used in the monitoring of human and veterinary pharmaceuticals in biological and environmental samples - trends and Perspectives, Molecules 25 (2020) 286.

2. N. Treder, I. Olędzka, A. Roszkowska, T. Bączek, A. Plenis, Control of retention mechanisms on an octadecyl-bonded silica column using ionic liquid-based mobile

phase in analysis of cytostatic drugs by liquid chromatography, J. Chromatogr. A 462257 (2021) 462257.

3. N. Treder, I. Olędzka, A. Roszkowska, P. Kowalski, T. Bączek, A. Plenis, Practical and theoretical considerations of the effects of ionic liquids on the separation properties of phenyl-based stationary phases in reversed-phase liquid chromatography, Microchem. J. (2022) in press.

Green Sample Preparation for the Analysis of High Carbon Content Matrices

Érico M. M. Flores*

Federal University of Santa Maria, Chemistry Department, Campus – 97105-900, Santa Maria, RS – Brazil

Abstract:

Even in trace amounts, the presence of some elements could be deleterious to refining processes, especially due to corrosion, catalyst poisoning and by affecting the quality of refined products or petrochemical products. Classical methods for sample digestion and further determination by atomic spectrometry involve the use of a relatively high volume of concentrated reagents (inorganic acids in case of further metals determination) and a relatively long time for digestion. The digestion efficiency of these systems presents some limitations for many matrices. In this sense, even using methods based on microwave-assisted closed vessels some drawbacks can occur for petroleum and high carbon-content matrices (as coke, coal, graphite, etc) and incompleteness of digestion is frequently reported. There is a trend for the development of methods requiring lower reagent consumption, less analytical steps and lower waste generation combined with high efficiency of digestion. It is important that digests are suitable for the determination techniques avoiding excessive dilution or higher blank levels. On this aspect, the main trends for sample preparation of petroleum and high carbon-content matrices will be presented for further metals and some non-metals determination. The use of diluted solutions using oxygen pressurized systems with or without UV radiation, use of combustion systems, etc, will be covered and the main aspects of sample preparation for the determination of metals and halogens will be discussed. Recent applications will be presented showing the advantages of methods using diluted reagents (combustion, UV digestion) for metals and non-metals determination using ICP-MS and ICP-OES.

Biography:

Érico M. M. Flores has a permanent position at Federal University of Santa Maria/Brazil as a Titular Professor. He was the Director of Analytical Chemistry Division of Brazilian Chemical Society and Vice-President of Analytical Chemistry Division of IUPAC. He has experience in the development of methods for sample preparation for element determination, speciation analysis and quality control using atomic spectrometry. He has published more than 390 papers, one book and many book chapters and patents (>8,700 citations, H-index 47). More than 30 students have received the PhD and more than 50 have received the MS degree under his supervision.

Real-time Raman Spectroscopy for Endoscopy Lung Cancer Detection

Haishan Zeng

BC Cancer Research Institute, University of British Columbia, Vancouver, Canada

Abstract:

Lung cancer is the leading cause of cancer-related deaths, with a five year survival rate of less than 20%. If lung cancer can be diagnosed earlier, the survival rate can be improved significantly (>70% for patients with stage 0 or 1A disease). Currently the most sensitive method for localizing lung cancers in central airways is autofluorescence bronchoscopy (AFB) in combination with white light bronchoscopy (WLB). The diagnostic accuracy of WLB+AFB for high grade dysplasia (HGD) and carcinoma in situ is variable depending on physician's experience. When WLB+AFB are operated at high diagnostic sensitivity, the associated diagnostic specificity is low. Raman spectroscopy probes molecular vibrations and gives highly specific, fingerprint-like spectral features and has high accuracy for tissue pathology classification. In this study we present the use of a real-time endoscopy Raman spectroscopy system to improve the specificity. A spectrum is acquired within 1 second and clinical data are obtained from 280 tissue sites (72 HGDs/malignant lesions, 208 benign lesions/normal sites) in 80 patients. Using multivariate analyses and waveband selection methods on the Raman spectra, we demonstrated that HGD and malignant lung lesions can be detected with high sensitivity (90%) and good specificity (65%). This is a significant improvement compared to WLB+AFB, which has a specificity of 18% -32% when the sensitivity is set at 90%. Point Raman measurement on lesions identified by imaging could become a new clinical tool for real-time detection of lung cancer.

Biography:

Haishan Zeng is a distinguished scientist with BC Cancer and professor at University of British Columbia. Dr. Zeng's research focuses on biophotonics and its medical applications. His group has pioneered the multiphoton-absorption based laser therapy and is at leading position in endoscopy imaging and Raman spectroscopy for noninvasive early cancer detection. He has published 185 refereed papers and holds 28 granted patents. Several medical devices derived from these patents including fluorescence endoscopy (ONCO-LIFE™) and rapid Raman spectroscopy (Aura™) have passed regulatory approvals. The Aura™ device was awarded the Prism Award in 2013 by the International Society for Optics and Photonics.

Automated Machine Learning Applied in Analytical Chemistry

Aderval S. Luna[1*]
Igor C. A. Lima[1]
Camilla L. Cunha[2]
Alexandre R. Torres[2]
Luís G. Nonato[3]

[1]Graduate Program in Chemical Engineering, Rio de Janeiro State University, Brazil
[2]Faculty of Technology, Rio de Janeiro State University, Brazil

[3]Institute of Mathematical and Computer Sciences, University of São Paulo, Brazil

Abstract:

This work aims to develop an auto-machine learning method using Mid-Infrared (MIR) spectroscopy data to determine the cold filter plugging point (CFPP) and kinematic viscosity at 400C biodiesel diesel and mixtures samples. The dataset was composed of 335 blends (biodiesel obtained from different biomass such as soy, corn, sunflower, and canola) with binary, ternary and quaternary mixtures, also mixtures of diesel-biodiesel and diesel-biodiesel-ethanol. The physical properties of the samples were obtained according to ABNT NBR 14747 and ABNT NBR 10441, respectively. The MIR Spectroscopy data were acquired from 7,800 to 450 cm-1, with a 4 cm-1 resolution and 20 scans. The dataset was split into 70% and 30% training and test sets, respectively. The kinematic viscosity of 400C of the biodiesel samples and their blends could be odelled using the MIR Spectroscopy dataset using different auto-machine learning algorithms. The RMSEP (Root Mean Square Error of Prediction) (≤ 0.02 mm2. S-1) was similar to the experimental error obtained after log transformation. The CFPP of the biodiesel samples and their blends could be odelled using the MIR Spectroscopy dataset by different auto-machine learning algorithms with an RMSEP (≤ 1.60C) similar to the experimental error obtained by traditional methodology. Based on the lower computational time and the same performance observed by the RMSEP and R2 (coefficient of determination) values from different algorithms, it is recommended to use Ridge or Ridge Cross-Validation Regression models for both physical properties using MIR Spectroscopy data.

Biography:

Graduated in Chemistry from the Rio de Janeiro State University (1975), MSc (1996), and Ph.D. in Chemistry from the Pontifical Catholic University of Rio de Janeiro (2000). He did a postdoctoral in Chemometrics at Universitat Rovira I Virgili, Spain (2009/2010). He is currently a full professor at the Rio de Janeiro State University. He has supervised 10 Theses and 33 Dissertations in the areas of Chemical Engineering and Analytical Chemistry and published more than 100 articles in scientific journals. He was editor of the book Chemometrics: Methods, Applications, and New Research and the author and co-author of 8 book chapters.

Quantitative Analysis of Biological Compounds using a Pillar Array Column

Makoto Tsunoda

The University of Tokyo, Japan

Abstract: Not Available!!!

KEYNOTE PRESENTATIONS

An Automated Multicycle Immunoaffinity Enrichment Approach Developed for Sensitive Mouse IgG1 Antibody Drug Analysis

Linlin Dong

Takeda Pharmaceuticals, Cambridge, MA

Abstract: Not Available!!!

Quantitative Immuno-Mrm of the Pd-1/Pd-L1 Axis Predicts Survival in Non-Small Cell Lung Cancer (NSCLC)

Vincent Lacasse[1,2]
Vincent Richard[1]
Hangjun Wang[1,4]
Georgia Mitsa[1,5]
Olivier Poetz[6]
Andreas I Papadakis[1]
Mounib Elchebly[1]
Victor Cohen[2,3]
Jason Scott Agulnik[2,3]
Gerald Batist[4,5,7]
Rene P. Zahedi[8,9]
Alan Spatz[1,4,7]
Christoph H. Borchers[1,2,4,5,7*]

[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, Quebec, Canada
[2]Department of Pathology, McGill University Faculty of Medicine and Health Sciences, Montreal, Quebec, Canada
[3]Department of Pathology, McGill University Health Center, Montreal, Quebec, Canada;
[4]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University Faculty of Medicine and Health Sciences, Montreal, Quebec, Canada
[5]Division of Experimental Medicine, Lady Davis Institute for Medical Research. Jewish General Hospital, McGill University Faculty of Medicine and Health Sciences, Montreal, QC, Canada
[6]Signatope GmbH, Reutlingen, Germany
[7]McGill University Centre for Translational Research in Cancer, McGill University Faculty of Medicine and Health Sciences, Montreal, Quebec, Canada
[8]Department of Internal Medicine, University of Manitoba, Winnipeg, MB Canada
[9]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB Canada

Abstract:

Checkpoint inhibitors (CPIs), such as anti-PD-1 drugs, have revolutionized lung-cancer treatment, but predictive biomarkers for reliably identifying patients who respond to

treatment are lacking. PD-L1 immunohistochemistry (IHC) is currently used for patient screening, but only 40-50% of PD-L1-positive patients respond to CPI treatments, while 10% of PD-L1-IHC-negative patients would actually benefit from them. PD-L1 IHC is heterogenous, is affected by post-translational modifications (PTMs) such as glycosylation and does not efficiently reflect the tumor immune microenvironment. We developed a mass spectrometry (MS)-based proteomic workflow for the "absolute" quantitation of the PD-1/PD-L1 axis proteins in formalin-fixed paraffin-embedded (FFPE) tumors, which provides the concentrations of six proteins as well as the percent modification of one glycosylation site each on PD-1, PD-L1, and PD-L2.

Unique, easily detected, proteolytic peptides were used as surrogates for the target proteins (PD-L1, PD-1, PD-L2, NT5E, LCK, and ZAP70). Protein extraction from FFPE lung cancer samples, digestion, peptide immuno-enrichment, chromatography, and multiple reaction monitoring (MRM) parameters were optimized to maximize recovery, increase target-specific signal, and reduce noise. We also assessed the glycosylation status of PD-L1, PD-L2, and PD-1.

The entire workflow was fully validated using 31 NSCLC FFPE tumors. PD-L1 quantitation by immuno-MRM (iMRM) was compared to PD-L1 immunohistochemistry clone 22C3. Although this first set of patients was not treated with CPI, survival data was available. A trend was observed between survival and the concentration of our targets, and an immunoscore based on the concentration of these proteins was calculated for each patient. The immunoscore alone could predict long-term survival.

Biography:

Borchers is a Professor in the Department of Oncology at McGill University, where he is also Director of the Segal Cancer Proteomics Centre. Dr. Borchers' expertise includes improvement, development and application of proteomics and metabolomics technologies with a major focus on techniques for quantitative proteomics and metabolomics for clinical diagnostics. Dr. Borchers is actively involved in promoting proteomics research and education through his involvement with HUPO (International Council Member), the British Columbia Proteomics Network, and the Canadian National Proteomics Network. He is also a member of the Canadian Academy of Health Sciences, with >300 publications in proteomics and metabolomics.

ORAL PRESENTATIONS

Targeting Out of Range Biomolecules: Chemical Labeling Strategies for Qualitative and Quantitative MS-based Detection

Sejallon-Cipolla Mylene[1]
Devel Laurent[2]
Subra Gilles[1]
Cantel Sonia[1*]

[1]IBMM, Université de Montpellier, ENSCM, CNRS, Montpellier, FRANCE
[2]SIMOPRO, Institut des sciences du vivant Frédéric-Joliot, Centre CEA, Saclay, FRANCE

Abstract:

In health sciences and particularly in –omics approaches, Mass spectrometry is of strategic importance for the detection and identification of specific molecules involved in biological processes, leading to a better understanding of physiological and physiopathological processes and consequently for diagnosis purposes. However, a large number of these relevant biomarkers remain undetectable due to several parameters, a low molecular weight, a weak abundance, their ionization potential or their localization in a complex environment. To overcome these limitations, labeling strategies have been developed. MS labeling require the development of diverse tags as versatile as possible, involving innovative chemistry, and targeting different functional groups such as amine, hydroxy groups or carboxylic acids. Specific probes, such as ABP have been designed to selectively label biomolecules of interest and to match the current need for in vivo labeling methods following the development of imaging techniques.

Biography:

Sonia Cantel obtained her PhD in 2004 in Chemistry of Biomolecules from the University of Montpellier, in the field of pseudo-peptide and solid phase organic synthesis. For the following two years as Postdoctoral Fellow in the Laboratory for Translational Research (Harvard Medical School, Boston, USA), she actively participated to biomedicinal projects and developed extensive skills in analytical techniques applied to peptide and protein engineering. She joined in 2007 the IBMM, taking advantage of her multidisciplinary experience to develop new projects at the interface of Chemistry, Biology and Analytical Sciences. She focuses her research on the development of chemical probes for specific and sensitive detection of peptides and proteins, and pharmacological studies (GPCR/ligand interaction) by MALDI Mass Spectrometry. Actively involved in peptide environment, she is currently president of the GFPP (Groupe Francais des Peptides et Protéines).

A Highly Sensitive and Simple-to-use 3D Protein Detection Platform

Huiyan Li*
Nikan Momenbeitollahi

[1]University of Guelph, Canada

Abstract:

Measuring proteins in body fluids such as blood plasma can advance our knowledge in disease biology, and help in disease management such as diagnostics, prognosis, and treatment monitoring. Different from other biomolecules, proteins are functional molecules in life, providing physiological and pathological information at functional levels. New methods have been developed based on metal enhanced fluorescence, but required complicated microfabrication, limiting their broad applications. Here, we have developed a 3D platform on nitrocellulose membranes with entrapped gold nanoparticles for highly sensitive protein detection based on metal enhanced fluorescence phenomena. Gold nanoparticles with different sizes from 5 nm to 10 nm were tested with different concentrations. Two cellulose membranes with different surface chemistry and pore

sizes were compared to achieve optimal fluorescence signal intensities for quantifying proteins in blood plasma samples. After optimization of the assay steps, we used the platform to measure protein levels in blood plasma and extracellular vesicles. Compared to conventional protein assays, an improved assay sensitivity up to four orders of magnitude was achieved using our method. The new platform offers a useful tool for highly sensitive protein detection. The assay can be performed in a biological lab with basic setups, enabling broad applications for biological researchers and clinicians.

Biography:

Huiyan Li obtained her PhD in Biomedical Engineering from McGill University. After postdoctoral training from Massachusetts General Hospital, Harvard Medical School, she joined the Biomedical Engineering program in the School of Engineering at the University of Guelph. Her research focuses on developing novel micro- and nanotechnologies and lab-on-a-chip systems for the study of health and diseases. Her work has been published in top peerreviewed journals in the research field and has been highlighted in major scientific magazines.

The crosstalk, Lipidomics and Redox Proteomics, for Understanding the Role of Dietary Lipids in Brain

Isabel Medina*
Lucía Méndez
Lorena Barros
Francisco Moreno
Salomé Lois
Verónica Castro

Institute of Marine Research, CSIC, Spain

Abstract:

Strategies based on healthy eating and nutrition are key in the prevention of chronic and neurodegenerative diseases that usually accompany the aging process. The crosstalk, lipidomics and proteomics, provide useful resources for understanding brain function and the role of diet on brain lipid pathways. In particular, lipid metabolism modulates neuronal function and may signal nutrient status to influence metabolism in key peripherical tissues (1,2). Recent research suggests that fatty acid sensing in neurons via accumulation of lipids or lipid metabolites may signal nutritional sufficiency and affect liver function. This talk presents an untargeted LC-MS/MS approach for the quantification of lipid metabolites in differential brain regions based on Mass Spectral Fragmentations. The extensive study of fragmentation patterns obtained by SPE-LC-MS/MS provides fingerprints to comprehensively elucidate and identify lipid mediators derived from PUFA in biological samples. The effect of dietary lipids on brain lipid composition and the local production of lipid metabolites was studied in an animal model of aged Wistar rats. Diet altered brain lipid profiles and lipid metabolism with regional differences. Moreover, complex interaction between oxidised phopholipids and brain carbolinated proteins

reveals a singular effect of dietary lipid composition. Results demonstrate that lipids affect pathways thought to be involved in the regulation of aging, making them promising candidates towards human diseases, nutrition or other applications.

Biography:

1. Tracey, Timothy J et al. 2018. Neuronal Lipid Metabolism: Multiple Pathways Driving Functional Outcomes in Health and Disease. Frontiers in Molecular Neuroscience. Vol. 11: 10. doi:10.3389/fnmol.2018.00010.

2. Ingeborg Huitinga, Maree J. Webster. 2018. Proteomics and lipidomics in the human brain, Handbook of Clinical Neurology. Vol. 150: 285-302. https://doi.org/10.1016/B978-0-444-63639-3.00020-7.

Stroboscopic Flashes on the Netherworld

Pier Giorgio Righetti[1*]
Gleb Zilberstein[2]

[1]Politecnico di Milano, Dept. of Chemistry, Italy
[2]SpringStyle Tech Design Ltd, Rehovot, Israel.

Abstract:

We describe here a modern tool for exploring documents pertaining to the world Cultural Heritage while avoiding their contamination or damage. Known under the acronym EVA, it consists of a plastic foil of Ethylene Vinyl Acetate studded with strong cation and anion resins admixed with C8 and C18 hydrophobic beads. When applied to any surface such foils can harvest any type of surface material, which is then eluted and analyzed via standard means, such as GS/MS (typically for metabolites), MS/MS (for peptide and protein analysis), X-ray (for elemental analysis). We briefly review here a number of past data, such as screening of original documents by Bulgakov, Chekov, Casanova, Kepler, while dealing in extenso with very recent data, pertaining to Orwell and Stalin and analysis of the skin of an Egyptian mummy. The technique was also successfully applied to paintings, such as the Donna Nuda at the Hermitage in St. Petersburg, attributed to Leonardo and his school. This novel methodology represents a formidable tool for exploring the past life of famous authors, scientist and literates in that it can detect traces of their pathologies and even drug consumption left by saliva and sweat traces on their original hand-written documents.

Biography:

PG Righetti earned his Ph. D. in Organic Chemistry from the University of Pavia in 1965. He then spent 3 years as a Post Doc. at MIT and 1 year at Harvard. He is now Emeritus Professor at the Milan's Polytechnic. On 590 published articles Righetti scores 31.636 citations, with a H-index of 84. In World Ranking he is No. 1161 and at a National Ranking

level he is No. 23. In 2012 he has won the Beckman medal. In 2014, in Madrid, he was given the HuPO award for proteomic research and, in Atlanta, the American Electrophoresis Society award.

Challenges in Sample Preparation Methods for Trace Element Determination by Multitechniques

Marcia Foster Mesko*

Federal University of Pelotas, Chemistry, Pharmaceutical and Food Science Centre, Pelotas, Brazil

Abstract:

Trace element determination has been performed to provide information about the influence of the elements in several fields, such as nutrition, health, and toxicology. Even with the significant developments in instrumentation, samples are generally introduced in the equipment as a solution. Classical sample preparation methods generally use a relatively high volume of concentrated reagents and take a long time for digestion. The use of concentrated reagents may require a dilution step of digests before the analyte determination, which could compromise the limits of detection. Even methods based on microwave-assisted digestion in closed vessels present some drawbacks, and incomplete digestions are frequently reported. Moreover, there are some elements, such as halogens, that can be lost in their unstable volatile compounds in acid medium. Considering these limitations, the development of green analytical methods, which require lower reagent consumption and waste generation, less analytical steps combined with high-efficiency digestion, is a trend. In addition, the suitability of the digests with the determination techniques is also important. On this aspect, the main advances for sample preparation in a variety of matrices will be presented in this lecture for further trace element determination by inductively coupled plasma mass spectrometric and ion chromatography with mass spectrometry detection.

Biography:

Mesko is a full professor at Federal University of Pelotas, and an affiliate member of the Brazilian Academy of Science, and a titular member of the Brazilian Academy of Pharmaceutical Sciences. She was the Director of Analytical Chemistry Division of Brazilian Chemical Society. She is an editorial board member of the Journal of Analytical Atomic Spectrometry. She has experience in the development of methods for food, pharmaceutical, and biological analysis using ion chromatography and atomic spectrometry techniques. She has presented national and international invited lectures, published more than 120 peer reviewed international papers, patents and book chapters in these fields.

Comparison of Chiral Separation Performance of sub-2 mm and Conventional Polysaccharide-based Chiral Columns

Brian He[1*]
Ling Zhang[1]
Nicole G. Kleinsorge[2]

[1]Chemical and Process Development, Global Product Development and Supply, Bristol Myers Squibb Company, New Brunswick, NJ 08903, USA
[2]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109

Abstract:

Introduction of UHPLC chiral columns packed with sub-2 mm particles is a major development in analytical chiral separations in the last decade. Like in achiral separations, using UHPLC chiral columns would help to develop chiral methods with much shorter analysis time. It is believed that chiral separations (including stereoisomeric separations) achieved on conventional chiral columns can be straightforward transferred to sub-2 mm UHPLC columns.

To examine this common belief, we launched a study to evaluate the performance of sub-2 mm and conventional polysaccharide-based chiral columns for the separation of enantiomers and diastereomers in four different separation modes, i.e., reversed-phase, polar organic phase, normal phase, and supercritical fluidic chromatography. In this presentation, preliminary results of our study will be presented and discussed. Pitfalls that should be avoided in application of sub-2 mm UHPLC columns will be highlighted.

Biography:

Brian He is an Associate Scientific Director in Chemical & Process Development in Bristol Myers Squibb (BMS) and has 16+ years of experience in pharmaceutical industry. He has been an analytical project team leader and subject matter expert for many BMS projects. He has published over thirty peer-reviewed papers and two book chapters. Currently Dr. He serves in the editorial boards of Journal of Pharmaceutical and Biomedical Analysis OPEN, Journal of Pharmaceutical and Biomedical Analysis and American Pharmaceutical Review.

Electrochemical Monitoring of Biomarkers using Nanochannels

Alfredo de la Escosura-Muñiz

NanoBioAnalysis Group-Department of Physical and Analytical Chemistry, University of Oviedo, C/ Julián Clavería, 8, 33006 Oviedo, Spain

Abstract:

The purpose of this talk is to give an overview on the recent trends in the use of

nanochannels for biosensing applications [1,2]. Some general considerations on the principles of the stochastic sensing, together with an overview about the common routes for nanochannels preparation before focusing on the applications for DNA, protein, virus, toxin and other analytes detection will be given. Special focus will be put in recent approaches for the in-situ monitoring of biomarkers for wound infection diagnosis [3,4]. The state-of-the-art of the developed technology may open the way to new advances in the integration of nanochannels with (bio)molecules and synthetic receptors for the development of novel bio detection systems that can be extended to many other applications with interest for clinical analysis, safety, and security as well as environmental and other industrial studies and applications. The financial support of the MCI-21-PID2020-115204RB-I00 project from Spanish Ministry of Science and Innovation (MICINN) and the SV-PA-21-AYUD/2021/51323 project from the Asturias Regional Government is gratefully acknowledged. The author also acknowledges the MICINN for the "Ramón y Cajal" Research Fellow (RyC-2016-20299). [1] A. de la Escosura-Muñiz, A. Merkoçi, ACS Nano 6(9) (2012) 7556. [2] A. de la Escosura-Muñiz, A. Merkoçi, TrAC - Trends Anal. Chem. 79 (2016) 134. [3] A. de la Escosura-Muñiz, K. Ivanova, T. Tzanov, ACS Appl. Mater. Interfaces, 11 (2019) 13140. [4] A. Iglesias-Mayor, O. Amor-Gutiérrez, C. Toyos-Rodríguez, A. Bassegoda, T. Tzanov, A. de la EscosuraMuñiz, Biosens. Bioelectron. 209 (2022) 114243.

Biography:

Alfredo de la Escosura-Muñiz holds a PhD in Chemistry (2006) from the University of Oviedo (Spain). Most of his post-doctoral career has been spent at Prof. Merkoçi's group at ICN2 (Barcelona, Spain), where he specialized in Nanobiosensors. He has participated in +25 national and international projects and is the coauthor of over 85 scientific publications (+2800 citations; h-index: 31) and 4 patents. As of June 2018, he holds a Ramon y Cajal Research Fellowship at the University of Oviedo. His research interests focus on the development of biosensing systems based on nanoparticles and nanochannels for point-of-care diagnostic applications.

Separation of Urolithin Glucuronides in Biological Samples by using Supercritical Fluid Chromatography

Ana M. Ares[1*]
Beatriz Martín-Gómez[1]
Laura Toribio[1]
Rocío García-Villalba[2]
Francisco A. Tomás-Barberán[2]
José M. Villalgordo[3]
José Bernal[1]

[1]TESEA group, I.U. CINQUIMA, University of Valladolid, Valladolid, Spain.
[2]CEBAS-CSIC, Murcia, Spain.
[3]Eurofins-VillaPharma Research, Fuente Álamo, Murcia, Spain.

Abstract:

Urolithins are a class of polyphenols that are formed due to the microbiota after the consumption of foods rich in ellagitannins. After their absorption, they are conjugated with glucuronic acid producing different regiosimeric isomers, being mainly present as urolithins glucuronides. The final produced urolithins has been reported depending of different metabotype. These microbiota metabolites seem to be responsible of health beneficial effects and they can be found circulating in plasma and reaching the different tissues. The different analytical methods developed to date for their determination are focusing in used reverse phase high performance liquid chromatography. However, look for new strategies are needed due to several coelutions of the different isomers of urolithin A and isourolithin A are presented in all methods. For that reason, supercritical fluid chromatography could be a greener alternative technique that should be considered. The analytical development using chiral columns have allowed to achieve the separation for the first time. The proposed method was applied to analyze the urolithin metabolites in human urine samples from different volunteers belonging to different metabotypes. In general, Urolithin A glucuronides isomers were detected in similar proportions, while one isomer of the isourolithin was most common than the other. This work could represent a significant advance to improve metabotype assignment and their implications in human health.

Biography:

Ana M. Ares studied Chemistry at the University of Valladolid (UVa, Spain) and graduated as MSc in 2011. She then joined the Separation Techniques and Applied Analysis research group (TESEA), at the Institute of Innovation Center in Chemistry and Advanced Materials (CINQUIMA) in UVa. She received her PhD degree in 2015 at the same institution. After five years working in Analytical Development and Validations in Pharmaceutical Industry, she obtained the full position of an Assistant Professor in Analytical Department at the UVa. She has published more than 40 research articles in SCI(E) journals.

A Preconcentration Method using Magnetic Dispersive Solid-Phase Microextraction with GO-γFe2O3 Nanoparticles for the Determination of Se in Fish Samples by FIA-HG-AAS

Jefferson S. de Gois[1,2*]
Mayara Cristina Leal do Nascimento[1,2]
Fernanda Nunes Ferreira[1]
Ana Paula Benevides[1]
Danilo de Castro da Silva[1]
Deborah Vargas Cesar[1,2]
Aderval S. Luna[1,2]

[1]Rio de Janeiro State University, Department of Analytical Chemistry, Rua São Francisco Xavier 524 – Maracanã, Rio de Janeiro, RJ, Brazil, 20550-013
[2]Rio de Janeiro State University, Graduate Program in Chemical Engineering, Rua São Francisco Xavier 524 – Maracanã, Rio de Janeiro, RJ, Brazil, 20550-013

Abstract:

This work describes the development of an analytical method for the preconcentration of Se in digested fish samples using magnetic nanoparticles of graphene oxide GO-γFe2O3 with detection by hydride generation atomic absorption spectrometry and flow injection analysis (FIA-HG-AAS). The magnetic nanoparticles (MNPs) were synthesized and the structural properties were characterized by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), and X-ray diffraction (XRD). The domain of the factors pH, MNPs mass, and adsorption time was optimized using a central composite design, as well as the flow of carrier gas, the concentration of hydrochloric acid (HCl), and sodium borohydride (NaBH4) for the hydride generation system. The optimized experimental conditions were obtained at pH 2, 60 mg of MNPs, and 30 min for the adsorption process, and 4.5 (v/v) % HCl, 0.19 (m/v) % NaBH4, and 273.5 mL min-1 of carrier gas flow for hydride generation. Under optimized conditions, the enrichment factor (EF), the limits of detection (LOD), and quantification (LOQ) were 70, 30 ng g-1, and 90 ng g-1, respectively. The short-term precision of the method, defined by the relative standard deviation (RSD) (n=10), was 7.54%. The accuracy of the method was assessed through recovery tests, as well as the analysis of certified reference materials (CRM). The recovery values ranged from 103.8 to 117.3% and the Se concentration determined in the CRMs agreed with the certified values through a t-test at a 95% confidence level.

Biography:

Jefferson Santos de Gois currently lives in Rio de Janeiro (Brazil) and works at Rio de Janeiro State University (UERJ). He obtained his doctorate in Chemistry (2016) from the Ghent University (Belgium) and Federal University of Santa Catarina, UFSC (Brazil). His research interests encompasses the determination of organic compounds (by chromatographic techniques) and chemometrics (design of experiments, pattern recognition, and multivariate calibration).

Enhancement of Sensitivity and Quantification Quality in the LC MS/MS Measurement of Large Biomolecules with Sum of MRM (SMRM)

Liang Tang*
Robert R. Swezey
Carol E. Green
Jon C. Mirsalis

SRI International, Menlo Park, California, USA

Abstract:

Liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) has become a mainstay analytical technique in pharmaceutical industry and biomedical research. There was a challenge for large molecules such as proteins and peptides in LC-MS/MS analysis, because they can exist in multiple charged forms, and this will reduce total analyte signal by distributing it into multiple ion peaks with different number

of charges in a mass spectrum. This presentation will discuss innovative technique to analyze large biomolecules by LC-MS/MS.

The novel SMRM technique and application of Charge Conveyance Effect of large biomolecules can enhance detection sensitivity to measure potent macromolecule drugs and biomarkers at trace-levels, expedite method development in the bioanalysis of large biomolecules, facilitate the application of LC-MS/MS in biotransformation research of large biomolecule drugs, enable the separation and quantification of large-biomolecule isomers individually, and enable LC-MS/MS to expand its applications in preclinical research and clinical development such as large molecules PK and TK studies to be alternative methods to ligand binding assay (LBA) methods.

The presentation will showcase the novel and combat-proven SMRM in the LC-MS/MS to audience.

Biography:

Liang Tang is a pioneer in the field of electrospray ionization mass spectrometry (ESI-MS). His early work with Professor Paul Kebarle on the research of electrospray ionization mechanism set up the foundation of ESI-MS theory. The Kebarle-Tang Equation (Anal. Chem. 1991, 63, 2709-2715) depicted the relationship of major parameters in ESI-MS. Their broad study from ions in solution to ions in the gas phase enriched the theory of analytical mass spectrometry (Anal. Chem. 1993, 65, 972A-986A), and is frequently referred in literature to explain many phenomena in LC-MS such as the matrix effect in bioanalysis. His recent interest includes the application of analytical mass spectrometry in pharmaceutical research (e.g. J. Chromatogr. B, 2022, 1193, 123165, and Anal. Bioanal. Chem. 2022, 414, 1933–1947). He is a Senior Principal Scientist at SRI Biosciences.

Pyrolytic Graphite Electrode in Nucleic Acid Electroanalysis

Ales Danhel*
Jan Spacek
Ondrej Hesko
Miroslav Fojta

Institute of Biophysics of the Czech Academy of Sciences, Kralovopolska 135, 612 00 Brno, Czech Republic

Abstract:

An innovative approach to label-free voltammetric analysis of DNA at a pyrolytic graphite electrode (PGE) within a broad range of potentials (from −2.0 to +1.6 V) in an acetate buffer (pH 5) is presented. Not only anodic oxidation, but for the first time also cathodic reduction of nucleobases was observed at the PGE. In addition, products of irreversible oxidation/reduction of the parent bases were shown to yield analytically useful, base-specific cathodic/anodic signals, making it possible to distinguish between the canonical bases (adenine, cytosine, guanine and thymine), uracil (U) and 5-methylcytosine (mC)

in DNA. [1] Furthermore, it was found that presence of the ambient oxygen in the electrolyte does not dramatically affect the redox signals of the nucleosides at PGE. It was demonstrated that all studied nucleosides can be analyzed using a simple ex situ (medium exchange) procedure. [2] Additionally, 2'-deoxynucleoside analogs that are parts of an artificially expanded genetic information system (AEGIS) were analyzed. [3] Last but not least, a method for fast detection of short polyG RNAs presented in a large overabundance of cGMP has also been developed. [4]

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[2] J. Spacek, M. Fojta, J. Wang, Electroanalysis 2019, 31, 2057–2066.

[3] J. Spacek, N. Karalkar, M. Fojta, J. Wang, S. A. Benner, Electrochim. Acta 2020, 362, 137210.

[4] O. Hesko, M. Fojta, J. Špaček, J. Electroanal. Chem. 2021, 901, 115773.

Biography:

Ales Danhel received Ph.D. degree in analytical chemistry from Charles University in Prague in 2012. Since then, he has been working as a researcher at the Institute of Biophysics of the Czech Academy of Sciences in Brno. Since 2019, he has been leading a research group: Nanostructured surfaces for biomacromolecule analysis. Foreign research stays were at Hong Kong Baptist University, S.A.R., at the FIOCRUZ, Rio de Janeiro, Brazil, and at the CNRS, Villers-les-Nancy, France. His research interest is focused on the development of novel electroanalytical methods and detection systems applicable in bioanalysis e.g. DNA, proteins, bioactive compounds.

Responsive Probe for Luminescence Bioanalysis and Imaging

Run Zhang*

Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland, Brisbane, QLD, Australia

Abstract:

Rapid advances in the chemical and biomedical studies stimulate the design of new bioanalytical probes for precise and accurate sensing and bioimaging of specific disease biomarkers. These analytical probes enable detection and visualization of the physiological and pathological functions of key biomarkers in living cells and organisms, thus contributing to early diagnosis of diseases and monitoring of their treatments. Of various approaches, luminescent molecular-/nano-probes that can specifically detect and visualize biomolecules have been recognized as one of the most promising technologies due to their high sensitivity and selectivity in sensing and high spatiotemporal resolution

in bioimaging. Nevertheless, conventional molecule and nanoparticle-based probes for biomarker detection is readily interfered by autofluorescence from complicated biological environments, leading to false positive/negative signals. The high reactivities of disease's reactive biomarkers (such as reactive oxygen/nitrogen species with less than one second lifetime) necessitates the development of new bioanalytical probes for background-free detection these unstable and highly reactive biomarkers in situ. In our research, we found that the optical output signals can be easily modulated to eliminate the autofluorescence signals via three strategies, including anti-Stokes upconversion luminescence, time-gated luminescence, and photoswitchable "double-checked" luminescence. In this presentation, research advances in the development of responsive probes for the determination of reactive biomolecules will be introduced, with a particularly focus on the contributions from my research group in the development of probes for luminescence analysis and imaging. The advances, challenges, and future research directions in the development of responsive luminescence probes will also be proposed.

Biography:

Run Zhang received his PhD from the Dalian University of Technology in 2012. He was a Postdoc Research Fellow in the Macquarie University (MQ) in 2012, then a MQ Research Fellow in 2013-2015. He joined the Australian Institute for Bioengineering and Nanotechnology, The University of Queensland (AIBN UQ), as a Research Associate in 2016. Here, he was awarded the ARC DECRA in 2017, NHMRC Investigator in 2020, and now he is a senior research fellow in AIBN UQ. Research interests of his group include the development of responsive molecules/nanomaterials for biosensing and imaging, early disease detection and treatment.

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8105, Rasor Blvd - Suite #112, PLANO, TX 75024

Tel: +1-469-854-2280/81; **Fax:** +1-469-854-2278;

Email: secretary@analyticon-conference.com

Web: https://unitedscientificgroup.com/conferences/analyticon/