

INTERNATIONAL CONFERENCE ON
**ANALYTICAL AND
BIOANALYTICAL
TECHNIQUES**

SEPT **05-06**



VIRTUAL EVENT

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BOOK OF ABSTRACTS

INTERNATIONAL CONFERENCE ON
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05-06^{SEPT}

INDEX

Contents

About Host	4
Keynote Presentations	6
Speakers Presentations	13
Poster Presentations	36
Participants List	39

ABOUT MAGNUS GROUP

Magnus Group (MG) is initiated to meet a need and to pursue collective goals of the scientific community specifically focusing in the field of Sciences, Engineering and technology to endorse exchanging of the ideas & knowledge which facilitate the collaboration between the scientists, academicians and researchers of same field or interdisciplinary research. Magnus group is proficient in organizing conferences, meetings, seminars and workshops with the ingenious and peerless speakers throughout the world providing you and your organization with broad range of networking opportunities to globalize your research and create your own identity. Our conference and workshops can be well titled as 'ocean of knowledge' where you can sail your boat and pick the pearls, leading the way for innovative research and strategies empowering the strength by overwhelming the complications associated with in the respective fields.

Participation from 90 different countries and 1090 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions along with workshops and poster presentations. Our organization runs promptly with dedicated and proficient employees' managing different conferences throughout the world, without compromising service and quality.



ABOUT BIOANALYTICA 2022

Magnus Group welcomes you to our Online Event entitled “International Conference on Analytical and Bio analytical Techniques” BIOANALYTICA 2022 scheduled on September 05-06, 2022 with the theme “Inspecting Innovations and Furtherance Impacting Analytical and Bioanalytical Techniques”

BIOANALYTICA 2022 is an international platform that amalgamates world renowned experts of both academics and industries within the discipline of Bioanalytical and Analytical Chemistry from all over of the world. This event brings together all the bioanalytical and analytical chemistry researchers to exchange and innovates new theories and practices of bioanalytical and analytical chemistry



KEYNOTE FORUM

INTERNATIONAL CONFERENCE ON

ANALYTICAL AND

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05-06 SEPT



Jose Bernal*, Jesus A. Tapia, Laura Toribio, Maria T. Martin, Beatriz Martin-Gomez, Adrian Fuentes Ballesteros, Ana M. Ares

Analytical Chemistry Group (TESEA), I. U. CINQUIMA, Faculty of Sciences, University of Valladolid, Valladolid

Chromatographic methods for authenticating bee pollen origin

Bee pollen has been used in the human diet for many centuries, and its ever-increasing consumption results from its nutritional value and health-promoting effects, like those relating to its antioxidant, anti-inflammatory, anticarcinogenic, antibacterial or anti-fungal properties. The nutritional value/quality and health properties of bee pollen are linked to its constituents, which include proteins, amino acids, lipids, carbohydrates, phenolic compounds, vitamins, or minerals, among several other compounds. However, its composition varies greatly according to several factors, like botanical and geographical origins, climatic conditions, the type of soil, or harvesting and processing conditions. This is quite important to prevent one of the main problems currently affecting the commercialization of bee pollen, and consequently the beekeeping industry; this is the fraudulent practice of adulteration with pollen from other sources/origins, for instance, pine pollen. As may be expected, studying the profile of a particular family of compounds (proteins, amino acids, lipids, phenolic compounds, or minerals) in bee pollen has been proposed, to specify/authenticate its origin and to evaluate the corresponding nutritional value or health-promoting effect.

Therefore, the main goal of this presentation is to investigate the potential of three families of bioactive compounds (amino acids, betaines and glucosinolates), some of them scarcely investigated in this matrix (betaines and glucosinolates, and amino acids), as bee pollen markers, by determining with different chromatographic techniques (high performance liquid chromatography (HPLC) and gas chromatography (GC)) and sample treatments (solvent extraction and solid-phase extraction) their respective content in bee pollen samples from experimental apiaries located within the same area (Marchamalo, Guadalajara, Spain); these were collected in three consecutive harvesting periods in the same year (April-May; June; July-August). It should be mentioned that in all cases, new analytical methods were proposed, which fulfilled some of the principles of the green analytical chemistry, and that they were fully validated according with current legislation. Results showed that bee pollen samples can be classified in most cases, by means of a canonical discriminant analysis (CDA) based on the content of the different compounds, according to the corresponding apiary of origin or the harvesting periods; the potential of these compounds as bee pollen markers may thereby be demonstrated, and subsequently, new tools for authenticating bee pollen origin were provided.

Audience Take Away:

- Audience will know that there is a growing problem related to the authentication of the origin of bee products, and of bee pollen in particular, because of the detected fraud in its commercialization.
- They will be firstly proposed some compounds as pollen markers (glucosinolates and betaines) which also possess some nutritional and bioactive properties. Therefore, it was necessary to propose new analytical methods that were also fully validated. In relation to amino acids analysis, they will be compared two commercial kits for HPLC and GC to choose the most convenient for obtaining a rapid amino acid profile.
- It will be also highlighted the potential of chromatographic techniques to determine those compounds, and the need of employing different approaches depending on the physico-chemical properties of the compounds.
- The need of using chemometric tools, like CDA, as a complement for the analytical methods in order to obtain more relevant conclusions.

Biography

Dr. Bernal studied Chemistry at the University of Valladolid (UVa, Spain), and graduated as MSc in 2003. He then joined the TESEA group (UVa) of Prof. Jose L. Bernal for his PhD stage. After that, he worked (postdoctoral fellowship) at Spanish National Research Council (Jan 2008-Oct 2010) under the supervision of Dr. Alejandro Cifuentes. Then, he obtained an Assistant Professor position in Analytical Chemistry (UVa; 2010), and since 2012 until 2020, he worked as Permanent Assistant Professor (UVa). Finally, he obtained an Associate Professor position (UVa) in 2020. He has published more than 100 research articles in SCI(E) journals.



Pieter Samyn

Hasselt University, Applied and Analytical Chemistry, Institute for Materials Research (IMO-IMOMEC), Agoralaan Gebouw D, Diepenbeek, Belgium

Raman spectroscopy and imaging in organization, processing and functionalization of polysaccharide materials

The Raman spectra of polysaccharide materials provide plenty information on the local organization of polysaccharides in biological materials, their structural variations during processing and surface composition upon functionalization. Each of these aspects are covered by three case studies in our laboratory. First, the organization of polysaccharides in a chitin-protein matrix of crustacean exoskeleton is monitored to reveal differences in microstructure and composition throughout the cuticle cross-section of different skeletal segments with mineral and polysaccharide regions. A Raman study on organized layers provides better insight in the structure of biological materials and consequent possibilities for their extraction. Second, the processing of cellulosic nanofibers from pulp fibers by swelling in ionic liquids is a favourable pre-treatment to facilitate fiber fibrillation. Therefore, the selection of an appropriate swelling medium and conditions should be based on monitoring the influence of ionic liquid composition on swelling efficiency and resulting cellulose properties after different processing time. The local structural variations in crystallinity and internal stress distributions are monitored by in-situ micro-Raman mapping at single fiber-level as a function of time, indicating variations between mild and severe pre-treatment with possible increase in crystallinity, while extreme degradation upon complete dissolution is noticed. Third, the functionalization of micro- to nanofibrillated cellulose by deposition of oil-filled organic nanoparticles provides an active system for tuning of the surface hydrophobicity, which is quantified and visualized as a controlled thermal release of oil from the fiber surface by Raman mapping. After melt-processing of the functionalized fibers with a biopolymer, the different crystallization kinetics within the polymer matrix can be followed from specific spectral bands. All observations from Raman analysis are further supported by complementary analytical techniques and/or theoretical calculations.

Biography

Dr. ir. Pieter Samyn received Ph.D. in Materials Science and Engineering 2007 at Ghent University in the field of polymer tribology and subsequently developed an academic career with several post-doc and assistant professor positions at University Ghent, Freiburg, and Hasselt. In 2021, he joined the collective research center Sirris as a Senior Research Engineer in Circular Economy and Renewable Materials. He has broad experience on the synthesis, processing and analytical characterization of bio-based materials for nanocomposites and coatings. His analytical experiences focus on several types of spectroscopy, thermal analysis, elemental analysis and chromatography. His research focusses on surface functionalization of natural materials and papers in particular for engineering applications, subsequently leading research projects on bio-inspired adhesion mechanisms, bio-based barrier-coatings for packaging papers and the development of functional (nano)composite materials from bio-based building blocks (cellulose, biopolymers) including melt-processing conditions. His work was awarded with a Robert-Bosch Juniorprofessorship, Baden-Württemberg Juniorprofessorenprogramm, Heinz-Maier Leibnitz Preis, FRIAS Fellowship and visiting scholar stipendia at several research institutes. Currently, he assists companies in implementation of bio-based coatings and paints for industrial application.



Victor Cerda^{1*}, Piyawan Phansi²

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Portable and laboratory analytical photometric and fluorometric systems based on the use of 3D printed devices

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.



M. J. Villasenor^{1,2*}, C. Montes^{1,2,3}, M. Bartolome^{1,2}, and A. Rios^{1,2}

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Electrochemical properties and sensing capacities of different carbon-based nanodots toward the detection of bioactives in complex matrices

Carbon-based nanodots are a new family of spherical dots (size below 30 nm) which are overall categorized into graphene quantum dots (GQDs), carbon quantum dots (CQDs) and carbon nanodots (CNDs). They possess unique physicochemical properties such as stable fluorescence, large specific surface area and surface grafting, but they can differ in their crystallinity, graphitized-core degree (sp² /sp³ hybridization), morphology and quantum confinement. Thus, these differences in their cores entail different electrochemical activities and photoluminescence behaviors, which are still in debate. Whereas many efforts were focused over their photoluminescence mechanisms enabling us to distinguish amongst the nanodot types and surface passivation, there is still a need about to perform systematic and comparative works addressing the electrochemical properties exhibited by these different carbon-based nanodots, explaining the subsequent role they play in electron transfer kinetics too. Thus, this speech pretends to give a deep comparative insight about the electrochemical behavior of GQDs, CQDs and CNDs containing similar functionalized surface (oxygenated groups), but different crystallinity, core hybridization, morphology, and quantum confinement. With this aim the three families were firstly synthesized following the top-down methodology and later thoroughly characterized both structural and electrochemically by means of well-known redox probes, surface sensitive in different degree to its chemistry and microstructure. Thus, this study has been directed toward the understanding of those factors controlling carbon dots electrochemistry overall and their heterogeneous transfer rate specifically, in an attempt to gain perspective for a rational design of different carbon-based electrodes with implemented analytical performance as a function of specific analytes. The electroanalytical capabilities of these carbon nanodots-electrodes as sensing electrochemical modifiers are also evaluated versus a set of significant bioactive target analytes, namely vitamins (Vit B₂, Vit B₆ and Vit C) and amino acids (L-tyrosine). Finally, attending to its valuable electrochemical features, modified GQD-SPCEs were selected to carry out the simultaneous detection of these bioactives in commercial nutritional supplements by differential pulse voltammetry (DPV). So, the present research tries to open new possibilities for the design and tailoring of sensing systems attending the specific chemistry of the sought analyte. Then, attending these previous studies, a composite nanomaterial assembled from graphene quantum dots functionalized gamma cyclodextrins and chitosan has been designed and synthesized to evaluate the global content of fluoroquinolones in diverse daily food products. This nanocomposite exhibits an extraordinary electrochemical behaviour towards fluoroquinolones oxidation due to the improved conductivity of GQDs incorporated on chitosan film and to gamma cyclodextrins activity, which became a powerful and selective recognition element size-based for fluoroquinolones electrochemical sensing.

Audience Take Away:

- Familiarization with different carbon-based nanodots species.
- Familiarization with useful electrochemical characterization parameters.
- Familiarization with structural and physic-chemical characterization tools of nanomaterials.

Biography

Dr Maria Jesus Villaseñor Llerena completed her PhD in Analytical Chemistry at 28 years old, at Castilla- La Mancha University in derivative spectrophotometry and electrochemistry fields. Later, she carried out two postdoctoral collaborations with the Institute of Organic Chemistry (CSIC) and the University of Amsterdam (Analytical Chemistry and Polymers Area) being specialized in gas chromatography-mass spectrometry and different modes of capillary electrophoresis respectively. Nowadays her research interests are focused on the development of new optical and electrochemical sensors nanomaterials-based and on the development, synthesis and analytical characterization of new organic nanomaterials within the research group SAMAN (Simplification Analytical Minuturization and Nanotechnologies). She is currently tenured professor in the Department of Analytical Chemistry and Food Technology in the University of Castilla- La Mancha, SPAIN.

SPEAKERS

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Mohsin Sattar*, Dr. Abdul Rahim Othman

Mechanical Engineering Department, Universiti Teknologi PETRONAS,
Seri Iskandar, Perak, Malaysia

Development of new creep prediction model for use through computational modelling for SS-304 material

With the increase of the operational parameters, structural components in power plant are suffering from elevated temperatures and pressures, which are high enough for creep to occur. This may lead to failure and fracture in components. Over the past several decades, considerable efforts have been made to gain a fundamental understanding of the creep mechanism. Much attention has been paid to life prediction of equipment to ensure safety and reliability in power plants. Based on the Norton- Bailey and Kachanov-Rabotnov constitutive models, a modified new model is proposed in this abstract to be able to describe the whole three stages of creep, i-e primary, secondary and tertiary stage. Numerical calculations with the modified constitutive model were performed to simulate the damage development of uniaxial specimens. The emphasis was laid on the effect of specimen dimensions and stress on the damage development. The proposed new model validation was executed by comparing the FE results with experimental creep results obtained by applying acoustic emission technique. The results show a good agreement of the novel model that complete creep curve can be obtained for any material and the stress have remarkable effect on the creep behaviour and damage development.

Audience Take Away:

- Audience will be understand the significance in predicting the material degradation due to creep failure.
- Conducting actual creep tests are time consuming and costly, finite element prediction gives near accurate results.
- The audience can expand the scope of the research work to high level by going in depth of the subject that will help in achieving their research goals and career.

Biography

Mr. Mohsin Sattar received his bachelor's degree in mechanical engineering from NED University Pakistan, master's degree in engineering design from Brunel University, UK and currently pursuing his PhD degree in mechanical engineering from Universiti Teknologi PETRONAS, Malaysia. His current research interests include fracture mechanics, creep modelling and creep life prediction models. He published 4 research articles in ISI/Scopus impact factor journals.



Jingpu Zhang

Scientific Research Center, Shanghai Public Health Clinical Center, Fudan University, Shanghai, China

Dna-templated silver nanoclusters light up tryptophan for combined detection of plasma tryptophan and albumin in sepsis

Tryptophan (Trp) as an essential amino acid plays critical roles in regulating multiple cell activities, and the changes of its circulating level usually indicate disease status such as the severity of acute inflammation sepsis. However, the current technology for Trp detection mostly relies on chromatography that cannot meet the rapid and simple detection requirement in monitoring sepsis. Herein, a label-free fluorescent nanosensor was constructed to detect Trp and its carrier protein - human serum albumin (HSA) in plasma. The nanosensor consisted of a cytosine (C) - rich signal probe of DNA-templated silver nanoclusters (AgNCs/DNA) and a Trp (Trp) aptamer - based capture probe with a guanine (G) - rich overhang. Trp was found to trigger G-rich sequence-mediated fluorescence enhancement effect for AgNCs/DNA under UV irradiation which offers energy to induce the redox process between limited Trp and silver ions bound on the DNA probes. Based on this photochemical property, the nanosensor exhibited a linear response in the range of 0.05 ~ 60 μM with the limit of detection of 0.43 μM for Trp, superior to the current fluorescence-based detection method, and it gave specific response to indole group. When applied in plasma detection, the nanosensor resisted physiological level of NaCl in plasma, but was quenched by trace volume of HSA, which facilitates the combined HSA detection using only 1 μL plasma sample. The simple procedure of “mix, exposure and detection” together with its ultralow sampling volume, time-saving, cost-effective, sensitive and selective properties endow the nanosensor great potentials for future Trp detection-based clinical use.

Audience Take Away:

- An interesting phenomenon was found that tryptophan (Trp) triggered fluorescence enhancement of DNA-templated silver nanoclusters (AgNCs/DNA) upon UV irradiation.
- Based on the above phenomenon, improved limit of detection for Trp was achieved for fluorescence - based detection.
- The combined detection of Trp and HSA was easily conducted merely by mixing and UV exposure.
- The nanosensor resists physiological level of NaCl in plasma, challenges the previous notion that AgNCs/DNA is easily quenched by NaCl.
- The simple method developed based on AgNCs/DNA enables the rapid combined detection of Trp and HSA, and thus could lay a foundation for sepsis diagnosis in the future, which is characterized by rapid changes in levels of Trp and HSA in plasma.

Biography

Jingpu Zhang studied biochemistry at Xi'an Jiao Tong University, China and graduated as MS in 2012. She then joined the research group of Prof. Daxiang Cui at School of Biomedical Engineering, Shanghai Jiao Tong University, China. She received her PhD degree in 2016 at the same group. Immediately after graduation, she obtained the position of research assistant at Shanghai Public Health Clinical Center, and works on the biomedical applications of DNA-templated silver nanoclusters since from her PhD study. She has published 5 research articles as first author in SCI(E) journals.



Hu Xiaofeng* and Zhang Zhaowei

Oil Crops Research Institute, Chinese Academy of Agricultural Sciences,
Wuhan, China

Nanomaterial-based intelligent point-of-care testing for food safety: Mycotoxins

Mycotoxins are typical pollutants that endanger foods and have harmful effects such as carcinogenic, teratogenic, and mutagenic. Aflatoxin B₁ is recognized as a class I carcinogen by the International Agency for Research on Cancer. Cyclopiazonic acid can easily cause degenerative diseases of the liver, pancreas, spleen, and kidney, and zearalenone is accessible to reproductive damage function. Mycotoxin pollution easily occurs in each grain and oil product, such as harvest, storage, transportation, and processing. Mixed mycotoxin pollution is more serious to people's life and health than single mycotoxin pollution because of its additive and synergistic effect. To prevent the frequent occurrence caused by mycotoxin pollution and ensure the food quality and safety "from farm to table", the key is to study and establish a point-of-care test (POCT) to find the mixed mycotoxins pollution in time and reduce the enormous economic losses. The existing detection technology is mainly based on extensive instrument analysis such as high-performance liquid chromatography and mass spectrometry, which are costly, time-consuming, and cannot transmit and share detection results in real-time. The combination of smartphones and POCT modules can realize new methods of intelligent POCT of mycotoxins. It has the advantages of low detection costs, short time, high sensitivity, high throughput, and sharing detection results in real-time. Given the scientific problems of poor detection sensitivity, low throughput, and difficulty in real-time transmission and sharing of detection results in the existing intelligent POCT for mycotoxins in foods, we studied a high sensitivity and high-throughput Intelligent POCT for multi-mycotoxins. We analyzed the sensitivity enhancement and noise reduction mechanism to provide a theoretical basis for intelligent POCT of multi-mycotoxins in foods.

Audience Take Away:

- The audience can learn about the status of mycotoxins contamination in food and current detection methods, which can help them expand their research or teaching.
- The audience can learn the sensitization and noise reduction mechanism of mycotoxins detection, which will help them better understand the theoretical basis of intelligent detection.
- The audience can learn about the combination of intelligent detection and food safety technology, which will help them understand intelligent detection and future research.

Biography

Dr. Hu Xiaofeng is a researcher at Chinese Academy of Agricultural Sciences. She completed her PhD in Food Safety in 2022. Facing extremely hazardous aflatoxin and other mycotoxins extensively existing in contaminated agricultural and food products and food so far, Enzyme-linked immunosorbent assay (ELISA), biosensor, liquid/gas chromatography, and mass spectrometry can hardly meet the request the needs of high-sensitivity and rapid detection from farm to table. Thus, Hu's research has applied basic research on Biosensors for food and feed safety and minimized analytical sensors in food safety and environment monitoring. Specifically, Hu has involved the development of critical antibodies with high affinity, tracing nanomaterials, novel biosensors, and their application in the agricultural and food industry. She published 17 papers, and authorized 1 American invention patent, 1 Australian invention patent, and 7 Chinese invention patents. She participated in the formulation of 6 Chinese national or agricultural industry standards. The rapid detection technology she developed has been widely used in Singapore, India, and 23 provinces in China.



Megha Sharma^{1*}, Kusum Sharma², Pallab Ray²

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Innovations in bio analytical techniques for diagnosing infectious diseases

Infectious diseases, especially bacterial, continue to haunt the healthcare system of most countries. Accurate and timely diagnosis of these bacterial infections is imperative to prevent the high morbidity, mortality, length of stay and cost associated with them. Though advances in molecular biology have shortened the time-to-diagnosis, they are limited by high cost and technical dependence. There is, thus, an unmet need to develop innovative ways that would shorten the turn-around-time of diagnostic tests, without additional burden on workflow, cost and technical requirement. The talk will include innovative ways by which bioanalytical tools like MALDI-TOF MS, and techniques like magnetic bead flocculation and broth microdilution were incorporated into routine workflow of a high-throughput microbiology lab and how they brought about a favourable change by not only improving the patient outcome but also reducing the time and cost involved. The talk will encompass the wide applications that can be harnessed from MALDI-TOF MS in a routine microbiology laboratory – from identification of organism to susceptibility testing, typing and dendrogram analysis. Innovative technique of detecting amplified nucleic acid using simple magnetic beads instead of gel electrophoresis and other costly dyes will also be discussed. The menace of bacterial infections in any healthcare center can be adjudged by the rate of multi-drug resistant pathogens (MDROs) reported, especially gram-negative bacterial that do not respond to any drug except colistin. Performing susceptibility testing for colistin has been a universal challenge but innovative way of pre-prepared frozen plates can be tried to achieve the difficult task. The talk will cover more similar aspects in detail.

Audience Take Away:

- Real-life personal experiences will be shared that would stimulate the audience to apply innovative methods to increase the productivity at their workplace.
- By applying these innovations using bioanalytical tools, the overall ability of the hospital/healthcare center can be improved as there would be prompt and accurate diagnosis of infectious diseases.
- Their simplicity of performance will enable several researchers/teachers/laboratory personnel to incorporate them into their workflow and gain more.

Biography

Dr. Megha Sharma studied Medical Microbiology (MD) from Postgraduate Institute of Medical Education and research (PGIMER), Chandigarh, India and then joined the All India Institute of Medical Sciences (AIIMS), Bilaspur, India as Assistant Professor in Microbiology. She has 7-yrs experience in research and teaching medical microbiology at leading medical institutes like PGI and AIIMS. Her keen interest in developing better diagnostic services to shorten the turn-around-time of laboratory services is exemplified by >50 publications in international medical journals. Gold medals in MBBS, MD and DNB vouch for her academic excellence.



Xin Wang

School of Pharmacy, Shanghai Jiao Tong University, Shanghai, China

Investigation of human micro physiological systems using mass spectrometry-based qualitative analysis combined with metabolomics

Prediction of drug metabolism, drug effects, and drug-drug interactions are mostly investigated in animals and need to be validated in human models. However, limited access to human tissues, especially those that have not been exposed to disease and drugs, has hampered these efforts. Over the past decade, development of micro physiological systems aiming to represent relevant human physiology and organ-specific functions has accelerated, but publications have utilized mostly simple methods of biochemical analysis. Herein, we investigated human micro physiological systems using mass spectrometry-based qualitative analysis combined with metabolomics. An in vitro model of human brain was developed; meanwhile, a sophisticated human multiorgan micro physiological system was established for the comprehensive study of tolcapone metabolite profiling and metabolomics. Twelve tolcapone metabolites were identified, three of which are newly reported. Untargeted metabolomics identified key biomarkers that were significantly changed in human brain in vitro model after tolcapone dosing, which were mainly associated with perturbation of tryptophan and phenylalanine metabolism, glycerophospholipid metabolism, energy metabolism, and aspartate metabolism. The strategy of integrating drug metabolism with metabolomics not only provides a powerful approach to identify drug metabolites and endogenous biomarkers, but also widens our insights into the metabolic pathways perturbed by drug treatment, which are important for the investigation of drug efficacy and toxicity in human brain.

Audience Take Away:

- Mass spectrometry could be considered as a powerful tool for the study of human microphysiological systems.
- Novel bioanalytical approach is developed by the combination of mass spectrometry-based qualitative analysis and metabolomics.
- This strategy of combining drug metabolism, metabolomics, and cell engineering opens a new window for applying analytical chemical methods to evaluate human responses to xenobiotics and other insults.

Biography

Dr. Xin Wang received the Bachelor degree (Science in Chemistry) from Wuhan University in 2010, and the Ph.D degree (Analytical Chemistry) from Peking University in 2015. During Ph.D study, she also visited the University of California, Berkeley as an invited Affiliate Graduate Student of Prof. Frantisek Svec. In September, 2015, she joined Prof. Steven Tannenbaum's lab at Massachusetts Institute of Technology (MIT) as Postdoctoral Associate, and has been promoted to Senior Postdoctoral Associate in 2018. In 2020, she transitioned to the role of Principal Investigator (PI), she is now working at Shanghai Jiao Tong University as an Associate Professor, as well as the Head of Group of Pharmaceutical and Biomedical Analysis.



Uma Kamboj*, Soniya, Neha Munjal

Department of Physics, School of Chemical Engineering and Physical Sciences, Lovely Professional University, Jalandhar, Punjab (India)

Near infrared spectroscopy as a quick tool to identify saw dust adulteration in coriander (*Coriandrum Sativum* L) powder

Near Infrared (NIR) Spectroscopy is a rapid, non-destructive tool to analyse the food products qualitatively and quantitatively. In the present study NIR is used to analyse the adulteration of Coriander (*Coriandrum Sativum* L.) powder. Coriander is considered an annual herb and spice since both its leaves and seeds are used as condiments. It is used in all of its components as a species (seeds, leaves and powder) and also used in cuisine as a flavouring agent. It is also known as Ayurveda medicine in the modern period. Saw dust was used as an adulterant. Three samples were prepared to do a pilot study on how the pure and adulterated samples behave in near infrared spectrum. It was observed that NIR spectra was sufficient to identify the pure sample, adulterant and adulterated sample using Principal Component Analysis. Further it was also studied does the water absorption bands are also affected by the adulterant used. Satisfactory results were obtained which revealed that NIR spectra alone were sufficient for classification of adulterated samples.

Biography

Dr. Uma Kamboj is working as an Assistant Professor at Department of Physics, School of Chemical Engineering and Physical Sciences, LPU. She has completed her PhD from AcSIR CSIR-CSIO, Chandigarh and Post graduated from Punjabi University, Patiala with Gold Medal. Her research interests are spectroscopy, chemometric, statistical analysis, qualitative and quantitative analysis, astronomy and space physics. She was CSIR-SRF fellowship awardee 2013 and also received AMIE Graduate Eminent award 2021 from Institution of Engineers, India. She had 30+ research papers to her credit and guided masters' students in the field of Astronomy and qualitative analysis of food products. Currently working in the field of qualitative and quantitative analysis of food products and beverages using Near Infrared Spectroscopy and Chemometrics. She is an Associate member of A.M.I.E., IEI (India) and Life Time Member of The Indian Science Congress Association.



Gomathi N^{1*}, Lavanya J^{1,2,3}, Varsha M V¹

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Graphene and MOF based materials for electrochemical sensing of biologically important analytes

The full potential of graphene sheets as electrode material in electrochemical sensing is limited by restacking, inert surface and high charging current which can be overcome by incorporating carbon spacers such as carbon nanotube (CNT), graphene nanoribbon (GNR) or any carbon-based nanomaterial, with graphene oxide sheets. We synthesized hybrid graphene using graphene nanoribbon as a carbon spacer between the graphene sheets and further modified with nitrogen containing groups through N_2/Ar plasma treatment, and hybridized with Ni nanoparticle and used the same for (i) ascorbic acid (ii) simultaneous detection of dopamine, uric acid and ascorbic acid and (iii) glucose respectively. Metal-organic frameworks (MOFs), an emerging class of highly ordered crystalline materials with high porosity, facilitates mass and ion transport. However, the inferior electrical conductivity and poor aqueous stability hinders its application in electrochemical sensing. Reduced graphene oxide (RGO), having more accessible plane and edge sites than graphene films, improves the direct interaction between RGO modified electrode and redox species. The synergic effect arising from the combination of RGO and MOF composites exhibit enhanced electrical conductivity, high specific surface area and multi-channels for ion transport for electrochemical sensing applications. Ni-MOF/RGO composite obtained by direct assembly of Ni-MOF and RGO by a simple sonication method was employed as an electrode modifier for the electrochemical sensing of caffeine.

Audience Take Away:

- This talk will give information about surface modification of graphene and MOF.
- This will provide new information about the material for electrochemical sensing of biologically important analytes.

Biography

Dr. Gomathi N studied M.Tech in Chemical Engineering at the Coimbatore Institute of Technology, Bharathiar University, Tamil Nadu, India in 1999. She then joined the research group of Prof. Sudarsan Neogi as Research Scholar at the Indian Institute of Technology Kharagpur, India and received her PhD degree in 2009. After 8 months of postdoctoral fellowship in the research group of Prof. Shika Varma, at Indian Institute of Physics, Bhubaneswar, India, she joined as Assistant professor in Department of Chemistry, Indian Institute of Space Science and Technology, Thiruvananthapuram, Department of Space, Government of India, India in 2010. Currently she is an Associate Professor in the same Institution. She has published more than 40 research articles and book chapters.



Cristina Gutierrez-Sanchez^{1*}, Tamara Guerrero-Esteban¹, Monica Revenga-Parra^{1,2,3}, Felix Pariente^{1,2,3}, Encarnacion Lorenzo^{1,2,3}

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Bifunctional CNDs to enhance electrochemiluminescence for the sensitive detection of analytes of clinical and environmental interest

Nitrogen-rich carbon nanodots (CD) have been synthesized with two functions: To provide functional groups for covalent immobilization of antibodies and to act as co-reactants in the electrochemiluminescent process. CD have been synthesized by a carbonization method microwave-assisted using biocompatible precursors carefully selected, such as D-fructose and urea as N-donor reagent to obtain peripheral enriched nitrogen CD, among others. The synthesized nanomaterials have been characterized by different techniques, that confirm the presence of size-regular amorphous structures with blue fluorescence when are irradiated with UV light. The carbon nanodots designed contain amine groups (N-CD) that can be electrografted onto carbon electrodes and, thus, easily covalently immobilized on these conductive surfaces, confirming the presence of aromatic amines. The highly stable immobilization of N-CD onto the electrode surfaces by electrografting provides hybrid electrodes with greater relative surface area and improved electron transfer properties. Figure 1 shows the strategy used to obtain the hybrid-carbon electrodes.

N-CD immobilized on carbon electrodes efficiently amplifies the electrochemiluminescence signal (ECL), which has allowed the development of a novel ECL biosensors for the sensitive detection of analytes of clinical [1, 2] and environmental interest [3], which contains an aliphatic amine that gives it co-reactant properties [4].

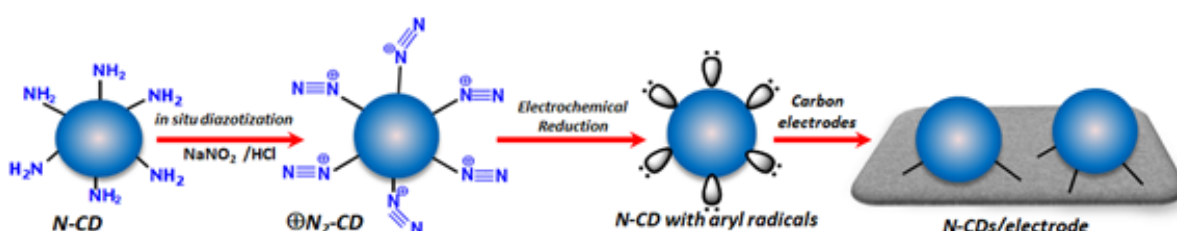


Fig. 1. Diazotized N-CD electrografting on carbon electrodes.

Audience Take Away:

- This informative talk will be of great interest to the rest of the researchers since it reports on a simple strategy to immobilize covalently nanometric carbon nanodots on carbon conductive surfaces, results that can be extended to other types of nanomaterials and that also present interesting detection applications. Carbon nanodots engineered from carefully selected precursors will contain amine groups that will allow its electrografting on carbon electrodes and, therefore, it can be easily covalently immobilized on these conductive surfaces. Resulting in highly stable surfaces which has allowed the development of promising disposable electrochemiluminescent immunosensors for detection of analytes of interest. In addition, the development of electrochemiluminescent processes will also be mentioned.
- The use of nanomaterials is currently very widespread. However, the immobilization of these nanomaterials on surfaces presents little stability since they can be desorbed. In this work, the development of a covalent immobilization

strategy of nanomaterials on the surface of carbon electrodes is shown.

- The selected nanomaterials have been carbon nanodots doped with nitrogen. Which have been synthesized for the first time in our laboratory using different precursors, so their synthesis will be shown. Some brushstrokes of the electrochemiluminescent processes will be explained to easily understand the process. Since the results of the development of electrochemiluminescent biosensors, specifically immunosensors, will be shown.
- The process described above will be clearly shown where researchers can take note of each of the stages followed in the development of these biosensors.
- The researcher will benefit from new information since the results that will be presented have been recently published.
- Results will be shown on the synthesis of novel carbon nanomaterials such as carbon nanodots, which have interesting properties since they are soluble in water, have a nanometric size, and are fluorescent. In addition, a simple synthesis has been developed using precursors abundant in nature and following the principles of green chemistry and the strategy developed for the design of highly stable surfaces with applications for the development of biosensors will be shown. The immobilization strategy of carbon nanomaterials has been designed for the first time, covalently, without the need to use linkers. That is, a covalent bond is formed directly between the nanomaterial and the carbon surface. This provides maximum stability for the development of nanostructured surfaces. The use of these nanomaterials has allowed us to design electrochemiluminescent biosensors. Basic knowledge of electrochemiluminescence will be clearly explained to understand the detection process. Specifically, we have designed immunosensors for the detection of analytes of clinical and environmental interest. All this will help the audience in their future research, since they can take ideas or develop the proposed methodology that will allow them to improve their work and thus their results.

Biography

Dr. Cristina Gutiérrez-Sánchez received her PhD degree from UNED, Spain in 2012. In the Bioelectrocatalysis laboratory of the Institute of Catalysis, CSIC, under the direction of Dr. Antonio Lopez De Lacey. She worked on the functionalization and characterization of surfaces using different techniques for the development of nanostructured enzyme electrodes. In 2013, she undertook her first postdoctoral contract at the University of Siegen, Germany. Subsequently, she moved to Marseille, France, to the CNRS Bioenergetics and Protein Engineering laboratory, for 2 years. Later, she joined the Bioelectrocatalysis group, CSIC in 2016. She is currently working in the group of Dr. Encarnación Lorenzo Chemical, Sensors and Biosensors group at UAM to carry out the Research Project in the Call for Talent Attraction. Her main research interests include areas as Analytical Chemistry, Bioelectrochemistry, Nanoscience and Materials Science. She has published more than 30 research articles.



Ana M. Ares^{*1}, Beatriz Martin-Gomez¹, Laura Toribio¹, Rocio Garcia-Villalba², Francisco A. Tomas-Barberan², Jose M. Villalgordo³, Jose Bernal¹

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Supercritical fluid chromatographic technique as an alternative to separate isomers of urolithin conjugates

Microbiota metabolites, which seem to be responsible of health beneficial effects, are produced in humans after the intake of foods. Urolithins are a class of them that can be found in foods that contain ellagitannins and ellagic acid. After their absorption, they are conjugated with glucuronic acid producing then different regiosimetric isomers, and being mainly present as urolithins glucuronides circulating in plasma and reaching the different tissues. Different metabolotypes have been reported depending on the final produced urolithins: Urolithin A, isoUrolithin A and Urolithin B whose glucuronides could be produced in diverse quantities with difference in regional isomers in individuals due to enzyme polymorphisms. However, the developed methodologies to date have some limitations due to not provide enough resolution to identify and quantify the different isomers in biological samples. Reverse phase high performance liquid chromatography analysis is the chosen technique in which Uro-A 3- and 8-glucuronide and isoUro-A- 9-glucuronide eluted together and only isoUro- A 3-glucuronide and Uro-B glucuronide are usually sufficiently resolved. For that reason, supercritical fluid chromatography using chiral columns is presented as an alternative technique to achieve the separation of the five urolithin glucuronides for the first time. The proposed method was applied to analyze these metabolites in urine samples from different volunteers belonging to different metabolotypes using a Whelk-O® 1 column in less than 15 minutes. In general, volunteers in who both isomers of Urolithin A glucuronides were detected are in similar proportions, while isoUro A-3-glucuronide is the most common isomer against isoUro A-9-glucuronide. This work could represent a significant advance to improve metabolotype assignment and their implications in human health.

Audience Take Away:

- Supercritical fluid chromatography could be considered as a greener alternative to traditional chromatographic techniques to separate isomers of metabolotypes with biological functions.
- The separation of the five urolithin glucuronides was achieved for the first time, which represent a significant advance in chromatography using lesser known columns than those used in reverse phase.
- Moreover, this work could be an important step to improve the urolithin metabolotype assignment and their implications in inter-individuals variations in ellagitannin metabolism and their effect in human health.

Biography

Dr. Ana M. Ares studied Chemistry at the University of Valladolid (UVa), Spain and graduated as MSc in 2011. She then joined the research group of Prof. José L. Bernal, Separation Techniques and Applied Analysis (TESEA group), 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 as postdoctoral position in Analytical Development and Validations in Pharmaceutical Industry (Curia global) and continuing linked at UVa as Associate Professor, 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.



Jefferson Santos de Gois*, Patricia Viana Rodrigues

Institute of Chemistry: Analytical Chemistry Department, Rio de Janeiro State University, Rio de Janeiro, RJ, Brazil

Trace-contaminants determination in glycerin samples after a simple dilute and shot approach for analysis by ICP-OES

Glycerol is an organic compound characterized as a thi-alcohol, with high viscosity (1.41 kg sm^{-1}) and density (1260 kg m^{-3} at 20°C), when compared to water. Glycerol represents around 10% of biodiesel production and it is widely used for sanitary formulations for sanitization. Therefore, contaminant determination in glycerol samples is an important task to be made to assure the quality and safety of this product. No analytical method was found in the literature for the determination of trace elements in the glycerin sample by inductively coupled plasma optical emission spectrometry (ICP-OES). Clasen et al (2015) evaluated the determination of Ca, Mg and K in a glycerin sample by atomic absorption spectrometry, however, the limit of detection is rather higher if compared to ICP-OES, moreover, ICP-OES presents the advantages of multielement determination. Therefore, the aim of this work was the development and validation of a simple dilute and shot method to determine the elements As, Ca, K, Cu, Mg, Na, P, Pb, S, and Zn in glycerin samples by ICP-OES. The effect of the glycerol sample matrix was studied for different glycerin sample masses with samples spiked with 0.5 mg L^{-1} . The developed method demonstrated that sample matrix is a major issue and oxidation with inorganic acids is rather dangerous, thus matrix matching standards were required for calibration using an internal standard (Sc). The accuracy of the method was accessed by recovery tests (ranging within the acceptable range of 80-120%). Different glycerin samples were analyzed and the concentration of these elements was accessed, demonstrating that, perhaps, the monitoring of contaminants in glycerin is an important factor to be considered.

Audience Take Away:

- Trace-elements determination in glycerol by ICP-OES.
- Sample matrix from glycerol may affect the determination by ICP-OES.
- Methods for diluted and shot analysis by ICP-OES.

Biography

Jefferson Santos de Gois currently lives in Rio de Janeiro (Brazil) and works at Rio de Janeiro State University (UERJ). He performs research in atomic absorption spectrometry (AAS), high-resolution continuum source atomic absorption spectrometry (HR-CS AAS), inductively coupled plasma mass spectrometry (ICP-MS) and high performance liquid chromatography (HPLC). His current research projects involve the application of nanomaterials for method development and removal of pollutants from the environment, the development of analytical methods for trace-element and organic compounds determination, sample preparation methods, the development of chemometric methods for multivariate calibration and classification, as well as the design of experiments.



Pier Giorgio Righetti^{1*}, Gleb Zilberstein²

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Stroboscopic flashes on the Netherland

The EVA methodology that will be presented consists in a hydrophilic polymer of ethylene-vinyl acetate (this is the origin of the acronym EVA) admixed with very fine particles of solid-phase sorbents (strong anion and cation exchangers added with hydrophobic resins such as C_8 and C_{18}). These diskettes, when applied to surfaces of items (paper, parchment, canvasses) belonging to the word Cultural Heritage, can capture ultra-minute amounts for proper chemical identification (such as via GC-MS, LC-MS, X-ray). The unique advantage of this probing technique is that it has been proven not to contaminate nor damage any of these precious items stored in museums, libraries, private collections, contrary to other harvesting techniques (e.g. by scraping or rubbing, such as in Collins's methodology) that are intrinsically damaging. The capture is secured via standard non-covalent bonding (ion-to-ion and hydrophobic interactions as well as hydrogen bonding). EVA is a peculiar chromatographic technique that could be classified as a mixed-bed column. It is based on the use of multiple sorbents mixed together and packed in a single column. Thus EVA diskettes can be assimilated to these mixed-bed packed columns except that they are in a form of a solid state cartridge. In a most recent version, also combinatorial peptide ligand library (CPLL) resins have been admixed to the standard sorbents described above. Thus this novel variant contains several millions of diversified beads able to capture, for instance, also very minor polypeptides in presence of high-abundance proteins. The EVA technique has been applied to the screening of manuscript from famous authors (Bulgakov, Chekhov, Casanova, Jack London, Kepler, Orwell, Stalin) as well as to archaeological items (Egyptian mummies, Dead Sea Scrolls, the Aleppo codex) with extraordinary and quite unexpected results.

Audience Take Away:

- Anyone in the audience will be able to synthesize their own EVA diskettes, since the chemistry is quite facile and all ingredients are commercially available.
- Any scientist interested in Cultural Heritage can propose the EVA technique and use it in any public or private collection, since this method is non-contaminating nor destructive. On the contrary M. J. Collins's rubbing method (Proc. Natl. Acad. Sci. USA 112, 2015, 15066-15071) will not have citizenship in any museum or public library since it will surely damage all items under investigation. Given the unique ability of these EVA diskettes to capture ultra-minute amounts of surface material, it will permit identification of, e.g., pigments adopted in canvasses, ink in famous scripts etc. via current instrumental analysis (e.g., mass spectrometry etc.). At present there does not seem to be any other alternative for exploring in full safety any precious document belonging to the word Cultural Heritage.

Biography

Prof. 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 (Cambridge, Mass, USA). He is now Emeritus Professor at the Milan's Polytechnic. On 590 articles reviewed by Mendeley Statistics, Righetti scores 31.636 citations, with an average of 47 citations/article and with a H-index of 84. During the years 2005-2013 he has received citations ranging from 1000 to 1200 per year. As a World Ranking he is No. 1161 and at a National Ranking level he is No. 23.



Vittoria Guglielmi

Department of Chemistry, University of Milan, Milan, Italy

Visible reflectance, Raman and FTIR spectroscopies in the scope of cultural heritage: Non-invasive and in-situ approaches

For many years now, artistic and archaeological research have been concerned with the contribution of scientific resources, especially with analytical techniques dealing with the chemical-physical characterisation of materials. In the same way as the artist applies themselves accurately with their artwork, the scientist devotes their expertise and efforts to the research of the chemical and physical properties of pigments, dyes, binders and other art materials and their identification in works of art and, more generally, in objects of historical and archaeological interest. In fact, the thorough and extensive comprehension of the materials utilised to create artwork is absolutely to be considered a plus. Indeed, it turns out to be another means for going deeper inside the comprehension of works of art themselves and their inherent value, other than the social and historical context to which they belong. One of the more relevant aspects of modern scientific resources in the field of cultural heritage is that the notable technological advances in recent years have permitted the application of increasingly effective analytical - especially spectroscopic - techniques. It is also to stress that a remarkable number of those methods are applicable in situ, i.e., directly on the works of art, and, therefore, without any need of sampling. Moreover, the increasing number of portable spectroscopic instrumentation allows researchers to investigate artwork directly in their regular locations, and this fact might be considered a breakthrough for the non-destructive and in situ study of artwork. In this work, some case studies concerning various types of artworks and consequently diverse kinds of investigated materials are presented, e.g. inorganic pigments, dyes and organic substances. Particularly, the spotlight is on the achievements of portable Raman, FTIR and visible reflectance spectroscopies.

Audience Take Away:

- The importance of interdisciplinary studies of humanities and applied sciences.
- Exploiting analytical techniques for the identification of artwork materials and archaeological findings.
- Application of portable and non-invasive spectroscopic instruments to the study of works of art. The explained analytical and spectroscopic methods are of the utmost importance in material science in general, not only in the scope of cultural heritage. Therefore, this is an opportunity for other scientists in the field of chemical-physical research to acquire new insights and ideas for their research work as well as for their teaching activities.

Biography

Vittoria Guglielmi is an Associate Professor of Analytical Chemistry in the Department of Chemistry at the University of Milan. She obtained her Master's Degree in Chemistry from the University of Milan and her PhD in Chemical Sciences from the same University. The research activity of Vittoria Guglielmi has been mainly devoted to the development and application of analytical methods via instrumentation, mainly employing spectroscopic and chromatographic techniques, for the investigation of both inorganic and organic materials in the field of cultural heritage. Her scientific activity has been reported in 70 publications and more than 50 contributions at conferences.



Marilena Giglio^{*1}, Angelo Sampaolo^{1,2}, Pietro Patimisco^{1,2}, and Vincenzo Spagnolo^{1,2}

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Breath and environmental relevant gas species detection based on Quartz Enhanced Photoacoustic Spectroscopy (QEPAS)

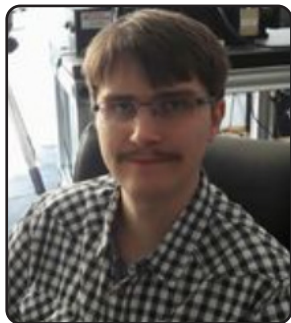
In this work we report on three gas sensors based on quartz-enhanced photoacoustic spectroscopy (QEPAS) technique and developed for environmental monitoring or breath sensing purposes. Spectroscopy has a crucial role in the development of chemical gas species detection, with a great impact in a wide range of applications. For example, the use of high sensitivity gas detectors is widespread in atmospheric science to measure different gas species, including greenhouse and ozone depleting gases, and detect harmful gases leaks; in oil and gas industry, detection of methane and heavier alkanes with their ratios and isotopes allows the evaluation of reservoir formation for guiding petroleum exploration and production estimate, and the identification of natural gas fugitive emissions; detection of volatile organic compounds in exhaled human breath is a pioneering tool for early-stage mass-screening diagnosis of cancer and diseases. Laser absorption-based gas sensors can provide non-invasive non-destructive highly sensitive and selective detection, with fast response time. In particular, QEPAS has been demonstrated as a powerful tool for the development of compact trace gas detectors. Moreover, the recent development of novel quantum cascade lasers (QCLs) and diode lasers (DL) fiber-amplifiers (FA) with high optical power output narrow emission linewidths and wide wavelength tunability allowed the QEPAS sensors detection performance to be boosted. All QEPAS-based sensors here presented were in-field demonstrated. The first detector is a laboratory workbench sensor, employing a non-commercial Vernier-effect quantum cascade laser (QCL), acting as an electrically tunable, switchable light source with emission clusters in the range 2100 cm^{-1} to 2220 cm^{-1} . CO , N_2O , CO_2 , and H_2O were detected in air. The second environmental monitoring purposes-detector is a compact, portable box-size sensor, employing commercial distributed-feedback QCLs to target CH_4 , H_2O and any gas molecule exhibiting absorption features in the IR-spectral range. The third one is a workbench sensor employing a commercial NIR DL and an erbium-doped FA to detect NH_3 in breath.

Audience Take Away:

- Quartz-enhanced photoacoustic spectroscopy as a high sensitivity and selectivity, robust, repeatable, real-time monitoring, non-destructive technique for gas sensing.
- Design of multi-gas detection sensors capable of detecting near-infrared absorption features of several gas species in sequence or simultaneously.
- Design of gas sensors specifically developed for environmental monitoring and/or breath sensing, with record minimum detection limits.

Biography

Dr. Marilena Giglio studied Physics at the University of Bari, Italy and graduated as MS in 2014 (cum laude) and as PhD in 2019. In 2012 she visited the group of Prof. van Leeuwen at the Academic Medical Center of Amsterdam, The Netherlands as a trainee. In 2016 she joined Prof. Tittel's group as Visiting Researcher at Rice University, Texas. After a 2-year Post-Doc at the Polytechnic of Bari, Italy she's currently an Assistant Professor in the same institution. She has published 34 research articles (Scopus), 1 review, 1 book chapter, more than 30 proceedings. She co-invented 1 patent.



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High pulsed power laser inducing phase change - Chemical transformations

High power laser interaction with matter is the tool key to both produce and analyse materials in a vast range from metals and oxides to complex polymers and biocomposites, from particulate matter (PM) in the atmosphere to thin films and bulk materials. The quality of the new materials produced by pulsed laser deposition technique involves the physico-chemical transformations and recombinations during laser ablation from ignition to plasma plume expansion and to the deposition. In order to achieve the desired quality, a consistent number of trials would be required until laser parameters specifically optimized. Also, analytical application of high power laser interaction with matter in LIBS (Laser Induced Breakdown Spectroscopy) and LIF (Laser Induced Fluorescence) requires laser parameters optimization as well. This is the gap that numerical simulation in COMSOL Multiphysics can fulfill, reducing the range of trials. And this is not all that a simulation of laser interaction with matter in COMSOL can provide in the context of a complex study. Developing numerical models using a set of variables and formula, analytical functions, parametric sweep, geometric construction with finite element and meshing accordingly to the needs of the study, physical phenomena and chemical reactions are anticipated and/or their occurrence is explained. The achievements of COMSOL numerical assisted analytic chemical spectrometric techniques establish the bases for a new strategy to enhance the benefits of the laser induced phenomena and processes to obtain new materials, to analyze a wide range of chemical compounds and to lead to a better understanding regarding their occurrence and behavior in certain conditions.

Biography

Dr. Alexandru COCEAN is a young researcher with experience in various projects, member of the Atmosphere Optics, Spectroscopy and Lasers Laboratory (LOA-SL) A. Cocean defended his doctoral thesis in 2019 obtaining the grade SUMMA CUM LAUDE. He has developed a series of experimental and theoretical investigations on the action of high power laser pulses on targets under various environmental and stress conditions. He develop finite element method (FEM) applied in COMSOL Multiphysics to study thermal effects of pulsed laser radiation on homogeneous and heterogeneous targets, as well as laser ablation and deposition simulating the PLD technique.



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Oxygen reduction reaction catalyzed by wired bilirubin oxidase: Fully enzymatic and self-calibrating pH biosensor

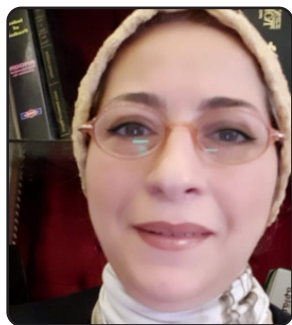
The oxygen reduction reaction (ORR) is important due to high electrochemical potential. Multicopper oxidases (e.g., bilirubin oxidase (BOx)) belong to a class of enzymes that catalyze ORR with low overpotential, and have attracted significant attention in designing bioelectronic devices, *viz.*, biosensors and enzymatic cathodes of biofuel cells. In this work, we present a new concept – an enzyme driven pH electrode system composed of two electrodes: A pH-sensitive BOx-based working electrode and pH-insensitive, a BOx-based reference electrode. ORR-driven pH monitoring was conducted by measuring the potential difference between the two electrodes. Moreover, the electrode system was self-supported and self-calibrating, and no additional electrodes (Pt counter or Ag/AgCl reference) were needed for measurements. The BOx-based pH sensor was tested in continuous and real-time pH monitoring with high accuracy. Also, we present an in-depth mechanistic study explaining the electrode potential-pH dependence, which brings new insights into the operational principle of bilirubin oxidase at different pH.

Audience Take Away:

- The principal action of pH biosensor will be understood.
- Electrode potential – pH dependency explanation based on Nernstian and sub-Nernstian dependency.
- In-depth explanation of BOx inhibition by fluoride.

Biography

Eimantas Ramonas received the B.Sc. and M.Sc. degrees in bioengineering from Vilnius Gediminas Technical University, Lithuania in 2016 and 2018, respectively. Currently, he is pursuing a Ph.D. degree in biochemistry at Vilnius University, Lithuania. His current research field covers fundamental studies of enzyme kinetics when immobilized using 3-D nanomaterials, as well as applied studies of various mono-/multi- enzymatic biosensors with carbon and/or gold-based nanomaterials for medical application.



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Development and validation of two robust simple chromatographic methods for estimation of tomatoes specific pesticides residues for safety monitoring prior to food processing line and evaluation of local samples

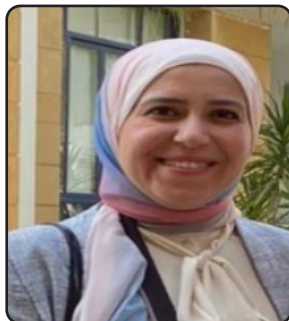
Plant infestation by pests is one of the worst effects of bacteria and fungi on human food. Plants as a primary food resource are critical for human muscle building and mental health. Many farmers worldwide misuse the pesticides' mixtures to keep crops, fruits, and vegetables uninjured, fight grown bacteria and fungi or produce abundant high-quality issues the pesticides' mixtures to keep crops, fruits, and vegetables uninjured, fighting grown bacteria and fungi or to produce abundant high-quality agricultural products. Detecting and analyzing pesticide residual traces could be a crucial issue. Much instrumental weather coupled with Mass or not could be used for the process of estimation. Not only is the estimation of residual insecticides critical in labs of official institutions in the authority of citizen health but also in labs on exporting-importing boundaries between countries. Fresh or processed tomatoes are the most common constituent in our dining tables. Combination of pesticides; acetamiprid, flutolanil and etofenprox are usually used for tomato fruits for protecting them against pest infection. Two specific simple sensitive chromatographic methods are developed for simultaneous estimation of the concerning pesticides' residues using simple economic steps of field sample preparation. The first method is HP- TLC method. Hexane: methanol: acetone: glacial acetic acid (8:2:0.5:0.1, by volume) is proposed as a developing system. The second one is RP- HPLC. Acetonitrile: water (75:25, v/v) is proposed as a mobile phase. The recommended methods are completely validated regarding ICH guidelines. Their means percentages and standard deviations of accuracy range 100.32 ± 0.89 to 99.27 ± 0.9 . The methods' repeatability and intermediate precision relative standard deviation percentages range 0.395–0.894. They are successfully applied for estimating the pesticides in pure and commercial forms and field samples.

Audience Take Away:

- Chemists, food controlling monitors and health and medical caregivers are the audience who can get benefits from the presentation. The presentation will give information about how to use instrumental analysis for estimation of chemical molecules used to destroy bacteria and fungi on food as a poisonous substance to man.
- The audience could use the proposed techniques in research or in quality control labs. By this research, the researchers could use it to expand their research using different techniques otherwise the old ones. The suggested methods may provide a practical solution to a problem that could simplify the microbiology field. It also makes an analyst do the job more efficiently. It will improve the accuracy of a method of analysis and provide added information to assist in an analysis problem.
- The presentation will give innovative ideas in food analysis for inspectors and quality control monitors, and for those who work and investigate nutritional therapy.
- It covers novelty the overlapping area of the food control and the bio-analytical chemistry.

Biography

Prof. Amira studied pharmaceutical sciences at the Cairo University, Egypt, and graduated with an MS in 2004. She then joined the research group of Prof. Raimer Loebenberg at the Drug Innovation Center, Edmonton, Canada. She received her Ph.D. degree in 2014 at the home institution after she got a scholarship at the University of Alberta as an award from her country for her excellence. She obtained the position of Associate Professor at the BSU. After one year, she got a postdoctoral clinical training program at Harvard Medical School. She has published many research articles in highly reputable and impacted journals.



Dina A. Ahmed* and Hayam M. Lotfy

Pharmaceutical Chemistry Department, Faculty of Pharmacy, Future University in Egypt, Cairo, Egypt

Green successive spectrophotometric resolution technique for the analyzing ternary medicine recommended to be used during covid-19 pandemic- purity study

This study presents a novel green spectrophotometric analytical approach for the analysis of ACE- Proxyvon® tablet dosage form recommended to be used in managing the aggressive symptoms of COVID-19 attack as well as dealing with the tiresome post vaccination symptoms. This study focused on the analysis of ternary mixture containing aceclofenac (ACE), paracetamol (PAR) and rabeprazole (RAB) in challengeable ratio; 10:50:1, respectively in the presence of the PAR's potential degradation product; 4-aminophenol (4-AP). A successful compromise was achieved between both resolution and in-silico sample enrichment techniques via employing successive manner based on the application of constant multiplication coupled with spectrum subtraction spectrophotometric method (CM-SS) to extract the parent spectrum for each proposed drug. The extracted parent spectra could be successfully used to monitor the purity of the drug and used effectively to detect counterfeit products. Synthetic mixtures and commercial medicine were constructively analyzed using the proposed technique while maintaining calibration graphs to be linear over ranges; 4.0-40.0 µg/mL for ACE, 2.0-14.0 µg/mL for PAR and 4.0-30.0 µg/mL for RAB. Additionally, methods' validation was confirmed via performing exhaustive statistical treatment of the experimental findings. Finally, method's greenness profile was finally guaranteed through analytical greenness (AGREE) metric assessment tool.

Audience Take Away:

- Giving an overview about the novel spectrophotometric approaches in the field of pharmaceutical drug analysis and the faced challenges compared to chromatographic techniques.
- How to solve and overcome the difficulty of analyzing active pharmaceutical ingredients found in critical ratio in their dosage forms via applying novel sample enrichment techniques.
- Talking about counterfeit products and how to detect them by simple and cost saving spectrophotometric methods.
- Talking about stability indicating assays and how to detect the purity of the pharmaceutical dosage form spectrophotometrically to ensure its freedom from undesirable degradation products.
- Shedding the light on greenness analytical techniques and the different tools used for greenness assessment.
- Application of the novel spectrophotometric method for the stability indicating assay of a ternary mixture in a dosage form recommended to be used to manage the aggressive symptoms of COVID-19 attack as well as dealing with the tiresome post vaccination symptoms.
- Finally, by the end of the talk, an overview will be presented on the problems that could be faced during analysis of different pharmaceutical dosage forms and how to overcome these obstacles by using novel, environmentally friendly, cost and time saving spectrophotometric techniques.

Biography

Dr. Dina is a lecturer in Pharmaceutical Chemistry department (Analytical Chemistry) in Faculty of Pharmacy, Future University in Egypt. She studied Pharmacy at Ain Shams University, Egypt and graduated in 2006. She then received Master (M. Sc.) degree in Pharmaceutical Sciences (Analytical Chemistry) from Faculty of Pharmacy, Ain Shams University in September 2015 then received Doctor of Philosophy (PH. D) degree in Pharmaceutical Sciences (Analytical Chemistry) from Faculty of Pharmacy, Cairo University in February 2020. She has published 8 research articles in different international Journals and attended 6 conferences (local and international) presenting her work as poster and oral presentations.



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Molecularly imprinted polymers for isolation of quinic acid from coffee beans coupled with UHPLC-MS/MS detection

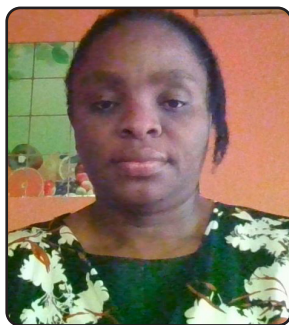
In this study, molecularly imprinted polymers (MIPs) were prepared for extraction of quinic acid (QA) a potent antioxidant and a precursor for the synthesis of many important compounds such as nicotinamide from coffee bean extract. Three different functional monomers were tested for imprinting; two of which were basic monomers (allylamine and 4-vinylpyridine (4-VP)), while the third monomer chosen was an acidic monomer; methacrylic acid (MAA). Rebinding studies revealed that the MIP prepared using 4-VP as functional monomer with template to monomer ratio of 1:5, had better binding performance than the MIPs prepared using the other monomers. Thus, it was chosen to be applied for selective extraction of QA from aqueous coffee extract. The optimized solid phase extraction procedure (SPE) was able to retrieve $81.918 \pm 3.027\%$ of QA with a significant reduction in the amount of other components in the extract. MIP reusability was also tested over ten adsorption-desorption cycles and showed a high recovery of QA (more than 93%) up to the fourth cycle. Selective extraction of QA was observed upon using the optimized SPE procedure on an equimolar mixture of QA, caffeic acid (CA) and chlorogenic acid (CGA). The recovery percent of QA was 82.30 ± 5.58 , compared to 23.71 ± 2.85 and 33.41 ± 0.90 for CA and CLA, respectively. A newly developed UHPLC-MS/MS method was used in the determination of QA. The method was validated according to the ICH guidelines in terms of linearity, limit of detection (LOD), limit of quantification (LOQ), inter- and intra-day precision and accuracy.

Audience Take Away:

- Plant extracts usually consist of a large number of closely related photoactive constituents. This imposes a challenge on the separation and extraction of a target constituent from plants. Molecularly imprinted polymers are polymers that are synthesized in a certain way that leaves recognition sites in the polymer matrix that have the ability to bind specifically to a wide variety of molecules ranging from small drug molecules to large peptides or proteins. In the presentation, the audience will be informed about the application of MIPs in the extraction of a target compound (QA) from plant extract (coffee beans aqueous extract). The synthesis process and the evaluation of the performance of the MIPs will be discussed. The optimization of solid phase extraction procedure for application to coffee beans extract will be thoroughly presented.
- This will help the audience in the design of similar approaches for isolation of other plant constituents, or for pre-concentration of certain constituents from different matrices.
- The audience will be shown how to design a cost effective, rapid, robust and reliable method for extraction of photoactive constituents.

Biography

Dr. Nesrine El Gohary graduated from the Faculty of Pharmacy, Ain Shams University in 2003. Following her graduation Dr. El Gohary was assigned as Organic Chemistry Teaching Assistant at the Faculty of Pharmacy, Misr International University. After wards, Dr. El Gohary worked as a Quality Control Analyst, Chromatography Unit, National Organization for Drug Control and Research (NODCAR). In September 2006, Dr. El Gohary was appointed as a Faculty member in the Pharmaceutical Chemistry Department at the Faculty of Pharmacy and Biotechnology, GUC. Dr. El Gohary earned both her Masters and PhD from the German University in Cairo in 2009 and 2015, respectively. Dr. El Gohary was the Principle investigator (2016-2017) for DAAD-BMBF funded project " Design and application of molecularly imprinted polymers as drug delivery vehicles". Dr. El Gohary currently holds the position of a lecturer at the Pharmaceutical Chemistry Department, Faculty of Pharmacy and Biotechnology, German University in Cairo.



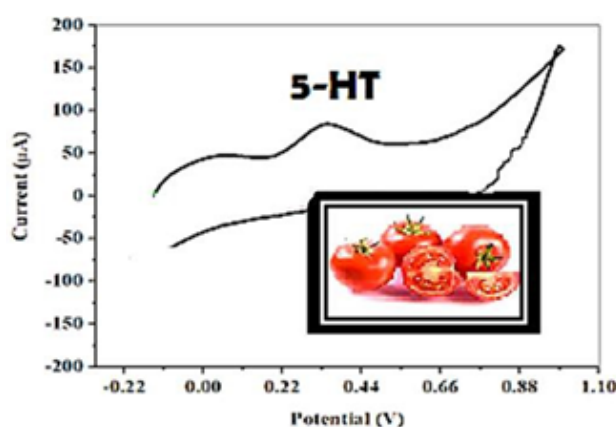
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Serotonin electrochemical detection in tomatoes at MWCNT-AONP nanocomposite modified electrode

This work reports on the successful synthesis of antimony oxide nanoparticles (AONPs) by hydrothermal method, acid treatment of multi-walled carbon nanotubes (f-MWCNTs), and fabrication of a MWCNT-AONP nanocomposite on screen-printed carbon electrodes (SPCE) to detect serotonin (5-HT) in tomatoes. The electro-analytic and electrocatalytic experiments were performed utilizing square wave voltammetry (SWV) and cyclic voltammetry (CV) methods. The SPCE-MWCNT-AONP modified electrodes showed better electron transport and improved current response towards detection of 5-HT when compared to other electrodes studied. The current response decreased in this manner, the SPCE-MWCNT-AONP (84.13 μA) > SPCE-fMWCNTs (33.49 μA) > SPCE-AONPs (24.40 μA) > SPCE-bare (2.89 μA).



The sensitivity, limit of detection (LoD) and limit of quantification (LoQ) for the SPCE-MWCNT-AONP modified electrode towards 5-HT detection was 0.2863 $\mu\text{A}/\mu\text{M}$, 24.6 nM, and 74 nM respectively, with linearity from 0.016 – 0.166 μM ($R^2 = 0.9851$) utilizing SWV. Real-sample analysis of 5-HT in tomatoes showed excellent recoveries ranging from 91.32 to 108.28%, with an average RSD (%) value of 2.57 ($n = 3$). The obtained results strongly suggest that the proposed novel sensor could be applicable in diagnosing point-of-care diseases and therapeutics.

Audience Take Away:

- The importance of using nanoparticles.
- Synthesis and characterization of nanocomposites.
- Application of fabricated electrochemical sensors.

Biography

Omolola Esther Fayemi is an Associate Professor of Analytical Chemistry and postgraduate coordinator in the department of Chemistry, North-West University, Mafikeng, South Africa. Her expertise in synthesis, characterization and application of nano-based materials through both chemical and green mediated synthesis. The synthesized nanomaterials are applied in electrochemical sensors for biological, environmental analytes and for wound dressing. She has published more than 55 research work in accredited journals, and her research outputs are recorded by Google Scholar and ResearchGate.

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Synthesis, characterization of a novel material Co-ZSM5 for supercapacitor

Zeolite composites derived steam-assisted crystallization method as electrode materials for supercapacitor applications has not been extensively reported. Although Zeolites exhibit exceptional surface area, high porosity, and well-controlled structure, they present relatively low conductivity, hindering their successful application in supercapacitor electrodes fabrication. In this work, we report the synthesis of Zeolitic composites (ZSM5, HZSM5) by the facile impregnation method. Among the alternative materials that show great potential for electrode material application, sulphides, nitrides, metal oxides, and other conductors are attracting particular attention. Moreover, other conductors or pseudo materials (Materials based on zeolites) may exhibit low conductivity but have other remarkable advantages such as high specific surface and multiple oxidation states during the electrochemical process. Enhancement of the specific capacitance in electrochemical double layer capacitors (EDLCs) is of high interest due to the ever-increasing demand for high power density energy storage devices. Zeolite templated carbon (ZTC) is a promising EDLC electrode material with large specific surface area and straight, ordered well-defined micropores. Furthermore, in electrochemistry, the application of Zeolites is somewhat limited because they have no redox metals in their structure. For this reason, it is therefore judicious to introduce or incorporate metals or metal oxides into the framework of the zeolite to initiate the retained activity. So, we synthesized zeolite ZSM5 and then impregnate with cobalt and the obtained material was Co-ZSM5. We did some analysis as BET, SEM, FTIR, XPS, XRD (will explained very well during the presentation). Then we did electrochemical analysis and we noticed that our novel material has a good specific capacitance compare to the literature and also maintained 98% retention after 5000 cycles. So, from this work, everyone who has a relation with supercapacitor will know that Co-ZSM5 is a good supercapacitor material. This will provide a practical solution to a problem that could simplify or make a designer's job more efficient because from this work, many professors could also expand this field trying to synthesize other catalysts based on zeolite with another metals. This material could provide energy storage and source balancing when used with energy harvesters and improve load balancing when used in parallel with a battery.

Biography

Mrs Saureille Ngouana Moafor studied Chemistry at University of Yaounde I, Cameroon and graduated for Master in 2018. She then joined the research group of Prof. Linda Jewell in 2020 at the University of South Africa, Florida campus, department of chemical engineering where she is doing her PhD between Cameroon and South Africa (sandwich program). She has not yet published but 2 manuscripts are ongoing.

POSTERS

INTERNATIONAL CONFERENCE ON
**ANALYTICAL AND
BIOANALYTICAL TECHNIQUES**

05-06 SEPT



Marius Butkevicius¹, Julija Razumiene¹, Justina Gaidukevic², Vidute Gureviciene¹, Ieva Sakinyte^{1*}

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Reagentless bioelectrocatalytic detection system for maltose and/or glucose, based on PQQ-glucose dehydrogenase immobilized onto modified reduced graphene oxide surfaces

Acute pancreatitis (AP) is an inflammatory injury, including edema, hemorrhage and necrosis in pancreas caused by tissue autodigestion in relation to various pathogens. Generally, AP is categorized into the mild AP (MAP), moderate severe AP (MSAP) and severe AP (SAP). One of the criteria for determining AP is the measurement of α -Amylases levels in the blood or urine¹. The main method for the determination of α -Amylases is colorimetric, but these methods are relatively slow and require expensive equipment and trained staff. α -Amylases (E.C.3.2.1.1) are enzymes that catalyze the hydrolysis of the internal α -1,4-glycosidic linkages, converting into low-molecular-weight products such as glucose, maltose, and maltotriose units. There is evidence in the literature that the form of AP correlates with glucose levels². Theoretically, maltose levels should also increase during AP. Our work discusses a bioelectrocatalytic system that would allow the rapid, easy and relatively inexpensive determination of glucose and/or maltose levels in urine, which would make it easier to monitor the course of AP. In our work we used PQQ-depend glucose dehydrogenase from microorganism, which was immobilized onto reduced graphene oxide (rGO) modified with organic dyes from three different classes (acridine, arylmethane and diazo) namely; neutral red (NR), malachite green (MG) and congo red (CR). All three rGO/organic dyes composites were characterized by a scanning electron microscopy, X-ray photoelectron spectroscopy and Raman spectroscopy. The impact of three rGO/organic dyes modifications employed in bioelectrocatalytic systems by forming biosensors on changes in enzyme activity and substrate selectivity were investigated in this work. An accuracy of the biosensor action was confirmed with colorimetric method.

¹ Carroll, J., Herrick, B., Gipson, T., & Lee, S. (2007). Acute pancreatitis: diagnosis, prognosis and treatment. *American Family Physician*, 2007, vol. 75, no 10, pp. 1513-1520.

² Sun, Y. F., Song, Y., Liu, C. S., & Geng, J. L. (2019). Correlation between the glucose level and the development of acute pancreatitis. *Saudi Journal of Biological Sciences*, 26(2), 427-430.

Audience Take Away:

- Possibility of applying non-specific PQQ-glucose dehydrogenase in the construction of carbohydrates biosensor.
- Possibility of alternative AP test method that would speed up disease detection.
- Modifications of graphene oxide with organic compounds and the possibility of their application in the design of biosensors.

Acknowledgements:

This research is funded by the European Regional Development Fund according to the supported activity 'Research Projects Implemented by World-class Researcher Groups' under Measure No. 01.2

Biography

Ieva Sakinyte received her Ph.D. degree from Vilnius University, Lithuania in 2017. He is research fellow at the Institute of Biochemistry, Life Sciences Center, Vilnius University. Her research interest includes electrochemical biosensors based on carbon nanomaterials and enzymes, nanotechnology and materials science. She has published more than 16 research articles.



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L-glutamate biosensor for in vitro investigations: Application in brain extracts

Abnormal transmission of glutamate can cause neurological diseases such as communication dysfunction, cognitive impairments, schizophrenia, Parkinson's disease, stroke and epilepsy. L-glutamate is known as the most common excitatory neurotransmitter in the mammalian central nervous system (CNS), thus investigations of L-glutamate release in rats and in mice could help to identify a novel, glutamate-related pathophysiological pathways. Glutamate content usually was assessed using microdialysis-HPLC method and only few electrochemical biosensors were designed. However, they act reliably for a sufficiently short time and their limits of detection for L-glutamate are very low and does not cover the full range of possible changes in concentrations in the study of the diseases mentioned above. In this work, we have proposed a biosensor that is easy to prepare, calibrate, and has adequate stability. The biosensor detects current generated during the electrooxidation of hydrogen peroxide released in the L-glutamate converting to α -ketoglutarate reaction catalysed by glutamate oxidase. The biosensor consists of semipermeable membrane with immobilized L-glutamate oxidase (EC 1.4.3.11), working Pt electrode, isolating corps and contact zone. Firstly, the glutamate biosensor was examined in PBS in terms to investigate sensitivity, reliability and stability. In order to demonstrate the applicability of glutamate biosensor in the analysis of complex real samples, quantification of L-glutamate in bovine brain extract was performed and the accuracy of biosensor was confirmed by alternative methods. Finally, the glutamate biosensor was approved for detection of L-glutamate in bovine and mice brain extracts.

Audience Take Away:

- Possibility of applying specific enzyme glutamate oxidase in the construction of L-glutamate biosensor.
- Possibility of alternative analysis method that would speed up investigations of potential glutamate-related pathophysiological pathways.
- This will provide a practical application for the investigations of CNS diseases.

Acknowledgements:

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Biography

Julija Razumiene Ph.D. is a Chief researcher at Vilnius University, Life sciences center, Institute of Biochemistry. Her research interest is investigations of biological systems structure and functioning, development and creation of new electrode materials, biosensors and analytical systems. In 2009 the work "Investigation and application of enzymatic and poly-enzymatic systems" was awarded by Lithuanian Science Award. Particular attention also has been paid on the development of reagentless biosensors. On a base of the research financing has been obtained for design of prototypes of analysers for hemodialysis monitoring, investigation of severity of acute pancreatitis as well as for fertilizer and industrial wastewater analysis.

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Amira M Hegazy Beni-Suef University, Egypt	30
Ana Maria Ares Sacristan University Of Valladolid, Spain	23
Cristina Gutierrez Sanchez Universidad Autonoma De Madrid, Spain	21
Dina Abbas Ahmed Mostafa Future University In Egypt, Egypt	31
Eimantas Ramonas Vilnius University, Lithuania	29
Gomathi N Indian Institute Of Space Science And Technology, India	20
Hu Xiaofeng Oil Crops Research Institute, China	16
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Jose Bernal University Of Valladolid, Spain	07
Julija Razumiene Vilnius University, Lithuania	38
Maria Jesus Villaseñor Llerena Castilla- La Mancha University, Spain	11
Marilena Giglio Polytechnic University of Bari, Italy	27

Megha Sharma All India Institute Of Medical Sciences, India	17
Mohsin Sattar Universiti Teknologi Petronas, Malaysia	14
Nesrine Abdelrehim El Gohary Mohamed German University, Egypt	32
Omolola Esther Fayemi North-West University, South Africa	34
Pier Giorgio Righetti Politecnico Di Milano, Italy	25
Pieter Samyn Hasselt University, Belgium	09
Saureille Ngouana Moafor University of South Africa, Florida campus/University of Yaounde I, South Africa	35
Uma Kamboj Lovely Professional University, India	19
Victor Cerda Sciware Systems, Spain	10
Vittoria Guglielmi University of Milan, Italy	26
Xin Wang Shanghai Jiao Tong University, China	18

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