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PROCEEDINGS OF

2nd ADVANCED CHEMISTRY WORLD CONGRESS

JUNE 14-15, 2021

Theme: “Latest Global Innovations and Market Insights in Chemistry”

ADV. CHEMISTRY 2021

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YOUR FIRST CHOICE FOR RESEARCH INGENUITY

PROGRAM-AT-A-GLANCE

ADV. CHEMISTRY
2021

DAY 1

MONDAY, JUNE 14, 2021

Scientific Program

BST – British Summer Time

09:45-10:00	**Opening Ceremony**

Sessions: Agricultural Chemistry | Chemical Engineering | Environmental Chemistry | Food Chemistry | Medicinal Chemistry | Nanomaterials | Natural Products, Amino Acids and Peptide Chemistry | Organometallic and Organometalloid Chemistry | Pharmaceutical Chemistry | Polymer Chemistry and Technology | Waste Recycling and Management

10:00-10:20	**Title: Elucidating leaching mechanism for sustainable metal extraction from sulfide ore minerals** **Fang Xia,** Murdoch University, Australia
10:20-10:40	**Title: Cholesterol removal in milk by beta-cyclodextrin: The effect of processing conditions** **Lukas Kolaric,** Slovak University of Technology, Slovakia
10:40-11:00	**Title: CRAC-Containing peptides derived from influenza virus-A protein M1 modulate cholesterol-dependent activity of cultured macrophages IC-21** **Antonina Dunina-Barkovskaya,** Lomonosov State University, Russia
11:00-11:20	**Title: Using model linked systems to study the role of chirality in the electron and energy transfer in biologically relevant processes** **Tatyana Leshina,** Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Russia
11:20-11:40	**Title: Wood leachates and their ecotoxicological impact on aquatic environment** **Klara Anna Mocova,** University of Chemistry and Technology Prague, Czech Republic

Refreshment Break 11:40-11:55

11:55-12:15	**Title: Effect of irrigation water containing iodine on the plant physiological processes and elemental concentrations of different vegetables** **Peter Dobosy,** Danube Research Institute, Hungary

12:15-12:35	**Title: Shape memory polymers in transition to programmable materials** **Thorsten Pretsch,** Fraunhofer Institute for Applied Polymer Research IAP, Germany
12:35-12:55	**Title: Resorc[4]arene-based site directed immobilization of antibodies for immunosensors development** **Francesca Ghirga,** Sapienza University of Rome, Italy
12:55-13:15	**Title: Inulin, a natural functionalizable PEG?** **Carla Sardo,** University of Salerno, Italy

Lunch Break 13:15-13:45

13:45-14:05	**Title: Polyaniline: Advances in synthesis and environmental applications** **Ermelinda Falletta,** University of Milan, Italy
14:05-14:25	**Title: Analysis of ethyl sulfate in wastewaters for estimation of alcohol consumption by the population: A national study conducted in Spain** **Miren López de Alda,** Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain
14:25-14:55 **Keynote Speaker**	**Title: Recent advances in microchip devices for sample treatment: Present and future** **Maria Ramos Payan,** University of Sevilla, Spain
14:55-15:25 **Keynote Speaker**	**Title: The role of mass spectrometry in optimizing the diagnosis and management of thyroid and adrenal diseases** **Steven J. Soldin,** National Institutes of Health, USA
15:25-15:45	**Title: Hollow fiber membrane contactors for post-combustion carbon capture: A review of modeling approaches** **Grigorios Panagakos,** Carnegie Mellon University, USA

Refreshment Break 15:45-16:00

16:00-16:20	**Title: Rhodium organometallics display antiviral activity against SARS-CoV-2** **Joseph S. Merola,** Virginia Polytechnic Institute and State University, USA
16:20-16:40	**Title: Hazardous waste mismanagement causes injuries and spill** **Neal Langerman,** Advanced Chemical Safety, USA

16:40-17:00	**Title: Design and biological activity of A_3 adenosine receptor modulators** **Kenneth A. Jacobson,** National Institutes of Health, USA
17:00-17:20	**Title: Galectin-1 therapy for use in muscular dystrophy** **Pam Van Ry,** Brigham Young University, USA
17:20-17:40	**Title: Impact of sex hormones on brain and colon cancer** **Sahar Eshghjoo,** Texas A&M University, USA

End of Day 1

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DAY 2

TUESDAY, JUNE 15, 2021

Scientific Program

BST – British Summer Time

Sessions: Analytical Chemistry | Biochemistry | Biological Chemistry | Chemical Engineering | Environmental Chemistry | Mass Spectrometry | Medicinal Chemistry | Medicinal Chemistry | Nanomaterials | Pharmaceutical Chemistry | Photo-Chemistry and Clean Energy | Waste Recycling and Management

10:00-10:20	**Title: Functionalization of chitosan with β-cyclodextrin for efficient removal of aspirin** **Norzita Ngadi,** Universiti Teknologi Malaysia, Malaysia
10:20-10:40	**Title: Functional expression of all human sulfotransferases in fission yeast, assay development, and structural models for SULT4A1 and SULT6B1** **Yanan Sun,** Tianjin University, China
10:40-11:00	**Title: ROS production and DNA damage induced by tailored Mn-doped ZnO nanoparticles in murine fibroblast cells** **Ioana Dorina Vlaicu,** National Institute of Materials Physics, Romania
11:00-11:20	**Title: Analysis of the qualitative evolution of groundwater in the Abouabou area in the Port-Bouët municipality (Abidjan, Côte d'Ivoire)** **Kouassi Innocent Kouame,** Nangui Abrogoua University, Ivory Coast
11:20-11:40	**Title: Developments and applications of chip-based mass spectrometry in glycomics of chondroitin/dermatan sulfate oligosaccharides** **Alina Diana Zamfir,** National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania
Refreshment Break 11:40-11:55	
11:55-12:15	**Title: Novel pH-responsive nanohybrid for simultaneous delivery of doxorubicin and paclitaxel: An *in-silico* insight** **Mohammad Dahri,** Computational Biology and Chemistry Group (CBCG), Iran
12:15-12:35	**Title: Gender justice in the energy transition era: Exploring gender and technology in the extractives sector** **Kennedy Chege,** University of Cape Town (UCT), South Africa
12:35-12:55	**Title: New high throughput reactor for biomass valorization** **Julien Thiel,** Deasyl S.A, Switzerland

12:55-13:15	**Title: Approaching multimodal analyses with high repetition-rate laser-induced plasma and associated strategies for complex data processing** **Yi You,** Federal Institute for Materials Research and Testing (BAM), Germany
Lunch Break 13:15-13:45	
13:45-14:15 **Keynote Speaker**	**Title: Personalized and Precision Medicine (PPM) as a unique healthcare model to be set up via biodesign and translational applications and upgraded business modeling to secure the human healthcare, wellness and biosafety** **Sergey Suchkov,** Sechenov University, Russia
14:15-14:45 **Keynote Speaker**	**Title: Adsorbate lateral interactions at patchwise topology: The lambert overall isotherms** **Michael Vigdorowitsch,** Angara GmbH, Germany
14:45-15:05	**Title: Back to Nature: Combating *Candida albicans* biofilm, phospholipase and hemolysin using plant essential oils** **Basem Mansour,** Delta University for Science and Technology, Egypt
15:05-15:25	**Title: Identification and characterization of volatile allosteric antagonists of mosquito odorant receptors** **Georgia Kythreoti,** National Centre for Scientific Research Demokritos, Greece
15:25-15:45	**Title: How to stop climate change?** **Karmen Margeta,** University of Zagreb, Croatia
Refreshment Break 15:45-16:00	
16:00-16:20	**Title: Design, Synthesis, Double effect as antimicrobial-anti-inflammatory and molecular docking of some new thienopyrimidinone glycosides derivatives** **Nesrin M. Morsy,** National research Centre, Egypt
16:20-16:40	**Title: The effect of zirconia phase structure on the production of lower olefins via fischer-tropsch** **Cemile Dut,** TÜBİTAK Marmara Research Center, Turkey
16:40-17:00	**Title: Enhancing the affinity of screen-printed carbon electrodes (SPCEs) towards nitrate and nitrite detection with metallic oxide nanopowders** **Alexandru Florentin Trandabat,** S.C. Intelectro Iasi SRL, Romania
Poster Presentations	
17:00-17:15	**Title: Synthetic search of hemostimulators in a family of novel 3,5-Diarylidenepiperidin-4-one derivatives** **Koshetova Zhanargul Abdrakhmanovna,** A.B. Bekturov Institute of Chemical Sciences, Kazakhstan

17:15-17:30	**Title: Glycolipidomics of human brain hemangioma by high resolution multistage mass spectrometry** **Raluca Ica,** National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania
17:30-17:45	**Title: Ion mobility mass spectrometry reveals the complexity of ganglioside structures expressed in human cerebrospinal fluid** **Mirela Sarbu,** National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania

E-poster Presentations

E-poster	**Title: Novel synthetic inhibitor of Ku/DNA interaction helps to reveal the mechanism of Ku-mediated regulation of HIV-1 transcription** **Sergey Korolev,** Lomonosov Moscow State University, Russia
E-poster	**Title: Development of a new method based microfluidic device liquid phase microextraction for compounds from ten different classes** **Maria Ramos Payan,** University of Sevilla, Spain

End of Day 2

Closing Remarks

BOOKMARK
YOUR DATES

3RD ADVANCED CHEMISTRY WORLD CONGRESS

MARCH 21-22, 2022
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2ND ADVANCED CHEMISTRY WORLD CONGRESS

June 14-15
2021

Keynote Presentations
Day 1

BIOGRAPHY

Steven J. Soldin earned his honors degree in Chemistry at the University of Witwatersrand in South Africa where he subsequently received his Master's degree in Organic Chemistry, and also his PhD in Biochemistry. He enrolled and obtained his boards in Clinical Chemistry at the University of Toronto and then accepted a tenured professor position at the University of Toronto in Clinical Biochemistry and Pharmacology. From 1988-2011, he worked as the Director of Clinical Chemistry at Children's National Medical Center in Washington, D.C. and was a tenured professor in the Department of Laboratory Medicine at The George Washington University School of Medicine. As he was developing his tandem mass spectrometry work, he moved to the Clinical Research Center at Georgetown University as Director of their Mass Spectrometry Core facility, where he still serves as adjunct professor in the Department of Endocrinology and Metabolism. In October 2011, he became a full time Senior Scientist at the Clinical Center Department of Laboratory Medicine where he additionally holds the position of a Deputy Director of Chemistry and Director Post-Doctoral Training Program and the laboratory Mass Spectrometry facility.

Steven J Soldin
National Institutes of Health, USA

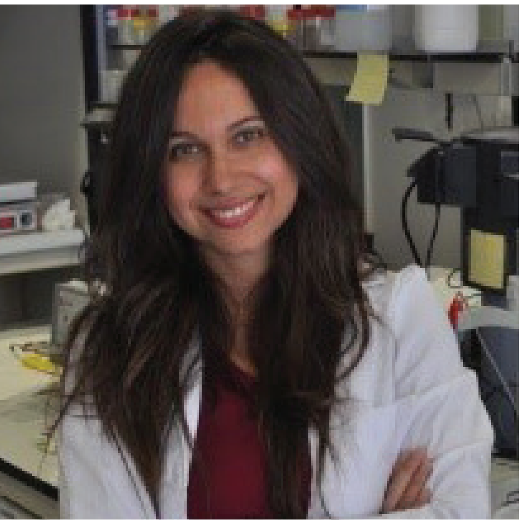
The role of mass spectrometry in optimizing the diagnosis and management of thyroid and adrenal diseases

This abstract covers 30y of work on the above topic. It illustrates that immunoassays currently used to diagnose thyroid and adrenal diseases are nonspecific but precise and frequently provide precisely the wrong diagnosis. We have shown this to be true for T3 and FT3 and also for CORTISOL. Immunoassays (IA) give the wrong results whenever the relevant binding proteins are high or low. Unfortunately for the patients being tested this is a very frequent occurrence especially in women as thyroid binding globulin is greatly increased in those women on the pill or on steroids for another reason. 65% of women between 14-49 years are on oral contraceptives (OCD's) in the USA. This gives inaccurate results for the active thyroid hormones T3 and for FT3. The same problem occurs for cortisol binding globulin, the concentrations of which are high when women are on OCD's. This should be no surprise to us as the Kd's for these binding proteins are close to those of the antibodies in the IA's and competition for these analytes is bound to happen. Renal diseases occur in about 15% of the population. Frequently this results in the loss of small molecular weight proteins in the urine, which include both TBG and CBG. This again results in inaccurate quantitation of the analytes previously mentioned. Here the incidence in men and women is similar.

This work started in 1988 when SJS was working at Children's National Medical Center together with the Head of Endocrinology Dr Wellington Hung, and AGK had not yet been conceived. Dr Hung kept complaining that the FT4's frequently did not agree with the TSH's. So SJS sent those samples to Esoterix for measurement of FT4 by equilibrium dialysis. After dialysis which removes the binding globulins the FT4 results agreed much better with TSH.

Messages: Listen to the clinician, and make sure that the results you obtain correlate with the patient's clinical state.

Question: Why has the FDA not heard that message for 3 decades and continues to license these inaccurate tests?



BIOGRAPHY

Maria Ramos Payán is Doctor in Chemistry (Ph.D) and she is Professor at University of Seville (Spain) at the Department of Analytical Chemistry. She has also developed her research at the University of Lund (Sweden), University of Copenhagen (Denmark), University of Chapel Hill (North Carolina, USA) and National Microelectronics Center (Barcelona). Her research interests focus on the development of new microextraction techniques and microfluidic devices for applications in the life sciences and pharmaceutical sciences. She has published over 40 scientific articles with Hindex 24 and her research line is world pioneer on simultaneous extraction of different compounds on microchip devices.

Maria Ramos Payan
University of Sevilla, Spain

Recent advances in microchip devices for sample treatment: Present and future

The complexity of biological and environmental samples requires analytical protocols that provide high selectivity, sensitivity, selectivity, clean-up, small volume samples, ability to parallelization and a decrease of the time analysis against the most commonly used drugs. Such requirements are closely linked to the miniaturization of analytical procedures which has been a tendency in recent years. The use of microchips for sample treatment becomes the new era in the field of analytical chemistry to carry out more rapid, portable and automated extractions. Microfluidic-chip has been developed for liquid phase microextraction (LPME) or Electromembrane extraction (EME). As known, the transport phenomena are faster at the micro-scale and extractions can be accomplished faster and they offer very high extraction efficiencies. The geometry of the devices is based on two working modes that can be used for both techniques: LPME and EME. Microfluidic devices address and solve sample preparation issues by developing a fast, reusable, efficient and simple-to-use μLPME and μEME applicable to biological and environmental water samples.

As a pioneer researcher in this line worldwide, the results of recent advances in this field will be discussed. For example, the study when both LPME and EME are implemented into a microfluidic chip for emergent pollutants determination by using poly(methyl methacrylate) devices. Comparison between different working modes and also simultaneous extraction of different families of compounds are demonstrated. The advantages of the microfluidic device used as sample preparation are discussed. In addition, the use of new membranes to make these devices more environmentally friendly, this line being one of the new short-term future objectives in this field.

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2ND ADVANCED CHEMISTRY WORLD CONGRESS

June 14-15
2021

Scientific Abstracts

Day 1

ADV. CHEMISTRY 2021

Elucidating leaching mechanism for sustainable metal extraction from sulfide ore minerals

Fang Xia
Murdoch University, Australia

Sulfide ore minerals are the main sources of important metals such as copper, zinc, nickel, cobalt, and lead. These metals are traditionally extracted from sulfide ore minerals by high temperature pyrometallurgical processes such as sintering, roasting, and smelting. These processes are not only energy intensive, but they also produce sulfur dioxide gas, which can cause environmental pollution. Sustainably metal extraction calls for the development of energy efficient and environmentally friendly processing techniques. In this regards, hydrometallurgical leaching at low temperatures is highly desirable, because leaching consumes less energy and produces elemental sulfur or sulfate salts instead of sulfur dioxide. However, leaching is often much slower than pyrometallurgical processes, limiting their widespread industrial applications. One main reason for slow leaching is the formation of surface phases on ore minerals and depending on the permeability of these phases surface passivation may occur during leaching. Yet, the mechanism of the formation of surface phases and their impact on leaching kinetics are still not adequately studied. In recent years, we conducted detailed investigations on leaching of sphalerite, galena, and chalcopyrite, aiming for gaining some fundamental understandings. The key findings are: (1) In all cases, surface phases are formed via the coupled dissolution-reprecipitation mineral replacement mechanism. (2) In chalcopyrite leaching, surface passivation due to elemental sulfur can be eliminated by adding sulfur dissolving agent such as tetrachloroethylene, but to prevent surface passivation due to jarosite formation, control of solution chemistry is important. (3) In sphalerite leaching, ferric nitrate and ferric methanesulfonate are more effective than ferric chloride and sulfate; surface passivation is not caused by elemental sulfur but by sulfate salts. (4) In galena leaching, ferric nitrate is more effective than ferric chloride, but the more promising lixiviant is citrate lixiviant with hydrogen peroxide at near neutron pH conditions.

Biography

Fang Xia is an Associate Professor at Murdoch University, Perth, Australia. He received his PhD degree from The University of Adelaide, Adelaide, Australia, and then he spent a few years as a postdoctoral research fellow at The Commonwealth Scientific and Industrial Research Organisation (CSIRO), Melbourne, Australia. He is interested in elucidating the mechanism and kinetics of dissolution, nucleation, crystallization, phase transformation, porosity generation and evolution, and surface passivation processes occurring in ore minerals leaching, aiming for developing environmentally more sustainable hydrometallurgical metal extraction strategies for processing ore minerals. His research utilizes conventional as well as advanced characterization techniques, including nano- and micro-tomography, synchrotron radiation *in situ* powder X-ray diffraction, and small angle neutron scattering.

Cholesterol removal in milk by beta-cyclodextrin: The effect of processing conditions

Lukas Kolaric and **P. Simko**
Slovak University of Technology, Slovakia

Cardiovascular diseases (CVD) are the leading cause of mortality in the world and the most frequently proposed mechanism for CVD consists of the increase of blood lipids content, especially total cholesterol. As milk and dairy products are rich in cholesterol and are consumed on a large scale, the production of low-cholesterol content products could decrease effectively high cholesterol intake what would be one of the crucial steps in CVD prevention. This study aims the suitable treatment conditions, especially the conditions of centrifugation and settlement, and β-cyclodextrin (β-CD) concentration on the measure of cholesterol removal in milk. The removal of cholesterol from milk is affected by treatment parameters such as centrifugation duration, centrifugation speed, and the settling of cholesterol-β-CD complex as well as β-CD concentration. The centrifugation speed significantly influenced the measure of cholesterol removal as the speed 70 g showed the least efficiency (44.1%) while 200 g the highest (77.8%). The measure of cholesterol removal decreased in higher speeds (400 and 600 g), suggested that the stability of the β-CD complex was lower. The time of centrifugation also affected final efficiency as 5 min showed the lowest (56.9%) and 20 min the highest value (81.1%). The important step in successful cholesterol removal in milk was the settling of cholesterol-β-CD complex at 4 °C after mixing. Without the settlement, the measure of cholesterol removal was only 79.2% while with 30 min of settling, it was 93.6%. The highest

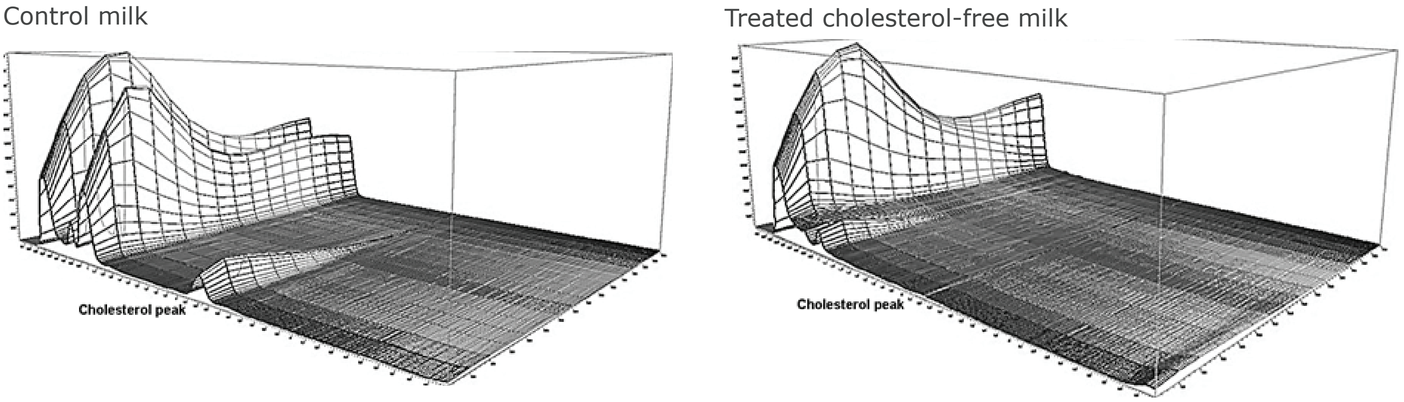
Control milk
Treated cholesterol-free milk

Figure 1: The 3D UV-DAD records of the analysis of control milk and treated cholesterol-free milk.

value (96.3%) was observed after 120 min. The optimal β-CD was monitored at 1.5% with an efficiency of 99.3%. Thus, this study confirmed the excellent possibility of the production of cholesterol-free milk by application of β-CD. The 3D UV-DAD record of the analysis of control milk and treated cholesterol-free milk is shown in Figure 1.

Biography

Lukas Kolaric was born in Bratislava, Slovakia. He is 26 years old and currently, He is a PhD student at the Faculty of Chemical and Food Technology, the Slovak University of Technology in Bratislava in department of Food Technology. His master thesis was describing the extraction of starch from sweet potatoes, its analysis of chemical composition and resistant starch content, and its application in pasta production. Recently, He is focusing on the analysis of cholesterol content in milk and dairy products, and the study of elimination of cholesterol from these products. His expertise is connecting to High-Performance Chromatography, spectroscopy, food sample preparation, food constituent's extraction and analysis, or the analysis of mechanical, rheological, and sensory properties of food products.

CRAC-Containing peptides derived from influenza virus-A protein M1 modulate cholesterol-dependent activity of cultured macrophages IC-21

Antonina Dunina-Barkovskaya[1], **Kh. S. Vishnyakova**[2], **V. A. Radyukhin**[1] and **L. A. Baratova**[1]

[1]*Lomonosov State University, Russia*
[2]*Russian Academy of Sciences, Russia*

Cholesterol is an integral component of an animal cell plasma membrane required for its normal functioning. Some pathogenic bacteria and viruses employ cholesterol dependent mechanisms for cell invasion. One of the hypothesis explaining protein cholesterol interactions suggests the existence of the Cholesterol Recognition Amino acid Consensus (CRAC) motifs characterized by a certain amino acid sequence with a polar, aromatic, and positively charged side groups. One of the ways to verify the significance of CRAC motifs in membrane proteins for cholesterol-dependent cell functions is to analyze the impact of CRAC-containing peptides on cholesterol dependent processes. In this context we studied the effects of synthetic peptides derived from influenza virus A protein M1, which contains several α-helices exposing CRAC motifs, on cholesterol-dependent interaction of cultured macrophages IC-21 with test 2-micron particles. Of four CRAC-containing peptides studied, peptide RTKLWEMLVELGNMDKAVKLWRKLKR (P4) containing two CRAC motifs was most efficient; in a micromolar concentration range it dose-dependently modulated the activity of macrophages and at 20–50 μM produced a cytotoxic effect. Extraction of membrane cholesterol by methyl-β-cyclodextrin lowered the toxic concentration of P4. Peptide obtained by substitution by serine of all CRAC-forming amino acids in P4 did not produce any effect at 0.5–50 μM. Neither was effective peptide with substituted aromatic amino acids in CRAC motifs. Peptide STKLWEMLVELGNMDKAVKLWRKLSR with substitution of cationic amino acids in the CRAC was as efficient as P4. Peptide EWGMAVLWERNRKLKKDLKVLKMLRT composed of the same amino acids as P4 but in a random order ("scramble") and possessing one CRAC motif was not toxic at 50 μM. Our results suggest an important role of CRAC motifs in the mechanisms of the peptide induced modulations of cholesteroldependent cell functions. Possibly viral proteins affect host cell functions in a similar way. CRAC peptides may provide new tools for regulation the activity of cholesterol-dependent proteins and for the design of antimicrobial and immunomodulating drugs.

Biography

A. Ya. Dunina-Barkovskaya was born in Moscow, Russia, in 1952. In 1975 he graduated from the Biology Department, Moscow Lomonosov State University, Russia. Since 1975 till now he has been working at the Belozersky Institute, Moscow Lomonosov State University, Moscow; now he is a senior research fellow. PhD thesis was defended in 1989. Scientific collaboration: Stuttgart University, Germany; Amsterdam University, Holland; NIH, Bethesda; University College London, UK. His field of professional Interest includes cell biology, biophysics, cell membrane, cell–cell communications; gap junctions; tight junctions; ion transport; membrane fusion, endocytosis, phagocytosis. Methods: intracellular microelectrode and microinjection technique, patch-clamp, double whole-cell recording; intracellular microfluorimetry, cell culture, fluorescent microscopy. He is an author/co-author of about 50 publications. Since 2006, a member of the Editorial Board of the journal Biologicheskie Membrany (Biological Membranes).

Using model linked systems to study the role of chirality in the electron and energy transfer in biologically relevant processes

Tatyana V. Leshina[1], **Aleksandra A. Ageeva**[1], **Simon V. Babenko**[1], **Ilya M. Magin**[1], **Victor F. Plyusnin**[1,2] and **Nikolay E. Polyakov**[1]

[1]*Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Russia*
[2]*Novosibirsk State University, Russia*

Photoinduced elementary processes in chiral linked systems, consisting of drugs and tryptophan (Trp) residues, attract considerable attention due to several aspects. First of all, these are models that allow one to trace the full and partial charge transfer underlying the binding of drugs to enzymes and receptors. On the other hand, Trp fluorescence is widely used to establish the structure and conformational mobility of proteins due to its high sensitivity to the microenvironment. It is commonly used to identify a variety of protein changes, e.g., ligand-substrate binding, folding-unfolding processes, etc. In particular, Trp fluorescence analysis helps with the diagnosis of the state of the lens of the eye, the study of abnormalities in the processes of protein folding, the study of the stereospecific activity of quantum dots with D and L-amino acids. It is currently believed that the aging of eyes lens and proteins folding are accompanied by the change of optical configuration (chiral inversion) of amino acids, first of all it is the transformation of L-Trp to D-isomer. However, what properties of D and L-Trp lead to a change in the properties of proteins, for example, influence the folding, remains unknown. In this regard, it is considered relevant to study the activity of enantiomers using examples of elementary processes. An analysis of the photo-chemically induced dynamic nuclear polarization (CIDNP) and Trp fluorescence quenching in (R/S)-naproxen-(S)-tryptophan and (R/S)-ketoprofen-(S)-tryptophan dyads carried out in this work allowed us to trace the intramolecular reversible electron transfer (ET) and obtain evidence in favor of the resonance energy transfer (RET).

Biography

Tatyana V. Leshina is Professor of Physical Chemistry in the Institute of Chemical Kinetics and Combustion Siberian Branch of the Russian Academy of Sciences. She has been working for many years in the area of spin chemistry and, in particular, she is the author of the discovery "A new pattern of radical reactions in solution" (1998), devoted to the observation and explanation of the nature of the influence of inner and external magnetic fields on radical reactions in solutions. Today she applies the spin chemistry and photochemistry methods to study the biochemically relevant processes, including chemical nature of the difference in medical activity of chiral drugs enantiomers on the examples of model processes.

Wood leachates and their ecotoxicological impact on aquatic environment

Klara Anna Mocova
University of Chemistry and Technology Prague, Czech Republic

Wood represents an important natural resource which has been used for various purposes. When wood logs are harvested and processed or branches of trees in urban areas are trimmed, a significant amount of wood waste or by-products arises. Woodchips can be used as mulch, fuel, substrate for biochar production and also as filling material in denitrification bioreactors.

From biological point of view, natural wood may serve as an ecological niche for various types of microorganisms. Thus, after wood harvest these microfungi and bacteria metabolize organic matter and numerous products and semi-products of decomposition emerge. Besides, original wood chemicals including phenolic compounds can be released into leachates when water percolates through the solid material. Wood leachates may have harmful effect on aquatic biota depending on the toxic compounds content.

Ecotoxicity of wood or woodchip leachates is influenced by various conditions, e.g. geographical area and climate, soil contamination, woodchips surface area, and storage conditions such as time duration and temperature. Toxicity also varies due to biological species of the tree both in conifers and deciduous or evergreen trees. Leachate quality is also dependent on the type of the woodchips material (i.e. white vs. brown vs. green chips) as well as the metabolic activity of the present microorganisms. According to the biological species and water quality fresh leachates as well as leachates from fresh wood samples can be acidic and contain higher amount of phenolic acids which leads to higher toxicity to aquatic organisms. Nevertheless, the chemical composition and pH of the leachates change in time. The dynamics of potential ecotoxicity of wood leachates can be easily monitored via experiments with suitable aquatic organisms, such as freshwater plant *Lemna minor L.*

Biography

Klara Anna Mocova studied first biology at Charles University Prague. After obtaining Master's degree she continued in doctoral studies at University of Chemistry and Technology Prague (UCT Prague) with a thesis "Phytotoxicity Tests and Their Application for Evaluation of Solid Samples". Recently she is an assistant professor at the Department of Environmental Chemistry of the Faculty of Environmental Technology at UCT Prague. She is a lecturer of Biology, Ecology and Ecotoxicology courses. Her scientific fields of interest are soil and aquatic phytotoxicity assessment; methods of digital image analysis in environmental sciences. Her latest experimental work has been focused on the ecotoxicological impact of wood leachates, construction materials and waste.

Effect of irrigation water containing iodine on the plant physiological processes and elemental concentrations of different vegetables

Peter Dobosy[1], **Anett Endredi**[1], **Sirat Sandil**[1], **Viktória Vetesi**[1], **Mark Rekas**[2] and **Gyula Zaray**[1]

[1]*Danube Research Institute, Hungary*
[2]*Institute for Soil Sciences and Agricultural Chemistry, Hungary*

Iodine is an essential element for human health, having an important role in the regulation of metabolic processes such as synthesis of thyroid hormones (triiodothyronine and thyroxine), which are involved in the synthesis of sugars, nucleic acids and proteins. The recommended dietary allowance for iodine ranges between 90-270 µg/day, for a normal adult person it is 150 µg/day. Iodine deficiency affects several regions of the world and vegetables have been proven to be an effective alternative way to increase iodine intake for humans by iodine enriched edible plants.

In our study plant physiological processes of different plants (bean, potato, cabbage, tomato, pea and carrot) cultivated on three soils (sandy, sandy silt, silt) applying irrigation water containing iodine in concentration of 0.1 and 0.5 mg/L were studied. After harvesting, the different plant organs (root-, aerial- and edible parts) were dried and their mass were determined. Iodine and essential element concentrations of homogenized samples were measured by inductively coupled plasma mass spectrometer following microwave-assisted acidic digestion.

Iodine treatment had no significant effect on the biomass production of potato, tomato, carrot and pea, the dry mass of cabbage was stimulated, while in case of bean plants a considerable reduction was observed. The highest biofortification with iodine was achieved in cabbage, and accumulation of other plants changed in the following order: carrot>tomato>bean>pea>potato. Depending on the applied iodine dosage and soil type the essential elemental concentrations varied in wide range and it was established that sand soil seemed to be the best cultivation medium for biofortification with iodine.

Biography

Peter Dobosy is a researcher in the Danube Research Institute of Centre for Ecological Research (Budapest, Hungary) where he is currently a research fellow. He obtained his M.Sc. and Ph.D. degrees of the Eötvös Loránd University in the field of environmental chemistry in 2012 and 2017, respectively. He is member of the Hungarian Chemical Society, and the leadership of the Hungarian Spectrochemical Society. His research interests focus on the chemical characterization of sediment and water in river, lake, wastewater and drinking water matrices; effect of trace element-enriched or even highly contaminated irrigation waters on the plant cultivation through the soil-plant, plant-human nutrient connections.

Shape memory polymers in transition to programmable materials

Thorsten Pretsch[1], **D. Schonfeld**[1], **D. Chalissery**[1], **M. Walter**[1], **J. Kobler**[2], **H. Andra**[2], **F. Wenz**[3,4] and **C. Eberl**[3,4]

[1]*Fraunhofer Institute for Applied Polymer Research IAP, Germany*
[2]*Fraunhofer Institute for Industrial Mathematics ITWM, Germany*
[3]*Fraunhofer Institute for Mechanics of Materials IWM, Germany*
[4]*IMTEK, University of Freiburg, Germany*

Shape memory polymers (SMPs) can retain an imposed temporary shape after a thermomechanical treatment. When exposed to heat, the one-way shape memory effect (1W SME) is triggered and the polymer almost completely returns to its permanent shape. Although the 1W SME has been known for a long time, it is still possible to identify applications where the material behaviour provides functional added value. Against this background, some examples will be given. Interestingly, with certain polyurethane-based SMPs that allow distinct 1W SMEs, a programming of two-way SMEs is also possible. Focusing the vision of self-sufficiently adaptable objects, novel systems were designed and SMPs synthesized, processed and demonstrators developed. We assume that this can initiate a paradigm shift in the future, in which the programming of a material is understood as the programming of a functionality. In fact, the internal structure of polyurethane-based SMPs can be controlled whereupon the material properties and behavior change reversibly according to a program. It is achieved by programming the reaction of the material to temperature signals into the polymer structure. In this way, completely new components with specific properties can be produced, which can be used in a wide variety of contexts. We gratefully acknowledge financial support from Federal Ministry for Economic Affairs and Energy, German Federation of Industrial Research Associations – AiF, grant numbers 19820 BR/1 and 20400 BG, and Fraunhofer Cluster of Excellence Programmable Materials CPM, grant numbers 630500 and 630519. T.P. wishes to thank the European Regional Development Fund for financing parts of the laboratory equipment at Fraunhofer IAP (project 85007031).

Biography

Thorsten Pretsch has received his doctorate in Chemistry from the Free University of Berlin in 2004 and has been conducting research for more than 13 years in the field of shape memory polymers. Currently, he is deputy scientific coordinator at Fraunhofer Cluster of Excellence Programmable Materials CPM and responsible at Fraunhofer Institute for Applied Polymer Research IAP for the division Synthesis and Polymer Technology and the working group Shape Memory Polymers.

Resorc[4]arene-based site directed immobilization of antibodies for immunosensors development

Francesca Ghirga, Deborah Quaglio, Francesca Polli, Gabriele Favero, Marco Pierini, Bruno Botta and **Franco Mazzei**
Sapienza University of Rome, Italy

One of the main problems in the development of immunosensors is to overcome the complexity of binding antibody to the surface of the sensor. In fact, antibodies need to be immobilized with a high density and good orientation to allow the easy detection of antigens. The influence of nonspecific bindings should be minimized to improve the detection performance. Most of immobilizing methods lead to randomly oriented antibodies on the surface, which results in a low density of binding sites and alleviation of immunoaffinity of the antibodies. Therefore, oriented immobilization is required for the improvement of the performance enhancement.

Calix[4]arene derivatives have been proposed as an alternative tool for the oriented immobilization of antibodies thanks to their unique three-dimensional surface, which can be functionalized at both the upper and lower rims with several functional groups.1 Within the calixarene family, resorcinol-derived cycloligomers, namely resorcarenes, behave as abiotic artificial receptors having enforced cavities of molecular dimension. 2

To ensure the orientation control of antibodies on the sensor surface, we synthesized several resorc[4]arene derivatives able to self-assemble onto gold surface thanks to the thioether groups present on their structure.3 After the spectroscopic characterization of resorc[4]arene self-assembled monolayers (SAMs) onto gold films, the surface coverage and the orientation of insulin antibody (Ab-Ins) were assessed by a surface plasmon resonance (SPR) technique and compared with a random immobilization method. Experimental results combined with theoretical studies confirmed the dipole–dipole interaction as an important factor in antibody orientation and demonstrated the importance of the upper rim functionalization of resorcarenes. Based on these findings, the resorcarene-based immunosensor is a powerful system with improved sensitivity providing new insight into sensor development.

Biography

Francesca Ghirga received the master degree in Medicinal Chemistry in 2010 and the PhD degree in Pharmaceutical Sciences (XXVI) in 2014 at Sapienza University of Rome. Her primary research interest is centered in the fields of natural products chemistry and supramolecular chemistry. From 2014 to February 2020, she is a Post-Doc at Italian Institute of Technology (CLNS@Sapienza). Research performed at the CLNS@Sapienza covers several challenging and highly multidisciplinary projects ranging from synthetic chemistry to host-guest studies. Since 2018, she is the task leader of the Joint Lab CLNS (IIT)-CrestOptics Project 2b 2018 – 2021 for the Rational Design of Tau Tangle-Selective Near-Infrared Fluorescent probes. In 2021, she was awarded and are managing a fellowship "BE-FOR-ERC", an initiative fielded by Sapienza University, for the development of a research project of excellence as principal investigator. She is the author of 54 publications and 5 patents.

PEERS ALLEY MEDIA

Theme: Latest Global Innovations and Market Insights in Chemistry

2nd Advanced
CHEMISTRY
WORLD CONGRESS
June 14-15, 2021

Inulin, a natural functionalizable PEG?

Carlo Sardo, T. Mencherini, P. Russo and **R.P. Aquino**
University of Salerno, Italy

Inulin (INU) is a natural polysaccharide, easily extracted from different vegetable sources. In recent years, INU is growingly being used as substrate to obtain advanced functional nanomaterials for drug and gene delivery. The advantage stems from its biocompatibility and the number of hydroxyls of the dangling fructose units which allow its functionalization [1,2].

One of the most peculiar characteristics of INU, if compared with other polysaccharides, is the fact that it does not incorporate any sugar ring in the backbone, which adds a high flexibility to the hydrophilicity and the good solubility in organic solvents and the uncharged character. Looking closer to the backbone, it can be noticed a high structural analogy between INU and PolyEthyleneGlycol (PEG), a synthetic gold standard among the hydrophilic polymers in the design of drug delivery vehicles. That structural similarity is also accompanied by an analogy in the physicochemical characteristics. Moreover, as well as PEG, INU is classified under the GRAS status by the FDA since 2002.

Thus, the question is: can inulin be considered as a naturally occurring functionalisable PEG? To tackle this question, we designed the first Inulin-poly-D,L-lactic acid INU-PLA copolymer to be compared with the already well known PEG-PLA counterpart in terms of ability in forming supramolecular nanosystems, ability to carry a model drug, the colloidal stability, degradability rate of the PLA block and the drug release. A ligand installation for targeted delivery has been also considered (Fig. 1).

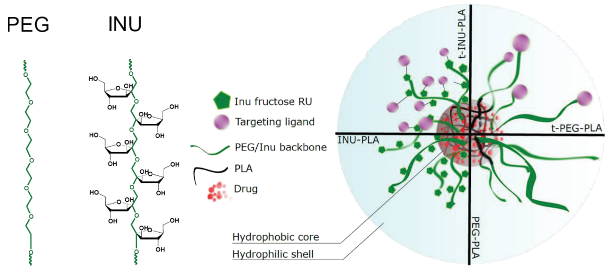

Fig.1. Structural analogy between PEG and INU and Schematic representation of nanosystems obtained from linear PEG-PLA and brush-like INU-PLA copolymers

The positive answer to our main question would open up opportunities never considered before, thanks to the alternative it would represent in those cases where a PEG immunity is an obstacle for a successful therapeutic outcome [3], as well as for the structural variety of the derivatives that could stem from using Inulin.

Biography

Carlo Sardo is an expert in the field of nanotechnologies for biomedical application, with special interest in Drug and Nucleic Acid Delivery. She's currently a researcher at the department of Pharmacy at the University of Salerno (Italy). She works on a technology platform for therapeutic strategies against resistant cancer (Project "Campania Oncoterapie", Combattere la Resistenza Tumorale: Piattaforma Integrata Multidisciplinare per un Approccio Tecnologico Innovativo alle Oncoterapie - POR Campania FESR 2014-2020).

She finished her PhD in 2015 (Palermo, Italy) on the synthesis and characterization of biocompatible polymers for drug and gene delivery. In 2012-2019 she was involved in the following projects: "Identification of optimal delivery systems for NABD and study of the mechanisms of action in some models of inflammatory and cancerous human diseases" (Palermo, Italy); "Development and characterization of nano-structured systems for the delivery of drugs for the treatment of retinopathies" (Palermo, Italy) and "Oligopod Composites nucleic acids and boron clusters – new material for bionanotechnology" (Lodz, Poland).

Theme: Latest Global Innovations and Market Insights in Chemistry

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June 14-15, 2021

Polyaniline: Advances in synthesis and environmental applications

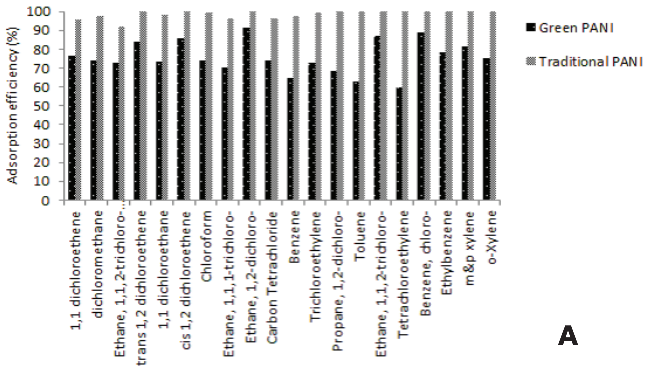
Ermelinda Falletta[1,2,3], M. Frias Ordonez[1], A. Bruni[1], M. Sartirana[1] and **C. Bianchi[1,2]**

[1]*University of Milan, Italy*
[2]*INSTM, Italy*
[3]*ISTM-CNR, Italy*

The chemical industry of the forthcoming years will be shaped by a number of emerging global megatrends strictly related to the growth and aging of the world population (nine billion people in 2050). This will result in demand of innovative materials able to solve new needs in different fields. Environmental deterioration and the scarcity of fresh water have become imperative global issues to be solved nowadays. Polyaniline (PANI) and PANI nanocomposites are innovative materials that have gained popularity in addressing water and air pollution issues.

These materials, combining electrostatic and hydrophobic segments in their backbone, showed promising results in the abatement of both remove organic (mainly hazardous dyes) and inorganic (mainly toxic metals) pollutants.

Even though many methods have developed to synthesized PANI of good quality in terms of conductivity, stability and porosity, all these approaches are based on the use of toxic stoichiometric oxidants (typically metals in high oxidation state) and lead to the production of carcinogenic coproducts (i. e. benzidine and *trans*-azobenzene) [1]. In line with the growing environmental sensitivity and the necessity of clean products, we have recently addressed our efforts on the development of environmentally friendly protocols to produce "green" PANI [2-4]. Herein, we report a brief overview of our results on the synthesis of PANI and its composites by environmentally friendly approaches and our recent goals in the abatement of VOCs [5] and NO_2 from air matrices and dyes [4], hydrocarbons [6] and metals from water [4].



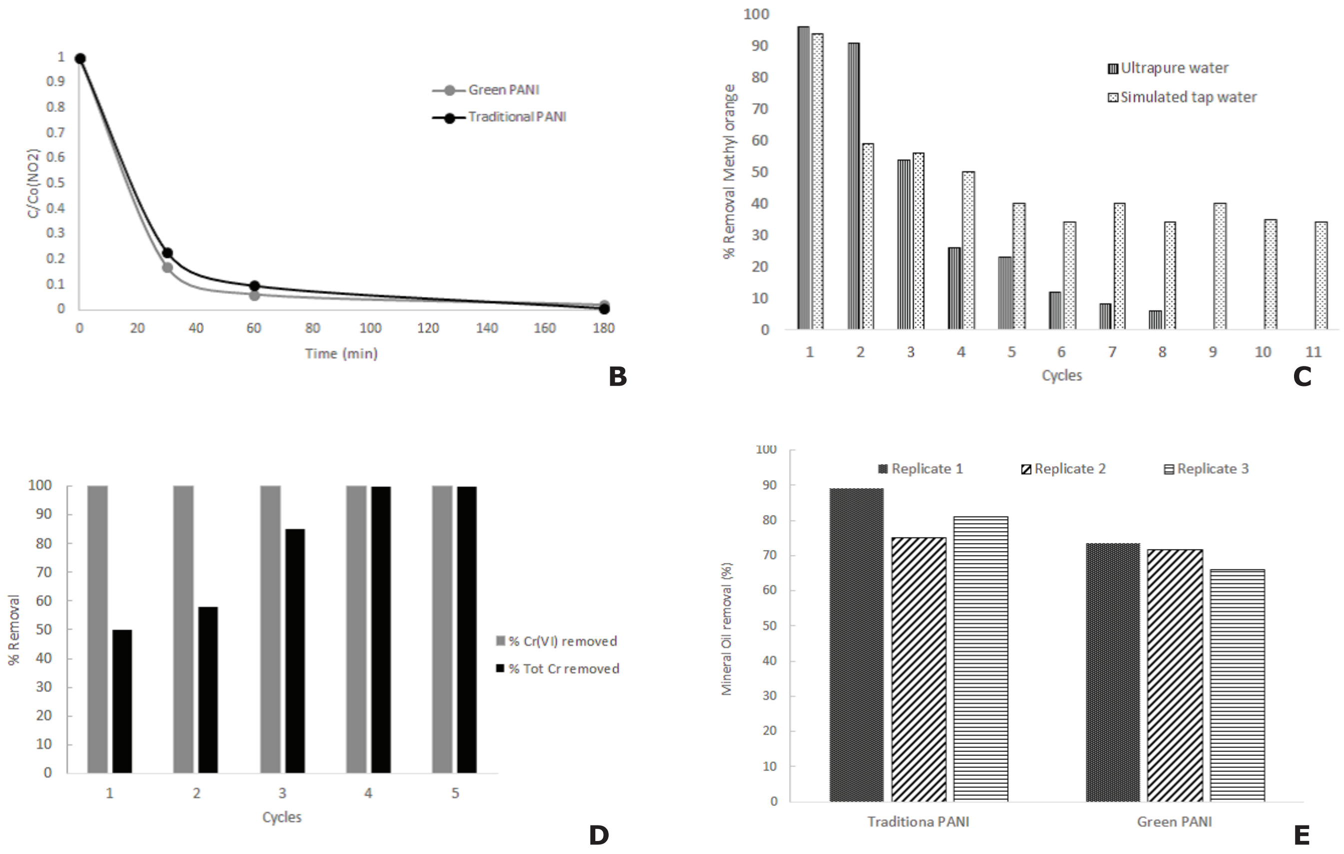


Figure: A) VOCs abatement by traditional and green PANIs
B) NO_2 removal by by traditional and green PANIs
C) Methyl orange sorption by green PANI in ultrapure water and simulated tap water
D) Chromium abatement by green PANI
E) Mineral oil sorption by traditional and green PANIs

Biography

Ermelinda Falletta is a researcher at the Department of Chemistry of the University of Milan. Her research activity deals with: i) development of innovative environmentally friendly approaches for the preparation of intrinsically conducting polymers and their composites and their application in the field of environmental remediation and piezoresistors, ii) development of heterogeneous catalysts for the selective oxidation of organic compounds and photodegradation of emerging pollutants, iii) development and optimization of new analytical methods (in particular UHPLC-MS/MS, GC/MS and SPME/GC/MS) for the identification and determination of target and non-target species in the environment and biological sectors.

She is author and co-authors of about 60 ISI papers, 3 books, 7 book chapters and 2 patents.

H-index: 23 (Scopus); 24 (Google Scholar).

Analysis of ethyl sulfate in wastewaters for estimation of alcohol consumption by the population: A national study conducted in Spain

Miren Lopez de Alda
Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain

The analysis of wastewaters as a means to investigate public health is gaining increasing acceptance and application worldwide. In the present study, we describe its application for evaluation of alcohol consumption habits by the population. The approach, known as wastewater-based epidemiology (WBE), consists in this case in measuring ethyl sulfate, which is a metabolite formed after alcohol consumption, in raw wastewaters collected at the entrance of wastewater treatment plants (WWTPs), and translating the concentrations measured into alcohol consumption data upon consideration of the metabolite excretion rate, the volume of water treated by the plant, and the population served by it. This approach was applied in Spain in a study where wastewater samples were collected daily during one week in a "normal" period (without special events or holidays) from 17 WWTPs located in 13 Spanish cities covering 12.8% of the Spanish population (see Figure 1).

The results obtained showed: (i) a variable geographic alcohol consumption, ranging from 4.5 to 46 mL/day/inhabitant; (ii) statistically significant differences in consumption between various cities and between weekdays and weekends (being higher in the latter case); (iii) comparable data in most cases with the official figures published by the corresponding regional authorities, which are based on other kind of methods/data such as interviews and medical and criminal statistics, as well as with the overall yearly consumption officially reported for the nation (4.7 L ethanol per capita (aged 15+) vs 5.7 ± 1.2 L ethanol per capita (aged 15+) calculated through the analysis of wastewaters). Studies conducted by the same authors in other investigations evidenced also conjoint consumption of alcohol and cocaine, and different increasing/decreasing trends in alcohol consumption throughout the years and during the pandemic.

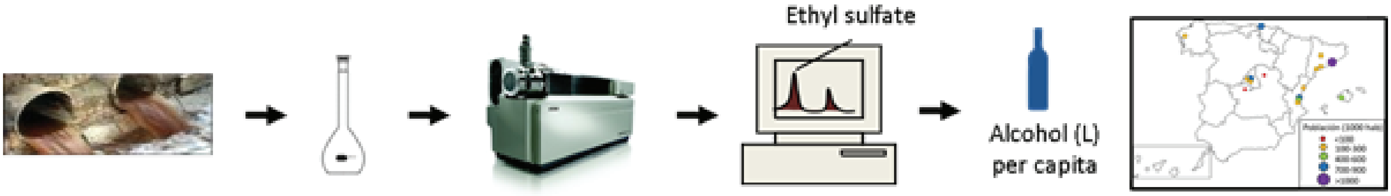


Figure 1. Steps of the study

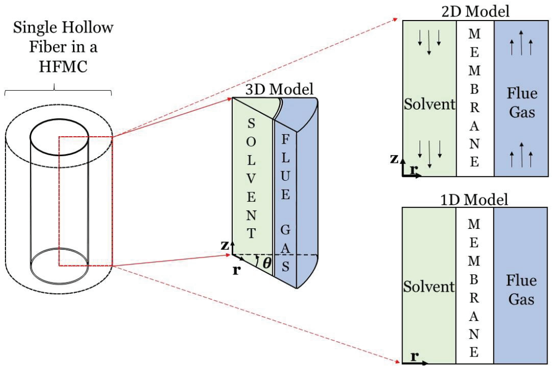
Biography

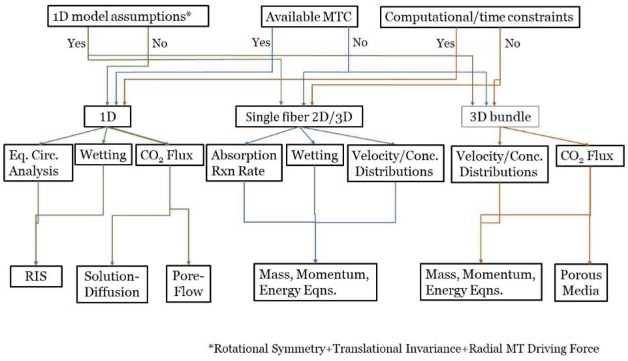
Miren Lopez de Alda is scientific researcher and Head of the consolidated research group ''Water and Soil Quality Unit'' at the Institute of Environmental Assessment and Water Research (IDAEA), that is part of the Spanish Council for Scientific Research (CSIC), in Barcelona, Spain. She has been working for many years on the environmental analysis of emerging contaminants (endocrine disrupting compounds, estrogens, illicit drugs, cytostatics, polar pesticides…), field where she has contributed many novel analytical methods and data in relation to their occurrence, risks for the environment and human health, and ways to eliminate them. She has published more than 200 SCI papers (Hirsch-index 68) and supervised 9 doctoral Thesis plus various DEA, TFG, and Masters. Mid-to-long term scientific interests focus on the investigation of anthropogenic contaminants and their transformation products, sewage-based epidemiology, water reuse, and contamination of the atmosphere, oceans and polar regions as transversal areas of study and application.

Hollow fiber membrane contactors for post-combustion carbon capture: A review of modeling approaches

Grigorios Panagakos[2], **Joanna R. Rivero**[1], **Austin Lieber**[1] and **Katherine Hornbostel**[1]
[1]*University of Pittsburgh, USA*
[2]*Carnegie Mellon University, USA*

Hollow fiber membrane contactors (HFMCs) can effectively separate CO_2 from post-combustion flue gas by providing a high contact surface area between the flue gas and a liquid solvent. Accurate models of carbon capture HFMCs are necessary to understand the underlying transport processes and optimize HFMC designs. There are various methods for modeling HFMCs in 1D, 2D, or 3D. These methods include (but are not limited to): resistance-in-series, solution-diffusion, pore flow, Happel's free surface model, and porous media modeling. This work discusses the state-of-the-art methods for modeling carbon capture HFMCs in 1D, 2D, and 3D. State-of-the-art 1D, 2D, and 3D carbon capture HFMC models are then compared in depth, based on their underlying assumptions. Numerical methods are also discussed, along with modeling to scale up HFMCs from the lab scale to the commercial scale.





*Rotational Symmetry+Translational Invariance+Radial MT Driving Force

Biography

Grigorios Panagakos' expertise stems from the area of computational fluid dynamics (CFD) and transport phenomena with applications ranging from carbon management and hydrogen technologies to energy storage and micro-fluidics.

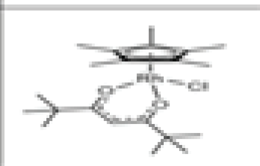
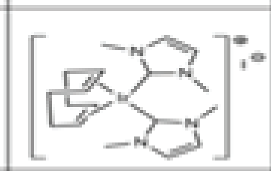
In the area of carbon management, his research includes modeling and simulations of separation systems like membranes and solvents for CO_2 absorption on intensified, advanced manufactured devices for improved performance and process optimization. Panagakos received his first degree in mechanical engineering and his MS in automation systems with emphasis on robotics from the National Technical University of Athens, followed by an MS in CFD at the University of Maryland. He is also holding a Ph.D. from the Technical University of Denmark working on Modeling and Structural Optimization of Solid Oxide Fuel Cells (SOFCs). After the Ph.D. he spent two years as a post doc at the CERTH and then joined NETL as an ORISE research associate, working on modeling SOFCs.

Rhodium organometallics display antiviral activity against SARS-CoV-2

Joseph S. Merola, Christina Chuong, Christine M. DuChane, Emily M. Webb, Pallavi Rai, Jeffrey M. Marano, Chad Bernier and **James Weger-Lucarelli**
Virginia Polytechnic Institute and State University, USA

SARS-CoV-2 emerged in 2019 as a devastating viral pathogen with no available preventative or treatment to control what lead to the current global pandemic. The initial wave of activity in the early days of the pandemic focused on development of vaccines, and rightfully so. However, we also need new therapeutics to treat those who become infected with the ability to lessen the severity and mortality of the viral disease. The continued spread of the virus and increasing death toll necessitate the development of effective antiviral treatments to combat this virus and, perhaps, provide a platform for the creation of antivirals for new, emerging viruses. We have been studying transition metal organometallic compounds for their anti-microbial activity against multi-drug resistant pathogens with some success. In addition, parallel studies show that these compounds are potentially safe for use in mammals – both *in vitro* and small animal studies.With this background, we evaluated a new class of organometallic compounds as potential antivirals. We demonstrated two rhodium complexes, coordinating with either 1,3-dicyclohexylimidazol-2-ylidene or dipivaloylmethanato, have direct virucidal activity against SARS-CoV-2. Subsequent *in vitro* testing suggested the dipivaloylmethanato complex was the more stable and effective complex and demonstrated both compounds have low toxicity in Vero E6 and Calu-3 cells. The complexes under study are eminently functionalizable holding the hope for tailoring them to have new anti-viral activity against new and mutated viruses. The results presented here highlight the potential for organometallics as antivirals and support further investigation into their activity.

Table 1. Organometallic complex structure and notation

Compound 1	Compound 2	Compound 3	Compound 4	Compound 5
				

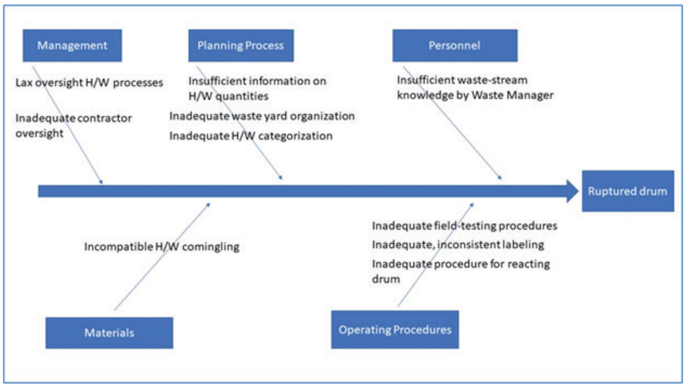
Biography

Joseph S. Merola received his Ph.D. in 1978 with Dietmar Seyferth at MIT. He joined the Corporate Research Laboratories of Exxon Research &Engineering Company in New Jersey. In 1987, he moved to the Department of Chemistry at Virginia Tech where he has remained since. He carries out work in the areas of transition metal organometallic complexes, primarily of rhodium and iridium and has published over 100 papers in this areas. This work began as an investigation into their catalytic activity and morphed into examining their biological activity. Professor Merola is a Fellow of the American Chemical Society and a Fellow of the American Association for the Advancement of Science.

Hazardous waste mismanagement causes injuries and spill

Neal Langerman
Advanced Chemical Safety, USA

Case studies are excellent tools to illustrate and expand implementation of fundamental concepts of chemical safety. This case study illustrates how inattention to established procedures and lax supervisory oversight work together to result in an adverse event. The report utilizes the "Five-Why's" method of Root Cause Analysis and illustrates the utility of this method for understanding the underlying causes of adverse events. The analysis is summarized in this fishbone diagram.



Biography

Neal Langerman is a chemist, earning a Ph.D. in biochemical thermodynamics at Northwestern University. He received a B.S. in Chemistry from Franklin & Marshall College in Lancaster, Pennsylvania. Following a NIH Post-Doctoral year at Yale, he joined the faculty of the Departments of Biochemistry and Pharmacology at Tufts University Medical School in 1970. In 1975, he went west and joined the Chemistry Department of Utah State University. At both Tufts and USU, he assumed responsibility for departmental safety programs. In 1979, Dr. Langerman learned of RCRA, and this started him on his career as a consultant.

Dr. Langerman established his first consulting company, Chemical Safety Associates, in 1980, in conjunction with other members of the USU faculty. He headed this firm until 1997, when he sold his interests in MSDS production and set up his current consulting firm, Advanced Chemical Safety.

Dr. Langerman's professional interests are in the prevention of chemical incidents and injuries. His professional time is spent consulting on chemical safety & security, and regulatory issues. He served as the Chair of the Division of Chemical Health and Safety of the American Chemical Society in 2004 and also, in 2004 and 2013, received the Tillsman-Skolnick Award for contributions to the field of chemical health and safety through the ACS from the Division. He is currently an Alternate Councilor for the Division.

Dr. Langerman is an avid SCUBA diver and photographer.

Design and biological activity of A_3 adenosine receptor modulators

Kenneth A. Jacobson, Dilip K. Tosh, R. Rama Suresh, Veronica Salmaso, Lucas Fallot and **Zhan-Guo Gao**
National Institutes of Health, USA

We synthesize and characterize new modulators of the A_3 adenosine receptor (A_3AR), a rhodopsin-like G protein-coupled receptor (GPCR). As an A_3AR structure is unavailable, we use homology modeling, docking and molecular dynamics simulations to computationally predict the receptor interactions of newly synthesized or planned orthosteric ligands, i.e. agonists, partial agonists and antagonists. Recently synthesized adenosine derivatives are highly selective A_3AR agonists (>3000-fold vs other ARs) by virtue of a rigid ribose substitution, i.e. a methanocarba (bicyclo[3.1.0]hexane) ring system that maintains an A_3AR-preferred conformation and lowers the binding energy barrier. Positive allosteric modulators (PAMs) and agonist prodrugs of A_3AR are also under development. Selective A_3AR agonists have anti-inflammatory effects *in vivo*. For example, our two prototypical A_3AR agonists are efficacious in clinical trials for psoriasis and for liver cancer and nonalcoholic steatohepatitis, without serious adverse effects. A_3AR agonists are also potentially useful for chronic neuropathic pain, through effects in the spinal cord, peripheral neurons and brain, as reported in collaboration with Daniela Salvemini (St. Louis University). We measured the real-time response to newly synthesized nucleosides administered orally in a mouse chronic constriction injury model (phenotypic screen). We introduced functional groups that enhanced efficacy and duration of the antiallodynic effects *in vivo*. A_3AR agonists that we have introduced show drug-like preclinical properties. A_3AR agonists reduce neuropathic pain arising from injury or cancer chemotherapeutic agents. When A_3AR agonists are combined with morphine, the opioid becomes safer and more effective for long term treatment. This promises to be a new approach to fulfill an unmet medical need, as chronic pain of various etiologies affects a large fraction of the population. If confirmed in clinical trials, this could become a key approach in combatting the opioid crisis. Thus, A_3AR modulation holds promise for chronic disease treatment, as demonstrated using highly selective ligands.

Biography

Kenneth A. Jacobson is Chief of the Molecular Recognition Section in the Laboratory of Bioorganic Chemistry at the National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health in Bethesda, Maryland, USA. Dr. Jacobson is a medicinal chemist with interests in the structure and pharmacology of G protein-coupled receptors, in particular receptors for adenosine and for purine and pyrimidine nucleotides. He obtained a Ph.D. in Chemistry from the University of California, San Diego. He has published more than 800 scientific publications and was inducted into the American Chemical Society's Division of Medicinal Chemistry Hall of Fame in 2009.

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Theme: Latest Global Innovations and Market Insights in Chemistry

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June 14-15, 2021

Galectin-1 therapy for use in muscular dystrophy

Pam Van Ry[1], **Mary L. Vallecillo-Zúniga**[1], **Matthew F. Rathgeber**[1], **P. Daniel Poulson**[1], **Spencer Hayes**[1], **Jacob S. Luddington**[1], **Hailie N. Gill**[1], **Matthew Teynor**[1], **Braden C. Kartchner**[1], **Jonard Valdoz**[1], **Caleb Stowell**[1], **Ashley R. Markham**[1], **Connie Arthur**[2] and **Sean Stowell**[2]

[1]*Brigham Young University, USA*
[2]*Center for Transfusion and Cellular Therapies School of Medicine, Emory University, USA*

Muscular dystrophies are a heterogeneous group of genetic diseases involving mutations in genes that compromise sarcolemma stability, muscle strength, and repair. Limb-girdle muscular dystrophy type 2B (LGMD2B) is a type of dysferlinopathy caused by mutations in the gene encoding dysferlin protein. LGMD2B is characterized by the following: diminished membrane repair, delayed removal of necrotic muscle fibers, loss of calcium sensitivity leading to signaling mis-regulation, muscle atrophy, increased inflammatory infiltrate, etc. The lack of a cure and treatment options for LGMD2B patients requires increased research to develop therapeutics. Galectin-1 (Gal-1) is a small 14.5kDa protein which can form monomers or dimers each with a carbohydrate recognition domain. Gal-1 has been proven to improve muscle repair capacity in Duchenne muscular dystrophy (DMD) models by increasing extracellular interaction resulted in healthier muscle fibers. Seeking to broaden the scope of use as a therapeutic, we chose to use this therapy in dysferlin-deficiency models postulating that rHsGal-1 would diminish disease endpoints. We found recombinant human Gal-1 (rHsGal-1) treatment promotes myogenic maturation and membrane repair capacity in both dysferlin-deficient myotubes and myofibers. Additionally, we discovered that the carbohydrate recognition domain of Gal-1 is necessary for observed membrane repair and was calcium-independent in both dysferlin-deficient and wild-type myotubes and myofibers . Similarly, one-week and one-month *in vivo* treatment with rHsGal-1 revealed significant improvement in membrane repair capability. Next, we developed several Gal-1 constructs to unravel the biologically relevant state of Gal-1 responsible for observed therapeutic befits in repair and in inflammation. We show a decrease in the canonical NF-kB pathway and modulation away from a chronic M1 macrophage phenotype with treatment. Together, our results reveal Gal-1 treatment improves membrane repair capacity, increases markers for myogenesis and decreases immune response in dysferlin-deficient models, thus indicting that Gal-1 is efficacious as a new protein treatment for LGMD2B.

Biography

Pam Van Ry is an Assistant Professor of Chemistry and Biochemistry at Brigham Young University in Provo, Utah. She is also an Assistant Director of the BYU MRI Facility. Dr. Van Ry earned her degree in Cellular and Molecular Pharmacology and Physiology at the University of Nevada-Reno in the Pharmacology Department. Her graduate investigated Laminin-111 and Galectin-1 protein therapies for different types of muscular dystrophies. Her post-doctoral work was funded by the Million Dollar Bike Ride Rare Disease Research and her current work is funded by the Jain Foundation. Dr. Van Ry's research shows evidence that Galectin-1 treatment improves membrane repair capacity, increases markers for myogenesis and decreases immune response in dysferlin-deficient models. Together her work shows that Gal-1 is efficacious as a new protein treatment for disease involving muscle repair and inflammation. Dr. Van Ry is passionate about training the next generation of researchers and medical professionals either in her lab and in her biochemistry classes.

Impact of sex hormones on brain and colon cancer

Sahar Eshghjoo[2] and **R. Ahmadi**[1]
[1]Hamedan Branch, Iran
[2]Texas A&M University, USA

Numerous studies have shown that sex steroid hormones affect cancer and non-cancer cells at cellular and molecular levels. This study aimed to investigate the proliferation effects of sex steroids on brain glioblastoma (A172), colorectal adenocarcinoma (HT29), and human embryonic kidney (HEK293) cells and Bax, Bcl-2, and KAI-1/CD82 gene expression in cell culture. Cell lines were randomly divided into control group (no exposure to hormone) and groups exposed to 0.001, 0.01, 0.1, 1, and 10 mg/ml of testosterone, progesterone, and estradiol valerate. The cytotoxic effect of the extract was measured using the MTT assay. qRT-PCR was used to evaluate Bax, Bcl2, and Kai genes expression levels.

Testosterone and progesterone indicated dose-dependent, proliferative or anti-proliferative effects on non-cancer Hek and colon adenocarcinoma cells; however, estradiol had anti-proliferative effects on Hek and colon adenocarcinoma cells. Testosterone and progesterone indicated anti-proliferative effects on brain glioblastoma cells; however, estradiol did not have proliferative or anti-proliferative effects on brain glioblastoma cells.

It can be concluded that the cytotoxic effects of testosterone and progesterone on colon cancer and brain glioblastoma cells are exerted through Bax-dependent apoptosis. Moreover, the cytotoxic effect of estradiol on colon cancer cells is exerted through Bax-dependent apoptosis. In glioblastoma cells, active anti-apoptosis induction prevents cells from cytotoxic effects of estradiol. The cytotoxic effect of testosterone on colon cancer and brain glioblastoma cells and the effect of estradiol and progesterone on brain glioblastoma cells did not trigger the anti-metastasis Kai1 gene expression. Furthermore, estradiol did not trigger anti-metastasis Kai1 gene expression; However, estradiol and progesterone exerted anti-metastasis Kai1 gene expression in colon cancer cells.

Overall, our data suggest that hormone therapy for cancer treatment is dose and cell-dependent and further studies are necessary to optimize treatments in this regard.

Biography

Sahar Eshghjoo research interests are Immunometabolism, Endocrinology, Nutritional and microbiota metabolites regulation, cell and molecular metabolism, and inflammation. Her undergraduate training first instilled her interest in diverse biomedical sciences. She worked at the International Endocrinology and Metabolism Research Institute (EMRI) in Tehran, Iran where She contributed to hormonal studies. Immediately after earning my B.Sc., She entered a Master's degree program to augment her knowledge in Medical Biochemistry. Her medical research laboratory placement was at Institute Pasteur of Iran working on "HIV Polytope vaccines loaded on Nanoparticles especially chitosan nanoparticle". After She successfully earned my M.Sc. She chose to pursue the next phase of my training in the United States. Soon after, She was recruited to join the graduate program at TAMU, where She completed her Ph.D. in Medical Sciences. She has recently started her post-doctoral training at Baylor College of Medicine in Texas Medical Center.

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Keynote Presentations
Day 2

BIOGRAPHY

Sergey Suchkov was born in the City of Astrakhan, Russia, in a family of dynasty medical doctors. In 1980, graduated from Astrakhan State Medical University and was awarded with MD. In 1985, Suchkov maintained his PhD as a PhD student of the I.M. Sechenov Moscow Medical Academy and Institute of Medical Enzymology. In 2001, Suchkov maintained his Doctor Degree at the National Institute of Immunology, Russia.

From 1989 through 1995, Dr Suchkov was being a Head of the Lab of Clinical Immunology, Helmholtz Eye Research Institute in Moscow. From 1995 through 2004 - a Chair of the Dept for Clinical Immunology, Moscow Clinical Research Institute (MONIKI). In 1993-1996, Dr Suchkov was a Secretary-in-Chief of the Editorial Board, Biomedical Science, an international journal published jointly by the USSR Academy of Sciences and the Royal Society of Chemistry, UK.

Contined next page

Sergey Suchkov
Sechenov University, Russia

Personalized and Precision Medicine (PPM) as a unique healthcare model to be set up *via* biodesign and translational applications and upgraded business modeling to secure the human healthcare, wellness and biosafety

Traditionally a disease has been defined by its clinical presentation and observable characteristics, not by the underlying molecular mechanisms, pathways and systems biology-related processes specific to a particular patient (ignoring persons-at-risk). A new systems approach to subclinical and/or diseased states and wellness resulted in a new trend in the healthcare services, namely, personalized and precision medicine (PPM).

To achieve the implementation of PPM concept, it is necessary to create a fundamentally new strategy based upon the biomarkers and targets to have a unique impact for the implementation of PPM model into the daily clinical practice and pharma. In this sense, despite breakthroughs in research that have led to an increased understanding of PPM-based human disease, the translation of discoveries into therapies for patients has not kept pace with medical need. It would be extremely useful to integrate data harvesting from different databanks for applications such as prediction and personalization of further treatment to thus provide more tailored measures for the patients and persons-at-risk resulting in improved outcomes and more cost effective use of the latest health care resources including diagnostic (companion ones), preventive and therapeutic (targeted molecular and cellular) etc.

Translational researchers, bio-designers and manufacturers are beginning to realize the promise of PPM, translating to direct benefit to patients or persons-at-risk. For instance, companion diagnostics tools and targeted

BIOGRAPHY

At present, Dr Sergey Suchkov, MD, PhD, is:

- Professor, Director, Center for Personalized Medicine, I.M.Sechenov First Moscow State Medical University and Dept of Clinical Immunology, A.I.Evdokimov Moscow State Medical and Dental University;
- Professor, Chair, Dept for Translational Medicine, Moscow Engineering Physical Institute (MEPhI), Russia
- Secretary General, United Cultural Convention (UCC), Cambridge, UK.

Dr Suchkov is a member of the:

- New York Academy of Sciences, USA
- American Chemical Society (ACS), USA;
- American Heart Association (AHA), USA;
- European Association for Medical Education (AMEE), Dundee, UK;
- EPMA (European Association for Predictive, Preventive and Personalized Medicine), Brussels, EU;
- ARVO (American Association for Research in Vision and Ophthalmology);
- ISER (International Society for Eye Research);
- Personalized Medicine Coalition (PMC), Washington, DC, USA
- All-Union (from 1992 - Russian) Biochemical Society;
- All-Union (from 1992 - Russian) Immunological Society.

Dr Suchkov is a member of the Editorial Boards of ***"Open Journal of Immunology", EPMA J., American J. of Cardiovascular Research and "Personalized Medicine Universe".***

therapies and biomarkers represent important stakes for the pharma, in terms of market access, of return on investment and of image among the prescribers. At the same time, they probably represent only the generation of products resulting translational research and applications. So, developing medicines and predictive diagnostic tools requires changes to traditional clinical trial designs, as well as the use of innovative (*adaptive*) testing procedures that result in new types of data. Making the best use of those innovations and being ready to demonstrate results for regulatory bodies requires specialized knowledge that many clinical development teams don't have. The areas where companies are most likely to encounter challenges, are data analysis and workforce expertise, biomarker and diagnostic test development, and cultural awareness. Navigating those complexities and ever-evolving technologies will pass regulatory muster and provide sufficient data for a successful launch of PPM, is a huge task. So, partnering and forming strategic alliances between researchers, bio-designers, clinicians, business, regulatory bodies and government can help ensure an optimal development program that leverages the Academia and industry experience and FDA's new and evolving toolkit to speed our way to getting new tools into the innovative markets.

Healthcare is undergoing a transformation, and it is imperative to leverage new technologies to support the advent of PPM. This is the reason for developing global scientific, clinical, social, and educational projects in the area of PPM and TraMed to elicit the content of the new trend. The latter would provide a unique platform for dialogue and collaboration among thought leaders and stakeholders in government, academia, industry, foundations, and disease and patient advocacy with an interest in improving the system of healthcare delivery on one hand and drug discovery, development, and translation, on the other one, whilst educating the policy community about issues where biomedical science and policy intersect.

BIOGRAPHY

Michael Vigdorowitsch Graduated from Moscow State Engineering Physics Institute (now National Research Nuclear University) in 1994, major in Theoretical and Mathematical Physics. Defended PhD thesis for Mathematical modeling in 1996 at alma mater and Doctor Dissertation (habilitation degree) for Physical Chemistry in 2000 at Institute of Physical Chemistry of Russian Academy of Sciences. Many years devoted to the real sector of economy. Since 2020 Principal Research Fellow at All-Russian Scientific Research Institute for the Use of Machinery and Oil Products in Agriculture and Professor of Mathematics at Tambov State Technical University. Place of residence: Düsseldorf. Areas of scientific intertest: adsorption theory, nano-materials,environmental science, epidemiological mathematics, theoretical tribology.

Michael Vigdorowitsch

Angara GmbH, Germany

Adsorbate lateral interactions at patchwise topology: The lambert overall isotherms

Taking into account the lateral interactions of the adsorbate species at a passage from a local to an overall adsorption function (AF) according to Eq. (1)

$$\Theta = \int_{-\infty}^{+\infty} \theta(\varepsilon,p)\, g(\varepsilon)\, d\varepsilon \qquad (1)$$

where θ(ε,p) and Θ(p) are local and overall AFs respectively, g(ε) is a functional distribution of adsorption centres on adsorption heat ε and p is pressure, did not appear yet to be successful for arbitrary distributions, since even one of the simplest local isotherms, Fowler-Guggenheim

$$p = \frac{1}{a(\varepsilon)} \cdot \frac{\theta(\varepsilon,p)}{1-\theta(\varepsilon,p)} \exp[-\alpha \cdot \theta(\varepsilon,p)] \qquad (2)$$

is an implicit function of pressure. For the Hill-de Boer local isotherm, some divergence of expansions on θ was reported with a general conclusion that problem (1) is analytically intractable [2]. Some approximate solutions were obtained just within the condensation approximation (CA, ACA) [1, 3].

In [4], expansions of Eq. (2) have been built which explicitly lead to sequences {θ_L^((n)) } and {θ_H^((n)) } convergent to θ as the lower and upper boundaries. The local AF (x=a(ε)p is dimensionless pressure and μ is approximation parameter) has been built:

$$\theta(x) = \begin{cases} x - \left[(\mu+2)e^{\frac{1}{2}\alpha} - \frac{3}{2}e^{\alpha}\right]x^2 + \left[(\mu+1)e^{\alpha} - e^{3/2\alpha}\right]x^3, & x < e^{-\frac{1}{2}\alpha} \\ 1 - \frac{e^{-\alpha}}{x} + \left[(\mu+2)e^{\frac{1}{2}\alpha} - \frac{3}{2}e^{\alpha}\right]\frac{e^{-2\alpha}}{x^2} - \left[(\mu+1)e^{\alpha} - e^{3/2\alpha}\right]\frac{e^{-3\alpha}}{x^3}, & x \geq e^{-\frac{1}{2}\alpha} \end{cases} \qquad (3)$$

It is asymptotically exact for both small and big p, has an intermediate reference point and, therefore, is essentially more accurate than ACA. It can be integrated in Eq. (1) with any distribution g(ε) of active centres (with gaussian s. results in Fig. 1).

Eq. (2) can be represented through the Lambert W-function [5] as

$$\theta=-1/\alpha\ W[\alpha(\theta-1)\cdot ap] \qquad (4)$$

Eq. (4) reproduces explicitly phase transitions depending on as W(x) is real at x<0 within the range -1/e<x<0 only and double-valued.

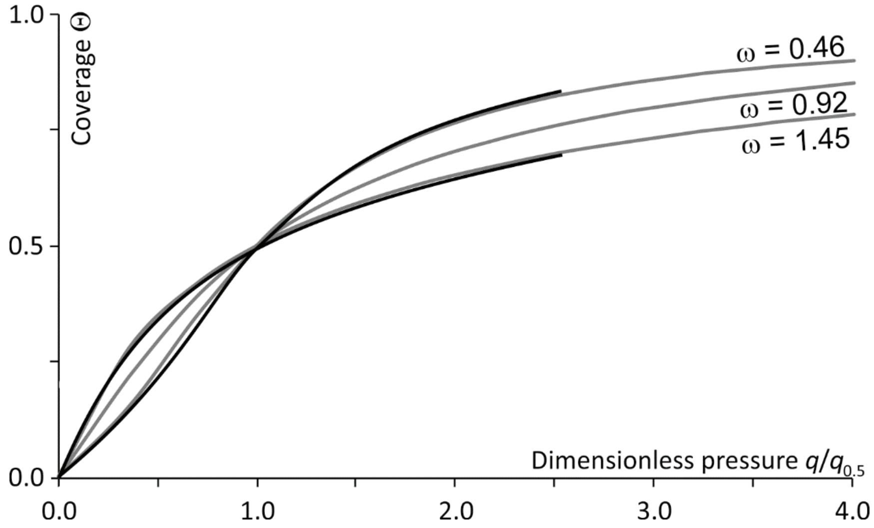

Fig. 1. Dependence of coverage on pressure. grey: analytical calculations (1), (3); black: classic computations (1964) [2] with the parameters of localised adsorption of Ar on hexagonal substrate (e.g., boron nitride) at 77.5 K corresponding to $\omega=\sigma/(kT)$ (square root from dimensionless dispersion of adsorption heat). $\Theta(q_{0.5}\approx 0.28)=0.5$ at $\alpha=2.57$, $\mu=2.6$)

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Functionalization of chitosan with β-cyclodextrin for efficient removal of aspirin

Norzita Ngadi and **Abu Hassan Nordin**
Universiti Teknologi Malaysia, Malyasia

Chitosan is a very versatile substance in terms of its usage. It has a number of uses ranging from agricultural to medicinal usage. In adsorption study, chitosan is a very promising material as it can be used to adsorb a variety of waste such as dyes, metal ions and pharmaceutical. This particular ability can be attributed to the presence of amino and hydroxyl group in its molecules. However, these reactive groups tend to form hydrogen bond with each other and greatly reduces the adsorption efficiency of chitosan. A lot of research have been done in order to improve the adsorption efficiency of chitosan. One of the methods used is by modifying the surface of chitosan with another chemical. Therefore, in this study, chitosan was modified with β-cyclodextrin by using impregnation method. This study was conducted to synthesize and characterize chitosan modified with β-cyclodextrin, to determine the adsorption performance of the adsorbent for aspirin removal. Chitosan was modified without using any harmful and hazardous chemical. The characterization of the adsorbents was conducted using Fourier transform infrared spectroscopy, point of zero charge, carbon, hydrogen, nitrogen and sulphur analysis, Field emission scanning electron microscopy and Brunauer-Emmett-Teller analysis. The maximum adsorption capacity of chitosan was 236.97 mg/g while the maximum adsorption capacity for β-cyclodextrin modified chitosan was 359.87 mg/g which is an increase of 51%. The best condition for the removal of aspirin is 10 minutes of contact time, pH 3, 30 ºC temperature, 500 mg/L initial concentration of aspirin and 0.05 g of adsorbent.

Biography

Norzita Ngadi is an Associate Professor in School of Chemical and Energy Engineering, Faculty of Engineering, Universti Teknologi Malaysia (UTM), where she has been a faculty member since 1999. She received her Ph.D. degree from University of Canterbury, New Zealand in 2010. She obtained her M.Eng in Chemical Engineering from UTM in 2002, after completion of her undergraduate study in Universiti Sains Malaysia. Her research interest includes wastewater treatment, catalytic reaction, renewable fuel and surface coating.

Functional expression of all human sulfotransferases in fission yeast, assay development, and structural models for SULT4A1 and SULT6B1

Yanan Sun[1,2], David Machalz[3], Gerhard Wolber[3], Maria Kristina Parr[2] and **Matthias Bureik[1]**

[1]Tianjin University, China
[2,3]Free University Berlin, Germany

Cytosolic sulfotransferases (SULTs) catalyse phase II (conjugation) reactions of drugs and endogenous compounds. A complete set of recombinant fission yeast strains each expressing one of the 14 human SULTs was generated, including SULT4A1 and SULT6B1. Sulfation of test substrates by whole-cell biotransformation was successfully demonstrated for all enzymes for which substrates were previously known. The results proved that the intracellular production of the cofactor 3'-phosphoadenosine 5'-phosphosulfate (PAPS) necessary for SULT activity in fission yeast is sufficiently high to support metabolite production. A modified variant of sulfotransferase assay was also developed that employs permeabilized fission yeast cells (enzyme bags). Using this approach SULT4A1-dependent sulfation of 1-naphthol was observed. Additionally, a new and convenient SULT activity assay is presented. It is based on the sulfation of a proluciferin compound, which was catalysed by SULT1E1, SULT2A1, SULT4A1, and SULT6B1. For the latter two enzymes this study represents the first demonstration of their enzymatic functionality. Furthermore, the first catalytically competent homology models for SULT4A1 and SULT6B1 in complex with PAPS are reported. Through mechanistic molecular modelling driven by substrate docking we pinned down the increased activity levels of these two isoforms to optimized substrate binding.

Biography

Yanan san presently doing her PhD in institute of pharmacy, Free University Berlin, Germany and also in School of pharmaceutical science and technology, Tianjin University, China from 09.2017-02.2020. She did her MPhil (09.2015-12.2016) from School of Pharmacy, Queen's University Belfast, UK. The Project that she did was Evaluating bioactivity of nigrocin-2-OV from the skin secretion of the Chinese bamboo leaf odorous frog, Odorrana versabilis. She also Complted her Bachelor (09.2011-06.2015) in School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, China in which her Major is Applied chemistry.

ROS production and DNA damage induced by tailored Mn-doped ZnO nanoparticles in murine fibroblast cells

Ioana Dorina Vlaicu[1], **Traian Popescu**[1], **Christien Oktaviani Matei**[2], **Ioan Tivig**[2], **Andrei Cristian Kuncser**[1], **Mariana Stefan**[1], **Daniela Ghica**[1], **Luminita Claudia Miclea**[2], **Tudor Savopol**[2], **Daniela Cristina Culita**[3] and **Mihaela Georgeta Moisescu**[2]

[1]*National Institute of Materials Physics, Romania*
[2]*Carol Davila University of Medicine and Pharmacy, Romania*
[3]*Ilie Murgulescu Institute of Physical Chemistry, Romania*

This paper reports the *in vitro* oxidative stress responses of non-malignant murine cells exposed to different surfactant-tailored ZnO nanoparticles (NPs). Two series of Mn-doped ZnO NPs have been prepared by surfactant-assisted coprecipitation method (in the presence of either polyvinylpyrrolidone (PVP) or sodium hexametaphosphate (SHMTP)). Their morpho-structural properties were were investigated by powder X-ray Diffraction, Transmission Electron Microscopy, Fourier-Transform Infrared and Electron Paramagnetic Resonance spectroscopic methods. Their textural properties in terms of specific surface area and porosity were determined by N2 adsorption-desorption analysis. Several morpho-structural and textural differences between the two series of ZnO NPs were considered when discussing the results: particle size, morphology, Mn-doping level (figure 1, left and center). cific surface area and porosity. g (figure 1, left side and center). Along with these, there were considered few other surfactant-dependent effects, like: particle size, specific surface area and porosity. The *in vitro* toxicity of the two series of Mn-doped ZnO NPs was assessed by studying the cell viability, intracellular reactive oxygen species (ROS) generation, and DNA fragmentation in NIH3T3 fibroblast cells (figure 1, right side).

The relationship between the surfactant dependent characteristics of the Mn-doped ZnO NPs and the *in vitro* toxicity responses was evaluated. There was observed a positive correlation between the specific surface area and the magnitude of the induced toxicological effects, but even so the Mn presence in the ZnO NPs exerted a protective effect on cells [1].

The conclusion of this study is that the *in vitro* toxicity of ZnO nanomaterials can be modulated by surfactant-controlled Mn-doping.

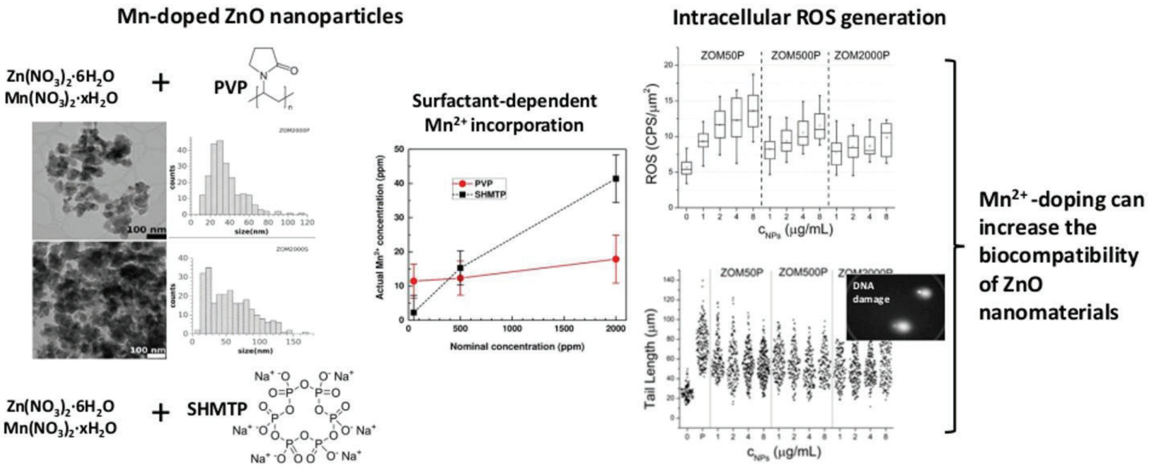


Figure 1. Morpho-structural characterization of ZnO:Mn nanoparticles and the effects induced in NIH3T3 fibroblast cells [1].

Biography

Ioana Dorina Vlaicu received her PhD (2014) in Chemistry from University of Bucharest – Faculty of Chemistry. She has ten years of experience in materials synthesis and characterization, experience gained starting as Research Assistant in 2011 at National Institute of Materials Physics, Magurele, Romania, where she is currently Scientific Researcher Rank III from 2019. Her specialization is materials chemistry and she has experience with different chemical synthesis methods for obtaining a wide range of materials for different applications (antimicrobials, optoelectronics, gas-sensors, energy harvesters, magnetism, and photocatalysis). Her portfolio contains 20 ISI papers of which 12 as principal author. All these 20 papers cumulated 144 citations (111 without self-citations) and a cumulated impact factor of ~ 65. Her interdisciplinary research results brought contributions in bioinorganic, inorganic and physical chemistry. Her scientific contributions illustrate her independent nature since she conceived and lead most of the reported studies.

Analysis of the qualitative evolution of groundwater in the Abouabou area in the Port-Bouët municipality (Abidjan, Côte d'Ivoire)

Kouassi Innocent Kouame, K. H. Konan, A. Dao, D. Noufe, J.T. K. Koffi and **B. Kamagate**
Nangui Abrogoua University, Ivory Coast

The study aimed to analyze the seasonal qualitative evolution of the Quaternary groundwater in the Abouabou area in order to see the capacity of this water to be used as a water supply by the populations. In-situ measurements (temperature, electrical conductivity, dissolved oxygen, turbidity and pH) and chemical parameter analyses (NH_4^+, Ca^{2+}, Mg^{2+}, K^+, Na^+, NO_3^-, NO_2^-, PO^{43-}, SO^{42-}, Cl^- and HCO_3^-) were performed on the 24 samples collected during the four (4) seasons of the year. The use of Kruskal-Wallis and ANOVA tests has allowed the monitoring of seasonal variations in hydro-chemical parameters in well and borehole water. Also, the Piper diagram permit to identify the main hydrochemical facies according to the seasons. Finally, the Kohonen Self Organizing Maps (SOM) method was applied to physico-chemical parameters in order to highlight the spatial distribution of groundwater quality in the Abouabou area. The results show that, based on the physico-chemical parameters analysed, the groundwater is of good quality due to meeting WHO standards for drinking water consumption during all seasons of the year. Significant seasonal variations were recorded in the values of the parameters like turbidity, pH and Cl^- for well water and turbidity, PO^{43-}, NO_3^-, NH_4^+, K^+, Cl^- for borehole water. The hydrochemical facies shows a seasonal variation. Analysis of Abouabou's water reveals the variation of its hydrochemical facies. Thus, bicarbonate, calcium and magnesium facies during the long dry and rainy seasons move towards the chlorine, calcium and magnesium facies during the short dry and rainy seasons. Four water groups have been identified using SOM method, including heterogeneous groups composed mainly of borehole water (I and III) or of well water (II and IV). Borehole and well water acquire most of their mineralization by the infiltration of surface elements. Drinking water from boreholes is of good quality.

Biography

Kouassi Innocent Kouame is a teacher-researcher and lecturer at the Nangui Abrogoua University (Abidjan, Ivory Coast). He is part of the Geosciences and Environment laboratory at the training and Research Unit of Environmental Sciences and Management. He is a specialist in Hydrogeology and Environment. He works mainly on the quality of groundwater intended for human consumption and also on the risks of groundwater contamination by anthropogenic sources of pollution.

Developments and applications of chip-based mass spectrometry in glycomics of chondroitin/dermatan sulfate oligosaccharides

Alina Diana Zamfir
National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania

Among glycosaminoglycans (GAGs), chondroitin sulfate (CS) and dermatan sulfate (DS) are found linked to a variety of proteoglycans with an extensive expression in the extracellular matrix. Since in CS/DS domains, sulfation is generated by a non-template driven process, undersulfated and oversulfated motifs also exist in nature and play major roles, including the mediation of the interactions with specific proteins, an event for which the sulfation status is a crucial determinant. The elevated structural diversity of CS/DS sequences, even within a single GAG chain, in which sulfation may occur not only at GalNAc but also at IdoA/GlcA in various combinations, triggered the development of an array of methods for their detailed analysis. Mass spectrometry (MS) with chip-based electrospray (ESI), introduced by our group in glycosaminoglycomics, demonstrated its capability to provide de novo information on CS/DS oligosaccharides, as well as on their noncovalent interactions with specific proteins. In combination with high resolution mass spectrometers or instruments able to perform multistage fragmentation of the chosen precursor ions, chip-electrospray offered a detailed structural elucidation of regularly, under- and oversulfated CS/DS domains at subpicomolar sensitivities and of minor species in complex mixtures, which very often represent valuable biomarkers. Hence, the present paper will highlight the microfluidics strategies developed by our group, which allowed a successful application of chip technology in combination with MS and fragmentation analysis by tandem MS (MS/MS) using collision induced dissociation (CID) for mapping and sequencing of CS/DS released from human decorin, biglycan and species expressed in brain tissue as well as the characterization of rare, previously undiscovered CS/DS motifs having biomarker value. The accomplishments of the developed methods in characterization of novel structures indicate that the advanced chip-based MS is also a powerful tools for early diagnosis of pathologies based on discovery of CS/DS molecular fingerprints.

Biography

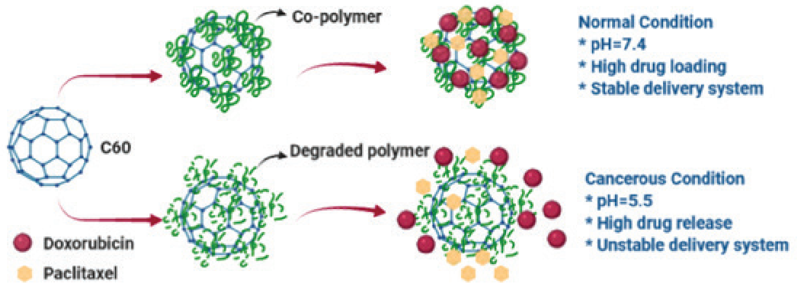
Alina D. Zamfir, PhD in Physics (2001), habilitation in Biophysics (2006), is Professor of Biophysics & Principal Investigator, Head of Biological Mass Spectrometry Group – National Institute for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania. Her research is focused on the development of novel mass spectrometry techniques implemented in glycomics. Dr. Zamfir published 114 articles (WOS) in prominent journals such as Angewandte Chemie, Lab Chip, Analytical Chemistry, Analyst, Analytical and Bioanalytical Chemistry, Glycobiology, Journal Am. Soc. Mass Spectrom., Biophysica and Biochimica Acta, Biochimie, Electrophoresis, Amino Acids, Carbohydrate Research, Analytical Biochemistry etc., which collected so far over 2200 citations, Hirsch index 28 and prestigious prizes. Dr. Zamfir and her group gave over 350 presentations at international scientific meetings held all over the world and published 15 book chapters with international publishing houses (Humana Press, Springer, Wiley, Elsevier, RSC, CRC Press etc).

Novel pH-responsive nanohybrid for simultaneous delivery of doxorubicin and paclitaxel: An *in-silico* insight

Mohammad Dahri[1,2]
[1]Computational Biology and Chemistry Group (CBCG), Iran
[2]Universal Scientific and Education and Research Network (USERN), Iran

Background: The distribution of drugs could not be controlled in the conventional delivery systems. This has led to the developing of a specific nanoparticle-based delivery system, called smart drug delivery systems. In cancer therapy, innovative biocompatible nanocarriers have received much attention for various ranges of anti-cancer drugs. In this work, the effect of an interesting and novel copolymer named "dimethyl acrylamide-trimethyl chitosan" was investigated on delivery of paclitaxel and doxorubicin applying carboxylated fullerene nanohybrid. The current study was run via molecular dynamics simulation and quantum calculations based on the acidic pH differences between cancerous microenvironment and normal tissues. Furthermore, hydrogen bonds, radius of gyration, and nanoparticle interaction energies were studied here. Stimulatingly, a simultaneous pH and temperature-responsive system were proposed for paclitaxel and doxorubicin for a co-polymer. A pH-responsive and thermal responsive copolymer were utilized based on trimethyl chitosan and dimethyl acrylamide, respectively. In such a dualistic approach, co-polymer makes an excellent system to possess two simultaneous properties in one bio-polymer.Results: The simulation results proposed dramatic and indisputable effects of the copolymer in the release of drugs in cancerous tissues, as well as increased biocompatibility and drug uptake in healthy tissues. Repeated simulations of a similar article performed for the validation test. The results are very close to those of the reference paper.

Conclusions: Overall, conjugated modified fullerene and dimethyl acrylamide-trimethyl chitosan (DMAA-TMC) as nanohybrid can be an appropriate proposition for drug loading, drug delivery, and drug release on dual responsive smart drug delivery system.



Biography

Mohammad Dahri was born in Tabriz, Iran at 1996. He is a doctor of Pharmacy and nanobiotechnology researcher. He got his PharmD from Shiraz University of Medical Science, one of the top medical universities in Iran.

Gender justice in the energy transition era: Exploring gender and technology in the extractives sector

Kennedy Chege and **Alaka Lugonzo**
University of Cape Town (UCT), South Africa

The world of technology is transitioning fast as a result of the so-called 4th Industrial revolution (referred to henceforth as "the 4IR") or digital revolution. This digital revolution is not only making fundamental changes to how we live, but it is also having a profound impact on how we conduct business. The global market is adapting to new trends and faster turnaround times, and all sectors, including the energy and extractives sector (oil and gas, and mining sectors), will be forced to adapt to the transition. This change aligns with the clean energy developments and the global transition to a low carbon economy, which is characterized by technological advancements.

The world is gradually discovering new things to do with technology, as its potential is beginning to be embraced. The present COVID-19 pandemic, for example, has altered the way we use technology, with many people spending more time online, thus creating the impetus to fast track the implementation of the 4IR. These changes will affect gender inclusivity and the future of work.

Apart from the above issues, this chapter examines the following aspects: why it is essential to include women in the workforce and along the different value chains, the need for automation in the extractives sector, and how it will affect the way that we work. Lastly, the proposed solutions to address the challenges of gender disparity and to promote inclusivity in the energy and extractives sector will be explored from the perspectives of the different role players in this sector, i.e. the public sector/governments; the private sector (including business entities); and Non-Governmental Organisations (NGO's).

Biography

Kennedy Chege is a Researcher and PhD Candidate at the NRF/DST SARChI: Mineral Law in Africa (MLiA) Research Chair at the University of Cape Town (UCT). His responsibilities at the Chair include: coordinating the programme for the Specialized LLM in the Law of Mineral and Petroleum Extraction and Use, lecturing in the courses under this programme; supervising LLM theses; participating in the research functions of the Chair, etc. For his Masters of Laws (LLM) Degree, he majored in Commercial Law, coupled with Mining Law. He also holds a Bachelor of Laws (LL.B) Degree, and a Bachelor of Social Sciences (BSocSc) Degree, majoring in Public Policy and Administration. Kennedy is also a practitioner at ENSafrica law firm in the Business Development Department, dealing with matters relating to Mineral & Mining Law, Energy Law, Competition/Antitrust Law, general corporate and commercial work, and other areas of law. Additionally, Kennedy is also in the Management Committee of the African Energy and Mining Management Initiative (AEMI), assisting with projects in both South Africa and Kenya, including: the Mentorship Programme, Legal Aid Programme, Women in Energy & Mining Empowerment Programme, and the Knowledge Centre Programme.

New high throughput reactor for biomass valorization

Julien Thiel[1], **Irene Malpartida**[1,2], **Pedro Maireles-Torres**[2], **Valentin Lair**[1], **Samy Halloumi**[1] and **François Lacoste**[1]

[1] *Deasyl S.A., Switzerland*
[2] *Universidad de Málaga, Spain*

The development of an innovative and sustainable high-throughput reaction platform allows optimizing a wide range of chemical processes (materials synthesis and catalysis, among others) to tackle the Green Deal. This tool unifies, for the first time, the benefits of mechanical energy, thermal and pressure activation in continuous flow with an induction *in situ* heating system, facilitating the incorporation of inputs (liquids, solids and gases) with controlled pressure. As a result of the synergistic effect of this simultaneous activation, this technology will: (i) shorten reaction times; (ii) decrease temperature; (iii) improve reactions kinetics as mass transfer limitations are reduced; (iv) minimize the use of solvents; (v) decrease the reaction steps; (vi) increase the volume treated, enabling a real scale-up; and (vii) enhance the yields and/or selectivity. This new high-throughput reactor is used for the synthesis of calcium diglyceroxide (CaDG), minimizing the reaction steps and cost, to obtain a pure CaDG. This heterogeneous catalyst is used for biodiesel production and valorization of the glycerol generated as a by-product. An efficient synthesis protocol of CaDG has been developed, requiring shorter time, without heating, and no need for a solvent. This new process facilitates oil–methanol mixing in the transesterification process, thus minimizing the mass transfer limitations associated with the immiscibility of reactants. In addition, this process has been optimized by using CaDG as a solid catalyst.

Biography

Julien Thiel is an Executive MBA graduate with analytical skills and demonstrated leadership. Recognized for excellent communication, problem solving, and teamwork skills. Known as a quick learner, with a keen eye for details; capable of analyzing issues and their implications and implementing solution. With strong entrepreneurial experience, CEO of Deeptech Startup with Easyl France and Deasyl Switzerland dedicated to provide cutting edge solutions for green chemistry and storage of renewable energies.

Approaching multimodal analyses with high repetition-rate laser-induced plasma and associated strategies for complex data processing

Yi You[1], **Boyang Xue**[1,2], **Andreas Bierstedt**[1] and **Jens Riedel**[1]
[1]Federal Institute for Materials Research and Testing (BAM), Germany
[2]Qilu University of Technology (Shandong Academy of Sciences), China

The use of high-power laser irradiation to generate elemental emitters has been well established into a systematic method, termed laser-induced breakdown spectroscopy or LIBS. While the repetition rates (rep.-rates) at 10-100 Hz are most commonly used, the advances in solid-state lasers offer an alternative route to achieve LIBS measurements at much higher rep.-rates, e.g., 20 kHz. A most straightforward expectation from the higher rep.-rate is the improved statistical validity by accumulating orders of magnitude more spectra per unit time compared to the low rep.-rate regimes; this resembles a linear response system of spectral emissions with respect to rep.-rates. However, experimental results suggested that example analytes were detected in a non-linear fashion if the laser rep.-rate exceeds a certain threshold. In our initial tests with the high rep.-rate laser-induced plasma (LIP) for underwater elemental detections, typical LIBS spectra that reflect the dissolved ions in water were yielded below a threshold rep.-rate of 8.5 kHz. However, rep.-rates higher than this threshold resulted in an additional type of spectra that contain emissions only stemming from water. Despite the interesting formation mechanism of H and O emitters in the high rep.-rate regime, the distinctive signal response of each spectral channel to the rep.-rate allows more flexible uses of LIP. Following the concept of correlation spectroscopy, it becomes possible to differentiate continuum emissions from elemental signals even if these are superimposed in the same spectral channel when the laser rep.-rate is modulated.

In this presentation, we will demonstrate continuum background removal through laser rep.-rate modulation without temporal gating. Associated workflow and algorithms will be presented, which exploit the information encoded in the rep.-rate domain for spectral reconstruction. In addition to elemental detection as conventional LIBS, the use of LIP as an ionization source for molecular detection through mass spectrometry will also be explored, where LIP modulations reveal the unique physiochemical properties of analytes.

Biography

Yi You hails from Shandong province in China. In 2010, Yi joined the Department of Chemistry and Biochemistry at Kent State University, U.S., to pursue his Ph.D. in atmospheric physics and chemistry. Yi's engineering background lead to his initial research endeavors focused on mass-spectrometer interface developments for atmospheric chemicals and associated data processing strategies. In 2014, Yi joined Prof. Jacob T. Shelley's research group as a Ph.D. candidate, orienting at novel hardware, software, and workflows for correlation mass-spectrometric methods. After Yi received his Ph.D. in 2017, he joined Dr. Jens Riedel's group at BAM as an Adolf-Martens Postdoctoral Fellow focusing on laser-based mass spectrometry and optical emission spectroscopy for multimodal analyte detections, as well as mass/optical spectral reconstructions through simultaneous orthogonal detections. Currently, Yi serves as an independent research scientist, pursuing his paths on instrument developments for molecular/elemental detections, phase-imaging techniques, and incorporating ultrasound into various analytical techniques.

Back to Nature: Combating *Candida albicans* biofilm, phospholipase and hemolysin using plant essential oils

Basem Mansour[1], **Ahmed M. El-Baz**[1], **Rasha A. Mosbah**[2], **Reham M. Goda**[1], **Taranum Sultana**[3], **Tanya E. S. Dahms**[3] and **Amira M. El-Ganiny**[4]

[1]Delta University for Science and Technology, Egypt
[2]Zagazig University hospitals, Egypt
[3]University of Regina, Canada
[4]Zagazig University, Egypt

Objectives: *Candida albicans* is the causative agent of fatal systemic candidiasis. Due to limitations of antifungals, new drugs are needed. Materials and method; The anti-virulence effect of plant essential oils (EOs) was evaluated against clinical *C. albicans* isolates including cinnamon, clove, jasmine and rosemary oils. Biofilm, phospholipase and hemolysin were assessed phenotypically. EOs were evaluated for their anti-virulence activity using phenotypic methods as well as scanning electron microscopy (SEM) and atomic force microscopy (AFM). Results; Among the *C. albicans* isolates, biofilm, phospholipase and hemolysins were detected in 40.4, 86.5 and 78.8% of isolates, respectively. Jasmine oil showed the highest anti-biofilm activity followed by cinnamon, clove and rosemary oils. SEM and AFM analysis showed reduced adherence and roughness in the presence of EOs. For phospholipase, rosemary oil was the most inhibitory, followed by jasmine, cinnamon and clove oils, and for hemolysins, cinnamon had the highest inhibition followed by jasmine, rosemary and clove oils. A molecular docking study revealed major EO constituents as promising inhibitors of the Als3 adhesive protein, with the highest binding for eugenol, followed by 1,8-cineole, 2-phenylthiolane and cinnamaldehyde. Conclusion; EOs have a promising inhibitory impact on Candida biofilm, phospholipase and hemolysin production, hence EOs could be used as potential antifungals that impact virulence factors.

Biography

Basem A. Mansour was born in 1973, in Dikirness, Daqahlya, Egypt. He is lecturer of pharmaceutical organic chemistry, faculty of pharmacy, Delta University for Science and Technology, Gamasa 11152, Egypt. He has got his B.Sc. in May 1996 from faculty pharmacy, Mansoura University, Egypt. Conferred his Master degree in Pharmaceutical Organic Chemistry at the same college in March 2014. Master thesis was entitled "Design and synthesis of novel benzimidazoles of potential anthelmintic activity". Enrolled to PhD program since 2014 through now at the same department he had granted his master from. PhD thesis entitled "Synthesis of certain Quinoline derivatives as antitumor agents".

Identification and characterization of volatile allosteric antagonists of mosquito odorant receptors

Georgia Kythreoti[1], **Nadia Sdralia**[1], **Panagiota Tsitoura**[1,4], **Dimitrios P. Papachristos**[2], **Antonios Michaelakis**[2], **Vasileios Karras**[2], **Stefan Schulz**[3] and **Kostas Iatrou**[1]

[1]National Centre for Scientific Research "Demokritos", Greece
[2]Benaki Phytopathological Institute, Greece
[3]Technische Universität Braunschweig, Germany
[4]Hellenic Pasteur Institute, Greece

Odorant-dependent behaviors in insects are triggered by the binding of odorant ligands to the variable subunits of heteromeric olfactory receptors. Previous studies have shown, however, that specific odor binding to ORco, the common subunit of odorant receptor heteromers, may allosterically alter olfactory receptor function and profoundly affect subsequent behavioral responses. We will report on the identification and characterization of several antagonists of the odorant receptor co-receptor of the African malaria vector Anopheles gambiae, AgamORco, in a small collection of natural volatile organic compounds (VOCs) using a relevant insect cell-based screening platform. The identified antagonist hits act as strong repellents against Aedes albopictus mosquitoes, which are capable of vectoring a number of infectious agents. Binding competition assays reveal the existence of othosteric and allosteric binding sites relative to a known agonist binding site. Specific binary and ternary combinations of orthosteric and allosteric antagonists produce increased inhibition of ORco function and enhanced behavioral effects *in vivo*. Evidence is also presented suggesting that the effects of the examined antagonists on Orco function are additive rather than synergistic. These findings demonstrate that a simple screening assay may yield new possibilities for enhanced indoor and outdoor protection against mosquito-borne infectious diseases and novel insights concerning the molecular aspects of receptor function.

Biography

Georgia Kythreoti graduated with first class honours from the Department of Chemistry, University of Manchester, from where she also acquired Doctor of Philosophy title in Molecular Biology. Her collaboration with DSM Anti-Infectives, during her PhD, and her brief stay at Mundipharma Pharmaceuticals thereafter, as a Quality Assurance senior officer, provided her with a spherical view of drug development and pharmaceutical market needs. Returning to research, at NCSR "Demokritos", she has integrated this perspective towards investigating, for example, "green" pathways for the synthesis of small bioactive molecules, and their subsequent biological activity. Her scientific interests involve incorporating a chemical approach towards understanding biological processes and the molecular characterization of biological macromolecules. Investigating how small molecules bind to their targets, in both prokaryotic and eukaryotic systems, in order to design novel affinity binding detection methodologies. Comprehending their mechanism of action and subsequent binding effects, as an aspect of designing new therapeutic agents.

How to stop climate change?

Karmen Margeta[1], **Zvonimir Glasnovic**[2] and **Nataša Zabukovec Logar**[3]

[1,2]University of Zagreb, Croatia
[3]National Institute of Chemistry, Slovenia

Humanity has become aware of the threat of climate change, but still does not know how to stop it. The policy resulting from the Paris Agreement, even after five years does not give results as global temperatures increase rapidly. In 2020, according to WMO data, it was 1.2 (± 0.1)°C, while the same source, for 2024, predicts reaching as much as 1.5°C! This alarming situation requires an urgent change in existing policies; which were predominantly set by economists (all with the intention of sustaining economic growth); into a completely new policy, based on technological solutions that will be able to realize the world's sustainable energy system and thus stop climate change because otherwise climate collapse is quite certain. The new climate agreement, which the authors called Climate New Deal, would be based on a top-down principle, and its application would be strictly binding for all countries. This new policy would be based on the criterion of fair distribution of the burden of climate care, both to developed and underdeveloped countries, with a deadline for its implementation by 2050. Special attention was paid to the radically new technology Seawater Steam Engine (SSE), as the most powerful "weapon" in the fight against climate change, which can simultaneously produce energy and drinking water. The problem of drinking water supply in the near future will be even greater than the problem of energy. SSE technology can also solve the problem of energy and drinking water storage, which enables the construction of sustainable cities/settlements. The authors of this paper will present the dynamic process of stopping climate change by 2050 (Figure 1) and analyse the management of possible risks. Saving the climate must become a priority for the survival of humanity.

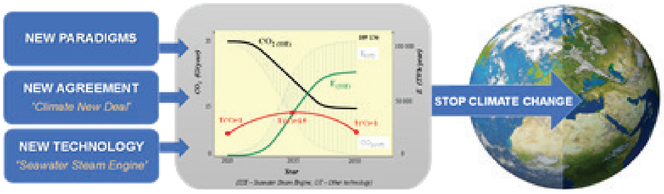


Fig.1. The dynamic process of stopping climate change by 2050

Biography

Karmen Margeta is Senior Scientist, received B.Sc., M.Sc. and Ph.D. degree in chemical engineering from University of Zagreb, Croatia. She has been working at the University of Zagreb in the field of water treatment and zeolite nanomaterial. She is expert in the field of chemical (analytical) testing and testing of the environment (water, air, soil, waste). She is involved in applied research related to the material science for energy technologies, desalination systems and water treatment technologies. She has published extensively and presented numerous papers on these topics. 2017 she published a book titled "Seawater Steam Engine as a 'prime mover' for the third industrial revolution", which technology is a scientific and technological breakthrough for stopping climate change. She has an international patent in this area.

Design, synthesis, Double effect as antimicrobial anti-inflammatory and molecular docking of some new thienopyrimidinone glycosides derivatives

Nesrin M. Morsy, Khadiga M. Abu-Zied , Ahmed S. Aly and **Abdelbaset M A Elgamal**
National research Centre, Egypt

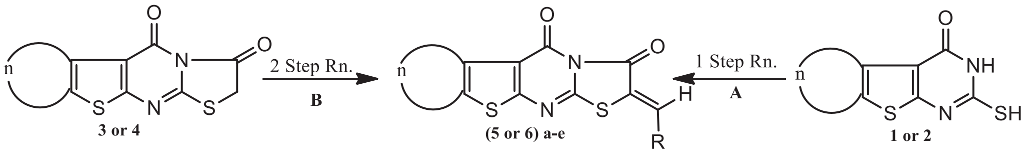
A novel series of thienopyrimidinone glycoside derivatives 5 or 6 a–e were synthesized from the reaction of 2-mercapto-2,3,6,7-tetrahydro-1*H*-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4(5H)-one (1) and 2-mercapto-2,3,5,6,7,8-hexahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(1H)-one(2) in the presence of chloroacetic acide, and pyridine/ piperdrine mixture(1:1) or 7,8-dihydrocyclopenta[4,5]thieno[2,3-d]thiazolo[3,2-a]pyrimidine-3,5(2H,6H)-dione (3) and 6,7,8,9-tetrahydro-2H-benzo[4,5]thieno[2,3-d]thiazolo[3,2-a]pyrimidine-3,5-dione (4) in the presence of absolute ethanol and triethyle amine (as a catalyst) with different aldo sugars either hexoses or pentoses. Based upon nuclear magnetic resonance (NMR), infrared (IR), and mass spectra. the structure of the newly obtained derivatives were elucidated. The target compounds 5 or 6 a–e were screened against 7 pathogenic bacteria followed by measurement of Minimum Inhibitory Concentration (MIC) and the results were very close to Gentamycin which was used as a standard , also all products were investigated against *Trichophyton schoenleinii* which is a fungus and some of the investigated compounds showed very good results when compared with the standard drug Amphotericin B, also we measured the MIC for these compounds . Docking studies were done on three compounds with height Inhibition zone and low minimal inhibitory concentration for bacteria and fungus. In our study we discover the anti-inflammation effect of these compounds where 14 samples were submitted for evaluation of their anti-inflammatory activity against Lipoxygenase “LOX”,cyclooxygenase “COX 1” cyclooxygenase “COX 2” and membrane stabilization. The results confirm high anti-inflammatory action for samples which is very nearest to standards. The tested samples have dual action as anti-microbial and anti-inflammatory agents, molecular docking study was also made as antimicrobial and anti-inflammatory agents give high indicators for the high activity of the samples.

Biography

Nesrin Mahmoud Morsy is an associate professor at National Research Centre, Organometallic and Organometalloid Chemistry Department , Cairo, Egypt. She had her Ph. D degree on advanced Organic Chemistry. She worked for 6 years ago at Collage of science and She was the head of chemistry department (girls branch), Al jouf University, KSA. She is interested in heterocyclic synthesis and applied chemistry. She has a number of International publications and books. She passed a lot of scientific workshops and training courses and still working in the field of research to discover new organic compounds with valuable biological applications.

The anti-inflammatory effect of the samples comparative to the standard

Parameter Samuels	Lipoxygenase LOX	Cyclooxygenase COX1	Cyclooxygenase COX2	Membrane stabilization
1	1.6	10.7	12.4	15.9
2	1.7	11..2	13.7	19.8
3	1.6	12	14.2	18.4
4	1.8	11.7	13.9	19.6
5	1.6	11.3	13.7	19.8
6	1.7	10.8	12.9	17.5
7	1.8	11.2	12.8	19.2
8	1.9	12.1	13.1	18.7
9	1.1	11.9	13.8	18.9
10	1.7	10.8	13.5	18.2
11	1.5	11.5	13.2	17.5
12	1.7	11	12.9	16.2
13	2.4	19	21	16.9
14	5	22	25	15.2
ST	1.5	10.2	12.7	14.3
	Ibuprofen	Ibuprofen	Ibuprofen	Indomethacin



No.	$n(CH_2)$
1	3
2	4
3	3
4	4
5	3
6	4

R=aldo-sugar(Hexsoses or Pentoses)

Scheme (1): Synthesis of New Thienopyrimidinone Glycosides Derivatives 5 or 6 a-e

The effect of zirconia phase structure on the production of lower olefins via fischer-tropsch

Cemile Dut[1,2], **G. Behmenyar**[2], **A.Z. Turan**[2] and **H.E. Figen**[1]
[1]Yıldız Technical University, Turkey
[2]TÜBİTAK Marmara Research Center, Energy Institute, Turkey

Production of lower olefins via Fischer-Tropsch (FT) reaction is a very favorable research topic due to the need of finding alternative pathways rather than conventional refinery processes. While iron-based species are generally regarded as the most promising active sites for FT reaction, support selection greatly affects the reaction mechanism and so the final product distribution. In this direction, this study focuses on the investigation of the effects of different zirconia structures to be used as catalyst supports on FT performance.

All catalysts were prepared via iron nitrate impregnation of different commercial zirconia supports namely, monoclinic (MC) and tetragonal (TG) zirconia, followed by drying, calcination and reduction. Catalytic activity was measured in a fixed bed test rig, while samples were subjected to XRD for characterization. As a preliminary investigation, different impregnation solvents (ethanol, water) were used, where the resulting catalysts exhibited similar performance. Next, a series of catalysts were prepared to explore the effect of calcination (450-750°C) and reduction (400-500°C) temperatures. No significant change in catalytic performance was observed at different reduction temperatures for the studied range. On the other hand, calcination temperature was found to be determinant in catalytic activity. Best CO conversion rates were obtained at 750°C calcination for MC and 550°C calcination for TG. In the final stage a parametric study (T=300-340°C; P=10-20 bar) was carried out using catalysts prepared at their optimum calcination temperatures already determined. Generally, the catalytic activity of TG was found to be better than that of MC, which suggests that structure of TG is more favorable for FT. XRD analysis showed that there is no significant tetragonal-to-monoclinic transformation in the studied range. Temperature and pressure affected CO conversion and olefin:paraffin ratio significantly. The optimum catalyst-operation pair considering a trade-off between better activity and better olefin production rate was found to be "TG-300°C-20 bar".

Biography

Cemile Dut is MSc. Chemical Engineering student at Yildiz Technical University and a MSc. Research Fellow at TUBITAK Marmara Research Center (MRC). Her main research interest is catalyst synthesis especially for the development of alternative fuel/chemical production methods. She currently works at Energy Institute of MRC within a project on the development of catalysts for the production of light olefins from synthesis gas, financial support of which is gratefully acknowledged (Project No: 5182102).

Enhancing the affinity of screen-printed carbon electrodes (SPCEs) towards nitrate and nitrite detection with metallic oxide nanopowders

Alexandru Florentin Trandabat[1], **A. Arcire**[2],
L.R. Popescu[3] and **R.E. Scutariu**[4]

[1,2]S.C. Intelectro Iasi SRL, Romania
[3,4]National Research and Development Institute for Industrial Ecology ECOIND, Romania

Exposure to nitrate/nitrite is associated with health effects such as methemoglobinemia, increased heart rate, and nausea. Some studies also suggest an increased risk of cancer, especially gastric cancer [1,2]. We are focusing here on a facile manufacturing method needed for mass production of these sensors able to detect toxicity threshold limits. Electrochemical sensors based on screen-printed Carbon electrodes (SPCE) have been used with success in electroanalysis, offering low-cost, precise, sensitive, rapid, quantitative information and laboratory equivalent results for *in situ* analysis [3-7]. In this paper, SPCEs were manufactured by screen-printing of multi-walled carbon nanotubes (MWCNT) ink on a flexible polymer substrate and dried at 90°C for 30 min. A 0.1 g of FeO_4 and ZnO nanopowder was dispersed in 100 mL of DMF and ultrasonicated for 120 min. A 1.5 uL of freshly made dispersion was drop cast on each sensor (on the active area of the working electrode) and dried at 55 C for 30 min. Electrochemical activation of the SPCE consisted of 25 repetitive voltammetric cycles at 10 mV s^{-1} in phosphate buffer (pH 7). SPCEs were modified with $Fe3O_4$ and ZnO nanoparticles to enhance the affinity of the sensor towards the analytes, all substances being commercially available. The modified sensors were investigated by differential pulse voltammetry (DPV) and square wave voltammetry (SWV), which proved to be much more efficient methods than cyclic voltammetry when comparing the electrochemical signal. Results showed that via DPV sensors modified with ZnO nanoparticles exhibited a stronger reaction to NO_2, while through SWV sensors modified with $Fe3O_4$ nanoparticles were more active in the presence of NO_3. Compared to the bare sensor, SPCE modified with metallic oxide manifested stronger clearer peaks. Sensor calibration showed good linearity with $R^2=0.9863$ for NO_3 and $R^2=0.9852$ for NO_2. For NO_2 LoD was $4x10^{-4}$M/l and for NO_3- 1x10-^{4}M/l, respectively.

Acknowledgment: All this work was realized with the support of Operational Programme Competitiveness 2014 - 2020, Project ID P_40_300, SMIS 105581, Subsidiary Contract 07563/2020.

Biography

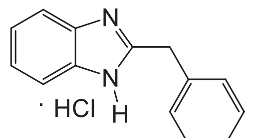
Alexandru Florentin Trandabat is the director of research department of S.C. Intelectro Iasi SRL, Romania.

Synthetic search of hemostimulators in a family of novel 3,5-Diarylidenepiperidin-4-one derivatives

Koshetova Zhanargul Abdrakhmanovna[1,3], **Yu V.K**[1], **Malmakova A.Ye.**[1,3], **Baktybayeva L.K**[2] and **Daulet G**[3]

[1]A.B. Bekturov Institute of Chemical Sciences, Kazakhstan
[2]Al-Farabi Kazakh National University, Kazakhstan
[3]Kazakh National Women's Pedagogical University, Kazakhstan

Introduction: Coronavirus infection has changed the life of the entire planet in general and each person in particular. COVID-19 is dangerous by the development of bilateral pneumonia and acute respiratory failure. The need to search for drugs for the treatment of immune diseases and diseases associated with the state of the immune system - infectious and oncological is extremely urgent [1,2].



Dibazol

The stimulus for conducting pharmaceutical screening for hematopoiesis stimulation of triazabicyclic structures with a required N-alkoxyalkylpiperidine fragment was the discovery of immunostimulating activity in 1-(2-ethoxyethyl) piperidine derivatives [3]. In addition, our attention was attracted by the diazol molecule, which increases resistance to oxygen starvation, poisons and some infections. It turned out that diazol activates the production of its own interferon in the presence of viruses or other respiratory infection, and also stimulates the production of antibodies after vaccinations.

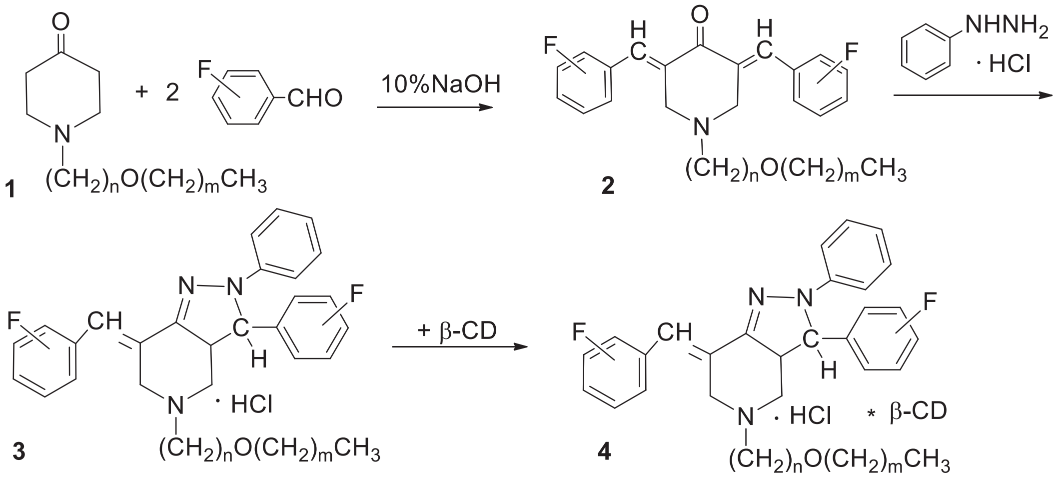
Objectives: We assumed that a preparatively simply obtained pyrazine-piperidine molecule with an N-alkoxyalkylpiperidine residue is quite "close" in structure to dibazol by the presence of a five-membered ring with two nitrogens. The synthesis and pharmacological evaluation of a family of new fluorinated pyrazine-piperidines became the goal of the study.

Used Methods: The synthesis of the target molecules had been carried out sequentially - via the Claisen-Schmidt reaction N-alkoxyalkylpiperidin-4-ones had converted into α,β-unsaturated derivatives, followed by cyclization of the latter with phenylhydrazine.

Hemostimulation studies in comparison with methyluracil had been carried out on white rats. Hemosuppression was induced by the cytostatic injection - sodium cyclophosphamide. The blood analysis had been carried out on the analyzer for laboratory animals "Abacus junior vet".

Results and Discussion: Under the action of fluorobenzaldehydes on 1-(N-alkoxyalkyl)-4-oxopiperidine (1) in the presence of alkali in a 2: 1 ratio, dienones (2) had been formed in 50-61% yield. Cyclization of the latter with phenylhydrazine leaded to pyrazine-piperidines (3) (40-55%).

In the IR spectra of dienones (2) were identified the C=O bands at 1667-1679 cm-1, as well as conjugated C=C bonds (1450-1509 cm^{-1}). The C=N band in (3) is observed at 1609-1614 cm-1. The absorption at 1190-1193 cm^{-1} is attributed to the C-F bond in 2 and 3. In the 13C NMR spectrum, the carbon C=O signal is observed at 186-188 ppm (2), while imine carbon resonates at 154-155 ppm (3). The carbon signal adjacent to F is a doublet at 161-164 ppm.



It turned out that β-cyclodextrin complexes of pyrazine-piperidines (4) exhibited an activity greater than or equal to the action of methyluracil, stimulating leucopoiesis, erythropoiesis, and thrombocytopoiesis. Acute toxicity (4) ranges from 250 to 500 mg/kg.

Conclusion: Novel fluorine-containing triazabicyclic structures with an obligatory N-alkoxyalkylpiperidine moiety with stimulate hematopoiesis had been synthesized.

Biography

Koshetova Zhanargul Abdrakhmanovna graduated from 2001-2005 - By the decision of the State Attestation Committee of Kazakh State Women's Teacher Traininig University awarded the degree of Bachelor of Science on 030340 –Chemistry and biology. 2005-2007 - By the decision of the State Attestation Committee of Kazakh State Women's Teacher Traininig University awarded the degree of Master of Chemistry Sciences on 6M060600 –Chemistry. 2018-2021 - By the decision of the competitive commission of the Ministry of Education and Science of the Republic of Kazakhstan dated on August 25, 2018 No. 696, the PhD degree in the specialty 6D060600-Chemistry was adopted. She has published more than 25 papers.

Labor activity:

2007-2008 Kazakh State Women's Teacher Training University, Faculty of Natural and Geographical Sciences, Senior Lecturer of Biology Department. (Almaty);

2008-2011 Kazakh State Women's Pedagogical University, office registrar of the natural-geographical faculty. (Almaty.);

Since 2012 Kazakh State Women's Pedagogical University, Senior Lecturer, Department of Chemistry (Almaty).

Febrary 2019 - at this time – engineer at Institute of Chemical Sciences named after A.B. Bekturov.

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Glycolipidomics of human brain hemangioma by high resolution multistage mass spectrometry

Raluca Ica[1,2], **Mirela Sarbu**[1], **Cristian V.A. Munteanu**[3] and **Alina D. Zamfir**[1,4]

[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania
[2]West University of Timisoara, Romania
[3]Institute of Biochemistry of the Romanian Academy, Romania
[4]"Aurel Vlaicu" University of Arad, Romania

Hemangioma is most commonly diagnosed by routine magnetic resonance imaging, specific detection can be accomplished by gradient-echo sequence MRI that is able to unmask small lesions that may otherwise remain undetected. A modern alternative is the early detection of hemangioma at an incipient stage, based on routine screening and biomarker discovery before manifestation of clinical symptoms. In the present study, we have optimized nanoESI Orbitrap MS and MS/MS for the discovery and characterization in human brain hemangioma of the biomarkers in the class of sialylated glicosphingolipids, known as gangliosides [1-3].

The native ganglioside mixture was extracted and purified from a hemangioma specimen. The tumor, located in the right hemisphere of the frontal cortex in an adult male patient, was removed by surgery. For MS analysis the sample were dissolved in methanol up to final concentration of 5 pmol/μL and subjected to high resolution (HR) nanoESI Orbitrap MS and HCD MS/MS in the negative ion mode for screening and sequencing. The product ion spectra were combined over scans acquired at variable collision energy within 35-65 eV range.

Following the exact mass calculation the total number of 62 ions identified in the sample mass spectrum were assigned to 52 distinct ganglioside species. Of these, one structure was found asialylated, belonging to the GA1 class, 14 monosialylated, of which eight GM1, one GM2, four GM3 and one GM4. The detailed fragmentation analysis performed by CID tandem MS provided information of structural elements related to the glycan core and ceramide moiety, which confirmed the molecular configuration of GD3 (d18:1/24:1) and GD3 (d18:1/24:2) species with potential biomarker role.

In conclusion, HR MS revealed that hemangioma is characterized by gangliosides of short glycan chains and reduced number of Neu5Ac residues, while MS^n provided data useful in structure elucidation and isomer identification in hemangioma ganglioside mixture.

Biography

Raluca Ica (b. 1983) obtained the BSc in Physics (2005), MSc in Optical and Spectroscopy of the LASER Materials (2007) and BSc in Physics-Informatics (2018). Since 2019 she is enrolled as a PhD student in Physics (supervisor Prof. Alina Diana Zamfir) at West University of Timisoara, Faculty Physics, thesis title ''Development of high-resolution spectrometric methods for the analysis of biomolecules with application in biophysics and biomedicine''. Mrs. Ica authored so far 4 articles in high impact factor journals, 1 book chapter and disseminated her results in 27 presentations at prominent international conferences held in Europe and USA.

Ion mobility mass spectrometry reveals the complexity of ganglioside structures expressed in human cerebrospinal fluid

Mirela Sarbu[1], **D.E. Clemmer**[2] and **A.D. Zamfir**[1,3]

[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Romania
[2]Indiana University, United States of America
[3]"Aurel Vlaicu" University of Arad, Romania

The proximity of cerebrospinal fluid (CSF) with the brain, its permanent renewal, and better availability for research than tissue biopsies, as well as ganglioside (GG) shedding from brain to CSF, impelled lately the development of protocols for the characterization of gangliosides and discovery of central nervous system (CNS) biomarkers expressed in CSF. Here, we have implemented for the first time ion mobility separation mass spectrometry (IMS MS) for the exploration of human CSF gangliosidome, to generate the first robust mass spectral database of CSF gangliosides. The normal lumbar CSFs investigated here were obtained from adult individuals exhibiting no signs of tumors. The extracted GG sample [2] of 5 pmol/μL in methanol was infused into a Synapt G2s and the signal was acquired in the negative ion mode at 1.6kV ESI voltage. IMS MS separation and screening revealed 113 distinct GG species in CSF; of these, more than 76% were found polysialylated, which is similar with the percentage of the polysialylated ganglioside species (over 78%) detected in human brain using same approach. In comparison with the brain tissue, we have discovered in CSF several components containing fatty acids with odd number of carbon atoms and/or short glycan chains. Additionally, IMS MS evidenced the presence of four O-Fuc GGs and five O-Ac GGs. Further, the structural confirmation of GD3(d18:1/18:0) and GD2(d18:1/18:0), exhibiting shorter carbohydrate chain, a feature of CSF, was achieved in the transfer cell by tandem MS using collision energies between 30-40 eV. A significant number of fragment ions diagnostic for both the glycan core and ceramide moiety of the postulated GD3(d18:1/18:0) and GD2(d18:1/18:0) were generated. Hence, human CSF and brain show a similar ganglioside pattern, a finding that might be useful in clinical research focused on discovery of ganglioside species associated to neurodegenerative diseases and brain tumors.

Biography

MIRELA SARBU (b. 1986), scientific researcher and currently principal investigator (PN-III-P1-1.1-PD-2019-0226), obtained in 2015 the PhD in Physics (Faculty of Physics, West University of Timisoara, Romania) with "Summa cum Laude" with the topic: "Development of chip ionization methods in combination with dissociation in radiofrequency field with biophysical and biomedical applications". Dr. Sarbu implemented IMS MS for the first time worldwide in human brain ganglioside research for biomarker discovery, and for monitoring the pathophysiological CNS changes. The research activity undertaken by Dr. Sarbu led to 12 national and international collaborations (USA, Germany) with important MS research centers and personalities in the field. The biomedical research conducted by Dr. Sarbu has resulted in 24 original/review articles in journal with an impact factor situated within 0.629 and 5.886 (cumulative IF of 62.997) and five book chapters. Hirsch index: 7 (Web of Science Core Collection), 7 (SCOPUS) and 8 (Google Scholar).

Novel synthetic inhibitor of Ku/DNA interaction helps to reveal the mechanism of Ku-mediated regulation of HIV-1 transcription

Sergey Korolev, E. Pavlova, O. Shadrina, A. Mantsyzov and **M. Gottikh**
Lomonosov Moscow State University, Russia

Human Ku protein participates in DNA double strand break repair and binds to free ends of DNA. Besides Ku can contribute to the transcription regulation of cellular and viral genes through interaction with proteins and DNA, including transcription of one og the most dangerous viruses – HIV-1 (human immunodeficiency virus). We investigated the effect of Ku intracellular concentrations on the transcription of the Firefly luciferase reporter protein gene under the control of the LTR HIV-1 promoter in a pGL3 vector. It was found that Ku is a positive transcription factor from the HIV-1 LTR promoter. We decided to use Ku/DNA interaction inhibitors to elucidate whether such an effect can be determined by the direct interaction of the Ku protein with the HIV-1 promoter. Using the available crystallographic structure of Ku/DNA complex we built a pharmacophore model describing key contacts of a DNA duplex with Ku and selected a series of the molecules fitting the pharmacophore via virtual docking. We carried out EMSA experimental screening on recombinant Ku and identified a new structural class of Ku/DNA interaction inhibitors with an IC50 within micromolar range. We showed that one of the compounds effectively blocked the repair of double-stranded DNA breaks in Hek 293T cells. However this compound was unable to influence on the transcription of HIV-1 LTR promoter. In this regard we consider that Ku regulates HIV-1 transcription in DNA independent way. Thus the series of new inhibitors of the interaction of Ku with DNA was discovered, which opens up prospects for further optimization of their structure in order to create even more active substances that can be used in the treatment of cancer, as well as gene therapy. The work was supported by Russian Science Foundation grant RSF 17-14-01107-P.

Biography

Sergey Korolev graduated with honors from the Chemistry Department of the Lomonosov Moscow State University in 2006. In 2010, Korolev S. P. defended his PhD thesis in bioorganic chemistry on the topic: "Development of approaches to study the mechanism of action and search for new HIV-1 integrase inhibitors". Since 2010 Sergey Korolev has been working in Department of Chemistry and Belozersky Institute if Physico-Chemical Biology of Lomonosov Moscow State University. The scientific activity of S. Korolev in recent years has been developing in two main directions. The first one is the search for HIV-1 integrase and reverse transcriptase inhibitors. The second field of the research is the study of the interaction of the human heterodimeric protein Ku with DNA and the search for the inhibitors.

Development of a new method based microfluidic device liquid phase microextraction for compounds from ten different classes

Maria Ramos Payan[2], Samira Dowlatshah[1,2], Mohammad Saraji[2], Rut Fernandez Torres[1] and **Miguel Angel Bello Lopez[1]**

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Frequent consumption of pharmaceuticals and personal care products (PPCPs) have emerged as a current problem that highlights the pressing need for new multi-residue analytical methods that allow their simultaneously determination to assess their overall effect on human health. In this regard and for the first time, a versatile microfluidic method base liquid phase microextraction (LPME) was developed for simultaneous monitoring of ten compounds from six different classes: amoxicillin, sulfadiazine, sulfamerazine, tiamphenicol, ethyl 4-hydroxybenzoate, flumequine, propyl 4-hydroxybenzoate, 5-hydroxydiclofenac, 3-hydroxydiclofenac and diclofenac. The microfluidic device was combined with a HPLC-UV system for the separation and determination of the model analytes in the sample. Under optimal method conditions, the extraction efficiency was between 85-100% for most compounds after 10 minutes extraction, and it was successfully applied in non-diluted human urine, with recoveries between 70-100% for all analytes except for sulfamerazine (52% recovery). In addition, the extraction of metabolites (3-hydroxydiclofenac and 5-hydroxydiclofenac) was also demonstrated in microfluidic systems with recoveries between 71-100% in human urine. The proposed method allowed consecutive extraction and only requires 5 μL of organic solvent and less than 15 μL of sample volume.

Biography

Maria Ramos Payán is Doctor in Chemistry (Ph.D) and she is Professor at University of Seville (Spain) at the Department of Analytical Chemistry. She has also developed her research at the University of Lund (Sweden), University of Copenhagen (Denmark), University of Chapel Hill (North Carolina, USA) and National Microelectronics Center (Barcelona). Her research interests focus on the development of new microextraction techniques and microfluidic devices for applications in the life sciences and pharmaceutical sciences. She has published over 40 scientific articles with Hindex 24 and her research line is world pioneer on simultaneous extraction of different compounds on microchip devices.

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Polypropylene/Lignin blend monoliths used as sorbent in oil spill cleanup

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With increasing industrial development, frequent oil spillages in water; therefore, it is imperative and challenging to develop absorbents materials that are eco-efficiency, cost-effective, and pollution prevention. In this study, sorbents obtained from Lignin incorporated with Polypropylene in different levels loading 0, 10, 20 % wt using thermally induced phase separation Technique (TIPS). The Polypropylene /Lignin blend monoliths were fabricated and compared in terms of morphological, thermal, and wetting characterizations. The successfully blending of different lignin concentrations with preserved the chemical structure of the polymer was confirmed by FTIR analysis. Thermogravimetric tests displayed that the existence of Lignin has changed the onset temperature (Tonset) of the blending sorbents, decreasing as the loading of Lignin is increased. The contact angle measurement showed a decrease in the hydrophobicity of sorbents with increasing lignin loading, Polypropylene/Lignin blend monoliths showed better absorption toward oils (soybean – engine) as compared to Polypropylene itself. PP10L showed an improvement in the oil sorption capacity around 2 times compared to the Polypropylene. These excellent features make Polypropylene /Lignin blend monoliths more competitive promising candidates than commercial absorbent.

Molecular docking, design, synthesis and biological evaluation of novel benzodioxole derivatives on various biological targets

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In this project 18 novel Benzodioxole derivatives (three different groups; benzodiazepine, aryl acetate, and acetic acid) were synthesized in order to evaluate their biological activities on various targets. The synthesized compounds were identified using FTIR, HRMS, ^{1}H-NMR, and ^{13}C-NMR techniques. The analogues were evaluated on AMPA receptor, COX, lipase, α-amylase, DPPH enzymes, as well as on different cancer cell lines. The group with benzodiazepine structures were active on AMPA receptors [1]. Aryl acetate derivatives showed potent activity on COX2 enzymes, while two compounds of acetic acid group were the most selective agents on COX2 over COX1 enzyme [2]. Three compounds of acetic acid and one compound from acetate group have potent activity against α-amylase enzyme with IC50 below the value of Acarbose positive control, as well as one compounds showed potent cytotoxic activity against MCF7 cancer cell line. However, these compounds showed very week or negligible activity on the lipase enzyme. Molecular docking studies were used to identify the Receptor–Antagonist interactions between Benzodiazpine compounds and AMPA receptor, and between aryl acetic acid group and α-amylase enzyme. A good correlation was obtained between the theoretical predictions of bioavailability using Molinspiration calculation, Lipinski's rule of five, and experimental verification. The current project provides possible drug candidates on AMPA receptor for various neurological diseases (benzodiazepine group), promising group of compounds having a Benzodioxole moiety against COX enzyme as novel Non-steroidal anti-inflammatory agents, as well as promising compounds against diabetes disease.

Characterization of a new natural fiber extracted from corypha taliera fruit

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This study deals with the determination of new natural fibers extracted from the *Corypha taliera fruit* (CTF) and its characteristics were reported for the potential alternative of harmful synthetic fiber. The physical, chemical, mechanical, thermal, and morphological characteristics were investigated for CTF fibers. X-ray diffraction and chemical composition characterization ensured a higher amount of cellulose (55.1 wt. %) content and crystallinity (62.5%) in the CTF fiber. The FTIR analysis ensured the different functional groups of cellulose, hemicellulose, and lignin present in the fiber. The Scherrer's equation was used to determine crystallite size 1.45 nm. The mean diameter, specific density, and linear density of the CTF fiber were found (average) 131 μm, 0.86 g/cc, and 43 tex, respectively. The maximum tensile strength was obtained 53.55 MPa for GL 20 mm and Young's modulus 572.21 MPa for GL 30 mm. The required energy at break was recorded during the tensile strength experiment from the tensile strength tester and the average values for GL 20 mm and GL 30 mm are 0.05381J and 0.08968J, respectively. The thermal analysis ensured the thermal sustainability of CTF fiber up to 230°C. Entirely the aforementioned outcomes ensured that the new CTF fiber is the expected reinforcement to the fiber-reinforced composite materials.

Hydrothermal synthesis of silver decorated reduced graphene oxide (rGO) nanoflakes with effective photocatalytic activity for wastewater treatment

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Graphene oxide (GO) was obtained through modified hummers method, and reduced graphene oxide (rGO) was acquired by employing heat treatment. Various concentrations (2.5, 5, 7.5, and 10 wt. %) of silver (Ag) were incorporated in GO nanosheets by adopting hydrothermal approach. Synthesized Ag decorated rGO photocatalyst Ag/rGO was characterized using X-ray diffraction (XRD) to determine phase purity and crystal structure. XRD patterns showed the formation of GO to Ag/rGO. Molecular vibration and functional groups were determined through Fourier Transform Infrared spectroscopy (FTIR). Optical properties and a decrease in bandgap with insertion of Ag were confirmed with UV-Visible (Uv-Vis) spectrophotometer and photoluminescence (PL). Electronic properties and disorders in carbon structures were investigated through Raman spectroscopy that revealed the existence of characteristic bands (D and G). Surface morphology of prepared samples was examined with field emission scanning electron microscope (FESEM). Homogeneous distribution, size, and spherical shape of Ag NPs over rGO sheets were further confirmed with the help of high-resolution transmission electron microscope (HRTEM). Dye degradation of doped and undoped samples was examined through Uv-Vis spectra. Experimental results indicated that photocatalytic activity of Ag@rGO enhanced with increased doping ratio owing to diminished electron-hole pair recombination. Therefore, it is suggested that Ag@rGO can be used as a beneficial and superior photocatalyst to clean environment and wastewater with no harmful effect on environment.

Use of Triphenylphosphine-Bromotrichloromethane (PPh3-BrCCl3) in the preparation of Acylhydrazines, N-methylamides, anilides and N-arylmaleimides from carboxylic acids

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In certain countries, many of the reagents used to transform carboxylic acids to acyl halides such as phosphorus trichloride, phosphorus tribromide, phosphorus pentachloride, phosphoryl chloride, thionyl chloride and sulfuryl chloride are difficult to come by. Against this background, the authors developed the reaction system triphenylphosphine (PPh3)–bromotrichloromethane (BrCCl3) to prepare acyl halides in situ. In the following, the use of this reagent combination is joined with the reaction of the *in situ* prepared acyl halides with nitrogen nucleophiles, specifically with hydrazines, methylamine and anilines. The reaction is also used in an intramolecular variant by the reaction of maleanilic acids to N-arylmaleimides.

Metal organic frameworks based mixed matrix membranes: A game changer for water purification

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The efficient removal of contaminants from drinking water requires highly permeable and selective processes and techniques. Membrane technology is a promising option due to its numerous inherent advantages such as cost effectiveness and low ecological footprint. Polymeric membranes are conventionally used for such purposes. However, the commercial use of polymeric membranes is limited due to their low separation and permeabilities. Inorganic materials, on the other hand, have excellent separation properties but are very expensive materials. Mixed matrix membranes, combining the advantageous properties of polymers and inorganic fillers, are a new class of membrane materials. Such membranes not only exhibit high rejection but they have also high thermal and solvent stability which is excellent considering the working conditions and parameters in practical and industrial applications. In this study, metal organic frameworks (Uio-66) was selected as filler for MMMs to enhance the separation performance. Uio-66 was synthesized at lab scale and was characterized by different techniques to determine its morphology, thermal stability, surface area and pore volume etc. Membranes synthesis was done by preparing PI supports followed by the coating of different percentage loadings of filler. Finally these membranes were tested by passing a contaminated drinking water. The results showed that the increased in the percentage of Uio-66 in polymer lead to increase in the pure water flux as well as the rejection of solutes from solution.

Design and synthesis of halogenated bis(imino) pyridyl chromium(III) complexes and their ethylene polymerization behavior

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Polyolefin materials are the most synthesized polymer used nowadays and symbolize the development level of the national petrochemical industry, in which polyethylenes are major along with alternative product α-olefins for co-monomer and substrates for fine chemicals. Likely operating catalysts such as Ziegler-Natta and metallocene meet all demanding of various polyethylene materials. Polyethylene is a thermoplastic polymer with a variable crystalline structure and an extensive range of applications depending on the particular type. It is one of the most widely produced plastics in the world (between 2018- 2019, world plastics production totaled around 359 million metric tons.) The industrial process (the Ziegler-Natta catalysts) that made PE such a success was developed in the 1950s by German and Italian scientists Karl Ziegler and Giulio Natta. Five unsymmetrical 2-[1-(2,4-dibenzhydryl-6-chlorophenylimino)ethyl]-6-[1-(arylimino)ethyl]pyridine compounds (aryl: 2,6-Me2Ph L1, 2,6-Et_2Ph L2, 2,6-iPr2Ph L3, 2,4,6-Me3Ph L4 and 2,6-Et_2-4-MePh L5) were prepared and characterized with FT-IR and $^1H/^{13}C$ NMR spectroscopy as well as elemental analysis. The treatment of L1 – L5 with $CrCl_3 \cdot 3THF$ afforded the corresponding chromium chloride complexes (Cr1 – Cr5) in excellent yields. On activation with either MAO or MMAO, Cr1 – Cr5 collectively displayed high activity (up to 14.96×10^6 g (PE) mol−1 (Cr) h−1 at 60°C) affording highly linear polyethylene with low molecular weight distribution (Mw/Mn) ranging from 1.06 to 2.81. Then a series of five examples of unsymmetrical Cr (III) chloride complexes (Cr1 – Cr5) each bearing 2-[1-(2,4-dibenzhydryl-6-fluorophenylimino)ethyl]-6-[1-(arylimino)ethyl] pyridyl (aryl: 2,6-Me2Ph L1, 2,6-Et_2Ph L2, 2,6-iPr2Ph L3, 2,4,6-Me3Ph L4, 2,6-Et_2-4-MePh L5) were prepared. The catalytic potential of all the complexes was investigated for ethylene polymerization and compared with the results of prototypal pre-catalyst. On treatment with MAO and MMAO co-catalysts, while the chromium complexes (Cr1 – Cr5) displayed exceptionally high activities as high as 20.14×10^6 g (PE) mol−1 (Cr) h−1 at 30°C).

Cytotoxicity and antimycobacterial properties of pyrrolo[1,2-a] quinoline derivatives: Molecular target identification and molecular docking studies

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Rani Channamma University, India

A series of ethyl 1-(substituted benzoyl)-5-methylpyrrolo[1,2-a] quinoline-3-carboxylates 4a–f and dimethyl 1-(substituted benzoyl)-5-methylpyrrolo[1,2-a]quinoline-2,3-dicarboxylates 4g–k have been synthesized and evaluated for their anti-tubercular (TB) activities against H37Rv (American Type Culture Collection (ATCC) strain 25177) and multidrug-resistant (MDR) strains of Mycobacterium tuberculosis by resazurin microplate assay (REMA). Molecular target identification for these compounds was also carried out by a computational approach. All test compounds exhibited anti-tuberculosis (TB) activity in the range of 8–128 µg/mL against H37Rv. The test compound dimethyl-1-(4-fluorobenzoyl)-5-methylpyrrolo[1,2-a]quinoline-2,3-dicarboxylate 4j emerged as the most promising anti-TB agent against H37Rv and multidrug-resistant strains of Mycobacterium tuberculosis at 8 and 16 µg/mL, respectively. *In silico* evaluation of pharmacokinetic properties indicated overall drug-likeness for most of the compounds. Docking studies were also carried out to investigate the binding affinities as well as interactions of these compounds with the target proteins.

Effect of *Opuntia ficus-indica* mucilage on the treatment of a textile wastewater by coagulation-flocculation

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In this work, the ability to remove a synthetic and a real textile wastewater using coagulation-flocculation (CF) process with aluminum sulfate, ferric chloride, industrial flocculant and a mucilage of *Opuntia ficus indica* as a natural flocculant aid has been investigated.

Experiments were performed to study the effect of operating parameters such as initial pH (3.5 – 10.5), coagulant dosage (50 – 500 mg/L), initial concentration of the dye (50 – 1400 mg/L), conductivity (2.5 – 6.5 mS/cm), industrial flocculant (5 – 150 mg/L), natural flocculant (2– 60 mL/L), contact time (5 - 120 min) and mixing conditions (150 to 250 rpm for 2 and 3 min mixing time for coagulation phase, 30 – 60 rpm for 20 and 30 min mixing time for flocculation phase).

Results showed that:

- The stirring velocity for coagulation must be fast (150 rpm - 3 min) and that of flocculation must be slow (30 rpm - 20 min).
- CF functions well, even with the highest dyestuff concentrations, up to 600 mg/L (1959 NTU) for aluminum sulfate (YTurb = 99 %) and 800 mg/L (2717 NTU) for ferric chloride (YTurb = 96.83 %) under initial pH ranging from 8.5 to 10.5.
- The optimal amount of ferric chloride and aluminum sulphate is of 250 mg/L.
- The optimal amount of the anion flocculant for the elimination of turbidity with aluminum sulphate is 50 mg/L, and that of ferric chloride is 5 mg/L.
- The optimal amount of the natural flocculant agent (juice of cactus) is 12 to 15 mL/L.
- By adding 3 ml/L of *Opuntia ficus indica* as a natural flocculant aid, the efficiency increased by 10 %.
- The application of the optimized parameters to a real textile wastewater showed an acceptable reduction of the turbidity (67 %), SS (57.33 %) and COD (94.81 %).

Development of μ-Thermo Electric Generators with high electrical power for a clean energy

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The ever-increasing number of connected objects requires novel ways to power them and make them fully autonomous. In this context, photovoltaic, piezoelectric or thermoelectric energy-harvesting technologies show great promises as they make possible the conversion of solar radiation, motion or thermal energy into useful electricity for charging micro-batteries for instance. Thermoelectric micro-generators (μ-TEGs) exhibit several key benefits, making them prime candidates for harvesting any temperature difference between their two exchange surfaces. However, their output power critically depends on the design of the μ-TEG, the minimization of the detrimental influence of the contact resistances and on the coupling of the μ-TEG with the heat source and heat sink. Here, we theoretically and experimentally demonstrate how these inherent difficulties can be mitigated using an innovative, smart flexible μ-TEG design based on bismuth telluride thin films. Our experimental findings show that an output power of 5.5 μW per thermocouple can be generated under a temperature difference of only 5 K, in excellent agreement with predictions based on three-dimensional finite element analyses. These remarkable results rank our μ-TEG among the best micro-generators currently available.

DFT/B3LYP and BP86 examination of mononuclear half-sandwich nd^7 metallo drug complexes based on n∩o dendritic scaffolds

Bikele Mama Desire
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In this paper, we have explored the bonding properties of a series of mononuclear half-sandwich nd7 anticancer complexes based on N∩O dendritic scaffolds using B3LYP and BP86 functionals. A generic basis set has been adopted: LanL2DZ and 6-311+G (d,p) respectively for nd^7 transition metals (as well as halogen atoms) and for others atoms. Computed results reveal that all complexes optimized have adopted the piano-stool environment with the nd7 metal atoms bound to the pentamethylcyclopentadienyl ligand (CP*), one halogen atom (Cl or Br) and N∩O chelating ligands (L). BP86 functional yielded overestimated the N-M-O bond angles compared to those obtained with the B3LYP functional. At the same time, this first functional underestimates the complexation energies by about 10.57 and 31.05 kJ/mol on average respectively for chloride cobalt complexes and their bromide homologues. Our results also show that the M...O, M...N and M...X interactions are closed-shell interaction nature. From the contribution of the ΔE_{orb} term in the ranges 4.06-98.61% (X=Cl) and 10.29-99.87% (X=Br), the nature of the $[MLCP^*]^n$ $(n=0(A;B;C),n=-2(D;E))$ ...X^- interaction turned out to be mainly dependent on the transition metal and halogen atom involved. The smallest back-donation observed for chloride complexes corresponding to the highest barrier to the formation of [MLCP*]-*X* bond traduces that chloride complexes are the least reactive. In the majority of cases, larger donation is obtained compared to back-donation showing that the possibility of $([LCP^{*}]^{-n}))^{\delta-} \leftarrow ([MX]^{+})\delta^{+}$ charge separation can be expected. For α rings of chloride complexes, B3LYP-calculated HOMA indexes are higher than those estimated by PB86 functional. Conversely, opposite results were found for their bromide counterparts.

Reaction kinetics in chemical engineering

Christo Boyadjiev
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In the lecture is presented a theoretical analysis of the role of the reaction kinetics in chemical engineering for the solution of the main problems in the chemical industry (biotechnology, heat energy), i.e. the optimal design of new devices and the optimal control of active processes. The thermodynamic and hydrodynamic approximations for the modeling of the industrial process rates are presented and analyzed. The industrial processes are the result of reactions, i.e. creation or disappearance of a substance and (or) heat as a result of chemical and (or) physical processes and their rate is determined by the reaction kinetics. The reactions deviate the systems from the thermodynamic equilibrium and as a result processes arise, who are trying to restore that equilibrium. The rate of these processes can be determined by Onsager's "linearity principle", where the rate of the process depends linearly on the deviation from the thermodynamic equilibrium. The Onsager's linearity coefficient can be determined after solving the hydrodynamics, mass transfer and heat transfer equations, where it is proportional to the mass transfer (heat transfer) coefficient. The relations between the Onsager's linearity coefficient and mass transfer coefficient are presented for different processes.

Biochemical insights into diet-induced vascular complications in diabetes

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An unprecedented rise in the global prevalence of diabetes and diabetes-related complications roughly parallels an increased consumption of sugar-sweetened or artificially-sweetened beverages. While substitution of sugars, and sugar-related products, with artificial sweeteners has been employed for better glycemic and caloric control, their impact on biochemical processes and cellular functions has not been intensely reported. Additionally, little is known about the similarity or dissimilarity in the changes in cardiovascular markers induced by these compounds. By employing animal-disease models and novel methodologies, which includes high-throughput technology coupled with molecular biology techniques, the molecular and biochemical changes induced by these compounds have been recently explored. This presentation will give an overview of sugar-induced vascular changes, and focus on recent research findings of artificial sweeteners on vascular complications in diabetes. Additionally, the presentation will also discuss the similarities and/or differences in the biochemical changes induced by natural and artificial sweeteners, and how they can translate into having physiopathological consequences. By understanding the critical biochemical changes these compounds potentially trigger in pathological and/or healthy conditions, we can endeavor to develop a rationale for regulation of high-dose consumption of sugars and artificial sweeteners.

Design, synthesis and *in vitro* evaluation of anti-TB drug analogs against an Infectious disease *Mycobacterium tuberculosis* (M.tb.) strains

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Tuberculosis (TB) is an infectious disease, which affects millions of people every year and is ranked as one of the top ten cause of human death. The current treatment regimen includes combination of four first-line drugs, namely, rifampicin, isoniazid, pyrazinamide, and ethambutol for a period of six months. Development of drug resistance against these conventional antibiotics is a matter of great concern requiring immediate attention. Since MDR- and XDR-TB have become serious problems worldwide, there is an urgent need to discover new anti TB compounds.

We have designed and synthesised some of the anti-TB drug analog derivatives, which shows better bactericidal activity. The efficacy of synthesized molecules against drug sensitive as well as drug resistance isolates of Mtb were carried out. We have screened these molecules and determined its active concentration by using rapid liquid based procedure called Luciferous Reporter Phages (LRP). It is one of the growth based assays which is being used to determine anti-Tb activity of existing as well as newer molecules. Moreover, we have also confirmed the efficacy of the molecules by conventional methods. In the conventional assay we have determined MIC of newer molecules by the Agar dilution method using 7middle brook 7H10 Agar plates and Minimum Bactericidal Concentration (MBC) for these molecules using Broth dilution method & subsequently plating it on middle brook 7H11 Agar plates. In conclusion, we have designed and synthesized novel anti-TB drug analog which showed more efficacy and less toxic.

Methodological approaches to the assessment of toxic pollution of fresh waters in arid climate

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The study aimed to address the relevant challenges associated with determining the concentration ranges of six heavy metals (Cd, Cu, Zn, Pb, Ni, and Cr) to create a regional scale for assessing water quality. The scale based on a long-term survey (1997-2017) of the relationship between the response of plankton communities to toxic pollution in 90 fresh water bodies of arid and semi-arid regions of Kazakhstan. Heavy metals measurements were performed by mass spectrometry with inductively coupled plasma using Agilent 7500 A. Hydrobiological samples were processed using standard methods. The distribution of heavy metals in water bodies was studied by statistical methods. The scale is represented by six classes of water quality, from extremely pure to the most polluted (Table).

Table. Regional ecological classification of the water quality in Kazakhstan water bodies (1) in the "Heavy Metals" section in comparison with the ecological classification of the surface lotic waters of Europe (2) using our color codes

When identifying water quality classes, we studied the background content of heavy metals, the content of heavy metals in water bodies with fluctuation of surface levels and the nature of anthropogenic pollution (Krupa et al., 2019), as well as the reaction of biological communities to toxic pollution in their natural habitat (Krupa, 2005; Krupa et al., 2018). Absolute values of all heavy metals' concentrations for each class of water quality in the regional classification are several times lower than in the ecological grades established for European temperate climate water bodies. The proposed methodological approach assesses not only the local content of heavy metals in water bodies of Kazakhstan but also the level of toxic pollution of vast areas of their catchment basins. The proposed methods can be applied to other arid regions with similar physical and climatic conditions.

Discovery of the oscillations in the RPV steel radiation embrittlement kinetics as an indication of nanostructure self-organizing

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Influence of neutron irradiation on reactor pressure vessel (RPV) steel degradation are examined with reference to the possible reasons of the substantial experimental data scatter and furthermore – nonstandard (non-monotonous) and oscillatory embrittlement behavior. In our glance this phenomenon may be explained by presence of the wavelike recovering component in the embrittlement kinetics. We suppose that the main factor affecting steel anomalous embrittlement is fast neutron intensity (dose rate or flux), flux effect manifestation depends on state-of-the-art fluence level. At low fluencies radiation degradation has to exceed normative value, then approaches to normative meaning and finally became sub normative. Data on radiation damage change including through the ex-service RPVs taking into account chemical factor, fast neutron fluence and neutron flux were obtained and analyzed. In our opinion controversy in the estimation on neutron flux on radiation degradation impact may be explained by presence of the wavelike component in the embrittlement kinetics. Therefore flux effect manifestation depends on fluence level. At low fluencies radiation degradation has to exceed normative value, then approaches to normative meaning and finally became sub normative. As a result of dose rate effect manifestation peripheral RPV's zones in some range of fluencies have to be damaged to a large extent than situated closely to core. Moreover as a hypothesis we suppose that at some stages of irradiation damaged metal have to be partially restored by irradiation i.e. neutron bombardment. Nascent during irradiation nanostructure undergo occurring once or periodically transformation in a direction both degradation and recovery of the initial properties. According to our hypothesis at some stage(s) of metal structure degradation neutron bombardment became recovering factor. Self-recovering section of RPV steel radiation embrittlement kinetics is an indication of material nanostructure self-organizing and intelligent behavior.

Stabilization of supramolecular membrane protein-lipid bilayer assemblies through immobilization in a crystalline exoskeleton

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Artificial native-like lipid bilayer systems constructed from unilamellar liposomes allow the reconstitution of transmembrane proteins into proteoliposomes, which mimic cellular membranes. Stabilization of these remains challenging because of their chemical composition, the hydrophobicity and structural instability of membrane proteins, and the lability of interactions between protein, detergent, and lipids within micelles and lipid bilayers. In this work we demonstrate that metastable lipid, protein-detergent, and protein-lipid supramolecular complexes can be successfully generated and immobilized within zeolitic-imidazole framework (ZIF). We describe a method for the thermal stabilization of blank 200 nm liposomes, purified transmembrane proteins, and 200 nm transmembrane protein-liposome supramolecular complexes (proteoliposomes) against chemical and thermal stressors through biomimetic nucleation in ZIF-L. We found that encapsulation of the proteoliposome complex generates thermodynamically stable bio-composites that can withstand exposure to high temperatures, aging, and common protein denaturants (Figure 1). Further, the ZIF-L coatings can be removed to afford pristine proteoliposomes, liposomes, and transmembrane protein micelle complexes of similar composition, morphology, structure, and catalytic activity to their native counterparts.

Development of heterostructures photocatalytic application to $Nb_2O_5/g\text{-}C_3N_4$ heterostructures as efficient photocatalyst

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The work focuses on the developments made in the photocatalytic applications. Many factors such as synthesis, the formation of heterostructures, doping, metallic deposition and charge carrier concentrations affect the efficiency. My work will focus on progression in this field and how a material can be engineered to make a suitable band position and a favourable surface area for efficient photocatalytic applications. Particularly, $Nb_2O_5/g\text{-}C_3N_4$ heterostructures will be focused on, as recently, I have synthesized $Nb_2O_5/g\text{-}C_3N_4$ heterostructures with suitable band positions and high surface area by using in-situ and ex-situ synthesis method. The combination of a Nb_2O_5 with a low charge carrier recombination rate and a $g\text{-}C_3N_4$ exhibiting high visible light absorption resulted in remarkable photocatalytic activity under simulated solar irradiation in the presence of various hole scavengers (triethanolamine (TEOA) and methanol). Moreover, I tried to activate reduction and oxidation potentials by adopting a novel technique which led to small water splitting. Currently, working on how the material could be engineered for efficient water splitting. The enhanced photocatalytic activity is attributed to a sufficient interfacial interaction thus favoring the fast photogeneration of electron-hole pairs at the $Nb_2O_5/g\text{-}C_3N_4$ interface through a direct Z-scheme.

1D and 2D hybrid plasmonic-photonic structures based on Cu-doped TiO_2

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The development of new photocatalytic materials with improved stability, low cost, and high photocatalytic activity under solar light are one of the current challenges for photo-electrochemical (PEC) water splitting. Research of TiO_2 photocatalysis is constantly develops and one of many goals is to find positive impacts of dopants. Very attractive approach is doping of TiO_2 with transition metals such as the very low-cost copper (Cu) [1]. This work deals with Cu-modified 1DTiO_2 microrods (MRs) and 2DTiO_2 leaves and their surface properties. The pristine lyophilized precursor Cu_1DTiO_2, prepared by an environmentally friendly cryo-lyophilization method, was further annealed in the temperature interval from 500 to 950°C. [2-3]. The microstructure of all samples was characterized by electron microscopy (SEM/EDS and HRTEM/SAED), X-ray powder diffraction (XRD), infrared spectroscopy, simultaneous DTA/TGA thermoanalytical measurement, and mass spectroscopy (MS). The morphology of all annealed samples was preserved, but their surface roughness varied due to anatase-rutile phase transformation and the change of the nanocrystals habits due to nanocavities formation after releasing of confined ice-water. All samples were tested for their UV absorption properties and H_2 generation by PEC water splitting. We presented a detailed study on the surface characteristics of Cu doped 1DTiO_2 MRs and 2DTiO_2 leaves due to gain a better idea of their photocatalytic activity. Last step was comparing all properties of 1DTiO_2 MRs and 2DTiO_2 leaves including morphology.

Enhanced characteristics of planar perovskite solar cells using (Al^{3+}, La^{3+}) co-doped SnO_2 as the electron transport layer

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Rapid increment of population and industrialization enhance the energy consumption day by day. Propelling our welfare and quality of life, the usage of fossil fuels as the primary energy source, but, it exacts a huge penalty on humankind as well as the environment. Solar energy is one of the most abundant, clean and renewable energy source. Perovskite solar cells based on lead-halide perovskites have attracted significant attention as prime candidates for next-generation solar cells because of their high-power conversion efficiency. Despite the high efficiency achieved using the mesoporous scaffold for organic-inorganic halide perovskite solar cells (PCS), the mesoporous configuration limits the stability, allowable preparation methods and use on flexible device. Hence, the planar configuration is deemed more favourable for commercial endeavors although the device efficiency is lower. In the present study, aluminium (Al^{3+}) and lanthanum (La^{3+}) metals were successfully co-doped into low-temperature processed SnO_2 electron transport layer (ETL). Our results showed that Al and La co-doped SnO_2 ETL exhibited synergistic effect of improved electrical conductivity and optical transparency compared to the pristine and individually doped SnO_2 ETL. Electro chemical impedance spectroscopy and photoluminescence analysis confirmed that AlLa-SnO_2 based device exhibited high recombination resistance, promoting fast electron extraction and transportation due to the better band energy alignment of ETL-perovskite. Moreover, small amount of trivalent dopants Al^{3+} and La^{3+} ions replaced the Sn^{4+} ions in the host SnO_2 lattice influenced the growth process of SnO_2 grains and induced the formation of good crystalline perovskite film on ETL leads to decrease the concentration of trap states. Superior device power conversion efficiency was achieved when AlLa-SnO_2 was used as the ETL of 19.13% compared to the pristine SnO_2 device of 17.21%. Mean while, the reproducibility of 20 fabricated AlLa-SnO_2 ETL device retained 91% of its initial PCE after storage at the relative humidity of 30 ± 2% for 30 days without encapsulation. From this work, we demonstrated that Al and La co-doping is a promising approach to fabricate excellent n-type ETL, which is a simple way to improve the efficiency, stability and reproducibility in planar PSCs.

The structure-reactivity relationship of Pt surface sites towards the glucose electro-oxidation in neutral solution

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Due to the possibility of developing implantable DGFC cells, as in an artificial heart, for example, glucose electro-oxidation is a subject of great relevance in electrochemistry. However, for this application to be possible it is necessary to oxidize glucose completely to CO_2, which is very difficult, especially due to the low selectivity and activity of the catalysts used in the reaction, especially in the anode, which is easily poisoned by the adsorption of species generated during the reaction. Additionally, we know that the real catalysts present in the fuel cells are in nanoparticulate form, and therefore contain sites of terraces, steps, kinks and defects with well-defined crystallographic orientations, which confer a specific local catalytic activity. Thus, in order to try to develop catalysts capable of efficiently electro-oxidizing glucose so that they can be used in implantable DGFC cells, we need to understand the specific reactivity of the catalytic sites under conditions similar to the physiological ones (pH 7), and, for that, it is done necessary to fully elucidate the reaction mechanism under these conditions.

In this perspective, our studies have been directed towards the investigation of the electro-oxidation of glucose in phosphate buffer solution (pH 7 - biological) on single-crystal Pt surfaces (low-index Miller and stepped surfaces) using cyclic voltammetry and *in situ* FTIR techniques, in order to investigate the reactivity of surface catalytic sites in neutral solution. Thus, in this presentation we will discuss the effects of the size of the terraces and the symmetry of the sites of the terraces and steps, that is, which sites favor or inhibit the formation and adsorption of species generated during the reaction process and how this influences the catalytic activity.

Distinct molecular formation in laser-induced carbon plasmas in air

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Laser-induced carbon plasma in air undergoes various physicochemical processes that affect the kinetic chemistry of species of the plasma plume. We report the time- and space- resolved characterization of carbon plasma produced by infrared nanosecond laser into air at atmospheric pressure. Investigating the laser fluence effect highlights dissociation for fluences > 40 J cm^{-2} and recombination processes in the fluence range of 10-40 J cm^{-2}. Emission intensities of C_2 and C_N molecules undergo an enhancement at specific spatiotemporal locations in the laser-induced plasma. At a value of 27 J/cm2 and 0.8 mm from the plasma ignition, molecular band formation is favored for the specific temperature and density values of 1.7×1015 cm^{-3} and 9502 K. The vibrational temperatures of molecules are determined using non-linear spectral data fitting program. The shock front between laser-induced carbon plasma and air may lead to a significant shock wave that affects the occurrence of molecular C_N and C_2 formation. This can be explained by the distinct temperatures exhibited by CN and C_2 molecules with laser fluence. The atomic carbon travels farther to react and form C_2, where the ionization-recombination process plays a significant role in its formation. Collisions of C with N neutrals and N_2 molecules are the plausible origin of CN generation. Moreover, the density of C_N in the plasma depends on C_2 molecules.

Anticancer furan-conjugated tripeptides

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Cancer is among the deadliest diseases of the present age which is advancing day by day causing around 8.8 million deaths worldwide. Currently used medicines are usually invasive and non-specific resulting in deterioration of normal cells along with the cancerous cells. To tackle such issues, discovery of molecules which specifically target and inhibit the growth of cancerous cell is an ultimate need of the day. Peptides are biologically active molecules which possess the tendency to specifically kill cancer cells. There are around 60 FDA approved peptide-based drugs present in market and hundreds of them are under developmental stages. But poor solubility, low bioavailability and sensitivity towards lower pH and proteolytic enzymes are the major limitations for peptide therapeutics. Introduction of some unusual amino acid residues, heterocyclic moieties or modification in the basic skeleton of peptides proves to be fruitful to overcome such issues with peptide therapeutics. In drug discovery, heterocyclic molecules are proving themselves to be very important pharmacophores and unique scaffold. In the current study, a library of new furan-based peptides is designed and synthesized on the Rink amide resin by using Fmoc strategy. Peptides were constructed from *C* to *N* terminus followed by capping by 2-furoyl moiety. The synthesized peptides were purified by recycling RP-HPLC and structures of all the peptides were confirmed by using ESIMS/FABMS, ^{1}H-NMR, ^{13}C-NMR and HR-FAB. The cytotoxicity of all the synthesized peptides 1-10 was determined against HeLa cancer cell line. One new peptide conjugate (4) was identified as potent anticancer agents against HeLa cancer cell line, with no toxicity against normal 3T3 fibroblasts and the other cancer and normal cell lines used in this study. This study disclosed a good structure activity relationship among various peptide conjugates. Peptide conjugate 4 in its branched form was found to be inactive. AFM and staining with rhodamine 123 and propodium iodide showed membranolytic effect of peptide conjugate 4 [1].

Extraction and antioxidant properties of second metabolites of (medicinal) plants-review

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There is a long list using various plants for different purposes by humans for ages. The focus will be on their second metabolites which have also many important functions narrowed to their effect on human health. To the second metabolites belong phenols (including flavonoids), terpenoids, vitamins, tannins, hormones and others. Before their study they should be extracted either specifically or in a mixture, and purified. Next step is analytical determination either as a group of compounds (total phenols, total flavonoids, and so on) or to find out the components of the mixture. Important properties of the components which should be determined belong solubility, pKa, antioxidant, antiviral, antibacterial properties, their effect on our metabolism, activation or inhibition of enzymes, synergic effects, and so on. When the dominant components are commercially available then they should be compared with the extracts.Our results are related to moringa, juniperus, and other medicinal plants to demonstrate various extraction methods. Antioxidant activity against several radicals (superoxide, hydroxide and nitritoperoxyl) and FRAP were determined in the extracts. Various radicals were studied due to their different effects and mechanisms of action. In evaluation of antioxidant activity we used novel correction and double phase system.

A surface patterning of 2DTiO$_2$ with nanocavities - application in methyl-parathion photomineralization

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The preparation of ultrathin two-dimensional (2D) TiO$_2$ nanomaterials have attracted an increasing attention for their unique physical and chemical properties. 2DTiO$_2$ nanomaterials with high specific surface-to-volume ratio demonstrated exceptional photochemical reactivity, as well as other supreme properties such as photocatalytic degradation of methyl-parathion (MP). MP is an organophosphorus pesticide from agriculture [1] that is difficult to remove from the environment.

A set of 2DTiO$_2$ photocatalysts samples with nanosheets morphology and dense regular polyhedral nanocavities inside were synthesized through a freeze-casting process [2-3]. We prepared cryogel TiO$_2$ precursor further annealed at 500, 650, 800 and 950°C for 1h. Thermal treatment induced the precursor to transform into vertically aligned arrays of 2D TiO$_2$ nanosheets composed of anatase (TiO_LYO_500, TiO_LYO_650, TiO_LYO_800) and anatase-rutile (TiO_LYO_950). In addition, TiO$_2$ nanocrystals with sharp nanocavities on their surface after the removal of ice were observed. These new nanomaterials were characterized by X-Ray Diffraction (XRD), Electron Microscopy (SEM, HRTEM) and tested for the photocatalytic mineralization of MP under UV light.

The method has demonstrated a remarkably high photocatalytic activity determined by measuring the kinetics of methyl parathion degradation. The activity increased with increasing annealing temperature in order of 500 °C < 600 °C < 950 °C < 800 °C. The most active photocatalyst was a well crystallized sample with anatase structure annealed at 800°C, followed by sample annealed at 950°C, where anatase-rutile mixture was obtained.

Synthesis of 3D structured graphene-based structures from stacked or electrically exfoliated graphene flakes

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Graphene roses or graphene flowers are a novel derivative of flaked graphene. Up to date only few reports have announced the possible self-assembling of randomly oriented nano-flakes of graphene to spherical 3D structures resembling blossoming rose, chrysanthemums or aster. Since first published papers announced similarity of such structures to roses, the current research material is also denoted as graphene rose. The report describes a thermally triggered re-structuration of stacked or preliminary exfoliated graphene flakes to 3D nanostructures resembling blossoming flower (rose). The size of graphene rose varies in the typical nonmetric range i.e. 50 to 150 cm (diameter). The fabrication method involves spraying of a graphene-containing suspension against a hot back-ground like a steel plate covered by a thin layer of PTFE. The elaborated method eliminates in fact oil as dispersive medium and is based on water supplemented with surfactant only. Graphene being in the sprayed suspension may be exfoliated preliminary by a chemical and/or electrochemical method (electroexfoliation). The resulting graphene-roses, despite a condense appearance, the roses exhibit advanced surface area up to 800 m^2/g and dominating mesoporosity. These basic structural properties along with excellent electric conductivity make graphene-roses an outstanding candidate for electrode fabrication applicable to electrochemical power generators/magazines.

A supramolecular probe of cyanine dye for Pb^{2+} detection based on the recognition of a G-quadruplex from DNA duplexes

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Cyanine-based probes are considered as the best candidates due to their controllable assembly and disassembly. Herein, we carried out the supramolecular self-assembly of cyanine dye (MTC) for the transformation between duplex DNA and G-quadruplex (T30695) for the highly selective and sensitive recognition of Pb^{2+} ions via Uv-Vis spectroscopy. A specific duplex DNA (duplex-a) consisting of a Pb^{2+} aptamer and its part complementary strand was constructed, which could be unwound to single-strand DNA to form a G-quadruplex in the presence of Pb^{2+}. The formed G-quadruplex could transform MTC H-aggregates into monomers, resulting in a specific recognition absorption signal.

Fig. 1. Structure of MTC and a schematic illustration of the mechanism for the detection of Pb^{2+} by using the MTC-duplex DNA system.

Long noncoding RNA SNGH7 is activated by SP1 and exerts oncogenic properties by interacting with EZH2 in ovarian cancer

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Long noncoding RNAs (lncRNAs) are key regulators or a range of diseases and chronic conditions such as cancers, but how they function in the context of ovarian cancer (OC) is poorly understood. The Coding-Potential Assessment Tool was used to assesse the likely protein coding poteintial of SNHG7. SNHG7 expression was elevated in ovarian tumor tissues measured by qRT-PCR. The online database JASPAR was used to predict the transcription factors binding to SNHG7. 24-well Transwell plates were used for invasion assays. RNA immunoprecipitation was performed to determine RNA-protein associations. EdU assay was introduced to detect cell proliferation. Chromatin immunoprecipitation was performed to confirm the directly interaction between DNA and protein. We discovered that in the context of OC there is a significant upregulation of the lncRNA SNHG7. Knocking down this lncRNA disrupted both OC cell invasion and proliferation, while its overexpression had the opposite effect. SP1 binding sites were present in the SNHG7 promoter, and chromatin immunoprecipitation (ChIP) confirmed direct SP1 binding to this region, activating SNHG7 transcription. We found that at a mechanistic level in OC cells, KLF2 is a probable SNHG7 target, as we found that SHNCCC16 directly interacts with EZH2 and thus represses KLF2 expression. In summary, this research demonstrates that lncRNA SNHG7 is an SP1-activated molecule that contributes to OC progression by providing a scaffold whereby EZH2 can repress KLF2 expression.

Unusual utilization of clinoptilolite and lignite in ecology and agriculture in Bulgaria – Review

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The industrial use of natural zeolites in agriculture began in the early 70s of the last century in MINERALAGRO, Bulgaria. N. Popov and G. Stoilov created the world's first zeolite substrate for growing plants - Balkanin, providing up to 2 times higher yield in greenhouse conditions. The other authors (Chakalov et al 1996, 1998; Filcheva et al., 1996b, 1999; Popova et al. 1998) proved the influence of clinoptilolite, on the physico-chemical properties and the transformation of organic matter to humic substances. Clinoptilolite changes the media's reactivity by controlling the exchangeable ions with acidic function: Al, Fe, H, Mn, Cu. K- zeolite has a particular influence on the limitation of exchangeable acidity. The NH^{4+} and Ca^{2+} -clinoptilolite accumulate high levels of exchangeable acidity. The differentiated natural fertilization of the zeolite determines the ability for ionization of the amphoteric hydroxides. Their ion-hydroxide equilibrium is determined by the degree of clinoptilolite influence on the exchangeable acidity; translocation of exchangeable H^+, Al^{3+} and Fe^{3+} ions in organic-mineral adsorbents. The variable charges of substrate adsorbent are responsible for organization of covalent connections-bridges with several elements. Composts with low level of T_A, accelerate T_A in meliorated soils and vice versa, i.e. the so called "mirror effect" is observed, which is well expressed in the case of measured Phosphate Buffer Capacity. The effect of these processes is also associated with a change in dehydrogenase activity. This provokes the problem on the production of humic substances with the help of zeolites. For this purpose, a method for their microbial activation has been developed. Clinoptilolite is a supporting agent of enzyme systems and a sorbent of excess metal cations and NH^{4+}.

These products also use turbomechanically activated zeolites. They are also used in gels for rooting cuttings.

In conclusion, it should be noted that worldwide the limitations are in the content of radioactive elements in some zeolite deposits.

Phytochemical screening and antioxidant activity of some medicinal plants' crude juices

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The present work was focused on evaluating the resultant crude juices from the mechanical pressing of some agricultural and food industries by-products i.e., pomegranate leaves and peels and leaves of fig, guava and olive as a source of naturalistic antioxidants. The results indicated that the amounts of polyphenols, flavonoids, tannins and anthocyanins in crude pomegranate peels juices were markedly higher than those of other crude juices under study. The polyphenolic constituents in fig leaves, pomegranate leaves and peels, guava leaves and olive leaves were distinguished using HPLC. The major compounds found in all crude juices were gallic acid, ellagic acid, naringenin, ferulic acid and methyl gallate, respectively. Pomegranate peels crude juice exhibited the highest antioxidant activity in comparison with other crude juices under study. In this context, pomegranate peels crude juice is a valuable source of health-promoting compounds, fulfilling concurrently the promising antioxidant activity that can be utilized virtually as food complements, to delay lipid oxidation and healing from particular ailments via its free radicals scavenging ability.

Influence of Cu^{2+} ions on the corrosion resistance of AZ31 magnesium alloy with microarc oxidation

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The objectives of this study were to reduce the corrosion rate and increase the cytocompatibility of AZ31 Mg alloy. Two coatings were considered. One coating contained MgO (MAO/AZ31). The other coating contained Cu^{2+} (Cu/MAO/AZ31), and it was produced on the AZ31 Mg alloy via microarc oxidation (MAO). Coating characterization was conducted using a set of methods, including scanning electron microscopy, energy-dispersive spectrometry, X-ray photoelectron spectroscopy, and X-ray diffraction. Corrosion properties were investigated through an electrochemical test, and a H_2 evolution measurement. The AZ31 Mg alloy with the Cu^{2+} containing coating showed an improved and more stable corrosion resistance compared with the MgO-containing coating and AZ31 Mg alloy specimen. Cell morphology observation and cytotoxicity test via Cell Counting Kit-8 assay showed that the Cu^{2+}-containing coating enhanced the proliferation of L-929 cells and did not induce a toxic effect, thus resulting in excellent cytocompatibility and biological activity. In summary, adding Cu ions to MAO coating improved the corrosion resistance and cytocompatibility of the coating.

Total remove amoxicillin from water using magnetic core functionalized with silver nanoparticles

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Remains of drugs, pesticides and other polluting substances are being found in sewage, rivers and other surface streams. These are the so-called emerging pollutants, compounds that are dumped into the water and are not regulated. Due to its impact on the environment, new processes of degradation or elimination of these pollutants in water are being studied [1, 2]. Amoxicillin is a drug widely used by humans, so the interest in proposing methods capable of eliminating this compound in water has been growing in recent years [3-5]. In this work a novel procedure for the total removal of amoxicillin, an emerging pollutant, from water samples using magnetic nanoparticles functionalized with nanometric silver (Fe_3O_4@AgNPs). Experimental conditions such as pH, contact time, temperature and adsorbate and adsorbent dose have been studied in order to achieve the total adsorption for different concentration of amoxicillin in water. For 10 and 100 mg/L of amoxicillin in water a maximum removal efficiency of 100% was reached at room temperature and pH=7 after 15 minutes of contact time between adsorbent and water samples under gentle shaking. The dose of adsorbent using to remove 10 and 100 mg/L of amoxicillin were 100 and 500 µL, respectively. Field emission scanning electron microscopy, energy dispersive X-ray spectroscopy, BET analysis, Fourier-transform infrared spectroscopy and differential scanning calorimetry were employed to characterize of the adsorbent. Recycling studies were carried out in order to desorbed and reused the adsorbent, the results shows that using 500 µL of NaOH solution 1 M during 15 minutes Fe_3O_4@AgNPs remain unaltered and can be used for two more additionally adsorption cycles and showing 93% adsorption efficiency after the third regeneration.

Nitric oxide, salicylic acid and kaolin effects on the biochemical traits and photosynthesis system of hazelnut cultivars during heat stress

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Hazelnut (*Corylus avellana L.*) is considered one of the essential nuts regarding the nutritional value and it generally is cultivated in temperate location to proper yield. Climate change is endangered hazelnut's optimum requirements and impose deleterious damage to the growth and yield production. However, the high temperature at Karaj was increased and fluctuated between 35-45, which is detrimental for development and growth. Nowadays, application of supportive chemicals as foliage spraying on plants for decreasing the effects of biotic and abiotic stresses has been of interest. This study was conducted on trees of six commercial hazelnuts under exogenous spraying of two phytohormones such as nitrogen monoxide (Nitric oxide), (salicylic acid), and inert silicate aluminum (kaolin (($Al_4Si_4O_{10}(OH)8$)). The experiment was conducted in a randomized complete block design with six replications in three-year-old hazelnut seedlings. In this study, nitric oxide (NO) was applied with three concentrations included (0 (control), 1.5 and 2.5 mM) salicylic acid (0, 1, 2.5), and kaolin (0, 3% and 6%) under 3 spraying program during July-August in 2017. Afterward, results demonstrated that photosynthetically active radiation PAR was improved under seedling's spraying by kA, SA, and NO treatment, respectively, in contrast, to control. Furthermore, KA 6% and SA 1 mM treatments positively affected about 50% increase in stomatal conductance compared to control, while NO did not significantly impact stomatal conductance compared to other treatments. In addition, 6% Kaolin and 2.5 NO improved chlorophyl content ((SPAD-5020) value nearly %15 and %10 compared to control. On the other hand, chlorophyll fluorescence significantly improved under the application of 6% kaolin, 2.5 mM NO, and 1 mM SA approximately 8%, 7%, and 5% compared to control. As a result, exogenous application of KA, SA and NO were ameliorated the adverse effects of high temperature through improve PAR distribution, photosynthesis system in a semi-arid location.

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Ionic Liquids: Unique extraction solvents for analytical sample preparation

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Ionic liquids, in older literature sometimes referred to as molten salts, are very valuable chemicals with extraordinary properties. By definition, they are ionic compounds with a melting temperature below 100°C. The low melting point and ionic conductivity are the two main characteristics, but many ionic liquids also have other unique physicochemical properties, such as nonflammability, negligible vapor pressure, thermal and electrochemical resistance, and the ability to dissolve organic and inorganic substances [1,2]. Within the last years, the attention to these compounds has rapidly increased, especially due to their universal applicability as solvents and the possibility to replace organic solvents, which are highly volatile, environmentally harmful and do not exhibit ionic properties. The physical and chemical characteristics mainly depend on the composition of the salt. As a result, it is possible to synthesize specifically designed ionic liquids for specific applications including analytical sample preparation, which is an essential step in modern analysis [3,4]. The main objective of analytical sample preparation is to isolate and if necessary enrich analytes of interest from complex matrices to ensure satisfying determinations by guaranteeing selectivity, accuracy, reproducibility and reliability of analysis [5,6]. A common sample preparation technique is liquid-phase microextraction, which has the advantage of both: isolation of analytes from interfering substances and high enrichment factors to enhance detection limits. In addition, this technique is faster, simpler and more environmentally-friendly than conventional liquid-liquid extraction methods [7]. Numerous scientific articles have already successfully applied ionic liquids as an extraction solvent in different liquid-phase microextraction techniques [8,9]. A relatively new class of ionic liquids are di(alkyloxy) imidazolium based room temperature ionic liquids, which have been successfully applied for the extraction of different analytes from various matrices by our working group and been published just recently [10–12].

Synthesis and *in-vitro* antimycobacterial activity of cinnamic acid hybrid of betulinic acid

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The purpose of the study is to develop new sets of efficacious anti-tuberculosis agent with multi-target activities against tuberculosis through the molecular hybridization of betulinic acid (BA) and cinnamic acid as Fig 1.

Methodology: The solvent directed synthesis of cinnamic derivative of betulinic acid at C-28 position was carried out successfully. The synthesized compounds were characterized by spectroscopic techniques and subsequently evaluated for antimycobacterial activity (MABA test, against $H_{37}RV$ [ATCC27294] and cytotoxicity (MTT test using Human embryonic kidney [HEK293] and Human hepatocellular carcinoma [HepG2] cell lines. Results: The synthesized compound above has anti-TB MIC values in the range of 85.20μM as against BA with activity of 109.48 μM and cinnamic acid with activity of 337.50 μM respectively. The cytotoxicity of the compound to the two human cell line (HEK 293 and HepG2) were in the range of $IC_{50} \geq 300$ μM, indicating low toxicity level and could serve as template for the synthesis of efficacious TB drugs.

Chemical ratchet in repressor binding to its operator mediated by one-dimensional diffusion

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One-dimensional diffusion of proteins along DNA is a unique DNA protein interaction that can kinetically enhance protein-DNA binding1. The diffusion eliminates the delay of binding, which is typically some seconds. Thus the diffusion is too rapid in regulating most of gene regulations unless it changes the binding affinity. However, the change is seemingly prohibited by the thermodynamic rule, detailed balance, which has been proved at binding equilibrium. According to hydroxyl-radical footprinting *in vitro, E. coli* TrpR repressor, showed a 10,000-fold change of its binding affinity for its operator, *trpO*, depending on the length of DNA harboring the site2, 3, which is called antenna effect. The detailed balance thus claims the possibility that a TrpR molecule can contact a looped DNA molecule at *trpO* and other sites on DNA, with the helix-turn-helix domain and other unknown protein surfaces. However, this looping mechanism was denied by an experiment using a short *trpO* connected to a long nonspecific DNA with phosphodiester or biotin-avidin interaction that likely inhibits one-dimensional diffusion3. Moreover, the diffusion mechanism was also suggested *in vivo* by the loss of TrpR repression activity by introducing a strong LexA binding site at various distances from the *trpO* to inhibit the diffuaion3. Thus, I collaborated theoretical chemists and noticed that experimental determination of the affinity requires only macroscopic equilibrium, but detailed balance requires the equilibrium at molecular level. In the presence of conformational changes with the timescale slower than or as slow as the binding2-4, binding equilibrium at molecular level is not required at macroscopic equilibrium. For example, TrpR-*trpO* complex is significantly dissociated by a slow DNA bending at the *trpO* site, the reaction is determined by alternating potential of mean force rather and described with two or more sets of kinetic schemes. In these cases, detailed balance is not guaranteed because the equilibrium at the molecular level has not been established. This mechanism is named "Chemical ratchet". Since, the deviation from detailed balance occurs at a molecular level, single-molecule evidence is required. We are going to show it.

In conclusion, chemical ratchet expanded the possible contribution of one-dimensional diffusion in biological regulations with much slower timescales of that of binding.

Solvent and solid phase extraction of rare-earth elements with Di-2-Ethylhexylphosphoric acid

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Rare earth elements (REE) are widely used in various branches of high-tech industry. Mineral ores are still the main source of REE. These ores are characterized by a low yttrium and lanthanides content in the presence of other components. For this reason, extraction remains the main method to recover them from complex water-salt solutions with low pH values. Industrial phosphoric acid solutions, obtained during apatite leaching by sulphuric acid, are used as a source of REE. These solutions are characterized by following composition: Ln (0,07-0,1%), where Ln – total REE content, P_2O_5 (16-22% or 3,08 mol/L H_3PO_4), SO_3 (1,3-1,5%), Al_2O_3 (0,1-0,2%), CaO (0,3-0,8%), Fe_2O_3 (0,1-0,2%), SiO_2 (0,7-1,4%), F (0,8-1,1%). The revealing of the thermodynamic and kinetic features of solvent extraction by di-2-ethylhexylphosphoric acid (D2EHPA) and solid-phase extraction of REE using Levextrel resin, contained D2EHPA, is the subject of this research. A weak dependence of the rate constant of liquid REE extraction on temperature and a significant dependence on the mixing rate was established, which characterizes the diffusion limiting stage. Extraction kinetics by Levextrel resin are described by Fick's second law equation, which establishes the laws of diffusion in the organic phase of the solid material grain. The factors impacting the concentration of heavy REE in the organic phase and their separation at the extraction and re-extraction stage are determined. Based on the revealed differences in the element extraction kinetics and thermodynamics of the extraction process, a conceptual scheme for the REE recovery from industrial solutions followed by separation into individual elements is developed. Resins chemically modified with grafted selective to REE ligands can be suggested for use in continuous processes with adsorption columns with a fixed or fluidized bed. The absence of significant amounts of flammable solvents, which accompany liquid extraction, complies with the principles of green chemistry.

Qualitative and semiquantitative determination of bromine in hybrid hydroxyurethanes poly(dimethylsiloxane) films containing phosphotungstates ([$PW_{12}O_{40}$]3-)

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In this study, hybrid poly(dimethylsiloxane)-derived hydroxyurethanes films (PDMSUr-PWA) containing phosphotungstic acid ($H3PW_{12}O_{40}$/PWA) were characterized using field emission gun scanning electron microscopy (FEG-SEM), in attenuated total reflectance Fourier transform mid-infrared mode (ATR FT-MIR), and analyzed using synchrotron radiation micro-X-ray fluorescence (SR-µXRF), synchrotron radiation grazing incidence X-ray fluorescence (SR-GIXRF), laser-induced breakdown spectroscopy (LIBS), and instrumental neutron activation analysis (NAA) in order to correlate the distribution patterns of tungsten and properties of PDMSUr-PWA films. PDMS constitute elastomers with good mechanical, thermal, and chemical (hydrophobicity/non-hygroscopy) resistance. Currently, products based on urethanes (e.g., polyurethanes) are widely used in many applications as plastics, fiber-reinforced polymers, high-performance adhesives, corrosion-resistant coatings, photochromic films, among others. The possibility to combine inorganic and organic components can produce a hybrid material with unique properties. PWA has an important role as agent against the corrosion of steel surfaces in different media, besides exhibiting amazing catalytic and photochromic properties in these films. PWA kept its structure inside of these hybrid films through interactions between the organic matrix of PDMSUr and silanol from the inorganic part (organically modified silica), as was shown using ATR FT-MIR spectra. The FEG-SEM/SR-µXRF/Wide-Angle X-ray Scattering (WAXS)/X-ray Diffraction (XRD)/Energy Dispersive X-ray results proved the presence of PWA in the composition of domains of PDMSUr-PWA films. At PWA concentrations higher than 50 wt%/wt, tungsten segregation across the thickness is predominant, while that at PWA concentrations lower than 35 wt%/wt, tungsten segregation at surface is predominant. Inhomogeneities in the tungsten distribution patterns (at micrometric and millimetric level) may play an important role in the mechanical properties of these films (elastic modulus and hardness).

Innovative photoactive admixtures for concrete and cement-based plaster finishes, to create self-cleaning surfaces

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This article presents research and development on innovative photoactive admixtures for concrete and cement-based plasters for the finishing of concrete surfaces. The goal was to provide the resulting surfaces of these newly developed materials with a self-cleaning ability stemming from photocatalytic reaction during exposure to UV radiation. This research and development was part of a project supported by the Czech Ministry of Industry and Trade, in the TRIO programme; and in cooperation with BETOSAN s.r.o., the Technical University of Liberec, the Institute of Inorganic chemistry of the Czech Academy of Sciences and the J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences. The first type of developed material is a photocatalytically active admixture in powder form, allowing the preparation of concrete surfaces with photocatalytic properties. The second type of developed material is a photocatalytically active cement-based plaster, intended primarily for application to a concrete substrate. Each of the materials has two final versions. In the case of the plaster this includes the preparation of two colour variants, specifically white and grey. For the powdered cement admixture we prepared two types based on their application. This means two different types of admixtures mixed throughout the entire volume of the concrete or only in the surface layer of the concrete. We envisage exterior applications on the self-cleaning outer shell of buildings, as well as treatment of the surface layer of various structures such as bridges, noise barriers, traffic barriers and tunnels. The materials created could also be used in interiors under specific conditions (UV LED lights), with anticipated uses in the healthcare and food processing industries.

Formation of surface self-assembled organosilicon nanolayers on carbon steel and its effect on electrochemical and corrosion behavior of the metal

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With the usinпg Fourier transformed infrared (FT-IR) spectroscopy, scanning electron spectroscopy(SEM) and energy dispersive x-ray spectroscopy(EDX), the adsorption of vinyltrimethoxysilane on the surface of carbon steel from an aqueous solution and surface self-assembled organosilicon nanolayers formation have been studied. The mechanism of formation of the surface self-assembled nanolayer is proposed. It have been shown that during adsorption organosilanes interact with hydroxil radicals of a metal surface with Fe-O-Si bonds formation. The effect of organosilicon nanolayers on the electrochemical behavior of carbon steel was studied by obtaining anodic polarization curves. It is shown that the presence on the surface of vinyl and diamine-containing siloxane nanolayers on the surface leads to a significant reduction in the critical passivation current of steel, i.e. surface organosilicon nanolayers contribute to passivation of steel. In addition, it have been found that in the presence of organosilicon nanolayers on a metal surface causes the shift of critical potential of pitting formation of steel to the region of positive values, which indicates the inhibition of localized anodic dissolution of the metal. Accelerated corrosion tests of steel samples in the climatic chamber were carried out and the corrosion inhibiting effect of vinyl-containing surface nanolayers was shown. It have been established that vinyl-containing soiloxane surface self-assembled nanolayer is resistant to anodic polarization action, which usually contributesunifiorm and localized dissoltution of metals. As have been shown by FT-IR spectroscopy, the surface nanolayer is presented on a metal surface after anodic polarization. The results obtained indicate on the stability of siloxane nanolayers to water and corrosion-active components of an electrolyte action and to change of surface morphology due to dissolution of surface metal atoms with the release of metal ions into solution.

In silico toxicity assessment of emerging fire resistant chemical released from e-waste materials

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Electronic waste (e-waste) sites are the key source for the emission of emerging brominated fire-resistant chemicals (NBFRs). These chemicals negatively affect the environment and human health because of its high environmental persistence and structural similarity with thyroid hormones. In this study, we have performed the reactivity profiling and thyroid disruption potency analysis of twelve NBFRs released from different e-waste sites.We have conducted screening and prioritization of NBFRs on the basis of their degree of bromination by using Quantitative Structure Activity Relationship (QSAR) based models. Further DFT based global reactivity analysis and molecular interaction with thyroid receptor (TR) β has been evaluated. Binding free energy values are proficient to interpret the interactions between the binding sites of the receptor and ligands. The results indicate that the presence of heteroatoms other than bromine also plays a crucial role in the toxicity of this series of NBFRs. Both structural and interaction studies have given evidence that NBFRs are potentially persistent in nature and have the capacity to disrupt the thyroid endocrine system.

A comprehensive review of the global efforts on COVID-19 vaccine development

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The outbreak of COVID-19 sparked an unprecedented effort around the world to discover effective treatments and vaccines against SARS-CoV-2 virus. Despite the Emergency Use Authorization (EUA) of a few therapeutics, safe and effective COVID-19 vaccines are necessary to mitigate the pandemic and allow a return to normalcy. To promote understanding of COVID-19 vaccinology, we provide an overview of the vaccine development landscape and summarize the advantages and challenges surrounding various vaccine platforms, including conventional platforms (live-attenuated and inactivated vaccines), recombinant viral protein-based platforms (protein subunit and virus-like particle vaccines), viral vector-based platforms, and nucleic acid-based platforms (DNA- and mRNA-based vaccines). We then discuss COVID-19 candidate vaccines in clinical trials and those recently approved. We also address the use of adjuvants and delivery systems relevant to COVID-19 vaccine development. In addition, we analyze research trends in published journal articles and patents related to COVID-19 vaccine development in the CAS content collection and provide a landscape of these documents. The novel platforms and technologies catalyzed by this pandemic may also shape future vaccine development when new viruses emerge.

Triazol ylimino-DNA interaction by UV–Vis spectroscopy

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To efficiently design improved therapeutic agent, study of molecule-DNA interaction is a crucial step. In our previous study, we investigated comprehensive mechanism of some 1,2,4 triazol-4-ylimino derivatives, and they exhibited excellent *in vitro* anti-cancer activities. Out of all compounds studied previously (E)-3-((4H-1,2,4 triazol-4-ylimino) methyl) benzene-1,2-diol (TMB) demonstrated the best anti-cancer activity. This prompted us to explore its action mechanism by interacting the compound with the Salmon Sperm DNA. UV–Vis spectroscopic technique was employed as a tool to study this mechanism at two different temperatures. A slight bathochromic shift along with a noticeable hypochromic effect appears signalling interaction of the molecules with DNA. Spectroscopic results indicating hypsochromic as well as bathochromic shifts in the peak maxima upon changed concentration of TMB in constant amount of DNA demonstrate that TMB-DNA binding took place. To interpret the TMB-DNA interaction mechanism, adsorption of TMB on various concentrations of salmon sperm DNA was investigated. It was found that the adsorption of TMB decreased with increased concentrations of DNA. Kb value for TMB-DNA complexation is in the range of 105 which suggests that this binding take place via intercalation mode. Electrostatic attraction between TMB and DNA, and interactions among TMB molecules deemed to play a role in the interaction mechanism. UV–Vis spectroscopic technique used as a tool to study TMB-DNA complexation mechanism at two different temperatures to evaluate thermodynamic parameters of complexation process. Thermodynamic data obtained indicates the thermodynamic feasibility of overall process. This work offered an insight to molecular mechanism of the interaction between TMB and tumour cells. It further offered a valuable standpoint to the design novel 1,2,4 triazol-4-ylimino derivatives based anticancer compounds.

Proteomics approach for COVID 19: New perspectives in target therapy strategies

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World Health Organisation declared COVID-19 a pandemic on March 11, 2020. It was temporarily named as 2019-nCoV then subsequently named as COVID-19 virus. A coronavirus is a group of viruses, known to be zoonotic, causing illness ranging from acute to mild respiratory infections. These are spherical or pleomorphic enveloped particles containing positive sense RNA. The virus enters host cells, its uncoated genetic material transcribes, and translates. Since it has started spreading rapidly, protective measures have been taken all over the world. However, its transmission has been proved to be unstoppable and the absence of an effective drug makes the situation worse. The scientific community has gone all out to discover and develop a possible vaccine or a competent antiviral drug. Other domains of biological sciences that promise effective results and target somewhat stable entities that are proteins, could be very useful in this time of crisis. Proteomics and metabolomics are the vast fields that are equipped with sufficient technologies to face this challenge. Various protein separation and identification techniques are available which facilitates the analysis of various type interactions among proteins and their evolutionary lineages. The presented review aims at confronting the question: 'how proteomics can help in tackling SARS-CoV-2'. It deals with the role of upcoming proteome technology in these pandemic situations and discusses the proteomics approach towards the COVID-19 dilemma.

Physicochemical and bioactivity characterization of *Moringa* gum: Prospects and perspectives for applications in food and therapeutics

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Moringa gum exudates are mucoadhesive polymers derived from the stem of Miracle tree, M. oleifera. Part from being used in various traditional medicines, properties of these gum exudates as suspending and binding agent has also been well established. Even though *Moringa* gum has a wide range of applications in food and medicine, but due to tedious harvesting methods and less knowledge of physicochemical properties, its uses have been restricted to the research laboratories only. Thus, in order to optimize uses of these gum exudates at industrial scale, a detailed knowledge about structural and physicochemical constituents is the first and foremost requirement, which can lead to prepare stable and non-reactive formulations. Thus, in this study comprehensive characterization of the *Moringa* gum exudates to gain detailed knowledge of its structural, chemical, physical and biological properties was performed. Being sparingly soluble in water, extracts of gum was prepared in different solvent systems using both hot and cold extraction methods. Further, deacetylation of gum was done to identify functional groups having central role in maintaining the structural integrity of the gum. The findings revealed that acetyl groups play important role in the structural integrity of the gum and its deacetylation resulted in formation of a mesh with scattered and fibrillar particles with reduced pore size (0.2 μm) than that of the aqueous gum (0.5 μm). This hydrocolloidal gum polymer was amorphous in nature and showed maximum thermal stability in alkaline solvent system. Carbohydrate derivatives constituted its major (>80%) part while other metabolites including terpenes and fatty acids were present in traces. The preliminary findings of this study have not only laid the foundation for its applications in preparation of drug formulations with sustained release, but has also confirmed its bioligand and gelling properties. Moreover, the non-toxic nature and inherent medicinal properties of the gum make it an excellent substitute for its conventional/ chemical counterparts in both food and therapeutic preparations.

Unravelling a potential bacteriocin produced by ethnophyto-microbiome originated *Bacillus Subtilis* (MK733983)

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Massive utilization of antibiotics has radically expanded the emergence of antibiotic-resistant microbes. Resistant microbes adapt multifarious mechanisms to survive various impacts of antibiotics. This is an alarmingly evolving health hazard threatening existing medical practices, global health, and economy. On the other hand, scarcity of novel antimicrobials in recent years is worsening the situation. Present research reveals an anti-mycobacterial bacteriocin (Antimicrobial peptide) of ethnophytomedicinal originated *Bacillus subtilis* (MK733983). The optimization of the microbe enhanced the bacteriocin activity by 33% and showed many stable characteristics. The bacteriocin was purified using RP-HPLC and elution with 65% acetonitrile showed highest antimicrobial activity with *Mycobacterium smegmatis*. Its specific activity and purification fold increased by 70.5% and 44%, respectively, compared to crude. Its molecular weight was estimated to be 3.40287KDa by LC-ESI-MS/MS analysis. The bacteriocin is non-hemolytic and exhibited a broad inhibition spectrum with standard strains of *Staphylococcus aureus, Pseudomonas aeruginosa, Klebsiella pneumoniae, Escherichia coli* and *Chromobacterium violaceum*. Scanning Electron Microscopy observations showed cell annihilation with pores in cell membranes of *S. aureus* and *P. aeruginosa* treated with the bacteriocin, implicating bactericidal mode of action. Antibiofilm capacity of the bacteriocin with prioritized standard strains has shown significant biofilm inhibition and eradication and was confirmed with scanning electron microscope observations. It exhibited remarkable synergistic potential with 9 front line antibiotics. MTT assay on 3T3 cell lines revealed its non-cytotoxic nature and was reconfirmed by trypan-blue staining. Bacteriocins are promising antibiotic alternatives and the findings of the present study are competent to be considered.

Assessment of DNA-damaging potential of quinones of bisphenol analogues: Quantum mechanics and molecular dynamics based approaches

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Bisphenol A (BPA) is largely used for consumer and industrial applications. Its occurrence as well as exposure has led to adverse impact. One such impact associated with BPA is genotoxicity, via the formation of DNA adduct by BPA quinone (BPAQ) metabolite. Recently, large number of analogues are developed to substitute BPA, which is leading to a high environmental exposure. This mass replacement has emerged as a matter of concern as the usage of these chemicals remains unregulated and unrestricted. Analogues like, 3,3′-dimethylbisphenol A (DMBPA) and Bisphenol F (BPF) are recently reported for their ability to act as genotoxicant. However, a mode of mechanism of genotoxicity remains unidentified. In our present study, we have proposed a tentative mode of mechanism as depicted in figure 1, which highlights the role of quinones leading to genotoxicity.

Thus, to investigate this, we have performed a complete reactivity profile calculation using DFT based QM approaches of quinones of BPF, DMBPA and compared with BPA quinone. Next, we have analyzed the quinone-DNA interaction using molecular interaction technique. Further, to check the stability of the quinone-DNA complex, Molecular Dynamics simulation for 50 ns was performed and lastly, using g_mmbpsa, different energies like non-polar solvation energy, polar solvation energy, potential energy, and average binding energy were calculated. With this, the nucleotide residues involved in ligand binding were also analyzed. A similar action spectrum was obtained for all the quinones as the electrophilicity index was observed to be high. With this, DFT based charge transfer calculation confirmed the flow of electrons taking place from nucleotides (Adenine and Guanine) to the metabolites. MD simulations revealed their structural intricacies of quinone-DNA interaction highlighting the role of different energies in stabilizing the complex. It was observed that structural similarity plays a major role behind the genotoxicity induced by Bisphenols.

Cytotoxicity of *Mimusops Caffra based* ursolic acid, oleanolic acid and derivatives against human cancerous and non –cancerous cell lines

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According to World Health Organization, cancer is still leading cause of death for humans worldwide. Although over 100 chemotherapeutic agents are currently available for the treatment of cancer patients, the overall long term clinical benefit is disappointing due to the lack of effectiveness or severe side effects from these drugs. The use of complementary and alternative medicinal products from plants has continued to increase in past decades, due to fewer side effects compared to synthetic drugs. The main aim of this study is to extract, isolate, identify, semi-synthesize and elucidate pentacyclic triterpenoids namely ursolic acid (1) and oleanolic acid (2) from *Mimusops caffra* and derivatives including 3-O-acetyl ursolic acid (3), methyl 3β-acetylurs-12-ene-28-oate (4) and methyl ursolate (5) with the evaluation of these compounds as anti-cancer therapeutic agents. *In vitro* cytotoxicity activities of compounds 1–5 against various cancer cell lines such as human breast adenocarcinoma cancer (MDA), human liver cancer (HepG2), human prostate cancer (PC3) and non-cancerous human fibroblast (KMST-6), using MTT assay (assessment of oxydoreductive activity of mitochondria measurement of capacity to decrease the stain in living cells) compared to 5 μM Camptothecin (standard drug) and untreated cells. The compounds 2 and 5 exhibited remarkable cytotoxic activities in all cancerous cells at IC50 values ranging 0.156–5 μM, while little or no cytotoxicity activities were observed on non-cancerous cell lines which indicate that the addition of methyl at C-28 of UA is essential to enhance its activity as a therapeutic agent for cancer. The remainder of the compounds (1, 3 and 4) showed moderate cytotoxicity against the different cancer cell lines. Moreover, these results suggest that ursolic acid, its isomer oleanolic acid and UA derivatives are potential therapeutic drugs for human breast, liver and prostate cancers. *In vivo* anticancer research of the studied compounds is recommended for future studies.

Carbon nanomaterials as “Electrochemical sensing surface” for the examination of body fluids of persons suffering from various diseases: A decennium study (2010 -2020)

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Determination of biomolecules and drugs in human body fluids” has a great role in the detection of diseases, sports doping cases, and poisoning cases. However, it is not so easy to translate biological information in the form of electronic signals because it is very difficult to connect the electronic device directly to the biological media. To overcome these problems nanomaterials modified electrochemical sensors are a good alternative to conventional devices as these are highly sensitive, selective, inexpensive, and quick resulting. These sensors can effectively translate the biological information into an electrical signal. Furthermore, the sensors using fullerenes, carbon nanotubes, and metal nanoparticles as surface modifiers offer the additional possibility of signal amplification that improves analytical performance. The carbon nanomaterials have good conductivity and stiffness, unique electrical and catalytic property that increases the overall efficiency of the detection system. These sensors are utilized successfully in the proposed study to determine a wide range of biologically important molecules like amino acid, bronchodilators, nucleic acid, steroids, neurotransmitters, pharmaceuticals, and doping agents in various sensing media such as urine and blood plasma samples. In this study, the real samples are collected from the patients suffering from carcinoma, depression, diabetes, angina, asthma and, pregnant women and, athletes abusing doping agents. These nanomaterials modified voltammetric sensors are simple, rapid, easy to handle, having a low cost, and can be used for on-site determinations. This study explores the uses of developed nanomaterials modified sensors in the field of doping, pharmacy, medical and health issues.

Biosensors for the detection of viruses and cancer cells- An emerging technology for point of care diagnostics

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Early diagnostic and effective therapy are two of the important benchmarks for the early detection of life threatening viruses and cancer cells. Exosomes from viral cells may be important candidates for reliable biomarkers for the detection evaluation of tumor. In this study, Human interferon α2 (IFNα2) and thymosin α1 (Tα1) are therapeutic proteins used for the treatment of viral infections and different types of cancer. Both IFNα2 and Tα1 show a synergic effect in their activities when used in combination. Furthermore, the therapeutic fusion proteins produced through the genetic fusion of two genes can exhibit several therapeutic functions in one molecule. In this study, we determined the anticancer and antiviral effect of human Interferon α2-Thymosin α1 fusion protein (IFNα2-Tα1) produced in our laboratory for the first time. We discuss the candidature of exosomal biomarkers for the detection of cancers, which can be employed for indicative diagnostic and treatment responses by incorporating IFNα2 and Tα1 with the cancer-derived exosomes on biosensors. Further electrochemical recognition of viral cells was done by chronampermoteric studies which comprise integrated scientific development of bioelectrochemical engineering and important figure of merits related with electrochemical aspects. Furthermore, advanced research directions and aspects in using viral-derived exosomes and recombinant with therapeutic proteins for point-of-care (POC) testing and bio sensory technology will be presented.

Free radical and oxidative stress in pathological processes in cardiovascular disease

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It is well known that atherogenesis is characteristic of the process of LDL oxidation in a special grade of atherogenesis by means of LDL oxidative alteration. The study recommends 15-lipoxygenase to be considered in the early ranges of atherogenesis for LDL oxidation, while the later stages of non-enzymatic arachidonate oxidation are more essential. In LDL atherosclerotic patients were observed an expansion of the product linoleic acid oxidization (hydroxy fatty acids). It was also found that development of relatively severe atherosclerosis and atherosclerosis regression in people depended on the production level and activity of the superoxides NADPH oxidase. Lactosylceramide glycosphingolopide supports atherosclerosis with NADPH oxidase activation.

High blood pressure ratio and low heat capacity ratio lead to aneurysm, hemorrhagic stroke and other neurological disorders

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Evidences are escalating on the diverse neurological disorders associated with COVID-19 pandemic. The theoretical discovery of internal flow choking (Biofluid / Sanal flow choking) in the cardiovascular system is a paradigm shift in the diagnostic science of asymptomatic stroke causing neurological disorders in earth and at the microgravity condition (human spaceflight). A critical review has been carried out herein for correlating the phenomenon of Sanal flow choking and hemorrhagic stroke. Herein, we show that when systolic-to-diastolic blood-pressure-ratio (BPR) reaches the lower-critical-hemorrhage-index (LCHI) the internal flow choking and shock wave generation occurs in the downstream region of the vessels, with sudden expansion, divergence, bifurcation, stenosis and/or occlusion, leading to pressure-overshoot causing aneurysm, brain hemorrhage and/or neurological disorders. The critical BPR for internal flow choking is uniquely regulating by the biofluid/blood-heat-capacity-ratio (BHCR). The BHCR is well correlated with BPR and blood-viscosity. The closed-form analytical model reveals that the relatively high and the low blood-viscosity are risk factors of internal flow choking causing aneurysm and hemorrhagic stroke. *In vitro* data shows that fresh blood samples of healthy subjects evaporate at a temperature range of 37 - 400 C (98.6 - 104^0 F) and generate carbon dioxide, nitrogen, and oxygen gases in the vessel. The single phase *in silico* results demonstrated the occurrence of Sanal flow choking and pressure-overshoot causing memory effect (stroke history) leading to progressive neurological disorders. We concluded that disproportionate blood thinning medication increases the risk of flow choking causing hemorrhagic stroke. The risk of brain hemorrhage and various types of neurological disorders in COVID-19 patients and others in earth and microgravity environment could be diminished by concurrently lessening the viscosity of biofluid/blood and flow turbulence by increasing the thermal tolerance level in terms of BHCR and/or by decreasing the BPR. The effect of Sanal flow choking is more severe in blood vessels with divergent/bifurcation regions because it leads to the shock-wave generation and the transient pressure-overshoot causing irreversible neuronal damage forming the core of infarction. We concluded that, for a healthy-life all subjects with high-BPR inevitably have high-BHCR for reducing the risk of the internal flow choking (biofluid/Sanal flow choking) triggering neurological disorders as results of infraction.

Poly(sugar acid): Novel acidic polysaccharide poly[3-(3,4-dihydroxyphenyl)glyceric acid] from medicinal plants of boraginaceae family, its synthetic analogues and their comparative anticancer efficacy

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The main chemical constituent of high molecular (>1000 kDa) water-soluble preparations from medicinal plants of *Symphytum asperum, S.caucasicum, S.officinale, S.grandiflorum, Anchusa italica, Cynoglossum officinale* and *Borago officinalis* (Boraginaceae) according to data of liquid-state 1H, 13C NMR, 2D 1H/13C HSQC, 2D DOSY and solid-state 13C NMR spectra was found to be poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] or poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA). The polyoxyethylene chain is the backbone of this regular polymer with the repeating unit 3-(3,4-dihydroxyphenyl)glyceric acid residue. PDPGA as a 3,4-dihydroxyphenyl derivative of poly(glyceric acid ether) belongs to a novel class of acidic polysaccharides [poly(sugar acids)] as well. Its basic monomeric moiety glyceric acid is a natural three-carbon sugar acid which is oxidative form of aldotriose glyceraldehyde. The monomer of PDPGA 3-(3,4-dihydroxyphenyl) glyceric acid was synthesized via Sharpless asymmetric dihydroxylation of trans-caffeic acid using a potassium osmate catalyst which is new finding in sugar acids. Methylated derivative of PDPGA was synthesized via ring opening polymerization of 2-methoxycarbonyl-3-(3,4-dimethoxyphenyl)oxirane using a cationic initiator (BF3•OEt2). Human Hyaluronidase (Hyal-1) degrades high molecular mass Hyaluronic acid (HA) into smaller fragments which have pro-inflammatory effects. PDPGA possesses the ability to inhibit the enzymatic activity of Hyal-1 completely. Consequently PDPGA exhibited anti-inflammatory efficacy. PDPGA and its synthetic monomer suppressed the growth and induced death in androgen-dependent (LNCaP) and -independent (22Rv1) human prostate cancer (PCA) cells. PDPGA induced apoptotic death by activating caspases, and also strongly decreased androgen receptor and prostate specific antigen (PSA) expression. In 22Rv1 xenograft model male athymic nude mice with 22Rv1 xenografts was administered orally of PDPGA. Plasma analyses revealed that PDPGA administration caused a strong dose-dependent decrease in PSA levels by 87%. Anticancer efficacy of PDPGA against PCA cells is more compared to its synthetic monomer. Methylated PDPGA did not show any activity against PCA. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity.

Synthesis and *in-vitro* anti mycobacterial activity of cinnamic acid hybrid of oleanolic acid

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The purpose of the study is to develop new sets of efficacious anti-tuberculosis agent with multi-target activities against tuberculosis through the molecular hybridization of oleanolic acid (OA) and cinnamic acid as Fig 1.

Methodology: The solvent directed synthesis of cinnamic derivative of oleanolic acid (OA) at C-28 position was carried out successfully. The synthesized compounds were characterized by using spectroscopic techniques and subsequently evaluated for antimycobacterial activity (MABA test, against H37RV [ATCC27294] and cytotoxicity (MTT test using Human embryonic kidney [HEK293] and Human hepatocellular carcinoma [HepG2] cell lines. Results: The synthesized compound above has anti-TB MIC values in the range of 48.05μM as against OA with activity of 42.04 μM and cinnamic acid with activity of 337.50 μM respectively. The cytotoxicity of the compound to the two human cell line (HEK 293 and HepG2) were in the range of IC50 ≥ 300 μM, indicating low toxicity level and may be a drug candidate for future.

Development of a cost-effective medium for *Photorhabdus temperata* bioinsecticide production from wastewater and exploration of performance kinetic

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To improve *Photorhabdus temperata* bioinsecticide production in wastewater (WS4), used as a low-cost feedstock, an experimental design was developed by response surface methodology. Box-Behnken design (BBD) was used to evaluate the effects of carbon to nitrogen ratio (C/N), sodium chloride concentration and inoculum size on *P. temperata* biomass production and insecticidal activity. For an enhanced bioinsecticide production, the optimum operating conditions were as follows: inoculum size=4%; C/N ratio=12.5 and [NaCl]=4 g/L for two responses. 1.95 and 2.75 fold improvements in oral toxicity and biomass production were respectively obtained in the cost-effective medium developed in this study (WS4 I) using the three variables at their optimal values. Under the optimized conditions, WS4 I-grown cells exhibited higher membrane integrity according to flow cytometry analysis since dead cells presented only 9.2% compared to 29.2% in WS4. From batch fermentations carried out in WS4 I and WS4, *P. temperata* kinetic parameters in terms of biomass production and substrate consumption rates were modeled. The obtained results showed that the maximum specific growth rate in WS4 I was of 0.43 h-1 while that obtained in WS4 was of 0.14 h-1. In addition, the efficiency of *P. temperata* to metabolize organic carbon was enhanced by optimizing the culture conditions. It reached 72.66% instead of 46.18% in the control fermentation after 10 h of incubation. Under the optimized conditions, *P. temperata* cells showed the highest specific consumption rate resulting in a toxin synthesis improvement.

Spectroscopic ellipsometry characterization of be-implanted gan epilayer: Effect of thermal annealing on optical properties

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Beryllium ions with an energy of 50 keV and a dose of 5 × 1014 cm^{-2} were implanted into gallium nitride thin films grown by low-pressure metalorganic chemical vapor deposition. After implantation, rapid thermal annealing was carried out for 40 s at temperature 600°C, 900 °C and 1100°C with N_2 as the ambient gas. The variable-angle spectroscopic ellipsometry measurements were carried out to study the surface roughness, the thickness, and optical properties of beryllium-implanted gallium nitride thin films in the wavelength range of 200-1600 nm. The thickness, refractive indices and extinction coefficients of the Be-implanted films were obtained both at room temperature and variable temperature. The mean depths of beryllium implantation acquired by the transport of ions in matter simulation are good agreement with spectroscopic ellipsometry fitting data. The crystal quality of samples was evaluated by a dual-beam ultraviolet-visible spectrophotometer, showing that the quality of the rapid thermal annealing sample is better than that of an unannealed sample. However, the thickness of the surface roughness layer increases due to partial surface decomposition in the process of thermal annealing. The bandgap of Be-implanted films follows the Varshni empirical equation and changes from 3.328 eV to 3.083 eV in the temperature range from 300 K to 850 K.

Bioanalytical method validation of acrylamide and glycidamide in dried blood spot using ultra high performance liquid chromatography tandem mass spectrometry

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Universitas Indonesia, Indonesia

Acrylamide (AA) is a carcinogenic compound that can be found in food, coffee, and cigarette smoke. When it enters the human body, acrylamide will be metabolized by CYP2E1 to glycidamide (GA) which can then react with DNA to form DNA adducts. To analyze acrylamide and glycidamide simultaneously in the blood, the biosampling technique commonly used is venipuncture which is invasive and requires special expertise. In this study, the biosampling technique used is dried blood spot (DBS) which is easy and non-invasive. Methods for analyzing acrylamide and glycidamide simultaneously using DBS have not been carried out in previous studies. Therefore, this study aims to obtain an optimal and validated method of acrylamide and glycidamide simultaneous analysis using propanamide as an internal standard. Samples were prepared by protein precipitation using methanol and water (1: 1). Separation of compounds used Acquity® UPLC BEH C18 column (1.7 µm, 2.1 mm x 100 mm), eluted at a flow rate of 0.20 mL/min under gradient conditions with a mobile phase of 0.2% formic acid in water and acetonitrile for 5 minutes. Quantification was performed using triple quadrupole mass spectrometry with positive electrospray ionization and multiple reaction monitoring (MRM) mode set at m / z 72.0> 55.02 for acrylamide, 88.1> 44.0 for glycidamide, and 74.01> 57.1 for propanamide. The lowest limit of quantification is obtained at 1 µg / ml for both acrylamide and glycidamide. The range of linear concentration is between 1 - 40 µg / ml. The analysis method is validated according to FDA 2018 guidelines.

Magnetic core-modified silver nanoparticles for removal of ibuprofen as emerging pollutant in waters

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Pharmaceuticals are products used in large doses in daily life considered as contaminants of emerging concern. Due to the large amounts of drugs consumed, the hydrogenic sources suffer from contamination processes that give rise to toxicological effects in humans despite its low concentrations 1,2. Many medicines considered as emerging contaminants are constantly detected in groundwater, wastewater treatment plants and water supply. The inefficiency of conventional methods used in water treatment plants to remove the contaminant motivates the development of effective methods to treat effluent contamination 3. According to the physico-chemical properties of drugs, their degradation products and the characteristics of the soils, these substances can reach the groundwater and contaminate the aquifers or remain retained in the soil, thus affecting the ecosystem and humans through the food chain [4]. Additionally, the portion of medicines not assimilated by the organism, as well as chemical substances administered to animals, usually become part of wastewater. Consequently, different ways of removing medicines in waters have been studied [5].

A novel procedure for ibuprofen adsorption from waters employing magnetic core-modified silver nanoparticles. We demonstrate that 93% adsorption of ibuprofen is achieved in 45 minutes by means of a simple method, for neutral pH and room temperature, also using a low dose of adsorbent, equal to 7 mg in 500 µL of suspension. The characterization of the adsorbent, before and after adsorption, was carried out by means of field emission scanning electron microscopy, energy dispersive X-ray spectroscopy, BET analysis, Fourier-transform infrared spectroscopy and differential scanning calorimetry. It is worth pointing out that ibuprofen can be desorbed and the adsorbent can be reused, remaining unaltered for the first three cycles, and showing 89.3% adsorption efficiency after the third regeneration. A three-parameter model and the Langmuir isotherm characterize the kinetics and isotherm of adsorption.

Extraction technique of trap states based on transient photo-voltage measurement

Z. Lin
Renmin University of China, China

I put forward a technique for extracting the density of trap states (DOST) distribution based on the transient photo-voltage (TPV) measurement result. We prove that when the TPV result is linear, the DOST distribution is exponential type and vice versa. Compared to the approach based on the space charge limited current measurement, the method given in this paper has the advantage of requiring less calculation. The results obtained by our method provides a guidance for preparing less trap states solar cells.

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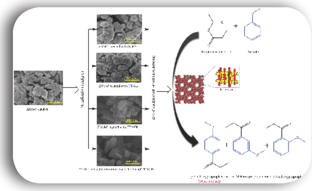

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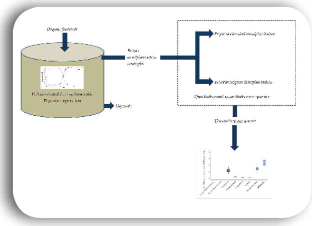

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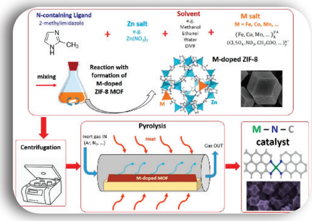

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