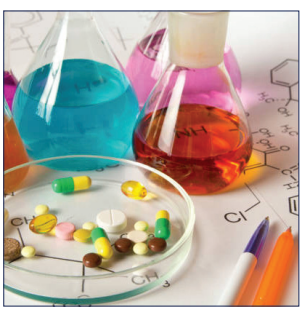
Scientific Tracks & Sessions
May 13, 2019

Chemistry 2019







9th World Congress on

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May 13-14, 2019 | Prague, Czech Republic

Sharina Abu Hanifah, Asian J Biomed Pharmaceut Sci, Volume:9
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Functional polymer for polymer electrolyte and biosensor applications

Sharina Abu Hanifah
Universiti Kebangsaan, Malaysia

For the past decade, much attention was focused on polysaccharide natural resources and methacrylate polymer for various purposes. Our group has been interested into functionalized polymer for exploring novel functions. Throughout the works, several efforts were done to prepare new function of chitosan by chemical modifications for biopolymer electrolyte. We focus on the synthesis of the chitosan derivative, namely, O-nitrochitosan which was synthesized at various compositions of sodium hydroxide. Its potential as biopolymer electrolytes was studied. We also have been working on functionalized polymer for the fabrication of Sunset Yellow and Tartrazine biosensors. The polymer used was in the form of thin film and microspheres for Sunset Yellow and Tartrazine biosensors respectively. The biosensor for Sunset Yellow was developed by coating a peelable poly (acrylamide-co-ethyl methacrylate) film with immobilized laccase prepared by photopolymerization on a glassy carbon electrode (GCE). Tartrazine biosensor was designed with a functionalized methacrylate-acrylate microsphere immobilized with laccase and gold nanoparticles composite coated on a carbon paste screen printed electrode. Both biosensors were analyzed by cyclic voltammetry (CV) and differential pulse voltammetry (DPV).

Speaker Biography

Sharina Abu Hanifah received her BSc (Chemical Technology) in 2004 and graduated her PhD (Chemistry) in 2008 from Universiti Kebangsaan Malaysia under the supervision of Prof Lee Yook Heng. During her PhD study, she was an invited researcher at the Institute of Biotechnology, University of Cambridge, United Kingdom. She specializes in functionalized polymer for various applications including sensor and polymer electrolyte. Currently she obtained a grant for endocrine disrupting chemical biosensor based on aptamer.

e: sharina@ukm.edu.my

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A comprehensive study on the bioactive compounds of pharmaceutical interest present in *Cannabis sativa L*.

Federica Pellati
University of Modena and Reggio Emilia, Italy

Cannabis sativa l. is a dioecious plant belonging to the *Cannabaceae* family. The main compounds present in this plant are represented by cannabinoids, flavonoids and terpenes. Among cannabinoids, Δ^9-tetrahydrocannabinol (Δ^9-THC) is responsible for Cannabis psychoactive effects. Other main cannabinoids include tetrahydrocannabinolic acid (THCA), cannabinol (CBN), cannabidiol (CBD) and cannabidiolic acid (CBDA). For what concerns other phenolic compounds, flavonoids have also been identified in C. *sativa*, belonging mainly to flavones and dihydrostilbenoids. In particular, cannflavin A and B represent *Cannabis*-specific methylated isoprenoid flavones. Terpenes represent the largest group of *Cannabis* components and they are responsible for its aromatic properties.

In this view, a detailed study on the above-mentioned compounds is highly recommended to guarantee a rational use of *Cannabis* for therapeutic purposes. In the light of all the above, the present work was aimed at the comprehensive analysis of the bioactive components present in C. *sativa* by means of innovative methods. In particular, the profiling of cannabinoids in extracts was carried out by means of a HPLC-UV/DAD, ESI-MS and MS^2 method, together with a selective extraction protocol, by taking advantage of the innovative fused-core technology of the stationary phase. A new RP-HPLC-UV/DAD, ESI-MS and MS^2 method, together with an optimized extraction procedure, was developed as well and applied for the determination of phenolics (including *cannflavin A, cannflavin B* and *canniprene*). The study on *Cannabis* volatile compounds was performed by developing a new method based on HS-SPME coupled with GC-MS and GC-FID.

The methods described above were applied to both drug-type and fibre-type *Cannabis* samples. These procedures were found to be suitable for the multi-component chemical analysis C. *sativa* inflorescences in order to ensure their quality, efficacy and safety.

Speaker Biography

Federica Pellati graduated cum laude in 2000 in Pharmaceutical Chemistry and Technology at the Faculty of Pharmacy of the University of Modena and Reggio Emilia. In 2004 she got a PhD degree in Pharmaceutical Sciences. Then she had a post-doctoral fellowship position in Medicinal Chemistry and in 2006 she got a position of Assistant Professor in Medicinal Chemistry at the University of Modena and Reggio Emilia. In 2014, she got the Italian Professorship Qualification (ASN 2012) as an Associate Professor in Medicinal Chemistry.

Her research activity is focused on the development of innovative techniques for the extraction and analysis of bioactive natural products, and on the isolation of new bioactive compounds of natural origin. She has a number of national and international research collaborations and she participates to peer-reviewed research projects.

She is the author of more than 60 papers in ISI indexed international journals, n. 3 book chapters, n. 4 proceedings in international journals, n. 2 patents and more than 90 congress communications (oral and poster). She is an associated editor, an editorial board member and a reviewer for international Journals in the area of Pharmaceutical, Plant and Food Analysis.

e: Federica.pellati@unimore.it

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Bioinspired membrane systems state-of-the art and innovative solution to overcome main limits

Rosalinda Mazzei
National Research Council of Italy, Italy

Nanostructured microporous membranes functionalized with biomolecules are very suitable for the development of biohybrid and biomimetic systems which find application in various fields including biocatalysis, biomedicine and biotechnology. The system simulates the biological membrane environmental like, where the biological system can be heterogenized inside/on the membrane and its passage can be regulated by controlled fluid dynamic conditions. Despite the advantages of nature simulation by bio-inspired materials application, there are some issues which need to be addressed in order to achieve the development of such systems. The main problems are related to both biomolecule stability as well as membrane cleaning and re-use.

Analyzing the use of membrane bioreactor (MBR) technology in patents development as well as their industrial application, it seems that the major development has been obtained by MBR for water treatment, whilst lower efforts have been devoted to MBR for pharmaceutical, food, cosmetics, etc. This is mainly due to more strict regulations that govern the discharge of waste water into the environment. However, the need to promote more sustainable processes for industrial production will force the development of MBR also in other fields, including biorefinery for bioderived chemicals.

In this work, alternative strategies to solve problems related to membrane stability/enzyme re-use will be described (e.g. the use of biofunctionalized nanoparticles integrated with membrane process). A deep understanding of biomolecule immobilization on membrane will be illustrated by using different biomolecule and functionalized membranes, to proof the concept of membrane versatility. In addition a biocatalytic multiphasic intensified membrane system, able produce and compartmentalize poor water stable antioxidant molecules will be also described, with the aim to provide alternative strategies for process intensification.

Speaker Biography

Rosalinda Mazzei received her PhD from University of Calabria (UNICAL) in 2009 and she is currently a researcher of the Institute on Membrane Technology since 2011. Her expertise is in the development of biohybrid membrane process for catalysis, integrated membrane process and in process intensification. She won different prizes in international conferences and she has recently started to collaborate with different Universities such as Leuven (Belgium), University of Federico Santa Maria (Chile), School of food Engineering Pontificia, Universidad Catolica de Valparaìso (Chile), Universidad Industrial de Santander (Colombia) etc. She published about 50 articles on international journal and more than 10 chapters on books.

e: r.mazzei@itm.cnr.it

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Hierarchical SERS substrate of Au Film over Nanosphere (AUFON) fabricated by Ion-Beam Sputtering Deposition

Hong Wang[1], Zongwei Xu[2], Ying Song[2], Liyang Wang[2] and **Zhen Yin[1]**
[1] Tianjin Polytechnic University, China
[2] Tianjin University, China

In this paper, basing on the method of ion-beam sputtering deposition and the self-assembly of polystyrene (PS) colloidal spheres, the preparation and characterization of Au film over nanosphere (AuFON) hierarchical Surface Enhance Raman Scattering (SERS) substrate were studied. Firstly, the influence of Au film thickness on the hierarchical SERS substrate of polystyrene nanospheres with diameters of 200nm was characterized. Experiments show that when the Au film thickness is 50nm, the density of nano-gaps between the PS colloidal spheres and the SERS substrates enhancement both reach the optimal level. The micro-morphological differences of AuFON SERS substrates prepared by electron beam deposition and ion-beam sputtering deposition were compared and analyzed from the perspective of coating atoms' energy and the polymer modification by ion bombardment. Furthermore, under the condition of optimal coating thickness, the absorption spectrum indicates that the frequency of LSPR (λmax=650, 656nm) is closest to the frequency of the excitation light in SERS spectra measured (λex=633nm). The FDTD simulation showed that the electromagnetic field intensity of the SERS substrate reached the maximum when the gaps between the coated spheres were about 5nm and the diameter of the Au clusters covering the PS sphere surface was about 20-30nm. Finally, the SERS substrates were used to detect the trace elements of melamine and Sudan III successfully.

Speaker Biography

Hong Wang, Dr. Engineering, Associate Professor, State Key Laboratory of Hollow Fiber Membrane Materials and Processes, School of Materials Science and Engineering, Tianjin Polytechnic University, China. Her main research interests include, Raman Spectroscopy, Surface Enhance Raman Scattering techniques, wastewater treatment by an electrocatalytic membrane reactor, etc.

e: waho7808@163.com

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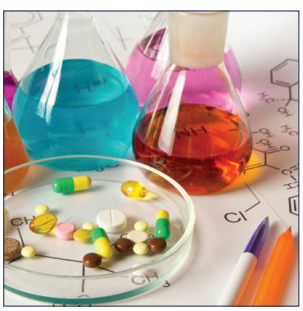

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Chemical characterization and evaluation of the antibacterial activity of essential oils from fibre-type *Cannabis sativa L*. (hemp)

Virginia Brighenti, Ramona Iseppi, Carla Sabia, Patrizia Messi, Stefania Benvenuti and **Federica Pellati**
University of Modena and Reggio Emilia, Italy

The main phytochemicals that are found in *Cannabis sativa L*. are cannabinoids and terpenes, reaching up to 42% of the identified molecules. Terpenes represent the largest group of *Cannabis* components and they are responsible for its aromatic properties. Even if many studies have been focused on cannabinoid components in *Cannabis*, little research has been carried out on its terpenic compounds

In the light of all the above, in the present work the phytochemical composition of seventeen essential oils from different fibre-type varieties of *Cannabis sativa* L. (hemp) was deeply investigated by means of GC-FID and GC-MS techniques. In total 89 compounds were identified and the semi-quantitative analysis revealed that α- and β-pinene, myrcene and β-caryophyllene are the major terpenes in all the essential oils analysed.

The antibacterial activity of hemp essential oils against some pathogenic and spoilage microorganisms isolated from food and food processing environment was also determined. The inhibitory effects of the essential oils were evaluated by both Agar Well Diffusion assay and Minimum Inhibitory Concentration (MIC) determination. By using the agar diffusion method and considering the zone of inhibition, it was possible to preliminarily verify the inhibitory activity on most of the examined strains. The results showed that the lowest MIC values were obtained, in particular, with six hemp essential oil against the Gram-positives bacteria, such as *Listeria monocytogenes, Staphylococcus aureus, Staphylococcus epidermidis, Enterococcus faecalis* and against *Bacillus* spp. spoilage bacteria.

The results obtained in this study demonstrate that hemp essential oils can reduce or inhibit bacteria proliferation, thus proving a valid support to reduce microorganism contamination especially in the food processing field.

Speaker Biography

Virginia Brighenti graduated in 2013 in Pharmaceutical Chemistry and Technology at the Department of Life Sciences of the University of Modena and Reggio Emilia. In 2018 she got a PhD degree in Clinical and Experimental Medicine. Currently she covers a post-doctoral fellowship position in Medicinal Chemistry at the Department of Life Sciences of the University of Modena and Reggio Emilia. Her research activity is mainly focused on the development of innovative techniques for the extraction and analysis of bioactive natural products, and on the isolation of new bioactive compounds of natural origin with antioxidant and antiproliferative activity. She is the author of 15 papers in ISI indexed international journals, and more than 20 congress communications (oral and poster).

e: virginia.brighenti@unimore.it

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Organic peroxides: From elusive intermediates to reagents and synthetic targets

Vera A Vil, Yana A Barsegyan, Maria V Ekimova, Oleg V Bityukov, Gabriel dos Passos Gomes, Igor V Alabugin and **Alexander O Terent'ev**
N D Zelinsky Institute of Organic Chemistry, Russia

For a long time, organic chemists thought about peroxides as an explosive high energy functionality that should be either avoided or used in selected niche applications as radical initiators, explosives, or oxidizing reagents. However, a recent revolution, illustrated by the 2015 Nobel Prize in Medicine, brought organic peroxide in the spotlight as a new promising class of medicinal and agricultural agents. In recent decades, interest to organic peroxides has been boosted by the discovery of their antimalarial, anthelmintic, antitumor, growth regulation, and antitubercular activities.

I will outline new methods that allow efficient preparation of new classes of organic peroxides. In particular, I will disclose the utility of BF_3-catalyzed H_2O_2-mediated cyclizations that transform a variety of acyclic precursors, β-ketoesters and their silyl enol ethers, alkyl enol ethers, enol acetates, and cyclic acetals into β-hydroperoxy-β-peroxylactones. The mild reduction of the respective β-hydroperoxy-β-peroxylactones opened access to previously elusive cyclic Criegee intermediates of Baeyer-Villiger reaction as stable β-hydroxy-β-peroxylactones. Despite the great importance of this >100-year old reaction in organic synthesis and industrial chemistry, these intermediates have never been isolated and structurally characterized. β-Peroxylactones, the new class of organic peroxides, are stable compounds that can be useful for further synthetic transformations, as well as new targets for medicinal chemistry and plant protection.

This study was supported by Russian Science Foundation (Grant № 18-73-00315).

Speaker Biography

Vera A Vil has completed her PhD at the age of 27 at the N. D. Zelinsky Institute of Organic Chemistry RAS, Russian Federation where she continues as a research scientist. Her studies focus on oxidational processes in organic synthesis, medicinal chemistry, and agrochemistry. She published over 30 publications that have been cited over 400 times (top 5 papers cited on average >50 times/paper).

e: vil@ioc.ac.ru

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Migration of toxic metals from wood and wax crayons: Exposure assessment of children in pre-school age

Nikola M, Jelena T, Djogo Mracevic, Danijela Djukic-Cosic, Marko Krstic and **Slavica Razic**
University of Belgrade, Serbia

Chemical exposure of children, especially from toys and crayons, as items in their every day use, is of increased concern in the last decades. In this study the concentration and migration of toxic metals from wood and wax crayons were determined, as well as their intakes which were assessed in the case of swallowing a part of crayon. Total concentration of Pb *(Lead)*, Cd *(Cadmium)*, As *(Arsenic)*, Cr *(Chromium)* and Ni *(Nickel)* were analyzed in 60 samples from 10 manufacturers of wooden and wax crayons of different colors. Microwave acid digestion followed by simulations of the saline extraction conditions was performed. Aim was to determine the concentrations of toxic metals that could leach out from the crayons during children's mouthing behaviours (chewing and sucking). Exposure assessment was conducted in accordance with methodology for toxic metals in children toys recommended by Holland institute for public health and environmental protection (RIVM). Method of evaluation was inductively coupled plasma optical spectroscopy (ICP-OES). The total concentrations of metals in the crayons ranged from 0.032-16.415 mg/kg, 4.31-614.75 µg/kg, 0.213-5.779 mg/kg, 0.163-11.174 mg/kg, 0.036-6.629 mg/kg for Pb, Cd, As, Cr and Ni respectively. Sb levels were 0.10-3.14 mg/kg and nondetectable in saliva. Availability studies showed concentrations ranging from 0.146-0.786 mg/kg, 3.73-100 µg/kg, 0.112-2.509 mg/kg, 0.084-4.037 mg/kg, 0.0112-0.4098 mg/kg for Pb, Cd, As, Cr and Ni respectively after saline extraction. For all measured values % TDI *(Tolerable Daily Intake)* for investigated metals is lower than 10% TDI, which is considered the upper limit for metal intake in this way. The obtained results have shown that in majority of tested samples the toxic metal content is below the WHO limits. The calculated levels of toxic metal intakes due to chewing or swallowing the parts of wood and wax crayons acceptable in all tested samples as well.

Speaker Biography

Nikola M is student on Faculty of Pharmacy, University of Belgrade, Serbia. Jelena T has comleted her Integrated academic studies from Faculty of Pharmacy, University of Belgrade, Serbia. They took part in 59th Serbian students' conference of biomedical sciences with international participation and in 52nd Days of preventive medicine. They presented this study which was conducted as part of a student scientific research work.

e: nikolamitrovic712@gmail.com
e: jtrisic94@gmail.com

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Engineered Metal Oxide Nanoparticles, Nano-Bio Interaction and Toxicology

Muhammad Furqan Danish
Antalya Bilim University, Turkey

Metal oxide nanoparticles (NPs) are usually utilized nanomaterials. The Nano-level size offer these metal oxides capability of novel properties resulting in top of the line advancements as well as in customer arranged applications. Nanotechnology is most recent undertaking, which has progressed hugely in most recent couple of years, however regardless it needs well laid rules and top to bottom toxicological investigations. How these metal oxide NPs and their ionic structure will respond in fluctuating organic interface and long-haul impacts are not very much characterized? In our exploration we have made an endeavor to think about the intense and ceaseless impacts of the normally utilized metal oxide nanoparticles, Al2O3 NPs and ZnO NPs in Drosophila melanogaster. The presentation portion incorporates 0.1-1mM NPs in Drosophila diet and flies were uncovered all through their life expectancy. Toxicological impacts post presentation was assessed on different parameters like: climbing capacity, fruitfulness, life expectancy, oxidative pressure, apoptosis and rate of deviant phenotype in ensuing ages. Critical decrease in climbing capacity was seen in parent flies on seven days introduction to these NPs. Critical increment in receptive oxidative species and apoptotic cells was seen in hatchlings hemocytes through DCF-DA and TUNEL test. Particular abnormal phenotypic changes like twisted portioned thorax, loss of wing, distorted body symmetry was seen in resulting age on ZnO NPs presentation. Perpetual introduction of Al2O3 NPs brought about flies with pigmented and sectioned thorax and disfigured legs. Our perceptions obviously delineated that these nanoparticles can make negative impacts consequent ages.

Speaker Biography

Muhammad Furqan Danish done BS organic chemistry from Pakistan. He completed his thesis work on the topic of synthesis of nanoparticles from sea weeds. He has 2 years pharmaceutical experience as a quality control analyst and handling multi instruments in pharmaceutical industry. And then he came turkey for higher education and got an admission Antalya Bilim University and doing MBA.

e: danish.furqan@yahoo.com

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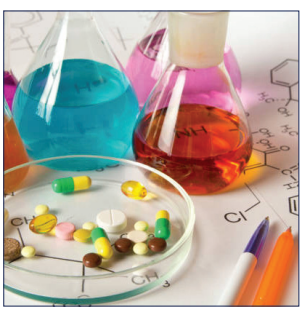

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Synthesis of Voltage Gated Sodium Channel Blockers (VGSCB)

Bölcskei H[1,2]
[1]Budapest University of Technology and Economics, Hungary
[2]Gedeon Richter Plc., Hungary

Voltage gated sodium channels play an important role in the physiological processes of the central nervous system. The main therapeutic areas are epilepsy, various types of pain, migraine and spasticity. In this talk the key aspects and difficulties (e.g. hERG activity) of the development of the new compounds with VGSCB activity will be demonstrated on three examples.

1) Company Gedeon RICHTER developed the centrally acting muscle relaxant Mydeton. Searching its derivatives, many aryloxy-alkyl-amines were synthetized, changing the aromatic moiety, the spacer, the amine function.
2) An HTS was the starting point of the development of NaV1.7 Subtype selective sodium channel blockers. Various members of an aryl- and heteroarylsubstituted benzyloxy-benzylamine compound family were prepared.
3) Targeting the obscessive compulsive disorder, compounds were prepared with dual activity: VGSCB and serotonin reuptake inhibitory activity. We focused on dextormethorphan derivatives. The best compounds were tested in vivo (marble burying test) too.

Speaker Biography

Bölcskei H has completed her MSc study as a chemical engineer from University of Technology, Budapest, Hungary. She received her PhD in 1979 at the same university, and her scientific degree "candidate of sciences" in 1988 from the Hungarian Academy of Sciences. Between 1973-2013 she worked as a researcher at the Hungarian pharmaceutical company Gedeon Richter Plc. Since 2009 she has been working as the associate professor of University of Technology and Economics, Budapest, Hungary. Her main research interest: alkaloid chemistry, organic chemistry, medicinal chemistry. She has over 60 publications that have been cited over 200 times.

e: h.bolcskei@mail.bme.hu

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20 years of G-quadruplex ligands: From synthesis to relevant biological activity

Marco Franceschin
University of Rome, Italy

G-Quadruplexes represent a group of unusual DNA secondary structures, based on Hoogsteen G–G paired hydrophobic planar rings consisting of four guanine units. Many studies have shown that G-quadruplex structures appear to be involved in several important biological processes, such as DNA replication, gene expression and recombination, as well as cell transformation. Some of the first G-quadruplex ligands (namely perylene and anthracene derivatives) were published by L.H. Hurleyand S. Neidle in 1998/1999. Starting from 2001, inspired by their works, we synthesized several perylene derivatives with different side chains and studied their chemical properties and biological activity, with the aim to understand the relevant molecular features. In the following years, based on these results and through improved syntheses, we prepared novel and more promising aromatic compounds: berberine and palmatine derivatives (from natural compounds), triazatruxene, xanthene and xanthone derived compounds, as well as, more recently, coronene derivatives. After 20 years, some of these compounds have shown very interesting biological effects, based on their ability to bind specific G-quadruplex structures, both on telomers, affecting therefore telomerase activity, and on oncogene promoting sequences, leading to antiproliferative effects and thus representing new potential selective anticancer drugs. In this Keynote Speech, an overview of the most interesting results will be given in order to understand future perspectives.

Speaker Biography

Marco Franceschin graduated cum laude from the 'Sapienza' in 2001, where he successively earned a PhD degree in Chemistry in 2005, including a significant period of research activity at the School of Pharmacy, University College London. Until 2011 he was a post-doc in the same University of Rome: with over 10 years research experience in the field of G-quadruplex ligands, leading to more than 30 international publications (h-index 18). His work included organic synthesis, characterization of the synthesized compounds and the study of DNA/ligand interactions by means of gel electrophoresis, spectroscopic techniques, molecular modeling simulations and mass spectrometry, as well as their biological activity. He has been qualified as associate professor of both Organic Chemistry and Medicinal Chemistry, holding a temporary teaching position as professor of organic chemistry for students in Biotechnology at the Faculty of Sciences of the University of Rome 'Sapienza' from 2014 to 2018.

e: marco.franceschin@uniroma1.it

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Membrane-based approaches for creating multifunctional tools for Neuronal Tissue-Engineering

Sabrina Morelli
National Research Council of Italy, Italy

Current research in neural tissue engineering is focused on the realization of *in vitro* advanced devices that enhance the neuronal growth and differentiation by mimicking specific features of the in vivo environment. Among the different devices used in neuroscience, membrane-based systems are promising approaches for culturing neuronal cells, offering a homogeneous environment in which the proper topographical, mechanical and biological conditions trigger the specific cellular organization. They offer a broad range of application in developing neuronal functional analogue or substitutes allowing cutting edge investigations in neuroscience field. Indeed, they represent both innovative devices to be used in restoring peripheral nerve damage by boosting its regeneration and valuable *in vitro* platforms for the investigation of new molecules for neurodegenerative diseases treatments.

Within this scenario, this talk will discuss the multifunctional role of biohybrid membrane systems in neuronal tissue engineering as innovative *in vitro* platforms with a well-controlled microenvironment, that enhance nervous system repair by guiding neuronal growth and differentiation. For the design of an advanced neuronal tissue-engineered constructs, membrane properties, including morphological, structural, mechanical, physicochemical, and electrical properties, are key elements in dictating cellular behavior and in controlling new tissue formation. An important challenge in neuronal tissue engineering is the optimization of the design parameters for the realization of novel instructive biomaterials able to promote neuronal outgrowth. To this purpose, different collagen-blend membranes were realized by combining collagen with chitosan (CHT) or poly (lactic-co-glycolic acid) (PLGA) to enhance their properties and thus create new biofunctional materials and permissive environment with great potential use for neuronal tissue engineering and regeneration. Collagen blending strongly affected membrane properties. It improved the surface hydrophilicity of both, pure CHT and PLGA membranes, reduced the stiffness of CHT membranes, but it did not modify the good mechanical properties of PLGA membranes.

Another challenging aspect in the field of neuronal tissue engineering is to create innovative tools capable of promoting cellular response in terms of neuronal orientation that may be used as investigational platforms for studying neurobiological events and neurodegenerative disorders. Our strategy was to develop high performing neuronal membrane bioreactors as a platform for the in vitro reconstruction of neuronal networks with defined functional, geometric, and neuroanatomical features. A novel membrane bioreactor was created to test the capacity of neuronal cells to react to topographical stimuli thus guiding their orientation and to provide a 3Dwell-controlled microenvironment for neuronal outgrowth. The peculiar component within the device namely the poly(lactic-L-acid) (PLLA) highly aligned and packed microtube array membrane, together with the perfusion system, offers a high grade of fidelity for cell growth and elongation thus leading cell polarisation and orientation. PLLA membrane bioreactor offers a continuous perfusion to the cells with oxygenated medium and removal of catabolites avoiding profile concentration and shear stress. It promotes long-term growth and differentiation of neuronal cells, and guided neurite alignment giving rise to a 3D neuronal tissue-like construct.

Our studies have provided new insights regarding the effects of membrane properties on neuronal behavior, and thus it may help to design and improve novel instructive biomaterials for neuronal tissue engineering.

Speaker Biography

Sabrina Morelli, Dr. in Animal Biology, is Researcher Scientist at the Institute on Membrane Technology of the National Research Council of Italy (ITM-CNR). She has expertise in the field of bioartificial membrane devices, especially in the realization of advanced membrane systems for creating 3D engineered tissues and organs for regenerative medicine, pharmacological screening, and as investigational platforms for studying physiological and/or pathological processes. She was scientific responsible for CNR of a PRIN project granted by Italian Ministry of Education, University and Research and she is also involved in several international projects, in the organizing committee of international conferences, in the referee pool of scientific journals. She is co-author of over 70 peer-review scientific papers published in international journals, chapters in books and encyclopedia.

e: s.morelli@itm.cnr.it

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Hydrogen-to-synfuels via Transition Metal Oxide (TMO) catalysts

Spadaro Lorenzo, Palella Alessandra and **Arena Francesco**
National Research Council of Italy, Italy

Growing concerns about environmental pollution and energy shortages have prompted new seeks in the field of chemistry and sustainable processes, for meeting human development goals while at the same time protecting the environment and preserving natural resources. On this address, European Community nations have adopted new Policies for a sustainable development, aiming to replace the fossil source and modify the traditional refinery by introducing renewable bio-feedstock. Furthermore, the utilization of CO_2 as "raw material" for the synthesis of value-added products (oils, solvents, chemicals, etc.) appears one of the most promising strategic route for a "greener economy". To meet these goals, it become imperative the design and development of novel advanced catalytic processes and materials, timely designed for the manufacturing of efficient, safe and environmentally benign fuels starting from various feedstock, ranging from bio-oil to carbon oxides. Many transition metals are differently active catalytic materials in the hydrogenation reactions, at temperatures between 180-360°C and pressure up to 100 bar. The chemical properties of the diverse transition elements can deeply affect the selectivity path of the hydrogenation reactions, modifying the products distribution and the hydrocarbon chain length of products. Therefore, a series of different catalytic formulations based have been proved and compared in the synthesis of green-fuels via hydrotreating processes. This work is aimed to ascertaining the feasibility of hydrogenation processes under industrial conditions for the advanced syn-fuel production, establishing the effect of the catalytic formulation on catalytic performance.

Speaker Biography

Spadaro Lorenzo is senior researcher and qualified professor of Industrial Chemistry. He has received his education at the Universities of Messina, Reggio Calabria, Turin and Rome, obtaining Ph.D. and Sc.D. in Industrial Chemistry and Chemical Engineering. Since 2007 he has been researcher of the National Research Council of Italy (CNR) and University Lecturer of several courses in Catalysis, Advanced Materials, Fuels and Renewable Energy, Green-Chemistry, Process Engineering and Chemistry. His main research activities concern the "Design of Catalysts and Industrial Processes for Energetic and Environmental Applications". He's co-author of about 300 technical-scientific documents and owner of several international industrial patents.

e: lorenzo.spadaro@itae.cnr.it

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Bioactive Natural Products

Severina Pacifico
University of Campania, Italy

Plants biosynthesize small organic compounds, known as secondary metabolites, which are an integral part of the plant's developmental program as they are involved in complex biotic and abiotic interactions, acting as signal, defense or protectant compounds. Several of these naturally occurring substances, broadly recognized to exert pharmacological or toxicological effects in humans and animals, are still the main source of lead molecules in modern drug discovery and development, and make the natural products research an endless and intriguing research field with multidisciplinary approach.

Nowadays, the research for secondary metabolites with health promoting effects in countering or slowing-down chronic and degenerative diseases (e.g. cancer, cardiovascular, and neurodegenerative diseases) identify phenols and polyphenols, widespread and mostly copious in dietary plant sources, as beneficial for human health. These compounds, as intrinsically antioxidant, are claimed as nutraceuticals with preventive efficacy in offsetting oxidant species over-genesis in normal cells, and with the potential ability to halt or reverse oxidative stress-related diseases. In this context, pure (poly)phenols and/or their herbal/food complex were found to exert both anti- and pro-oxidant activities, suggesting also a promising chemopreventive efficacy. In fact, different evidences further highlight their ability to induce apoptosis, growth arrest, DNA synthesis inhibition and/or modulation of signal transduction pathways. Indeed, a full understanding of the phenolic and polyphenolic composition of plant species, which still now represent their inestimable and worth exploring source, is an important challenge, which today can and must be favourably pursued in the consciousness that the bioactivity of a plant extract is always in its chemistry.

This talk will deepen into polyphenol research, focusing on biosynthesis, analytical approaches and exploitable activity of plant extracts rich in antioxidant and anti-inflammatory polyphenols and/or pure isolated polyphenols, which could significantly benefit human health and wellbeing towards non-communicable diseases.

Speaker Biography

Severina Pacifico is associate professor in Food Chemistry at the University of Campania "Luigi Vanvitelli" (Italy). Her research interest, in the field of Natural Products and Food Chemistry primarily aims to the phytochemical study of medicinal and/or edible plants; to the chemical characterization of secondary metabolites by spectroscopic and spectrometric techniques; to UHPLC-HRMS/MS metabolic profiling and fingerprinting of natural extracts; and to the evaluation of antioxidant, chemopreventive and neuroprotective properties of natural products (phytocomplexes and secondary metabolites therein).

e: severina.pacifico@unicampania.it

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Innovative carbon-based materials for solid state hydrogen storage and energy storage

Milanese Chiara
University of Pavia, Italy

Alkali cluster-intercalated fullerides (ACIF) consist in crystalline nanostructures in which positively charged metal clusters are ionically bond to negatively charged C_{60} molecules, forming charge-transfer salts. These compounds have been recently investigated with renewed interest, appearing as a novel class of materials for hydrogen storage, thanks to their proved capability to uptake reversibly high amounts of hydrogen via a complex chemisorption mechanism. In this presentation, after a short summary on the hydrogen storage topic, the synthesis, the structural investigation and the hydrogen storage properties of Li, Na and mixed Li-Na clusters intercalated fullerides belonging to the families $Na_xLi12_{-x}C_{60}$ ($0 \le x \le 12$) and $Na_xLi\ 6_{-x}C_{60}$ ($0 \le x \le 6$) will be presented. By manometric and thermal analyses it has been proved that C_{60} covalently binds up to 5.5 wt% H_2 at moderate temperature and pressure, thanks to the catalytic effect of the intercalated alkali clusters. Moreover, the destabilizing effect of Na in the co-intercalated Na_xLi_6-xC_{60} compounds leads to an improvement of the hydrogen-sorption kinetics by about 70%, linked to a decrease in the desorption enthalpy from 62 to 44 kJ/mol H_2. The addition of Pt and Pd nanoparticles to Li fullerides increases up to 5.9 wt% H_2 the absorption performances and of about 35 % the absorption rate. The ammonia storage properties of Li_6C_{60} have also been investigated, resulting quite appealing. Being the price of C_{60} quite high for large scale practical applications, new cheaper C based materials are under examination. In particular, porous biochar from agricultural waste are giving quite interesting results as electrode materials for high-performance supercapacitors.

Speaker Biography

Milanese Chiara is associate professor of Physical Chemistry at the Chemistry Department of the University of Pavia (Italy). Her main research interests regard the synthesis of innovative nanomaterials for solid state hydrogen storage and for energy storage, their physico-chemical characterization and the evaluation of their storage performance. In the last 5 years, her attention was mainly focused on C-based materials, in particular fullerene derivatives and biochar. She is author of 165 papers on materials science topics and she is expert of the IEA Task 40 "Energy storage and conversion based on hydrogen".

e: chiara.milanese@unipv.it

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Silver and copper nanoparticles by the pulsed plasma in liquid and their antibacterial properties

Emil Omurzak
Kyrgyz-Turkish Manas University, Kyrgyzstan

One of the most important properties of silver nanoparticles is their antimicrobial action against several bacteria, fungi, and viruses. Surprisingly, nano Ag are safe and non-toxic to human and animal cells at low concentrations because the possible toxicity of silver nanoparticles to the environment is considered extremely low as compared to other materials.

Silver and coppr nanoparticles were prepared by using pulsed plasma in liquid method. This is a low voltage pulsed spark discharge in a dielectric liquid. The electrodes of about 2 mm in diameter and about 10 mm in length made of pure silver rods were submerged in a 50 ml pyrex beaker filled with deionized water and plasma (200 V, 50 A (peak), 10 μs) was generated between the silver electrodes for about 15 min. Polyvinylpyrrolidone (PVP), Cetyl trimethylammonium bromide (CTAB), Sodium n-Dodecyl Sulphate (SDS) were used as a stabilizing agents.

The XRD spectra of the prepared samples indicated the face-centered cubic crystalline structure of metallic silver nanoparticles. Spherically shaped silver nanoparticles of diameter 2.2 ± 0.8 nm were synthesized by the pulsed plasma in aqueous solution with PVP surfactant. Similarly, silver nanoparticles of diameter 1.9 ± 0.4 nm size were obtained with SDS surfactant. *In vitro* antibacterial properties of all the synthesized silver nanoparticles against the Gram-negative bacteria Escherichia coli were examined by Kirby–Bauer disk diffusion susceptibility method. It was noticed that the stabilized with SDS silver nanoparticles demonstrated a better antibacterial activity against bacterial strains as compared to the silver nanoparticles stabilized with PVP, CTAB.

Speaker Biography

Emil Omurzak, Dr. Industrial Enginering, graduated from Physics and Electronics Department, Kyrgyz State National University in 2002. He worked for the National Academy of Sciences of Kyrgyzstan in 2002 – 2004 at the Institute of Physics, Laboratory of Plasma Technologies and Institute of Chemistry and Chemical Technology, Laboratory of Nanotechnology as scientist. From 2004 until 2008, he studied PhD course at the Kumamoto University, Graduate School of Science and Technology and obtained Doctor of Engineering degree in 2008 for the dissertation work "Synthesis of Nanomaterials by Impulse Plasma in Liquid". After that he worked as postdoctoral fellow at the central laboratory of Kumamoto University Innovation Collaboration Organization. From 2009 to 2015, he worked as specially appointed Assistant Professor at the Kumamoto University. Since 2015, he is Assistant Professor of the Chemical Engineering Department, Faculty of Engineering, Kyrgyz-Turkish Manas University. He has published more than 30 papers and 10 patents. His research is focused on the synthesis of nanomaterials by the pulsed plasma in liquid method and studying their physical and chemical properties for bio-medical, physical, chemical applications.

e: emil.omurzak@manas.edu.kg

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H_2S producing enzyme, 3-mercaptopyruvate sulfurtransferase

Noriyuki Nagahara
Nippon Medical School, Japan

3-Mercaptopyruvate sulfurtransferase (MST, EC 2.8.1.2) is a cystine-catabolizing enzyme involved in the mercaptopyruvate pathway and evolutionarily related to mitochondrial rhodanese (TST, EC 2.8.1.1). MST is a 33 kDa simple protein enzyme, which catalyzes transsulfuration reaction. An active site Cys^{247} is the site of persulfide formation during catalysis (Nagahara *et al*., J Biol Chem, 2005, Nagahara & Sawada, 2006, Nagahara *et al*., J Biol Chem, 2007). MST is found in all the tissues in rat and mouse; however, its activity differs in each tissue. Subcellular fractionation analysis revealed that eukaryotic MST activity was observed in both the cytoplasm and mitochondria (Nagahara *et al*., Histochem. Cell Biol, 1998, Tomita *et al*., Molecules, 2016). Interestingly, it is distributed in both prokaryotes and eukaryotes. MST has been demonstrated to serve multiple roles (Nagahara et al., Methods Enzymol, 2015, Nagahara, Bri J Pharmacol, 2018) as H_2S and polysulfide production (Ida *et al*., Proc Natl Acad Sci USA, 2014, Kimura *et al*., Sci Rep, 2015, Mikami *et al*., Biochem J, 2011, Shibuya *et al*., Antioxid Redox Signal, 2008, Yadav *et al*., J Biol Chem, 2013, Nagahara *et al*., Biochem Biophys Res Commun, 2018), antioxidant action (Nagahara and Katayama, J Biol Chem, 2005, Nagahara *et al*., J Biol Chem, 2007), possible SOx production (Nagahara *et al*., Antioxid Redox Signal, 2012), and possible anxiolytic-like effect (Nagahara *et al*. Sci Rep, 2013).

It has been reported that hydrogen sulfide and polysulfides were produced by cystathionine β-synthase (EC 4.2.1.22) (Abe and Kimura, J Neurosci, 1996), cystathionine γ-lyase (EC 4.4.1.1) (Hosoki *et al*., Biochem Biophys Res Commun, 1997), TST (Kimura *et al*., Sci Rep, 2015; Mikami *et al*., J Biol Chem, 2011) and MST. As to antioxidative function, MST activity is regulated by thioredoxin-dependent redox-sensing molecular switches; one switch is a catalytic site cysteine forming a low redox potential sulfenate under oxidized conditions which is reversibly converted to an inactive form MST. The other one is exposed cysteines outside enzyme forming a disulfide between MSTs under oxidized conditions to be inactive dimeric form. We are now investigating physiological role of MST using MST-knockout (KO) and double TST and MST-KO mice. Recently, we further reported H_2S and polysulfide production by MST *in vitro* (Nagahara *et al*., Biochem Biophys Res Commun, 2018).

Speaker Biography

Noriyuki Nagahara, MD., PhD., Biochemistry and Pathological Chemistry, is associate professor of Nippon Medical School. He makes a special study of medical biochemistry, molecular biology and organic chemistry, especially reaction mechanism and enzyme kinetic study on a transsulfuration enzyme, mercaptopyruvate sulfurtransferase (MST). He first purified rat MST to homogeneity and succeeded cloning. He found MST was evolutionarily related to mitochondrial rhodanese via substitution of amino acids in the active site by genetic engineering techniques. He certified that MST was an antioxidant enzyme. Recently, he produced MST-knockout mouse to clarify physiological roles of MST and a pathogenesis of congenital metabolic disease caused by deficiency of MST, mercaptolactate-cysteine disulfiduria.

e: noriyuki@nms.ac.jp

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A Theoretical Study of Copper Sulfide Nanoalloy Clusters: Density Functional Approach

Tanmoy Chakraborty
Manipal University, India

Importance of Nano clusters of Copper sulfides (CuS) is well known due to its interesting properties. Our group have studied nanoalloy clusters of (CuS)n; (n = 1–8) in terms of Conceptual Density Functional Theory (CDFT) based descriptors, aiming to explore its electronic and other properties. Global DFT based descriptors have been computed for ground state configurations and low-lying isomers of (CuS)n clusters. Our computed HOMO-LUMO energy difference, lying in the range of 1.25–3.53 eV, indicate possibility of utilization of (CuS) n clusters as renewable energy sources specially in photocatalysis and solar cell applications. A statistical regression analysis has been made between electronic and photo-catalytic properties of copper-sulfide clusters with their computational counterparts. The close agreement between experimental and computed data strengthens our analytical approach.

Speaker Biography

Tanmoy Chakraborty, PhD, is associate professor in the Department of Chemistry at Manipal University Jaipur, India. He has been working in the challenging field of computational and theoretical chemistry for last nine years. He has completed his PhD from the University of Kalyani, West-Bengal, India, in the field of application of QSAR/QSPR methodology in the bioactive molecules. He has published a large number of international research papers in peer-reviewed international journals with high impact factors. In addition, he has edited a number of research books. He served as an international Editorial board member of the International Journal of Chemoinformatics and Chemical Engineering. He is the recipient of prestigious Parameswar Mallik Smawarak Padak, from Hooghly Mohsin College, Chinsurah (University of Burdwan), in 2002.

e: Tanmoy.chakraborty@jaipur.manipal.edu

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