

Pharma

VIRTUAL 2020

November 16-17, 2020

“

Theme:

To Foster the Strategies of Pharmaceuticals
and Novel Drug Delivery Systems

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NOVEMBER 16-17, 2020

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To Foster the Strategies of Pharmaceuticals and Novel
Drug Delivery Systems

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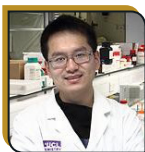
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Thank You
All...

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About **MAGNUS GROUP** |

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

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

About **Pharma Virtual 2020** |

PDDS welcomes all the participants to attend "PHARMA VIRTUAL 2020" which will be held during November 16-17, 2020 focussing on the theme "To Foster the Strategies of Pharmaceuticals and Novel Drug Delivery Systems"

Pharma Virtual 2020 is an international webinar, attracting global participant's intent on sharing, exchanging and exploring new avenues of Pharmaceutics and Novel Drug Delivery and latest developments.

Join our webinar to share and globalize your work with included advantages of special sessions on latest updates and analysis of pharmaceutical sciences related with COVID-19.

KEYNOTE FORUM-I

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1

SESSIONS ON:

BIOTECHNOLOGY AND BIOENGINEERING AND
PHARMACEUTICS AND DRUG DELIVERY SYSTEMS

PHARMA
VIRTUAL 2020

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2020

PHARMA VIRTUAL 2020





Hector M. Alvarez

Instituto de Biociencias de la Patagonia (INBIOP), FCNyCS, UNPSJB, CONICET, Comodoro Rivadavia, Chubut, Argentina

Bioengineering single-cell oil production by oleaginous *Rhodococcus* spp. to enlarge their application spectrum

Global oils, wax esters and biofuels demand is forecasted to increase in the next years. In order to meet this growing demand, the exploration of new ways of obtaining these products is required. In this context, microorganisms (bacteria, yeasts, fungi and microalgae) are now seriously considered as alternative oils and wax ester sources. Among bacteria, the oleaginous property is limited to a few specific species identified mainly from the genus *Rhodococcus*, such as *R. opacus* and *R. jostii*. These rhodococcal species are able to use a wide diversity of substrates for oil production, including industrial wastes such as glycerine, olive mill wastes, carob and orange residues, lignocellulosic material, whey, among others. Cell engineering to increase lipid production provides a good opportunity for designing a scalable and commercially viable oil-producing system. In addition, metabolic engineering allows expanding the capacity of the biochemical platform of rhodococci towards the synthesis of new bioproducts. Oleaginous rhodococci accumulate significant amounts of triacylglycerols (TAG) from gluconate or other carbon sources, but they are not able to produce detectable amounts of wax esters (WE) due to their inability to produce a significant pool of fatty alcohols in cell metabolism. In order to provide a pool of fatty alcohol moieties available for WE synthesis, we performed the heterologous expression of a gene encoding a fatty acyl-CoA reductase from the marine Gram-negative *Marinobacter hydrocarbonoclasticus* VT8 into the oleaginous *R. opacus* PD630. Recombinant cells produced ca. 46% of WE and 54% of TAG (of total WE + TAG) from gluconate compared to the wild type strain which produced 100% of TAG. Moreover, the cultivation of engineered *R. opacus* on residual whey, an inexpensive waste material from dairy industries, also resulted in the production of WE in addition to TAG, without affecting cell growth. These results demonstrated that the metabolism of oleaginous rhodococci is robust enough to successfully incorporate heterologous reactions and pathways to expand the range of lipids with commercial interest. On the other hand, the manipulation of rhodococcal genetics and biochemistry also allows expanding the lipogenesis ability to new growing conditions. We identified an interesting regulatory mechanism in *R. jostii* and *R. opacus* that couples the expression of several genes of lipogenesis to the activation of a regulatory system that provides alternative sources of nitrogen, when cells are cultivated under nitrogen-limiting conditions. This response is mediated by a protein called NlpR, which is a global regulator that provides a strong redirection of carbon flux toward lipid metabolism. NlpR is able to activate the expression of some genes involved in fatty acid biosynthesis (FASII) and the Kennedy pathway for TAG synthesis, including genes encoding AGPAT, PAP2 and DGAT enzymes, in addition to those encoding nitrate/nitrite reductase systems. Overexpression of *nlpR* gene improves TAG synthesis in oleaginous rhodococci under nitrogen-rich conditions. Thus, NlpR provides a new target for engineering single-cell oil production by rhodococci using nitrogen-rich industrial wastes. These results demonstrate that the application of molecular engineering to oleaginous rhodococci to improve lipid production and enlarge their application spectrum is possible.

Audience Take Away:

- The presentation will provide the audience with a comprehensive overview on single-cell oil production by oleaginous *Rhodococcus* spp. Bacteria
- The audience will learn about concrete molecular engineering strategies applied to oleaginous bacteria for improving oil production

- The audience will learn about molecular procedures applied to oleaginous bacteria to enlarge their range of applications
- This research will be of interest for all colleagues working on biofuels, biolubricants and oleochemical production

Biography

H.M. Alvarez studied Biochemistry at the University of Patagonia San Juan Bosco (Argentina) and graduated in 1993. He received his PhD degree in 1998 at the same institution. Between 1993 and 1997 he performed doctoral research at the Institute of Microbiology, Georg-August University of Göttingen, and the Institute for Molecular Microbiology and Biotechnology (IMMyB), Westfälischen Wilhelms University in Münster, Germany supervised by Prof. Alexander Steinbüchel. Between 2000 and 2001 he conducted postdoctoral research at the IMMyB, WWU Münster, Germany. He obtained the position of an Full Professor at the UNPSJB. He has published more than 55 research articles in SCI(E) journals.

SPEAKERS-I

DAY
1

SESSIONS ON:

BIOTECHNOLOGY AND BIOENGINEERING AND
PHARMACEUTICS AND DRUG DELIVERY SYSTEMS

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Carlos J.C. Rodrigues, Carla C.C.R. de Carvalho*

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Improving bioprocesses by using adaptation strategies of *Rhodococcus*

Rhodococcus are characteristic of the taxon mycolata which includes the genera *Mycobacterium* and *Nocardia*. These cells have a cell envelope characterized by the presence of long chain -alkyl- -hydroxy fatty acids, called mycolic acids. These lipids increase the tolerance of *Rhodococcus* cells to the presence of toxic compounds and challenging environmental conditions [1]. These cells are also able to modulate the composition of the fatty acids of the phospholipids of the cellular membrane as response to stressful conditions [2] and to produce specialized lipids [3]. *R. erythropolis* may be adapted to survive high osmotic stress and conditions that are usually considered extreme [2, 4]. Additionally, *Rhodococcus* cells contain efflux systems able to extrude toxic compounds [5]. These features, together with the large set of enzymes that *Rhodococcus* cells contain, make the cells very interesting for biocatalysis and bioremediation processes [6, 7]. Furthermore, the cells may survive when placed at 16°C and at 100°C for up to 15 min by adjusting the fluidity of the cellular membrane. These properties may be used to improve bioprocesses using toxic compounds such as the bioremediation of petroleum hydrocarbons under saline conditions. In this presentation, several adaptive mechanisms of *Rhodococcus* cells, and how they may be exploited to improve biotechnological processes, will be discussed.

Audience Take Away:

- Insights on phenotypic adaptation of *Rhodococcus* cells to toxic compounds and challenging environmental conditions.
- How to use bacterial survival mechanisms to improve the efficiency of bioprocesses.
- The impact of bacterial adaptation to human activities.

Biography:

Carla C.C.R. de Carvalho graduated in Chemical Engineering in 1998 and did a Master in Biotechnology (Biochemical Engineering) in 1999 at Instituto Superior Técnico (IST), Universidade Técnica de Lisboa (UTL). She completed a PhD in Biotechnology at UTL in 2003. She was awarded 2 Post-doctoral grants (2004-2006, IST-UTL; 2007-Feb 2008, IST-UTL and UFZ, Leipzig, Germany). In 2008, she was awarded a FCT 'Ciencia2007' 5-year contract and in 2014 she received a 'FCT Investigator 2013' 5-year contract as Principal Investigator. Since 2019, she is Assistant Professor at IST, Universidade de Lisboa. She published ca. 90 research papers in international peer reviewed journals and wrote 13 book chapters.



Siguna Mueller

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Towards a better comprehension of present and future Cyberbiosecurity Vulnerabilities Fostered by an Interdisciplinary Security Approach

The cyber-physical nature of biotechnology has led to fascinating advances in the biological, medical and life sciences but has also raised concern for new risks and potentials for misuse. Just as the emergence of the internet some decades ago led to a major revolution - which, by necessity was paralleled by the field of cyber-security - we are now facing the era of cyberbiosecurity with its own security vulnerabilities.

Although the DNA synthesis industry has, since the invention of gene-length synthesis, worked proactively to ensure synthesis is carried out securely and safely, the larger life-science and bio- logical community has largely remained unaware of the many forms of vulnerabilities that arise at the cyber-physical interface of virtually all of the involved technologies, systems, and applications. The convergence of advances in biotechnology with laboratory automation, access to data, and computational biology has led to a sheer unimaginable host of risks and vulnerabilities. Cyber- security attacks and data breaches in the health care industry have reached hospital IT systems and critically impacted biomanufacturing processes. However, the concern is not 'only' about data protection. Current and future threats range from the potential for weaponized bioengineered pharmaceuticals and biomedical agents, to toxic plants and food products masquerading as certified goods.

Comprehending these new dangers and determining where vulnerabilities reside, is no longer an option but of paramount and ultimate importance. Novel skills and approaches are needed to explore the unique cyberbiosecurity challenges at the nexus of cybersecurity, cyber-physical security and biosecurity as applied to biological and biomedical-based systems.

Yet, cyberbiosecurity is just emerging as a new discipline and many of the new risks and vulnerabilities are poorly understood. To complicate matters, the life-science and medical community is not trained and 'wired' to anticipate or analyze intrusions, infringements, and crime. This leads to the critical challenge, how immediate and emerging risks even can be conceived and conceptualized. It is suggested that a theoretical approach that utilizes ideas underlying the development of the early internet (without the explicit protocols per se) can give a different perspective, leading to a better comprehension of previously unrecognized vulnerabilities, and also provide potentials for risk mitigation.

Audience Take Away:

Historically, while the biotechnology and bioengineering community has placed considerable focus on safety issues (i.e., how might a product or service accidentally harm yourself or others), there has not been enough concern about security implications (i.e., how something could be used to intentionally harm others). Several programs and efforts, both within the United States and also internationally, have recognized the importance of developing a security mindset throughout the evolving bioengineering landscape and infrastructure. The Engineering Biology Research Council (EBRC) in the United States recently held a workshop funded by the Department of Homeland Security (DHS) and stressed the necessity of educational efforts. In addition to teaching security awareness to (young) researchers, it highlighted the potential value of asking in grant applications that, in addition to considering the safety implications of proposed work, applicants also demonstrate they have considered issues pertaining to security.

- Identify critical roadblocks to successful clinical trials.

- In this light, this talk introduces the potentials of ideas underlying (traditional) cyber-security
- Principles as a tool for both education and exploration, to
- Disclaim the prevailing misconception that cybersecurity-related concerns in the bioeconomy can be dealt with using IT solutions alone;
- Help develop an increased understanding of and insights into dual-use possibilities fostered by emergent tools in biotechnology and bioengineering.
- Illustrate, when/how cyber-physical vulnerabilities could benefit from insights and lessons
- Learned in the cybersecurity field.

Biography:

Dr. Mueller was among the first women in Austria to receive the Habilitation in Discrete Mathematics and Cryptography (2002). The following 15 years she spent at the Centre for Information Security and Cryptography Research at the University of Calgary, as Assistant Professor at the University of Wyoming (UW), and where, following her life-long passion in the life-sciences, she completed her second dissertation (PhD in Biomedical Sciences, 2014), the latter of which UW in part claimed priority as a U.S. patent. After major health challenges, she ardently devotes her experience to the exploration of critical objectives in the biomedical and life-sciences.



Mohammed Amine Serghini*, Khadija Lachguer, Mohamed Lachheb, Soumaya El Merzougui, Mohamed Ben El Caid and Imane Boudadi

Laboratory of Biotechnologies and Valorization of Natural Ressources, Faculty of Sciences, Ibn Zohr University, Agadir, Morocco

Molecular marker characterization and petal valorization of saffron 'Crocus sativus L.'

Saffron is very appreciated as a spice, as a product for therapeutic use and as a natural coloring. It consists of the dried stigmas of the flower of *Crocus sativus* L., an iridaceae with corms. Its exorbitant price of up to \$30/g frequently exposes it to fraud and requires the use of effective controlling methods to guarantee its authentication. The pruning of saffron flowers generates waste at the rate of 350 kg per kg of stigmas. This waste is discarded without any recovery.

The use of molecular markers such as SSRs and ISSRs is undertaken with the objective of finding a molecular identity of saffron from different countries and those of accessions belonging to the same country to distinguish them and trace the exact origin of saffron.

The search for SSRs at the level of the available genomic sequences of *C. sativus* made it possible to identify 26 pairs of primers which are used for the PCR amplification of 12 accessions of Moroccan saffron originating from the regions of Taliouine (province of Taroudant) and from Taznakht (province of Ouarzazate) and Greek and French saffron. These saffron samples are also used as a template for the PCR amplification of 10 ISSRs.

The data analysis made it possible to obtain a polymorphism of 40.38% despite the mode of vegetative propagation of this species, to clearly distinguish by these molecular markers, French saffron and certain Moroccan accessions and to draw up a dendrogram for the studied genotypes.

The use of the pruned saffron flowers for the production of bio-dye has involved aqueous extraction and treatments with different combinations of concentrations, temperatures, pH and dye times on cotton and wool. The parameters followed concern color yield, fastness to washing, dry and wet friction, acid and alkaline perspiration and light stability. It emerges from this study that the dyeing of wool and cotton by the extract of the petals of saffron flower is better with a concentration of 10% of dye, an acid pH (pH = 3) of the bath, a temperature of 90 ° for wool and 98 ° for cotton, for one hour. The dye is well fixed by wool than by cotton. The use of mordants increases wash resistance. It accentuates the coloring with only 3% of the dye and made it possible to obtain a wide range of colored tints from yellow to brown and green which shows that saffron petals waste can be a good natural dye for the cotton and wool textile industry.

Key words: Saffron, *Crocus sativus* L., Molecular markers, Flowers waste, Bio-dye.

Biography:

Mohammed Amine Serghini, born in 1964, holds a thesis from the Louis Pasteur University of Strasbourg, France and a PhD from Ibn Zohr University of Agadir, Morocco in molecular plant virology. Currently, he is a professor of higher education and director of biotechnology and genetic resources team in the faculty of sciences – Ibn Zohr University, Agadir. In terms of research activities, Prof. M.A. Serghini carries out several national and international research programs in the field of plant biotechnologies. He has supervised more than twelve doctoral theses and has published around forty publications in national and international journals.



Manisha Mandal¹, Shyamapada Mandal^{2*}

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Bioinformatic approaches on differential gene expression in scrub typhus compared to some other acute febrile infections

Concerning the acute febrile infection (AFI) development of improved diagnostics, particularly the molecular diagnostic intervention with therapeutic potential, is an urgent need for infection control and treatment management. Scrub typhus (caused by *Orientia tsutsugamushi* infection), without eschar development, is a febrile illness that mimics malaria, dengue, and other rickettsioses. Comparative analysis of microarray gene expression profiles of GSE16463 dataset, obtained from *Orientia tsutsugamushi* infected monocytes, was performed to identify transcriptional signatures in scrub typhus discriminated from other acute febrile infections, accompanied by functional pathways and enrichment analysis in disease pathogenesis. The GSE16463 expression profile was downloaded (www.ncbi.nlm.nih.gov/geo/), extracted with GEO2R tools, PPI network constructed by STRING, modules and hub genes identified using MCODE and CytoHubba plugin of Cytoscape, functional enrichment using GO and Reactome analysis. There were 333 differentially expressed genes ($\log_2FC > 1$, adjusted p value < 0.01) among scrub typhus ($n=65+85=150$), dengue ($n=189+233=422$), murine typhus ($n=37+27=64$), and malaria ($n=45+39=84$); n = upregulated + downregulated = total genes. Among the genes, 32 were common to all four diseases, and STAT1, ISG15, IFIT3, TRIM21, respectively were the candidate gene of each group. A unique 39 genes belonged to scrub typhus that could be used as signature genes to distinguish scrub typhus from other febrile illnesses compared. The biological process and functional pathways significantly enriched by the scrub typhus genes were respectively for defense response to the pathogens and interferon signaling, which could further help in diagnosis, treatment, and vaccine development as well.

Audience Take Away:

- Pathogenesis of scrub typhus and other acute febrile infection, such as malaria, dengue, and murine typhus compared?
- Provides clue of new tools to diagnose patients with scrub typhus.
- New effective therapeutics and vaccines for scrub typhus.

Biography:

Dr. Shyamapada Mandal is a Professor at the University of Gour Banga, India. His research interest is on infectious diseases, probiotics, genomics and bioinformatics. Did pre-PhD, PhD, and post-PhD research under the guidance of Professor Nishith Kumar Pal at Calcutta School of Tropical Medicine, India. He has published 110 articles and seven book chapters. He is life member of IAMM and IASR, India. Seven national academic and research awards have been conferred to him. He has guided 47 post graduate students; three MPhil and three PhD students have been awarded the degree, and five PhD students are working under the guidance of him.



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Biotechnological approach to valorize emissions: Biological conversion of styrene to polyhydroxyalkanoates using two-phase partitioning bioreactors

Styrene is an important pollutant released from chemical industry. Manufacturing of reinforced plastic, synthetic rubber and resin is the main source of styrene to atmosphere. These industrial activities consume about 15 million tons per year of styrene. In the best of scenarios, styrene emissions are recycled in 60 % and released to atmosphere in 20 %. However, in Mexico, all styrene emissions are released to atmosphere due to lack in emissions legislation. In order to promote sustainable processes to treat emissions from industrial sources in Mexico, this research work is focused to valorize styrene emissions using biotechnological processes to produce high added value products. To achieve this, the use of two-phase partitioning bioreactors (TPPB) which combine aqueous medium with a hydrophobic non-aqueous phase liquid (NAPL) is proposed. Firstly, the NAPL will increase the solubility of styrene into liquid medium because styrene is hydrophobic. Secondly, the use of NAPL will avoid the inhibition of styrene to microorganisms which can be toxic at high concentrations. Thus, NAPL will work as a mass transfer vector of styrene from gaseous to liquid medium and as a reservoir which will reduce the risk of styrene inhibition to microorganisms. This strategy has been successful in the biodegradation of hydrophobic gaseous pollutants, but, TPPB has not been proved in the conversion of this type of pollutants to biopolymers. In order to test the assumptions detailed, two NAPL such as silicon oil and ionic liquids and the strain *Pseudomonas putida* S12 were chosen. *P. putida* S12 has been reported to consume styrene and produce polyhydroxyalkanoates (PHAs, a high added value biopolymer). After caring out affinity to target compound, biodegradability and toxicity tests to choose the best NAPL to consume styrene and produce PHAs, it was found that ionic liquid absorbed 7.5 times more styrene than silicon oil ($H_{sty/IL} = 0.0030$; $H_{sty/SO} = 0.0226$; 28 °C) and both silicon oil and ionic liquid were non-biodegradable by *P. putida* S12. However, the ionic liquid caused inhibition to *P. putida* S12 in contrast to silicon oil which was not toxic for the strain. Then, it was concluded that silicon oil is the best NAPL for the TPPB experiments. Kinetic experiments were performed with and without NAPL to know if the addition of this increases the rate to produce the biopolymer. Results show that styrene removal rate and production rate of biopolymer in the presence of silicon oil were two times greater than control experiments in one phase (without silicon oil). Finally, the use of TPPB is a good alternative to valorize emissions of hydrophobic gaseous pollutants like styrene to produce high valuable products such as PHAs. However, investigations of this technology to show its viability in large scale are need.

Audience Take Away:

- Countries where treatment of gaseous pollutants is scarce
- A novel biotechnological strategy to treat and valorize hydrophobic gaseous pollutants
- Industrial sector interested in valorizing gaseous effluents to produce value added products via sustainable processes.

Biography:

Mr. Víctor Alonso studied Environmental Biochemistry Engineering at the Autonomous University of Campeche, Mexico. During Bachelor studies, He studied the sequestration of carbon in mangroves. Currently, He is studying a master's degree in Environmental Sciences at IPICYT, Mexico. He is learning about treatment and valorization of gaseous effluents using biotechnological processes.



Itzel Covarrubias-Garcia^{1,4*}, Guillermo Quijano², Aitor Aizpuru³, Jose Luis Sanchez-Garcia⁵, Jose Luis Rodriguez-Lopez¹, Sonia Arriaga⁴

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Implementation of conductive materials: Reduced graphene oxide adorned with Fe₃O₄ nanoparticles for biogas upgrading

During the biological process of biogas upgrading, H₂ and CO₂ are converted into CH₄ and H₂O, however the main limiting factor is the low mass transfer of the gaseous H₂ in the liquid phase, resulting in a low production rate of CH₄. The addition of some nanoparticles (NPs) in anaerobic digestion (AD) process can present a negative or positive effect on the production of CH₄ and biogas. Casals et al. (2014), reported an increment in biogas production of 180% and 234% in CH₄ production, when magnetite NPs (100 ppm, 7 nm) were added. They say, that small iron oxide NPs at non-saturation conditions slowly dissolve and boost bacterial activity in AD. On the other hand, Lin et al. (2017) added three different concentrations of graphene (0.5, 1.0 and 2.0 g/L) in an AD degrading cellulose. They found that the addition of 1 g/L resulted in the highest biomethane yield (695 ± 9.1 mL/g) and production rate (95.7 ± 7.6 mL/g/d), corresponding to an enhancement of 25% in biomethane yield and 19.5% in production rate. This study hypothesized that materials with higher conductivity play a significant role in promoting the direct interspecies electron transfer. The benefic effects of the addition of several nanomaterials during the biological upgrading of biogas were studied, in order to improve CH₄ production. The synthesized nanomaterials were magnetite nanoparticles (MNPs), reduced graphene oxide (rGO) and reduced graphene oxide decorated with magnetite nanoparticles (rGO-MNPs).

The results showed that MNPs and rGO at the three concentration tested (50, 100 and 200 ppm) did not boost the CH₄ production. Otherwise, the synergistic combination of the rGO-MNPs showed a higher CH₄ production compared with the control (without the nanocomposite); corresponding to an improvement of 47%, 28% and 33% for 50, 100 and 200 ppm, respectively. Based on the results, the improving in biogas upgrading process was linked to the sorption capacity of the nanomaterials, to the electron shuttling capacity provided from the addition of conductive materials like rGO-MNPs into the process and to the release of Fe²⁺ in the media which permitted to adsorb more H₂ and at the same time served as a dietary supply to stimulate microbial activity.

Audience Take Away:

- They will learn about the relationship between conductive nanomaterials and biological systems.
- They will know advantages that the addition of nanoparticles can provide to biological systems.
- They will think about the importance of the recovery of nanomaterials to prevent their released to the environment.
- Analyze that other nanomaterials can be added to improve a biological process.

Biography:

Ph.D. student Itzel studied Chemical Engineering at the Universidad Autónoma de San Luis Potosí (UASLP), Mexico and she graduated as MS in biotechnology and environmental sciences in Instituto Potosino de Investigación Científica y Tecnológica (IPICYT), Mexico at 2016. After finishing the MS, she started her Ph. D. in Advanced Materials at the same institution. She count with stays abroad in Denmark and Canada, at Aalborg Universitet (AAU) and Institut National de la Recherche Scientifique (INRS), respectively. She has published research articles related with biotechnology and nanomaterial



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Assessment an umbilical cells induced neuroplasticity in patients with schizophrenia using functional MRI

Purpose: To evaluate changes in the brain activation patterns using fMRI in patients with schizophrenia underwent an umbilical cells injections.

Materials and Methods: 15 patients (males, aged 20-40 years) with schizophrenia were included in the study. Remission of schizophrenia with a predominance of asthenic disorders was confirmed by psychiatry examination. Patients received intravenous infusions of group and rhesus compatible umbilical cord blood cells at the average dose of 250 x 10⁶ viable cells per infusion (4 injections at 2 week intervals). Patients also received standard neuroleptics therapy in maintenance doses. A functional MRI scans (3.0 T MRI scanner) with dual task paradigm were performed. Backwards counting by 7 from 100 was used for cognitive load, and in the same time patients were asked to keep a random word in memory as a working memory task. MRI was performed twice (before and in 3 months after treatment). SPM12 was used for data processing and analysis.

Results: Patients with schizophrenia before treatment showed deactivation of the anterior component of the verbal working memory loop in the left frontal cortex (P FWE corrected <0.001 for all activation and deactivation zones in this abstract). The deactivation cluster included Brodmann areas 9 and 10. Also we found deactivation zone in the left limbic lobe in the left posterior cingulate gyrus, Brodman area 23. However, patients showed a moderate activation zone in the posterior language system in the left inferior parietal cortex. After treatment deactivation zone in the left frontal cortex significantly decreased in volume and moved to the left and right Brodman area 10. Part of that zone including left Brodman area 9 and anterior part of the left insula was revealed as activation area. Additional activation zone in the anterior component of the verbal working memory loop was detected in the bilateral supplementary motor area.

Conclusion: Functional MRI revealed significant changes of brain activation patterns in patients with schizophrenia underwent an umbilical cells injections. This data is important for further evaluation of the pathophysiology of stem cell exposure in patients with schizophrenia.

Audience Take Away:

- The audience will learn about the possibility of intravenous administration of umbilical cord blood in patients with remission of schizophrenia and about the efficacy assessment using neuroplasticity evaluation by functional MR
- Changes of the cortical activation patterns evaluation can be considered as method for umbilical cells therapy effect assessment but now it is rather research and non-practical approach
- This will help for further research planning in this field to understand the effect of a novel stem cell therapy method in schizophrenic patients

Biography:

Dr. Dmitry Ustyuzhanin studied Medicine at the Moscow State University and graduated as MD in 2001. He then joined the research group of Prof. Sergey Ternovoy at the National Medical Research Center of Cardiology, Moscow, Russia. He finalized postgraduate residency in Radiology. He received his PhD degree in 2006 at the same institution. After that, he obtained the position of researcher at Department of tomography, National Medical Research Center of Cardiology, Moscow, Russia. He has published 55 research articles in Russian Citation Index and 23 in Scopus.



Mansureh Ghavam

Department of Range and Watershed Management, Faculty of Natural Resources and Earth Sciences, University of Kashan, Kashan, Iran.

An overview of RSV antiviral medicinal plants that may be key to Coronavirus

Medicinal plants have traditionally been used by Iranian scientists such as Ibn Sina and Zakaria Razi to treat infectious diseases. New research also shows the antiviral effect of a group of medicinal plants. Acute respiratory viral illness is the most common infectious disease in humans. Coronavirus is also a member of a large family of viruses that can cause respiratory infections. So far, there have been few reports of children being infected, and one percent of children with the virus are under 10 years old. Since there is no preventative or curative drug for coronavirus, traditional treatments and herbs can be used in children. One of the best options in traditional medicine is medicinal plants, which have been shown to have antiviral effects in laboratory studies on similar viruses. In children, the human respiratory syncytial virus (HRSV) is one of the most common airway viruses. The most common age of onset is under 2 years of age. Medicinal plants that are effective against this virus are *Origanum vulgare* L., *Glycyrrhiza glabra* L., *Rosmarinus officinalis* L., and *Zingiber officinale* Roscoe, which can be recommended for the treatment or prevention of coronavirus in children.

Keywords: RSV, Antiviral, COVID-19, Traditional medicine, Children

Introduction: Viruses are the most important cause of respiratory infections in humans and death is a significant percentage of children due to respiratory infections (Zhang et al., 2009). Respiratory tract infections are one of the most common infections and one of the leading causes of hospitalization worldwide (Chidekel et al., 1997). These infections are associated with childhood morbidity and mortality. The respiratory syncytial virus is one of the most important etiologies known (Vijgen et al., 2005). One of the most common childhood infections is RSV infection, which is most common in those under 2 years of age. RSV has a global spread, so that in all the geographical areas studied, there is evidence for the presence and occurrence of this infection. Manifestations of the disease are in the form of acute lower respiratory infections such as bronchiolitis, pneumonia, and croup, and are most common in infants with bronchiolitis (Remington et al., 2001).

Coronaviruses are a large family of viruses that can cause respiratory infections, from colds to more severe illnesses such as Mers 2 and SARS 8. The virus has recently been dubbed COVID-19; The outbreak of the new virus began in December 2020 in Johann, China (World Health Organization, 2020). The coronavirus also spread in Iran and quickly endangered mental and physical health. The symptoms of the virus range from mild to severe. Signs and symptoms of infection include fever, cough, and difficulty breathing (Wu and McGoogan, 2020). SARS-CoV-2 has not been shown to be a new virus, biological, epidemiological, pathogenic and immune. Efficient, fast, and accurate identification methods are still lacking. Specific drugs and vaccines were still being researched. As a special group compared to adults, children show different clinical features. Therefore, it is an important challenge for the medical community to diagnose and treat children with COVID-19.

In traditional medicine, it is tried to use chemical compounds in plants or by mixing different parts of several plants to find a suitable alternative to synthetic drugs. In other words, because herbal medicines have a wider range of effects than chemotherapeutic and synthetic drugs available in medicine, they have received more attention (Van, 2009). Medicinal plants have traditionally been used in a variety of cases, including infectious diseases. New research shows that some medicinal plants used in traditional medicine have antiviral effects. Therefore, there is no doubt that traditional medicinal plants can be

a very good tool for the discovery and production of antiviral drugs in the future (Vlietinck, 1991). This feature is especially noticeable in plants that contain alkaloids, flavonoids, tannins and terpenoids (Rocha Martins et al., 2011 and Krishnan et al., 2010).

In laboratory studies on various plants, the extract of 5 medicinal plants with antiviral effect against RSV has been identified. Since the RSV mainly affects children, the present study is designed to review these 5 medicinal plants and their effective compounds on this virus, so that perhaps more research on these plants can be used to prevent or treat coronavirus in children.

COVID-19 infection in children: The first child with a serious illness infected with COVID-19 has been reported in China. A one-year-old and one-month-old baby is born with an epidemic without a family history of contact. The clinical signs were the onset of diarrhea and vomiting, which quickly progressed to acute respiratory distress syndrome, sepsis, shock, and acute renal failure. During hospitalization, nucleic acid was detected 3 times, but only the third time showed a positive result. In addition, it should be noted that his family members did not have any clinical symptoms, so a free transfer should be considered (Chen et al., 2020). Therefore, although most children have mild clinical symptoms and a good prognosis, we should not overlook the possibility of these children in serious and dangerous conditions, especially people with atypical manifestations, major illnesses, long-term use of immunosuppressive drugs, and Children with immune system. The prevalence of COVID-19 in children is 2.4%, according to the 2019 report, and it is worth noting that some cases of latent infection may not be detected (Tang et al., 2020 and Chen et al., 2019b). Very few deaths have been reported in infants (Zhu et al., 2020).

Studies have shown that children show milder symptoms than adults, which is also seen in the early outbreaks of SARS-CoV and MERS-CoV infections (Wang et al., 2020; Wei et al., 2020 and Chen et al., 2020). In addition, this study suggests that mild or no symptoms in children may lead to misdiagnosis and lead to the need for testing for SARS-CoV-2, and therefore, asymptomatic children may develop the disease. Expansion (Guan et al., 2020) A study has shown that SARS-CoV-2 can be found shortly after testing for negative throat and nose swabs. However, the highest number of children infected with SARS-CoV-2 has been found as part of the cluster family prevalence. This is also consistent with the previous prevalence of SARS-CoV and MERS-CoV, which reported 50 to 80% and 32% of children, respectively, are infected with household contact (Wang and Al., 2020).

Children are twice as likely as adults to be infected with SARS-CoV-2, although they have milder symptoms or are completely asymptomatic. However, the role of children in the spread of the virus has not yet been discovered. Also, so far, there is no evidence of vertical SARS-CoV-2 transmission from mother to infant (Chen et al., 2020).

In Iran, less than 10 children have died of corona, all of which had underlying disease, meaning that children were not healthy or had respiratory or blood disease, which unfortunately had low immunity due to the underlying disease and they died. Currently, the number of children infected in southern Iran has increased (Ministry of Health and Medical Education).

Effective plants against RSV: *Origanum vulgare* L. is traditionally used as an anti-flatulence, diuretic, diaphoretic, regularizing, expectorant, and antiseptic (Omidbaigi, 2007; Amin, 2006 and Mozafarian, 2012). According to traditional medicine, this plant is warm and dry in terms of nature. In India, its leaves and seeds are used as an astringent, breast emollient and tonic (Mir-Heidar, 2002). The phenolic antioxidants of this plant have a variety of biological effects, for example, anticonvulsant, anti-inflammatory, anti-diabetic, antiviral, and anticonvulsant (Saxena et al., 2012), and this effects is believed that they are responsible for health. The main constituents of this plant are volatile essential oils (carvacrol, gamma-terpinene, p-cymene, and thymol), flavonoids (quercetin, apigenin, and apigenin) and caffeic acid derivatives, especially rosmarinic acid (Zhang et al., 2014 and LaGow, 2004).

In a laboratory study of antiviral activity in the ethanol extract of air-dried whole plant, only the combination of apigenin showed moderate to poor inhibitory activity against high RSV pressure with an IC₅₀ value of 23.1 μ M (Zhang et al., 2014). Also the combination rosmarinic acid of extract of this plant has HSV-1 antiviral activity (Sokmen et al., 2004). The results

of ethnobotanical studies in Iran showed that this plant is used for colds and antitussives in northern Iran (Gholipour et al., 2014) and also as a disinfectant for respiratory, anticonvulsant and cough painkillers in southern Iran (Dolatkhahi and Ghorbani Nohooji, 2013). Due to the traditional use of this plant by the Iranian people as a disinfectant and also the effect of apigenin combination of this plant against RSV virus, the extract of this plant can be used as an option for making antiviral drugs, including for the prevention and treatment of coronavirus in children.

Past sources have cited the use of *Glycyrrhiza glabra* L. for symptoms of viral respiratory infections such as dry cough or hoarseness and symptoms of hepatitis (Khanahmadi et al., 2013). In today's studies, modern medicine has shown the effects of licorice and its active components on the respiratory system and relieving cough, asthma and chest infections (Saxena, 2005). Native Americans have used echinacea since the early 17th century to treat gum and mouth disease, colds, coughs, blood poisonings, sore throats, stomach and intestinal aches and this plant was included in the list of the book National Formulary (American Society of Health-system Pharmacists, 2001).

Glycerin is the most important sweetener, 50 times sweeter than sugar (Bode and Dong, 2015). In the root extract of this plant, glycyrrhizic acid has an antiviral effect against influenza A / H1N1 virus (Baltina et al., 2015) and glycyrrhizin has a good inhibitory effect against HRSV (Yeh et al., 2013) and SARS-related coronavirus (Cinatl et al., 2003 and Hoefer et al., 2005). The people of northern Iran traditionally use a concentrated decoction of the root of this plant to relieve cough (Mirdilmi et al., 2015). *Origanum* herbal pills, made from marjoram and licorice, are taken three to two times a day three times a day after meals in cases of shortness of breath, bronchitis and severe cough (URL)

In traditional medicine, *Rosmarinus officinalis* L. is used for anti-asthma effects, digestive, sedative, headache reliever (Fu et al., 2007), circulatory disorders, increased visual acuity, anti-rheumatism (Toyoshi et al., 2006) and memory stimulant (Darshan, 2004). Pharmacological effects such as nerve growth factor stimulation (Martinez-Lirola et al., 1996), and inhibition of liver toxicity (Larrondo et al., 1995) has been reported for this plant. The plant contains essential oils, oleoresin and tannins, amyric acid, epinephrine, carnosol, cryptotanshinone, epizemanol, isorhamnetin, neptin, rosmarinic acid (Fu et al., 2007).

In one study, among the biologically active compounds tested of *R. officinalis*, carnosic acid showed the strongest anti-hRSV activity and was effective against both type A and B viruses. Carnosic acid effectively suppressed hRSV proliferation in a concentration-dependent manner. Carnosic acid effectively suppressed viral gene expression without inducing the production of type I interferon or affecting the survival of suppression, while not affecting the proliferation of influenza A virus, indicating that its antiviral activity is specific to hRSV (Shin et al., 2013). Also the effect of this plant extract and essential oil on HSV-1 virus has been proven. The main cause of this effect was phenolic compounds (Mancini et al., 2009; Vijayan et al., 2004 and Yousefi Kordestani and Parsania, 2015).

Today, Ginger (*Zingiber officinale* Roscoe) is considered a medicinal plant in North America in addition to food consumption. Many cold and flu supplements in the United States and Canada contain ginger extract as a major ingredient (Iwami et al., 2011). The immunomodulatory role of Ginger oil in mice has been investigated and it has been shown that ginger oil is effective in responding to humoral immunity in mice that have been discontinued (Carrasco et al., 2009). Ginger has very few side effects and is one of the most commonly known safe plants (Generally Recognized as Safe) on the US FDA list (Rehman et al., 2011). Accordingly, ginger can play an important role in health, prevention and treatment of various disorders and diseases. Fresh but not dried Ginger, ginger is effective against HRSV plaque formation in the airway epithelium by blocking the connection and viral infection. Gingerol, as the predominant ingredient in fresh and dried ginger, which had no effect on HRSV (unpublished data) Therefore, active compounds should be those that are only present in fresh ginger that should be identified in the future (Chang et al., 2013).

Conclusions: Although coronavirus has little effect on children, statistics in Iran in the summer show that many children are currently infected with the virus. Although the nature of the respiratory syncytial virus in children differs from that of COVID-19, both viruses involve the infant's respiratory tract. There is currently no cure for the virus, but it may be possible with traditional care to prevent or treat coronavirus. Iranians have used medicinal plants and traditional medicine in many diseases of infants such as bloating, jaundice and diarrhea, and its effect has been quite obvious. Licorice, ginger, marjoram

and rosemary are widely used in traditional Iranian medicine. Although the effect of the active ingredients of these plants on coronavirus has not been proven, but considering the laboratory results of the effect of these 4 plants on RSV virus and also the history of consumption of these four plants in traditional medicine for the treatment of respiratory diseases, these plants for further study. Drug detection is recommended for the treatment or prevention of coronavirus, especially for children. Clinical studies will certainly be responsible in the future

Biography:

Mansureh Ghavam graduated from Isfahan University of Technology in Iran in 2004 with a degree in Natural Resources Engineering. She completed a PhD in field of medicinal plants at University of Tehran in 2013. Her doctoral dissertation was in the field of genetics, cytogenetics and phytochemistry of medicinal plants, which was accepted with honors. She has been officially employed by University of Kashan since 2013 and is researching the antioxidant and antimicrobial properties of medicinal plants, nanotechnology of medicinal plants, and cultivation and propagation of medicinal plants. Her first research was accepted entitled "Effects of ecological factors on the antioxidant potential and total phenol content of *Scrophularia striata* Boiss." in Scientific Reports in November 2019. Due to this research skill, she now has a partnership agreement with the University of Cagliari



Rohit Bhatia^{1,*}, Raj K. Narang², Ravindra K. Rawal³

ISF College of Pharmacy, India

Coumarin-dihydropyrimidinone hybrids: design, virtual screening, synthesis and cytotoxic activity against breast cancer

Breast cancer is the most invasive form of cancer in women. It is characterized by over production of oestrogens which is mainly mediated by over-expression of aromatase. In the presented work we have designed a library of fifty coumarin-dihydropyrimidinone hybrids and screened them virtually for their aromatase inhibitory potentials through molecular docking tools. Docking was carried out against human aromatase (PDB Id: 3S7S) using exemestane as standard drug. Six compounds with best docking scores and interactions were selected and also analysed for in silico drug likeliness and toxicity. Further these six compounds were synthesized and characterized through spectrometric techniques. Further these were evaluated for cytotoxic potentials against breast cancer cell lines using MTT assay. Compounds CD8 and CD28 were found most potent among the all. The synthesized compounds must be explored further for discovery of a suitable therapeutic candidate against breast cancer.

Audience take Away:

- Audience will be able to know how to select drug design approaches.
- The presentation will be helpful to the audience to apply CADD tools in drug design by combining them with molecular hybridization approach to design multitarget directed therapeutic agents against cancer.

Biography:

Dr. Rohit Bhatia is currently working as Assistant Professor in Department of Pharmaceutical Chemistry, ISF College of Pharmacy, Moga; India. He has pursued his PhD from MRSPTU, Bathinda; India. He has a total of 6 years of research experience. His area of expertise is computer aided drug design, medicinal chemistry and bio-analysis. He has more than 40 publications in reputed International and National Journals. He has won several awards in National and International awards.



Nada F. Abo El-Magd*, Salma M. Eraky

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The molecular mechanism underlining the preventive effect of vitamin D against hepatic and renal acute toxicity through the NrF2/ BACH1/ HO-1 pathway

Aim: Drug-induced liver and kidney injuries are worldwide problems that cause restrictions in the use of drugs. The injury is highly mediated by oxidative stress and inflammation pathways. So, demonstrating the role of the natural compound (Vit.D) on the prevention of acetaminophen (APAP) overdose toxicity and the molecular mechanism through NrF2/BACH1/HO-1 pathway is promising.

Experimental: Male Sprague Dawley rats (40 rats) were divided randomly into 4 groups: Normal, APAP, APAP +Vit.D (500 IU/kg) and APAP+Vit.D (1000 IU/kg). The APAP toxicity caused by 2 g/kg (orally) on day 7.

Key findings: Vit D decreased significantly liver and kidney functions: serum ALT and AST activities ($P < 0.0005$); creatinine and urea ($P < 0.0005$) concentrations; liver and kidney histopathological scores. Furthermore, Vit.D ameliorated APAP-caused oxidative stress through the liver malondialdehyde concentration's decrease and the total antioxidant capacity's increase ($P < 0.0005$). The molecular mechanism of Vit.D may include the prevention of high deteriorating increase of oxidative stress mediators: hepatic and renal NrF2 and BACH1 tissue expression in addition to serum HO-1 ($P < 0.0005$); the increase of inflammatory mediators; hepatic and renal NF- κ B tissue expression, serum interleukin-10 ($P < 0.0005$) and TNF- α ($P < 0.05$). The 500 IU/kg Vit.D administration caused better protection results especially on the histopathological and immunohistochemical results than the 1000 IU/kg Vit.D administration.

Significance: Vit.D ameliorates APAP-induced liver and kidney injury that may be attributed to its ability to moderately increase antioxidant status to counteract the toxicity without the massive destructive increase in the anti-oxidant pathway (NrF2/HO-1/BACH1). So, this work represents a great prophylactic role of Vit.D against drug-induced liver and kidney injury. With the current epidemic COVID-19, the importance of Vit.D and acetaminophen had a great interest thus, may be combining them together will decrease the side effects of acetaminophen overdose.

Biography:

Dr. Nada Fawzy Abo El-Magd had B.Sc. of pharmaceutical sciences-Mansoura University, Egypt-May 2012; grade excellent with honors (2nd achiever). In 2012, She started academic work at Biochemistry Department, Faculty of Pharmacy, Mansoura University, Egypt. She received master's degree (biochemistry) in 2015 then Ph.D. (Clinical Biochemistry) in 2018 from the same home institution. In 2019, She traveled as a visitor postdoctoral fellowship at Robert Gordon University, Aberdeen, Scotland, UK for 6 months. She returned to her job as lecturer of Biochemistry and started her postdoctoral research at her home institute in different disciplines related to the molecular pathways underlying diseases and the effect of natural compounds and drugs in modulating these pathways.

POSTER DAY
1

SESSIONS ON:

BIOTECHNOLOGY AND BIOENGINEERING AND
PHARMACEUTICS AND DRUG DELIVERY SYSTEMS

PHARMA
VIRTUAL 2020

NOVEMBER 16-17
2020

PHARMA VIRTUAL 2020





Medina-Pino, L. M.^{1, 2*} Martínez-Vaquero, J. L.², Santellán-Olea, M. del R.²

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Obtaining blue fluorescent protein through a novel technique

Fluorescent proteins have been used like molecular tools since a few years ago. They have been used like reporter genes, localization markers, etcetera. Because of the research needs, a huge variety of fluorescent proteins have been generated, most of them have their origin on the *Aequorea victoria* GFP. Some of these proteins have been conferred improvements in their structural properties or their color emission has been modified. The laboratories, which employ these techniques, spend a lot of time and money. The first one, due to the prolonged obtaining process and the second one because they need to have more than one kind of fluorescent proteins coding genes and they have an expensive cost. In this work we obtain a GFPuv color variant, using a low cost cloning techniques that increases the usual speed of the process. We use *E. coli* DH5α for the plasmids propagation and assembly. For the color responsible amino acid codons modification we made a site-directed mutagenesis, we add to our PCR mutagenic primers. The primers were designed for having between them homolog regions in their 5' extreme to recircularize the PCR fragment by in-vivo recombination. We transformed the bacterial strain by thermal shock. The recombinant protein was expressed in the same bacterial strain, this bacteria was cultured in LB agar supplemented with 2% L (+)-arabinose and 100 ug/mL ampicillin for 24 hours at 37 °C. When we illuminated them with UV light of 390 nm, we observe the mutants bright blue.

In conclusion, this work gives us the basis for an efficient and practical strategy to generate a variety of fluorescent proteins, we will have many colors having only one gene. Through this method we substantially decreases costs and time in this process.

Audience Take Away:

- The audience will learn about a forgotten cloning technique that is not commonly used, but increases the speed of the cloning process.
- With this technique, they could obtain a huge variety of proteins from one gene and with a pair of primers for each color.
- They could obtain many variants of fluorescent proteins quicker with a lower cost.

Biography :

Lucelly studies Biotechnology at the Benemérita Universidad Autónoma de Puebla, México since 2018. She works in the research group of Dra. María del Rayo Santellán Olea at the Micoplasmas Laboratory on the Research Center for Microbiological Sciences.

KEYNOTE FORUM-II

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SESSIONS ON:

BIOTECHNOLOGY AND BIOENGINEERING AND
PHARMACEUTICS AND DRUG DELIVERY SYSTEMS

PHARMA
VIRTUAL 2020

NOVEMBER 16-17
2020

PHARMA VIRTUAL 2020





Daniela Monti

Department of Pharmacy, University of Pisa

Nanostructured Formulations in Skin Cancer: Challenges and Perspectives

The incidence of skin cancer, the most common malignant disease that mainly affects the Caucasian population, is increasing worldwide. There are three main types of skin cancers: basal cell carcinoma (BCC), squamous cell carcinoma (SCC) and melanoma. The first two are grouped as non-melanoma skin cancers: BCC is characterized by local tissue damage and seldom leads to metastasization while SCC can recur and metastasize. Melanoma is a cancer with dark pigment that develops from the pigment-containing cells known as melanocytes. Surgical excision of these malignancies has been the preferred treatment of patients for decades. However, the decision to perform surgery can be affected by various considerations, including comorbidities of the patient, the anatomical site of the lesion and potential intolerance for repeated excisions. Topical treatment of skin cancer may therefore be more appropriate in certain instances, e.g. when the patients present with field cancerization or multiple clinical and subclinical lesions over a large anatomical area. Topical treatment potentially allows for higher drug levels at the tumour site, and may result in less overall toxicity than systemic agents. Despite the numerous positive aspects, the topical way is also not without limitations, such as poor bioavailability, undesirable local side effects compromising the therapeutic efficacy (erythema, paresthesia, rash, edema, contact dermatitis). An ideal treatment should be developed taking into account the good patient compliance, a better overall efficiency of the treatment, a toxicity as low as possible, a high ability to reach the target site in an amount sufficient to give the therapeutic effect. The success of the topical therapy depends on both the pharmacologically active substance and the formulation strategy. Researchers have focused on developing new drugs and new combination of molecules, such as conventional cancer chemotherapeutics and phytochemical compounds promising as anti-cancer drugs or as lead compounds in the synthesis of new drugs. The physicochemical properties of molecules, such as size and Log P, are important issues in selecting a candidate for topical delivery. Nanotechnology based formulations can help in achieving our goal: enhancement of drug bioavailability and reduction of skin irritation by avoiding direct contact of the drug with the skin's surface. Delivery of drugs using nanotechnologies, not only, can improve drug stability, but also can help to overcome the stratum corneum, main barrier to penetration. The assessment of the drug penetration profile into the skin layers can be performed with in vitro penetration studies on porcine ear skin, allowing the determination of the amount of penetrated drug within the stratum corneum, epidermis and dermis and hair follicles and the relative penetration depth. .

Biography

Dr. Monti graduated in Chemistry and Pharmaceutical Technology in 1987 and received the PhD in "Design, Development and Bio-evaluation of Drugs" in 1993 and continued to work in the technological and biopharmaceutical field. In 2000, she became Assistant Professor of Pharmaceutical Technology at the Department of Pharmacy, University of Pisa. Her scientific research is oriented towards the study of drug delivery systems to the cutaneous, ungual, ocular, vaginal and buccal site, the use of cell cultures to evaluate toxicity on corneal epithelium cells of ophthalmic excipients and the cosmetic field, by focusing attention on the irritating and corrosive effect, on the one hand, and cutaneous permeation/penetration of cosmetic ingredients, on the other one. From 1997 to 2000 he participated in the European project BIOMED-2, (BMH4-97-2324) entitled "Evaluation of oculotoxicity of drugs in vitro" with the following European partners: University of Tampere (Finland), University of Bremen (Germany), University of Ioannina (Greece), Orion Corporation Ltd. and Oy Star AB, (Finland). She is also responsible for several research projects involving international companies. Furthermore, she is the author of many publications in international journals with referee, of patents and presented her research at national and international meetings. She has been reviewer for many scientific journals such as International Journal of Pharmaceutics.

KEYNOTE FORUM-I

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SESSIONS ON:
CHEMISTRY AND MATERIAL SCIENCE

PHARMA
VIRTUAL 2020

NOVEMBER 16-17
2020

PHARMA VIRTUAL 2020





Vakhtang Barbakadze*

Tbilisi State Medical University, Georgia

Poly(sugar acids): Acidic Polysaccharide Poly[3-(3,4-Dihydroxyphenyl) Glyceric Acid] from Medicinal Plants of Boraginaceae Family, its Synthetic Analogues and their Potential Therapeutic Effect

Natural polysaccharides have long been studied and widely used in medicine and pharmaceuticals. A new polysaccharide is 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 , ^{13}C NMR, 2D $^1\text{H}/^{13}\text{C}$ HSQC, 2D DOSY and solid-state ^{13}C 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 biopolymer. 3,4-Dihydroxyphenyl and carboxyl groups are regular substituents at two carbon atoms in the chain. The repeating unit of this regular polyether is 3-(3,4-dihydroxyphenyl)glyceric acid residue. On the other hand PDPGA as a 3,4-dihydroxyphenyl derivative of poly(2,3-glyceric acid ether) belongs to a class of an acidic polysaccharides [poly(sugar acids)] as well. Its basic monomeric moiety glyceric acid is oxidative form of the aldotriose glyceraldehyde. In this case poly(2,3-glyceric acid ether) chain is the backbone of this polymer molecule and 3,4-dihydroxyphenyl groups are regular substituents at carbon atoms in the chain. Every repeating structural unit of PDPGA contains three reactive functional groups, two phenolic hydroxyl groups in ortho-position and one carboxyl group. Multifunctionality of PDPGA should be a reason of its wide spectrum of biological activities.

PDPGA exhibited immunomodulatory (anticomplementary), antioxidant, anti-inflammatory, burn and wound healing and anticancer properties. The racemic monomer 2,3-dihydroxy-3-(3,4-dihydroxyphenyl)propionic acid (DDPPA) and its enantiomers (+)-(2R,3S)-DDPPA and (-)-(2S,3R)-DDPPA were synthesized for the first time via Sharpless asymmetric dihydroxylation of trans-cafeic acid derivative using a potassium osmate catalyst and enantiocomplementary catalysts cinchona alkaloid derivatives (DHQ)2-PHAL and (DHQD)2-PHA as chiral auxiliaries, respectively. These compounds are a new finding in sugar acids. Methylated derivative of PDPGA was synthesized via ring opening polymerization (ROP) of 2-methoxycarbonyl-3-(3,4-dimethoxyphenyl)oxirane using a cationic initiator $\text{BF}_3 \cdot \text{OEt}_2$. Oligomers of PDPGA was synthesized by "green" ROP enzymatic polymerization of methyl 3-(3,4-dibenzyloxyphenyl)glycidate using lipase from *Candida rugosa*. The size-exclusion chromatography, MALDI-TOF analyses and deprotection showed the formation of oligomers with degree of polymerization up to 5. Enzymatically obtained oligomers of natural polyether cause interest for diverse biological tests. 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 racemic monomer DDPPA suppressed the growth and induced death in androgen-dependent (LNCaP) and -independent (22Rv1) human prostate cancer (PCA) cells, with comparatively lesser cytotoxicity towards non-neoplastic human prostate epithelial cells PWR-1E. 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 human PCA cells is more compared to its synthetic monomer. Methylated synthetic analogue of PDPGA did not show any activity against PCA. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity. (about 250 - 500 words)

Audience take Away:

Background: Natural polysaccharides have long been studied and widely used in medicine and pharmaceuticals. Besides, within the field of pharmacologically active biopolymers the area of stable polyethers seems rather new and attractive.

Objective: The goal of this research was to study main chemical constituent of high molecular preparations from medicinal plants of Boraginaceae family and investigation of their therapeutic efficacy: immunomodulatory (anticomplementary), antioxidant, anti-inflammatory, burn and wound healing and anticancer properties.

Methods: Structure elucidation of biopolymers under study was carried out by different techniques of NMR spectroscopy.

Results: The main chemical constituent of high molecular (>1000 kDa) water-soluble preparations from medicinal plants *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 biopolyether. PDPGA as a 3,4-dihydroxyphenyl derivative of poly(2,3-glyceric acid ether) belongs to a class of acidic polysaccharides (sugar acids) as well. Its basic monomeric moiety glyceric acid is a natural three-carbon sugar acid which is oxidative form of aldotriose glyceraldehyde. PDPGA 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%.

Conclusion: Thus, this study identifies PDPGA as the first representative of a new class of natural polyethers. PDPGA as a poly(2,3-glyceric acid) belongs to a class of an acidic polysaccharides (sugar acids) as well. Overall, PDPGA is nontoxic compound with efficacy against PCA that supports its further pre-clinical and clinical testing.

Biography

Dr. Vakhtang Barbakadze has his expertise in isolation and structure elucidation of biologically active plant polysaccharides and polyethers. In 1978 and 1999 he has completed his Ph.D and D.Sci., respectively. He is the Head of Department of Plant Biopolymers at the Tbilisi State Medical University Institute of Pharmacochimistry. In 1996 and 2002 he has been a visiting scientist at Utrecht University (The Netherlands) by University Scholarship and The Netherlands organization for scientific research (NWO) Scholarship Scientific Program, respectively. He has published more than 100 papers in reputed journals. In 2004 he was Georgian State Prize Winner in Science and Technology.

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Roaa A. Tayeb*¹, Saleh O. Bahaffi², Alaa M. Khedr³

King Abdulaziz University, Saudi Arabia

Impact of Concomitant Administration of Apixaban and Rifampicin on the Pharmacokinetics of Apixaban in Rat Plasma Using Developed HPLC/MS Method

Apixaban (AP) is a novel oral anticoagulant drug that select and prohibit the active site of F-Xa factor. AP is metabolized mainly through hepatic enzymes CYP3A4 and P-glycoprotein. Co-administration of AP with Rifampicin (RF) antibiotic drug that act as an inducer of CYP3A4 and the P-gp substrates, it would be expose AP to drug-drug interaction. The main goal of the present study was to examine the impact of RF on the pharmacokinetics of orally administered AP in rat plasma. 10 mg/kg AP was administrated to sixty male rats that were divided into two groups. The rats in control group received only AP therapy, while rats in treatment group receive 10.2 mg/rat RF therapy for eight days before AP dose. Plasma samples were collected at 0.25, 0.5, 0.75, 1, 2, 4, 6, 8, 12, and 24 h after oral administration of AP. The concentration of AP in rat plasma were quantified by developed LC/MS method. The developed method was sensitive, selective and robust for both AP and RF with linear calibration curve. The separation was achieved on C-18 column with a gradient mobile phase system, that consist of 20%:80% ACN-Water with 0.1% formic acid. %R > 96% of SPE procedure that was performed on C18-100 mg cartridges. The pharmacokinetics of AP for both control and treatment groups after a single oral administration were calculated using non-compartmental method. The statistical t-test shows that the plasma curve of AP in treatment group is significantly difference than control group and p value < 0.001 at 95% CI. This study concluded that RF inhibit the metabolism of AP in rat plasma, and management of dose should be considered in the co-administrated of AP with RF.

Audience take Away:

- Determination and separation of candidate drug in rat plasma sample.
- Impact of Rifampicin drug on the metabolism of Apixaban.
- The developed method was simple and robust to applied in drug analysis.
- Management of drug-drug interaction according to the obtained results.

Biography:

Roaa Tayeb a PhD student in chemistry department at King Abdulaziz University, Jeddah, Saudi Arabia. I have A master's degree in chemistry from KAU in 2013. I published two articles on ISI journals in drug analysis by developing HPLC methods and separation of combined drugs. I employed as a lecturer on Jeddah University, Jeddah, Saudi Arabia. Then I joined PhD program in chemistry-analytical department especially chromatography. I am professional on HPLC instrument and Mass detector.



Dr. K. M. Lokanatha Rai

University of Mysore, Mysuru

Organic Synthesis under Solvothermal condition

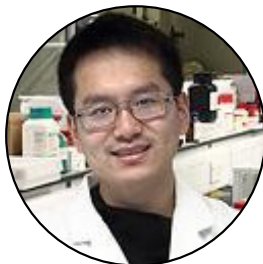
The chemistry of solvothermal reactions involves two major actors namely, high temperature and pressure. On record, water is the most common solvent used for many reactions. Many reactions underneath the earth's crust take place under high temperature and pressure and in this context; water plays an important role, viz., and crystal growth of minerals. Geologists and mineralogists to describe reactions, which takes place at high temperature and pressure in the presence of water, have used the word hydrothermal for many years. G. Demazeau et al have proposed to use the word solvothermal, whatever be the solvent used in such reactions. "Solvothermal reactions can be defined as reaction or a transformation of reactive in a closed system, in presence of a solvent at a temperature higher than its boiling point. Consequently these reactions can be developed in supercritical or in sub critical conditions". These reactions have been developed in Material Sciences – using aqueous or non-aqueous solutions in different areas. Some of the reaction proceed at slow rates under normal pressure can be enhanced by increasing the pressure. This can be achieved by heating the reaction mixture under sealed condition. The development of solvothermal reaction is of interest because they offer the possibility of environmentally benign reaction conditions by reducing the burden of organic solvent disposal. Solvothermal process involves the heterogeneous chemical reaction, which occur at solid-liquid or solid-liquid-gas interfaces under high temperature and high pressure.

During 1986, for the first time I have converted the lactone to amide by heating the amide with liquor ammonia in a sealed glass tube at water bath temperature. This prompted my group to carry out intramolecular 1,3-dipolar cycloaddition of oxime with olefins to isoxazolidines via nitron intermediate successfully in a sealed tube at 100 °C using benzene as solvent, while conversion of aldehyde semicarbazones to bishydrazones by thermolysis under reduced pressure was achieved in 90–95% yield using ethanol as solvent. For the first time we have attempted the synthesis of aromatic ketones via decarboxylation of aryl carboxylic acid in presence of alkyl nitrile under solvothermal conditions. We have successfully synthesized of substituted isoxazoles and pyrazoles from α,α -dioxoketene dithioacetals under solvothermal conditions. A simple method for the synthesis of benzhydryl derivatives is proposed by my group using anisole and substituted benzaldehydes in the presence of a salen metal catalyst at high temperature and pressure using Morey autoclave.

Thiocarbonyl containing molecules are versatile synthetic intermediates which find many applications in the synthesis of complex natural products. Though there are a number of reagents available for the thionation of esters or amides, they have some disadvantages. The various thionating reagents used for thionation reaction includes Lawesson's reagent, hydrogen sulfide, phosphorous pentasulfide, hexamethyldisilathiane, $R_3OBF_4/NaSH$, R_2PSX , $(Et_2Al)_2S$, bis(tricyclohexylstannyl) sulfide/boron trichloride, thiourea etc. For instance, many of these reagents require more reaction times, high temperatures, or inconvenient reaction condition for their execution and are often accompanied by painful chromatographic separation to remove spent reagents from desired products. This prompted to use thiourea as thionating agent for the conversion of 1, 3, 4-oxadiazole to 1, 3, 4-thiadiazole under solvothermal reaction condition. My group further proved that thiourea is an efficient reagent for the conversion of esters or amides to thioesters or thioamide respectively under solvothermal condition. In a typical synthesis, equimolar quantities of thiourea and ester were taken in a stainless steel SS316 Morey type of autoclave provided with a teflon liner of 30 ml capacity. On usual workup, it yields 85 to 90% of ethylthiobenzoate. Rai et al observed that under solvothermal condition, reaction of aryl aldehyde with ethanolamine in the presence of thiourea yielded 2-aryl-thiazoline while in the absence of thiourea yielded 2-aryl-oxazoline derivatives in almost quantitative yield.

Biography:

Prof. Lokanatha Rai, born in 1954, in Madavu village of Puttur taluk. He received his M. Sc., and Ph. D degrees from the University of Mysore. He joined Department of Studies in chemistry, University of Mysore as Lecturer in 1982, and moved upto become Reader in 1995 and Professor in 2003. He was a post-doctoral fellow at Bar-Ilan University, Israel from 1987-89. Dr. Rai has done outstanding research in the field of synthetic organic chemistry, particularly in the field of podopyllotoxin, solvothermal reactions, 1,3-dipolar cycloaddition reactions and [4+2] hetero Dies alder cycloaddition reactions. His contributions in different areas of chemistry reflect in the form of over 204 research publications in reputed National and International journals with over 3062 citations, h-index of 29 and i10 index 61. Most of his research papers are well cited in Books, National and International journals including Fieser's "Reagents for Organic Synthesis, Merck Index, Chemistry of Lignans, Aldrich and Lanchester Chemical catalogue. He served as an associate editor for many International Scientific journals of high repute. So far he has successfully guided 24 students for Ph. D., degree, and 05 students for M. Phil degrees. Dr. Rai was instrumental in developing M. Sc., Organic chemistry at Manasagangotri Campus. Prof. Rai has taught reaction mechanism, photochemistry and pericyclic reactions, bonding in organic chemistry, natural products, spectroscopy for M, Sc., students.

**Dr. Guanjie He***

University of Lincoln, London

Development of electrocatalysts and their structural evolution

The oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) is a critical process in the electrolysis of water and many other applications. Recently, much effort has been dedicated to developing low-cost, highly efficient, and stable electrocatalysts. Transition metal nitrides and phosphides are investigated intensively due to their high electronic conductivity and optimized absorption energy of intermediates in acid electrolytes. However, the low stability of metal nitrides and phosphide materials in air and during electrocatalytic processes causes a decay of performance and hinders the discovery of specific active sites.

In this talk, recent materials study in our group, such as the bimetal nitrides and phosphorus-modified monoclinic CoMoO₄, will be presented, we have developed as a low-cost, efficient, and stable OER and HER electrocatalyst for in alkaline media. The optimized catalyst shows a small overpotential with high stability in KOH electrolyte. Combined computational and in situ spectroscopic techniques show the evolution and the active sites of the materials and the work will guide further discovery of these electrocatalytic materials.

Audience Take Away:

- The synthesis and design strategy of the electrocatalysts for oxygen evolution and hydrogen evolution reactions will be benefit for researchers in the same fields.
- Other faculty could use to expand related knowledge from this talk for their research or teaching
- Materials techniques will be used for other materials chemistry and chemical engineering aspects
- New collaborations are expected to be established in this conference

Biography:

Dr. Guanjie He is a Senior Lecturer in Chemistry, University of Lincoln and an Honorary Lecturer in University College London (UCL). Dr. He's research focused on materials for electrochemical energy storage and conversion applications, especially electrode materials in aqueous electrolyte systems. Dr. He has published over 70 papers in peer-reviewed journals, with total citation of over 1900, and an h-index of 24 (Data from google scholar). Dr. He received his PhD degree in Chemistry Department, UCL. Before current appointment, he worked in Electrochemical Innovation Lab in Chemical Engineering Department, UCL as a Research Fellow



Aleksandra Kosińska^{1*}, Tom Kunde², Bernd M. Schmidt³, Artur Kasprzak⁴

Warsaw University of Technology, Poland^{1,4}, Heinrich-Heine-Universität Germany^{2,3}

Ferrocenylated molecular cages bearing triazine moieties

Syntheses of a ferrocene-templated molecular cage bearing triazine moieties will be presented. The formation of a symmetric cage-type structure is yet to be confirmed, but elemental analysis and IR spectra showed promising results. The synthesis of such molecular cages may be challenging, many reactions have been prepared, most of which recovered substrate, but no product has formed. First attempts were based on formation of triferrocenyl-substituted 1,3,5-triphenylbenzene¹. Reactant as 1,3,5-tris-(4-aminophenyl)triazine is structurally similar to 1,3,5-tris-(4-aminophenyl)benzene, hence the assumption that both those reagents will react in a similar way. It seems, however, that nitrogen in the benzene ring limits the reactivity of the compound and a product bearing this triazine moiety is likely much more difficult to obtain.

Alcohols as solvents have not given any positive results. However, results of syntheses have showed that triazine moieties are better used with aromatic solvents. Reactions with o-dichlorobenzene and butanol as solvents have given yet the best results. Such reactions have been prepared with 1,3,5-tris-(4-aminophenyl)triazine and also with a fluorinated triazine. In both cases precipitate is formed with high yield. The potential product has been tested in solubility and did not dissolve in any common solvents used, which made NMR analysis impossible, but IR spectra suggested that the potential product is formed. More analyses such as PXRD, SEM etc. are planned to confirm the formation of a molecular cage.

Audience Take Away:

- Audience will be able to expand their research horizons
- How to prepare new structures consisting of molecular cages
- Effect of different solvents on reactions
- Differences of reactivity between triazine moieties and benzene analogues
- Which analysis to use when you have an insoluble product

Biography:

Aleksandra Kosińska studies Chemical Technology at the Warsaw University of Technology, Poland and is now a student of the last, seventh semester of studies. She is a member of Dr. Artur Kasprzak's Group of the Functional Organic Compounds. Her research interests are focused on the synthesis of a molecular cage containing ferrocenyl groups.



Huda A. Shaheen*¹ Saleh O. Bahaffi ², Alaa M. Khedr³

King Abdulaziz University, Saudi Arabia

A sensitive high-performance liquid chromatography-tandem mass spectrometric method for determination of bisoprolol after derivatization with 3-bromomethyl-propyphenazone: Application to rat serum

A sensitive liquid chromatography-tandem mass spectrometric (LC-MS) method was developed to determine bisoprolol in rat serum. Bisoprolol (BIS) was monitored after labeling with 3-bromomethyl-propyphenazone (BMP). The MS response of BIS-MP was matched with dansylated bisoprolol (BIS-DNS). The BMP reagent proved its effectiveness in the complete derivatization of BIS and its superiority to BIS's process of derivatization over dansyl chloride (DNS-Cl). The LC-MS method was optimized and validated using rat serum as a matrix. The developed method showed enough selectivity and sensitivity to assay BIS in rat serum at the picogram scale. Orally administered BIS was extracted from rat serum using Sep-Pak vac C18-100 mg, followed by coupling with BMP. The calibration curve showed a regression coefficient value of 0.999 within a concentration spanning a range of 0.01-5000 ng/mL.

The limits of detection (LOD) and quantitation (LOQ) were 4 pg/mL and 12 pg/mL, respectively. The intraday and inter-day precision (% RSD) was ranged from 3.13E-3 to 6.91%, while the accuracy (% Er) was ranged from -3.63 to -0.50%. The method was successfully applied to rat serum after administration of only one dose of BIS and sampling at a time interval of zero to 8 h. The pharmacokinetic parameters were; 15.28 ng/mL for maximum concentration of BIS-MP (C_{max}) at 1h (t_{max}). The elimination half-life of the drug (t_{1/2}) was found to be 0.83 h, and the area under the curve (AUC_{0-t}) value found was 41.64 ng/mL.h.

Audience Take Away:

- The derivatization reagent are used for trace analysis of toxicological or biogenic materials, or metabolic pathway of drugs.
- Finding such derivatization compounds is the key role in noval scan of drug metabolites or disease biomarker in biological matrix.
- In this work, we targeted the preparation of new derivatization reagent and to test the reactivity of reported reagent.
- The study include optimization of reaction conditions with compounds bearing reactive functional groups like -OH (alcoholic, phenolic, carboxylic), and -NH groups.
- Improvement of selectivity and separation, enhancement of ionization efficiency, improvement of structural elucidation by LC-MS, and facilitation of isomer separation.

Biography:

(Huda PhD candidate, studied Chemistry at King Abdulaziz University, Saudi Arabia and graduated as MS in 2013. She has published 2 research articles in Journal of molecular liquids. Participated as a speaker by oral presentation entitled "Selective adsorption of gold ions from complex system using oxidized multi-walled carbon nanotubes" at the "11th Asia Pacific Diabetes Conference and Expo" held on July 11-12, 2016 in Brisbane, Australia and at the "BIT's 6th Annual World Congress of Nano Science & Technology (Nano S&T-2016)" held on October 26-28, 2016 in Singapore).

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Loai Aljerf

Damascus University, Syria

Factors Affecting Foam Stability and Behavioral Description of Dynamic Surface Tension for Polysiloxane-Polyether Copolymers in Polyol

Surface-active agents (surfactants) are one of the most commonly used compounds in both daily life as well as in diverse industrial processes. The ability of surfactants to partition at the interface, makes them ideal candidates for influencing the surface properties even in very small concentrations. Aqueous foaming solutions have significant dynamic surface tensions in the 0.001- to 0.1-second range. Taking into consideration that excess surface concentration can flow from low to high surface tension, how can the expansion of surface foam be overcome? And has surface elasticity any effect on foam production? Gibbs-Marangoni surface-elasticity effect gives a virtuous interpretation of foam stability. However, the question which merits the current discussion is: What is the best description of the dynamic surface tension for polysiloxane-polyether copolymers in polyol? To answer this question, viscous polyol (LG 56) has been used. Surface tension was assessed using the following procedure: the drop weight (w) against the three-fourths power of the reciprocal of the drop time $(1/T)^{0.75}$ ($= 0$ for pure solvent) was plotted and the slope (S) of the linear equation was determined. S is related to the viscosity of similar liquids, surface tension (σ), and density of the solution. The accuracy of the σ was 0.1 dyne cm^{-1} . The dynamic surface tension behaviors of the branched copolymers (A, B, and C) and linear copolymers (E-J) which are all nonionic surfactants, were studied. Rate constants (k) were compared for three branched copolymers at different concentrations and the equilibrium surface tensions (σ_e) were defined from the relation (surface tension, dyne cm^{-1} vs. drop time, seconds) in the concentration range 0-2% of polyurethane (PUR) foam. The σ_e was proportional to the extent of lowering.

The linearity of $\log(\sigma - \sigma_e)$ vs. T for the branched copolymer was above 5 seconds while the dynamic surface tensions of some solutions were higher than the equilibrium surface tension of the polyol alone in less than 5 seconds. The rate of attainment of surface tension has been affected by: (1) critical micelle concentration (c.m.c) of the surfactant, (2) molecular weight (contrary to polysiloxane (the lyophobic)), and (3) bulk concentration. Surprisingly, similar copolymers in molecular weight and percentage of polysiloxane have shown unlike surface activities. We found at 23 dynes cm^{-1} , an insufficient depression of surface tension for an effective Gibbs-Marangoni surface elasticity to operate.

Polydimethylsiloxane (PDMS) in linear copolymers that exhibits lower surface free energy has increased molecular weight and caused a reduction in the rate. Linear copolymers which show much sharper c.m.c's than the branched copolymers, discontinuities in the k/c plots are very noticeable at the c.m.c. Nevertheless, for equal concentrations, regardless of the c.m.c., the copolymers with the highest proportion of siloxane have the fastest rates of surface tension lowering. Linear copolymers showed worse foams (associated with temperature rises during formation and increasing of bulk concentration) and surface elasticity than branched copolymers. We believe that our study of dynamic surface tension has shown that too rapid a drop-in surface tension with time is detrimental to foam stability.

Audience take Away:

- The presentation is a beneficial meal for experts in polymer and surface chemistry where it offers better understanding of the difference in the applications of branched and linear copolymers for producing optimum foams and their capabilities in lowering the surface tension. The factors controlling these behaviors were determined which can highly be appreciated in polyurethane industry.

Biography

Loai Aljerf is a Prof in the Department of Chemistry, Faculty of Sciences/Damascus University. He is a specialist in analytical and industrial chemistry. He obtained many awards and published more than 50 peer-reviewed papers (two of them in French). He is a partner in Advances in Cleaner Production Network, and a member of the German Chemical Society e.V. (GDCh), Asian Chemical Society, and the American University of Beirut, the higher committee of the International Workshop-Advance in Cleaner Production (and in more than 60 conference organizing committees. He is editor of more than 80 journals and a reviewer for Top journals.

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Loai Aljerf^{*1}, Ukaogo Prince Onyidinma², Suhasini Bhatnagar³

Damascus University, Syria¹, Abia State University, Nigeria², Swaroop Enterprises and Biotech Pvt. Ltd., India³

Crystallization Behavior of Biodegradable Polyurethane Films Based on Glycols-Hexamethylene Diisocyanate

Polyurethanes (PURs) are solid hydrogens with glycols and hexamethylene diisocyanate (HMDI) form a class of solids known as quantum crystals. Their elastic properties are parameterized in terms of the elastic constants, is introduced to describe the anisotropic behavior of the lattice at the melting of highly crystalline PURs. The effective thermal conductivity can be reversibly transitioned between anisotropic and isotropic states. The mechanical properties of these materials are controlled by restriction of crystallization of polymer glycols. These combinational products are characterized by the property that the amplitude of the zero-point lattice vibrations is an appreciable fraction of the lattice constant, as a result of the small mass of molecules and the relatively weak intermolecular forces. Hydrogen bonding (NH O) in PUR structures is informative and eminently usable. It is, in a sense, a Rosetta stone that unlocks a wealth of information from the language of crystallography and makes it accessible to all scientists. In the X-ray pattern, the sharpness and intensity of the (200) interference characterizes the degree of ordering of the polymer chains in two-dimensional networks, in which the bonds are predominantly hydrogen bonds. While, (002) interference is associated with packing of the two-dimensional networks into three-dimensional aggregates and so that the bonds between the networks are formed by van der Waals forces. For study of the mechanism of melting of crystalline PURs, polymers from HMDI with ethylene glycol (EG), diethylene glycol (DEG), triethylene glycol (TEG) and butylene glycol (BG) were used.

The polymers prepared by the direct reaction of the components. Glycols and HMDI were added over a period of ½ to 1 hr. to the reaction vessel, while gradually increasing the temperature beyond the melting points of each polymer. The specimens were held at a temperature 20° above the melting point for 30 minutes in order to obtain complete melting. The melt was then cooled slowly to room temperature at a rate not greater than 1 degree/min. The X-ray diffraction curves of these specimens were recorded. Melting points were measured using a polarizing microscope equipped with an electrically heated stage. The partial degrees of crystallinities of each polymer rich in hydrogen bonds characterizing the hydrogen bonds and van der Waals bond were calculated, considering the angles of reflection of the (200) and (002) interference respectively, I_1 and I_2 the total intensities at the angles θ_1 and θ_2 respectively, and I_{cr1} and I_{cr2} the intensities of the crystalline parts of the spectrum at the angles θ_1 and θ_2 . X-ray analysis showed all polymers were highly crystalline with noticeable anisotropic behavior of the lattice and crystallinity is dependent on temperature. The maximal degree of ordering is reached close to the melting point while melting of the crystal lattice of PURs begins at the van der Waals bonds and hydrogen bonds are destroyed over a narrow range of temperature. The elastic vibrations of the elements of the lattice about its center of equilibrium increase. Besides, hydrogen bonds do not permit development of large amplitudes of vibration in the two-dimensional network.

Audience take Away:

The presentation has investigated the relationship between the degree of crystallinity of polyurethanes and the temperature of heat treatment, in addition to study the main characteristics of PURs during melt. The situation at which the lattice is being completely broken-down, has been determined. This information is very important for researchers and chemists working in polyurethane industry domain.

Biography:

Loai Aljerf is a Prof in the Department of Chemistry, Faculty of Sciences/Damascus University. He is a specialist in analytical and industrial chemistry. He obtained many awards and published more than 50 peer-reviewed papers (two of them in French). He is a partner in Advances in Cleaner Production Network, and a member of the German Chemical Society e.V. (GDCh), Asian Chemical Society, and the American University of Beirut, the higher committee of the International Workshop-Advance in Cleaner Production (and in more than 60 conference organizing committees. He is editor of more than 80 journals and a reviewer for Top journals.

**Ioana Stanciu***

University of Bucharest, Romania

Rheological behavior of olive oil used as biodegradable lubricant

The main objective of a lubricant is to reduce friction and wear. But also, it is responsible for heat evacuation. Taking into account their nature, there are mineral, synthetic, vegetal or animal lubricants. Until the XIX-th century, the manufacturing process of lubricants has been based on vegetal and animal resources. In southern country, the olive and corn poppy oils were used meanwhile in northern country the rapeseed oil was used. These oils have a high degree of biodegradability even today. But when mankind has discovered that oil could be processed for having lubricants and fuels at acceptable costs, the importance of vegetal resources had been reduced, but these petroleum-based lubricants have a strongly negative impact on the environment. This proposes three relationships of dynamic viscosity temperature dependence for olive oil. The purpose of this study was to find a polynomial or exponential dependence between temperature and dynamic viscosity of olive oil, using the Andrade equation changes.

Equation constants A, B, C and D were determined by fitting polynomial or exponential. Thousands of years, this oil was used for cooking, cosmetics and soap, but also as fuel for lamps. This proposes the relationship to describe the dependence of the dynamic viscosity of a olive oil, on the temperature. Experimental data for one type of olive oil were used to calculate the accuracy the proposed models. Equation constants were determined by exponential or polynomial best curves obtained at different shear rates using the program Origin 6.0. The correlation coefficients thus obtained varied between 0.8754 and 0.9999.

Audience Take Away:

- Stanciu I., 2020, Dependence viscosity of temperature and shear rate for vegetable oil used as biodegradable lubricant, Oriental Journal of Chemistry, 36(3), 563-566, (Factor impact 0.3700) <http://dx.doi.org/10.13005/ojc/360329>
- Stanciu I., 2020, Correlation between dynamic viscosity and shear rate for vegetable oil, Oriental Journal of Chemistry, 36(1), 33-36, (Factor impact 0.3700) <http://dx.doi.org/10.13005/ojc/360105>
- Stanciu I., 2020, Assessment of rheological behaviors of coconut oil, Journal of Science and Arts, 1(50), 183-186, (Factor impact 0.6750)

Biography:

I am a teacher of chemistry and physics in middle school. I graduated from the Faculty of Chemistry of the University of Bucharest in 1998. Studies Master we made in the same college and we have completed in 2001. I obtained a Ph.D. in chemistry in 2008 after 6 years of research stage, in which we obtained multi-grade oils based on synthetic polymers. Since 2005 has participated in numerous national and international conferences, has papers publishing in journals national and international for study multi-grade oils, canola oils and sunflower oil. I continued the research by studying oils and get new rheological models describing their behavior.



Alexander Ikechukwu Ajai*, Jimoh, Oladejo Tijani, Abdulrahman, Ali Yusuf

Federal University of Technology, Nigeria

Impacts of Artisanal Mining Activities on Heavy Metal contents in Soil, Water and Selected Food Crops

The concentrations of Ni, Fe, Zn, Pb and Cd in the soil, water, guinea corn, soya bean and millet around an artisanal mining site in Jatau-Garin Gabas community Niger State, Nigeria were determined during the dry and wet seasons using Atomic Absorption Spectrophotometry. The results from the study revealed that the soils profile was sandy loam in nature and some physicochemical properties and heavy metal contents of the soil and water samples determined where higher in the dry than the wet season. The mean heavy metal content in the soil ranged from 2.54 to 154.58 mg/kg and 2.11 to 52.29 mg/kg in the dry and wet season respectively. The speciation of the soil indicated higher concentrations of the heavy metals at the mining site and a sharp decline before and after it.

The soil pollution load indices ranged from 0.90 - 4.55 and 0.59 - 5.78 while the geo-accumulation indices from -0.51 - 1.11 and -0.92 - 1.35 for the wet and dry seasons respectively. The mean metal contents of the water samples ranged from 0.04 - 25.55 mg/L and BDL - 1.45 mg/L, in the dry and wet season respectively. The values for guinea corn, soya bean and millet ranged from 0.23 - 29.26, 0.73 - 25.13, 0.03 - 32 mg/kg; and from 0.12 - 25.26, 0.35 - 15.42, 0.07 - 15.62 mg/kg in the dry and wet seasons respectively. This study showed that the soils, water and food crops planted within the vicinity of the mining site were polluted with heavy metals. This calls for proper regulations and monitoring of mining activities in the area.

Audience Take Away:

- More informed on the impacts of artisanal mining activities on;
- Food crops
- Water
- Environment
- Health of immediate inhabitants
- Decision making by regulatory agencies and policy formulators

Biography:

Dr Alexander Ajai Ikechukwu is an Associate Professor and a Lecturer in the Department of Chemistry, Federal University of Technology Minna, Nigeria. He has his PhD in Analytical Chemistry from the same institution in 2011 and his M.Sc. Industrial Chemistry from University of Benin, Nigeria (1994). He is a member of the institution's Directorate of Research Innovation and Development (DRID) Grant Proposal evaluation committee and a Research Team Leader of the Heavy Metals and Pesticide Residues Unit of African Centre of Excellence for Mycotoxin and Food Safety. He has over twenty five (25) publications in various International peer reviewed Journals.



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Evaluation of ecofriendly compounds performance as corrosion inhibitors for mild steel in molar hydrochloric acid: Electrochemical study and theoretical approach

Mild steel has been extensively used in several industrial processes due to its distinctive characteristics. However, it can unavoidably be corroded due to the harsh environment around it. Recently, the use of organic corrosion inhibitors is the most effective and economical approach of all anticorrosive methods. The corrosion inhibition performances of two ecofriendly compounds (amino acids) (P1) and (P2) for mild steel in 1.0 M HCl solution were investigated using potentiodynamic polarization and Electrochemical Impedance Spectroscopy (EIS) techniques. Data obtained from EIS studies were analyzed to fit inhibition process through appropriate equivalent circuit model. The results of the electrochemical methods showed that the studied molecules imparted high resistance and behaved as cathodic type inhibitors. The inhibition efficiency for the optimal concentration of 10-3M was 87% and 89% for P1 and P2 respectively. Both thermodynamic and kinetic parameters were calculated and discussed. The adsorption of the inhibiting molecules on mild steel surface was found to be chemisorption and followed the Langmuir isotherm. Surface analyses were also carried out by the mean of SEM-EDX and FTIR to confirm inhibiting process. The reactivity of P1 and P2 was quantum chemically analyzed by the DFT method to investigate the effectiveness of these water soluble Green inhibitors.

Keywords: Amino acids, HCl, Mild steel corrosion, Electrochemical techniques, SEM-EDX, FTIR, DFT.

Audience Take Away:

- Audience will understand new corrosion inhibiting mechanism using green compounds.
- Audience (mainly industrials) could be interested in identifying and using new corrosion inhibitive molecules and appreciate the way they act in.
- International exchange and future collaborations could be beneficial.

Biography:

Dr. M. Oubaaqa is presently associate researcher in materials and environment chemistry department in the sciences faculty of Kénitra at Ibn Tofail University. In 1997, he graduated from Sciences faculty at Cadi Ayyad University of Marrakech. He previously worked on electrochemical heavy metals analysis and removal in wastewaters and urban sludges. Since 1996, he is member of the International Humic Substances Society, and since 1997 he is member of the Mediterranean Scientific Association for Environment Protection. Now, his research area is also turned towards the synthesis and study of new green inhibitors for mild steel corrosion in acid medium.



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Organic/ Inorganic hybrid materials for catalytic applications.

During the last decades, nanomaterials (NMs) have attracted intense research interest due to their multiple applications in various fields of science and technology, including medicine and catalysis. To enhance their applicability, it is well demonstrated that size matters and that the preparation of hybrid organic/inorganic materials will enlarge their applicability. The Catalysis & Fine Chemistry research group of the Coimbra University (Portugal) has accumulate experience to produce diverse functionalized materials at the nano and micrometer scale, including silica particles, carbon nanotubes, nanodiamonds and magnetic nanoparticles.

In this communication, our latest achievements, regarding the preparation of hybrid organic/inorganic nanomaterials and their application in the activation of small molecules, namely carbon monoxide, carbon dioxide and hydrogen will be presented. Such hybrid nanomaterials, prepared via covalent linkage of organometallic and porphyrin type complexes onto the surface of several inorganic supports, including carbon nanotubes, nanodiamonds and magnetic nanoparticle materials will be discussed. New approaches for functionalization of these materials and their covalent attachment to appropriately functionalized organic ligands, such as porphyrins, phosphines and C-scorpionate type molecules will be presented and discussed.

We highlight the application of catalytic hydroaminomethylation reaction as an innovative strategy to promote the covalent linkage of vinyl type ligands with amine-functionalized nanomaterials (10.1016/j.cattod.2019.05.045). The developed organic hybrid nanomaterials revealed to be highly active, selective and reusable catalysts in hydroformylation, oxidation/epoxidation, CO₂ cycloaddition reactions to epoxides (10.1002/cctc.201800397). In addition, Rh/P and Fe/C-scorpionate complexes immobilized onto iron-magnetic nanoparticles revealed to be highly active and reusable catalysts to promote the sequential hydroformylation/acetalization of olefins. Furthermore, the use of hybrid silica-metalloporphyrins in antibiotic degradation using H₂O₂ as green oxidant will be discussed. We have been able to promote the degradation of trimethoprim, one of the most worldwide prescribed antibiotics, aiming to prevent antimicrobial resistance caused by its environmental presence (10.1016/j.apcatb.2020.119556). Experimental details regarding the synthesis of the catalysts and their reutilization will be presented and discussed.

In sum, in this communication we highlight our most recent contributions in the preparation of hybrid organic- inorganic materials for application as reusable efficient catalysts both to create added value in fine chemistry and to aid in the eradication of polluting agents in the environment.

Audience Take Away:

- new techniques for immobilization of organic ligands onto solid nanomaterials including hydroaminomethylation as alternative tool
- strategies for reutilization of the immobilized catalysts onto nanomaterials
- importance and versatility of new sustainable catalytic systems that produce value added compounds and are used in environmental remediation

- examples of immobilized catalysts onto materials and their application/reutilization in fine chemistry will give the audience the opportunity to learn about how sustainable Catalysis/Chemistry are pivotal nowadays.
- solutions for environmental remediation through sustainable catalysis will be a good topic to discuss the wide applicability of these heterogeneous systems.

Biography:

Fábio M. S. Rodrigues (Portugal, 1990) received his Bachelor's degree in Industrial Chemistry (2013) and his MSc in Advanced Chemistry with specialization in Industrial Chemistry (2015), both from the University of Coimbra. Currently he is finishing his PhD in the Coimbra Chemistry Centre with a Catalysis and Sustainability PhD program fellowship. His research interests involve the development of new catalytic systems and new hybrid nanocatalysts for sequential processes. He is author and co-author of 5 scientific international publications in journals of high impact, 2 book chapters, and near 20 (oral/poster) participations in scientific meetings.



Nouha siragi*, Mohamed el hadri, Moulay ahmed el idrissi raghni, Hamid Aahamdane

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Synthesis and characterization of copper-doped forsterite as new blue ceramic pigments

In the field of ceramic pigments, one research trend is the exploration of new white matrixes that can serve as ceramic pigments by hosting different transition metals as chromophores. One example is Forsterite Mg_2SiO_4 : This thermally and chemically stable matrix can offer a large pallet of colors when Mg is partially substituted, in two inequivalent octahedral sites, for metals such as Co, Ni, Mn, Fe, Cu... In this work, we report on the potential use of Cu-doped Forsterite as new blue ceramic pigments.

$\text{Mg}_{2-x}\text{Cu}_x\text{SiO}_4$ solid solutions were successfully synthesized via a novel sol-gel method, and characterized using X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and UV-Vis Diffuse Reflectance Spectroscopy (DRS), to investigate their crystalline structure, microstructure, and optical properties. The color of the pigments was characterized using the CIE $L^*a^*b^*$ color space. The obtained crystalline powders are of high purity for substitution rates up to 20%. They are light blue in color for $x < 15\%$ turning green at higher substitution rates.

Audience Take Away:

- The audience of this presentation will be introduced to the important physical aspects governing the optical behavior of ceramic pigments.
- This presentation will also shed some light on the beneficial use of Sol-Gel route in the synthesis of ceramic pigments.

Biography:

Nouha received an engineering degree in “Process and Ceramic Materials Engineering” at the National School of Applied Sciences in Safi, University of Cadi Ayyad - Marrakech in 2015. She later joined the Laboratory of Materials Science at the Faculty of Sciences Semlalia of the same university as a PhD student, and is currently working on the elaboration, via Sol-gel route, and the characterization of new ceramic pigments.



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Vertical and Horizontal cell structural appraisal of a 9-Year Cedrela Odorata L. (Miliaceae) for pulp and paper making

Paper is a material of importance in human life and produced from wood. However, is not all wood that have the qualities to be used for paper production. This study assesses the suitability of a 9-year old *Cedrela odorata* wood along both vertical (bottom to top) and horizontal (sapwood to heartwood) directions for pulp and paper making. Specifically, we evaluated the variations in fibre dimensions and other derived technical requirements needed for wood to be used for paper production. Franklin's maceration process was adopted for the study. Collected data was subjected to statistical analysis using IBM Statistical Package for Social Sciences (SPSS) version 17.00. Mean fibre length was found to be short (i.e. ranged from 0.822 ± 0.142 mm – top heartwood to 1.142 ± 0.144 mm – base heartwood) which were all less than 1.6mm (1600 μ m). Runkel ratio was highest in top heartwood (0.26 ± 0.08); Flexibility Coefficient was highest in bottom sapwood (0.83 ± 0.05); and Slenderness Ratio was highest in bottom sapwood (49.18 ± 10.42). The derived fibre values were all within acceptable standard ranges for wood to be used for paper production: runkel ratio (< 1.0), Coefficient of Flexibility ($> 75\%$), and slenderness ratio > 33 indicate that the 9-year old *Cedrela odorata* hardwood in Ghana is a potential species to produce pulp and paper of desired qualities, especially when it is mixed with other long fibre wood species. Thus, the 9-year fast grown *Cedrela* wood species is recommended for consideration among other known species for paper manufacturing in Ghana and elsewhere.

Keywords: Ghana Paper, Wood fibres, Wood maceration, *Cedrela odorata*, Runkel ratio.

Biography:

Dr. Peter Kessels Dadzie is a Ghanaian professional teacher and holds BEd. Technology Education in Wood and Construction (2002), MSc. Wood Technology and Management (2007) and PhD. Wood Science and Technology (2014) from the University of Education, Winneba, and Kwame Nkrumah University of Science and Technology, all in Kumasi, Ghana. Currently, he is a senior lecturer at the Interior Design and Materials Technology Department of Kumasi Technical University, Kumasi, a member of the Society of Wood Science and Technology (SWST) and Forest Products Society (FPS) and has published over 17 research articles in various very reputable journals.



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Numerical analysis of ZnS/SnS Hetero junction solar cell

Materials for thin film solar cells are currently the subject of multiple researches in order to reach the highest ratio efficiency/cost. Tin sulfide (SnS) is one of the most promising solar cell absorber materials because it has appropriate optoelectronics properties and cost-effective. Zinc sulfide (ZnS) is the most common material for buffer layer of a heterojunction solar cell. In this work, we study the electrical characteristics of ZnS/SnS solar cells (Current density J_{sc} short circuit, open circuit voltage V_{oc} , $P(V)$, and $C(V)$). The one-dimensional SCAPS-1D is used to analyze numerically the performances of ZnS/SnS thin film solar cells.

Keywords: ZnS/SnS solar cells, short circuit, open circuit voltage, simulation, SCAPS-1D.

Biography:

Dr. Zaidi working as Asso. Prof. in Dept. of Physics at the University of Batna 1. He obtained a doctorate in Physics at the University of Annaba in 2014. He has published a number of research papers in reputed journals, has written three books on solar cells. He acted as an Editor-in-Chief of IJMSA (From 2017 to 2018). He is a potential reviewer for reputed journal papers. He participated in many international conferences serving as a referee, PC member... etc. He is also an Editorial Board member of numerous journals.



Dr. Mastura A .Abdalshafie EfHEMA*

Omer Al - Mukhtar University El-Beida, UK

Effect of flame retardants and 1% stabilizer on melting and melting dripping behaviour of pp thermoplastic polymers

This study is aimed to understand the mechanism of combining the action of different types of flame retardants (FR) on melting and melt dripping behaviour and its moderation of the Polypropylene polymer (PP). PP Polymer was chosen to be blended in a twin screw extruder with the flame retardants and an additive, which is a 1% Stabilizer, to investigate Polypropylene's melting and melt dripping behaviour moderation, to reduce its melting and melt dripping. This test, which is known as Furnace test, was applied in this study with a variety of conditions. A Carbolite tube furnace, which the calibration and design of is by Mastura A. EfHEMA, was used to provide non-burning conditions, as well as to prepare chars of polymers at different temperatures (2000C – 5000C) under isothermal heating conditions for 5 minutes.

In order to test the melting and melt dripping behaviour of the seven PP polymer samples, specific samples have been prepared. Then following the results, we can distinguish which of the PP polymer sample drips longest, the maximum length of train and velocity that is required could be known. The study also indicates that the melting behaviour of thermoplastic materials is an important characteristic in fires which should be taken into account in the development of modelling. To study melting and melt dripping behaviour, the methodology of melting is developed. The results from this test have been analysed to draw a relationship between melting and melt dripping behaviour. Most of previous works on melting and melt dripping behaviour was concentrated on study of fire operating conditions, and modelling of the thermal process, however, no work has been reported on quantitative relationship between melting and melt dripping behaviour of thermoplastic polymers.

Biography:

Mastura A .Abdalshafie EfHEMA is a reliable and punctual woman who enjoys working within a team. I consider myself to be cheerful, polite, and able to listen and I can follow instructions precisely. I am honest and trustworthy, self motivated and able to motivate others around me. I am a good organizer who is both patient and hardworking. Also have extensive academical and practical experience in experimental labs work in Physics, Theoretical physics, material sciences and sciences Engineering. Education/Training 2012-2013: NANO research grant – Created, analysed and monitored molecular projects and F95 codes via various computer science programmes. Work Experience 2009-2011: Arabic School of Life Science and physics in Manchester, Year 9, 10 and 11 physics teacher. Interests: Reading, Travelling and socialising with others.

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