3rd International Conference on

MASS SPECTROMETRY, PROTEOMICS AND POLYMER CHEMISTRY

May 20-21, 2019 | Rome, Italy

MASS SPECTROMETRY CONGRESS 2019

SCIENTIFIC TRACKS & ABSTRACTS

DAY 1

DAY 1 SESSIONS
MAY 20, 2019

Chromatographic Techniques | Mass Spectrometry in Forensic Science | Mass Spectrometry in Drug Discovery and Development | Mass Spectrometry in Proteome Research | Stereo Chemistry of Polymers

SESSION CHAIR

Magnus S Magnusson
University of Iceland, Iceland

SESSION CO-CHAIR

Anupam Chanda
Indian Institute of Packaging, India

✔ SESSION INTRODUCTION

Title: SWATH mass spectrometry as a tool for quantitative profiling of the bone marrow plasma from alcoholic liver disease

Renu Goel, Translational Health Science and Technology Institute, India

Title: Metabolomics profiles of autistic children's urine reveals altered dopamine and noradrenaline levels.

Federica Gevi, University of Tuscia, Italy

Title: Characterization of disease in preclinical cancer research using Desorption Electrospray Ionization Mass Spectrometry (DESI-MS)

Alessandra Tata, University of Toronto, Canada

Title: Chemical tools for selective detection of Monomethyl Lysine PTMs

Monika R, Auburn University, USA

Title: Porous polymers and metallic nanoparticles: A hybrid wedding toward innovative supported catalysts

Daniel Grande, East-Paris Institute of Chemistry and Materials Science (ICMPE), France

Title: Evaluation of chlorinated biphenylene air concentration after a fire

Silvia Mosca, CNR – IIA (Italian National Research Council – Institute for Atmospheric Pollution Research), Italy

Title: Prediction of mechanical properties of PP/EVA polymer blends governed by EVA phase change in the presence of environmentally friendly inorganic tungsten disulfide nanotubes (INT-WS2)

Reza Nikoomanesh, Jam petrochemical Complex, Iran

SWATH MASS SPECTROMETRY AS A TOOL FOR QUANTITATIVE PROFILING OF THE BONE MARROW PLASMA FROM ALCOHOLIC LIVER DISEASE

Renu Goel, Dhananjay Kumar, Ankur Kumar and **Anupam kumar**

Translational Health Science and Technology Institute, India

Alcoholic hepatitis is characterized by acute or acute-on-chronic hepatic failure and associated with a high mortality. Specific therapies should be considered for those at high risk of mortality. Model for End-Stage Liver Disease (MELD) score is a marker of disease severity and mortality in persons with chronic alcoholic liver disease. Author's aim is to find out a diagnostic biomarker for disease severity along with the MELD score which can be used as a predictor of short term mortality in persons with alcoholic hepatitis. Understanding molecular pathogenesis is pivotal in managing the disease. They employed sequential window acquisition of all theoretical mass spectra (SWATH-MS) to seek crucial proteins involved in disease progression. Bone marrow plasma is taken from chronic liver disease patient as a part of stem cells therapy clinical trial. In this study, a quantitative proteomic of bone marrow plasma with low and high MELD scores were compared with normal bone marrow plasma from non-cirrhotic portal hypertension patient whose liver function test was normal using a SWATH-MS strategy. In total, 232 proteins were differentially expressed in all groups. 17 proteins are down regulated and 81 up regulated in patients with MELD score <15 with control. Moreover, 37 proteins are down regulated, 59 up regulated while comparison of MELD score >15 with control. Inhibition of coagulation, complement and intrinsic prothrombin pathways are revealed by functional analysis. Humoral immune response, immune cell trafficking and inflammation pathways are enriched under physiological system development. Proteins preliminarily discovered in this study may be associated with dysregulation bone marrow microenvironment during disease progression. To the author's knowledge, this study presents the most complete view of bone marrow plasma in low and high MELD score, identifying hundreds of differentially expressed proteins, which together form a rich resource for novel drug targets or diagnostic biomarker discovery.

BIOGRAPHY

Renu Goel has obtained her M.Tech and PhD degree in Biotechnology from Institute of Bioinformatics, India with Prof. Akhilesh Pandey, Johns Hopkins University, Maryland. Her research group is working on identifying pathways or proteins involved in early stages of progression of diseases such as type II diabetes, liver diseases and dengue fever by using proteomics, metabolomics and bioinformatics approaches. She has also worked on draft map of human proteome published in Nature. During this period she has published around 30 research articles in high impact factor international journals. She is an Editorial Board Member for many journals.

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METABOLOMICS PROFILES OF AUTISTIC CHILDREN'S URINE REVEALS ALTERED DOPAMINE AND NORADRENALINE LEVELS

Federica Gevi, Fanelli Giuseppina, Antonio Belardo, Sara Rinalducci and **Timperio Anna Maria**
University of Tuscia, Italy

Autism spectrum disorders (ASDs) are a group of neurodevelopmental disorders consisting of a delayed or altered language development and difficulties in social interactions. Beside clinical and social tests, metabolic abnormalities are frequently associated with ASD and their knowledge could help clinicians to provide earlier and more reliable diagnosis. A considerable number (16,704) of urinary altered metabolites were recorded in autistic children, with 222 displaying the largest differences (p-value ≤ 0.05 and fold change ≥1.5) between young ASD children and controls. Several altered metabolic pathways have been implicated in the disease, such as tryptophan, purines and pyrimidine's; however, in this paper, altered level of the most important neurotransmitters have been discussed. The highest levels of dopamine and its metabolite, homovanillic acid, indicated a dopamine β-hydroxylase enzyme block, probably due to presence of 4-cresol together with a higher level of vitamin C, all revealed in the urine of autistic children. Moreover, the incorrect synthesis of the active form of vitamin B6, pyridoxal-5'-phosphate was also detected, which is an essential co-factor for the biotransformation of glutamate into GABA. The accumulation of glutamate and lower concentrations of GABA were found in all of the autistic children examined.

BIOGRAPHY

Federica Gevi has completed her PhD in cellular biology at University of Tuscia, Italy. Currently she is a research RTDa of Tuscia University, Italy. She has 10 years of experience in the field of mass spectrometry-HPLC (MALDI TOF, Orbitrap, Q-TOF, amaZon ETD) in protein identification, metabolomic and lipidomic characterizations in various biological samples. She has 23 publications that have been cited over 300 times and her publication H-index is 10.

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Note:

CHARACTERIZATION OF DISEASE IN PRECLINICAL CANCER RESEARCH USING DESORPTION ELECTROSPRAY IONIZATION MASS SPECTROMETRY (DESI-MS)

Alessandra Tata[1] and **Arash Zarrine-Afsar[2]**
[1]University of Toronto, Canada
[2]University of Health Network, Canada

There is a clinical need for new technologies that would enable rapid cancer diagnosis based on molecular signatures. New developments in ambient ionization mass spectrometry suggest that this technique will soon become a routine medical tool for cancer diagnosis. In particular, desorption electrospray ionization mass spectrometry (DESI-MS) is very successful because it does not require extensive tissue preparation; the data collection and analysis can be done within a few seconds. Generally, tissue smears are used in rapid intraoperative pathology workflows coupled quick staining methods to characterize cancer tissues. The author evaluated the combination of rapid DESI-MS detection with rapid tissue smear preparation for cancer detection. Principal component analysis (PCA) was performed to evaluate the concordance between DESI-MS profiles of breast cancer from tissue slices and smears prepared on various surfaces. During tumour resection, margin assessment is of extremely importance. This is usually done by H&E staining. To this aim, we demonstrated the utility of combined polarimetry and DESI-MS for accelerated identification of tumor boundaries. Polarimetry images are made available considerably faster than H&E images proposed for guiding DESI-MS. Therefore, a multi-modality combination of polarimetry and DESI-MS appears capable of accelerating the acquisition of MS data. Finally, patients affected by stroma-rich tumours exhibit a poor prognosis and a higher chance of relapse. As such, there is a need for a technology platform that allows rapid determination of the tumour stroma ratio. To this aim, we provided a proof of principle demonstration that DESI-MS can be used to determine tumour stroma ratios. This proof of principle demonstration is encouraging and must be further validated using human samples and a larger sample base. At maturity, DESI-MS thus may become a molecular pathology tool providing an alternative rapid cancer assessment without the need for time consuming staining and microscopy methods, potentially further conserving human resources.

BIOGRAPHY

Alessandra Tata received her master degree in Pharmacy (2006) and PhD in Pharmaceutical Sciences from University of Rome "Sapienza" in 2010. During her PhD studies, she did her internship as visiting scholar at Purdue University joining Dr. R.G. Cook's group in 2008. She has been a post-doctoral fellow at ThoMSon Mass Spectrometry Laboratory at the State University of Campinas, Brazil during 2011-2014 where she applied the MALDI-MS technique to develop methods for the rapid and sensitive detection of lipid profiles in oocytes, embryos, uterus and semen utilized in the *in vitro* fertilization. In 2014 she joined Prof. Demian Ifa's Lab at York University, Canada to apply DESI-MS techniques to the study of microbial networking and then moved to University of Health Network, Canada to develop methods for the rapid detection and characterization of tumor margins by ambient mass spectrometry with Prof. Arash Zarrine Afsar. She has just left research to start up her own company in Italy.

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CHEMICAL TOOLS FOR SELECTIVE DETECTION OF MONOMETHYL LYSINE PTMS

Monika R[1] and **Yonnette Sim[2]**
[1]Auburn University, USA
[2]Seton Hall University, United States

Selective modification of biomolecules provides scientists with an effective tool for a multitude of bio analytical, therapeutic, biological and bioengineering applications. However, chemical strategies that can target a particular functional group at a single site in the presence of reactive amino acid side chains on protein surfaces are limited. We have developed a multicomponent bioconjugation approach for selective labelling of proteins containing secondary amines. This method does not require any genetic engineering of the protein target and protection of the side chains of other amino acids. The resulting bioconjugation reaction leads to the formation of a highly stable C-C bond at the site of the conjugation. The broad utility of the bioconjugation reaction is demonstrated by conjugation of various probes such as dye, peptides and PEG on different proteins containing a proline at the N-terminus such as creatine kinase and aldolase. This method is employed for labelling monomethyl lysine containing post-translational modifications (PTMs) on proteins with various cargoes. The dysregulation of monomethyl lysine PTMs has been linked to a variety of different biological malfunctions, yet the chemical methods for selective detection of monomethyl lysine PTMs are still lacking. This selective tagging methodology can effectively detect monomethyl lysine PTMs thus has a potential to further our understanding of the role of monomethylated lysine containing PTMs in regulating various cellular signalling processes.

BIOGRAPHY

Monika R has completed her PhD in 2009 from Indian Institute of Technology, Kanpur, India and she completed her Postdoctoral from New York University, USA. Currently she is working as a Professor at Auburn University, USA.

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POROUS POLYMERS AND METALLIC NANOPARTICLES: A HYBRID WEDDING TOWARD INNOVATIVE SUPPORTED CATALYSTS

Daniel Grande, Benjamin Le Droumaguet and **Benjamin Carbonnier**

East-Paris Institute of Chemistry and Materials Science (ICMPE), France

Over the last decade, the generation of organic porous (nano) materials with tunable pore sizes and desired functionalities has been the subject of increasing attention in materials science. Interest in such porous frameworks originates from the large variety of applications in which they are involved, e.g. size/shape-selective nanoreactors, monoliths for advanced chromatographic techniques, nanofiltration membranes, high specific area catalytic supports, as well as 3-D scaffolds for tissue engineering. Porous monolithic polymers may represent suitable supports for the immobilization of metallic nanoparticles, thus allowing for the generation of hybrid materials having particularly interesting features for heterogeneous supported catalysis. Such porous materials indeed present some undeniable advantages over their inorganic counterparts, namely their synthesis is cost-effective and their mechanical properties as well as the chemical nature of the pore interface can be finely tuned. In this context, we have developed different polymer-based hybrid systems based on porous polymers that were suitably functionalized so as to successively immobilize gold nanoparticles. This presentation will particularly emphasize on recent studies developed in our laboratory on this topic. It will focus on hybrid systems based on three main types of porous polymers: Nanoporous polystyrene frameworks arising from polystyrene-block-poly(D,L-lactide) diblock copolymers with a cleavable functional group at the junction between both blocks; bulky macroporous monoliths prepared from a selectively cleavable disulfide dimethacrylate monomer; functionalized doubly porous poly(2-hydroxyethyl methacrylate)-based networks. Such functional hybrid materials have been successfully applied as efficient and versatile heterogeneous supported catalysts in miscellaneous model organic reactions, including hydride-mediated reduction of nitroaromatic compounds, C-C homocoupling of benezeneboronic acid derivatives and reduction of dyes. We have notably demonstrated that cascade reaction processes consisting of two successive nanogold-catalyzed reactions are efficiently implemented with these novel porous polymer-supported catalysts.

BIOGRAPHY

Daniel Grande is currently working as a CNRS Research Director at the East-Paris Institute of Chemistry and Materials Science (ICMPE) in France. He received his PhD degree in Polymer Chemistry from the University of Bordeaux, France and the University of Coahuila, Mexico in 1998 and then he spent about two years at Emory University, USA as a NIH post-doctoral fellow. His research interests include the development of functional polymer materials with a broad range of porosity scales and the whole spectrum from their design to their potential applications is investigated. He is the co-author of about 110 peer-reviewed publications in international journals, 40 proceedings, 14 book chapters and 11 patents.

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EVALUATION OF CHLORINATED BIPHENYLENE AIR CONCENTRATION AFTER A FIRE

Silvia Mosca, V Colapicchioni, M Cerasa and **E Guerriero**

CNR – IIA (Italian National Research Council – Institute for Atmospheric Pollution Research), Italy

A wide variety of chlorinated aromatic compounds are released intentionally and/or unintentionally in the environment. Polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) and polychlorobiphenyls (PCBs) are well known environmental contaminants. Another class of organochlorinated compounds consists of polychlorinated biphenylenes (PCBPs), whom toxicity is comparable to PCDDs and shows the same mechanism of action. It is known that the formation of PCBPs is strictly correlated with the release and combustion or pyrolization of capacitor and transformer fluids, office furnishings and computers. Despite these assumptions, there are very limited and dated studies on these toxic chemicals except observations on building fires. 2,3,6,7-TeCBP concentrations (the most common congener) have been investigated in air sampled in an industrial building containing electric material after a fire, in an extended time, in order to evaluate the persistence. The concentration was monitored over an extensive range of time and compared to ambient air levels.

BIOGRAPHY

Silvia Mosca has completed her Chemistry Degree and PhD from Sapienza University of Rome, Italy and she works as a Full Researcher at the Institute for Atmospheric Pollution Research of the Italian National Council (CNR-IIA) since 2004. Her research is focused on sampling strategies, analysis and diffusion in the environment. She is the author of national and international papers and she is peer-reviewer for international journals in the field of environmental pollution.

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PREDICTION OF MECHANICAL PROPERTIES OF PP/EVA POLYMER BLENDS GOVERNED BY EVA PHASE CHANGE IN THE PRESENCE OF ENVIRONMENTALLY FRIENDLY INORGANIC TUNGSTEN DISULFIDE NANOTUBES (INT-WS2)

Reza Nikoomanesh

Jam petrochemical Complex, Iran

Anticipating dynamic mechanical behavior of polymeric materials over long period of time and under different frequencies is the first step to be taken to afford loadbearing applications. Nevertheless, what we know about dynamic mechanical behavior of polymers is only limited to experiments, which necessitates large pools of data spending too much money, time and energy. Environmentally-friendly inorganic tungsten disulfide nanotube (INT-WS2), was introduced to polypropylene/ethylene vinyl acetate copolymer (PP/EVA, 75/25 wt/wt) blends through melt mixing and dynamic mechanical analysis (DMA) frequency sweep tests were performed to obtain master curves based on time-temperature superposition (TTS) theorem. The influence of EVA phase change (solid, semi-solid and melt domains) on the creep and recovery behavior of nanocomposites in linear region was then studied. It was found that using INT-WS2 along with PP-g-MA results in distinctive improvement in creep-recovery response of nanocomposites. Burger and Weibull models were used to mimic viscoelastic behavior of the nanocomposites. Creep compliance master curves predicted creep compliance, while analysis of cyclic creep-recovery at 30 8C revealed almost constant permanent strain parameters for sample having 5wt% INT-WS2 and PP-g-MA after three times repeating test cycles. Influence of phase change phenomenon of EVA domains on creep-recovery behavior of nanocomposites was mechanistically demonstrated.

BIOGRAPHY

Reza Nikoomanesh has completed his Masters from Islamic Azad University, Iran in the field of Chemical-Polymer Engineering. He is the Head of Physical Mechanical Laboratory of Jam Petrochemical Complex, Iran.

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YOUNG RESEARCHER FORUM

DAY 1

DIFFERENTIALLY REGULATED URINARY PROTEINS AND THEIR MODIFICATION STATUS SERVE AS NON-INVASIVE BIOMARKER FOR EARLY DIAGNOSIS AND CHARACTERIZATION OF DRUG-INDUCED LIVER INJURY (DILI)

Md Shabir Hussain[1], Parul Saini[1], S K Sarin[1], Shasthry S M[1], Ram Kumar[2], Priyanka Jain[1]
and **Sherin Thomas[1]**
[1]Institute of Liver and Biliary Sciences, India
[2]University of Delhi, India

Background & Aim: DILI is a frequent side effect of many drugs, but the diagnosis is mainly by exclusion of other causes as there are no specific biomarkers to diagnose DILI. This is the non-invasive methods to identify proteomic signature and determine urinary micro-albumin (µA).

Materials & Methods: Early morning urine samples from successive patients with biopsy proven DILI (n=40), age and sex matched healthy controls (HC), (n=40) were collected at ILBS from September 2017. Out of the 40, 10 had hepatocellular, 15 cholestatic and 15 mixed types of DILI based on 'R' value >5, <2 or between 2-5 respectively at baseline LFT and concentrate 50 ml of urinary by 3 kDa filter tube for label free quantification-mass spectrometry (LFQ-MS) and urinary µA analyses were done.

Results: Urinary µA level was significantly higher in DILI [50 mg/dl] compared to HC [0.17mg/dl] (p<0.05) at baseline. The author did LFQ-MS analysis of urine samples from each individual group and they identified more than 1900 proteins. And they have done the comparative analysis in different three types of DILI with HC and they found as 1292 were common, 235 found only in HC and 333 different in DILI, in cholestatic compared to HC, 57 common and 21 unique to cholestatic. Also they have analysed cholestatic with hepatocellular, cholestatic with mixed type of DILI. We further analysed samples abundance, Venn diagram, PCA plots, abundance plot and biological process. He used STRING pathway of differentially expressed proteins to characterization, significant function and clinical role of differentially expressed proteins in DILI, which were unique to DILI, like protein AMBP, Zinc-alpha-2, Kininogen, Mannan-binding lectin, Fibronectin, CD59 glycoprotein etc. functions were assessed in the Uniprot database.

BIOGRAPHY

Md Shabir Hussain has completed his PhD in Biomedical Sciences from Sai Nath University, and ILBS, India. He is the SERB National Post-Doctorate Fellow and Principal Investigator of the Project "Proteomics Study of Drug-Induced Liver Injury (DILI) For Identification of Non-Invasive Biomarkers" which has been funded by SERB, DST, Government of India. He has 11 publications that have been cited over 110 times and has published several original research articles in high impact factor international journals. His area of interest is in Multi-OMICS and he is doing his research on Proteomics, transcriptomics and metabolomics.

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SCIENTIFIC TRACKS & ABSTRACTS

DAY 2

DAY 2 SESSIONS
MAY 21, 2019

Applications of Mass Spectrometry | Applications of Bio-Polymers | Polymer Science | Isolation Techniques

SESSION CHAIR	**G A Farzi** Hakim Sabzevari University, Iran
SESSION CO-CHAIR	**Shrikaant Kulkarni** Vishwakarma Institute of Technology, India

✅ SESSION INTRODUCTION

Title: Synthesis of rigid polyurethane and effect of silicon surfactant on its properties

M Shafiq Randhawa, University of the Punjab, Pakistan

Title: Identification of hydroxytyrosyl and tyrosyl oleate in olive oils and olive oil by-products

Cinzia Benincasa, CREA Research Center for Olive, Italy

Title: Quantitative analysis of phosphorus containing nucleating agent in polymer resin by ICPMS

Birbal Bajia, Indian Oil Corporation Limited, India

Title: A study on the influence of water on the L-leucine fragmentation

Baliulyte L, Vilnius University, Lithuania

MASS SPECTROMETRY, PROTEOMICS AND POLYMER CHEMISTRY

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SYNTHESIS OF RIGID POLYURETHANE AND EFFECT OF SILICON SURFACTANT ON ITS PROPERTIES

M Shafiq Randhawa
University of the Punjab, Pakistan

Rigid polyurethane foam has been synthesized from high functional crude MDI and blending poly-l for a wide range of surfactant concentration with R141b blowing agent. Cream time, gel time and take free time increase as the concentration of surfactant is increases. The foam density decrease as the concentration of surfactant is increases the decrease in density due to the increase blowing efficiency with surfactant. Surface tension also rapidly decreases in accordance with cell size decrease and close cell content rapidly increase at low surfactant concentration. The decrease of cell size was accompanied by the decrease of thermal conductivity. Today, numerous building blocks and polymer structures are available to chemists and engineers for the synthesis of polyurethanes by the poly-addition principle. Because the manufacturer of polyurethane articles converts low-molecular weight raw materials into finished polymers at the production site, author have place special emphasis on the brief history and some basic concepts about the raw materials and chemistry of polyurethane. He also covers the manufacturing techniques and processing equipment's in this research article, reviews physical, chemical, mechanical and electrical properties and also cover the applications of all types of polyurethanes for a wide range of industries.

BIOGRAPHY

M Shafiq Randhawa has completed his PhD course work from University of the Punjab, Pakistan in Polymer Technology and Engineering. He is the General Manger of Relaxo Pvt. Limited (Chawla group of Industries).

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IDENTIFICATION OF HYDROXYTYROSYL AND TYROSYL OLEATE IN OLIVE OILS AND OLIVE OIL BY-PRODUCTS

Cinzia Benincasa, Pierluigi Plastina, Massimiliano Pellegrino and **Enzo Perri**
CREA Research Center for Olive, Italy

Although olive fruit is rich in phenolics, only 2% of the total phenolic content is found in the oil. The main fractions are found in olive mill waste water (OMWW) and pomace. Hydroxytyrosol (HTy) and Tyrosol (Ty) are two of the major phenolic components of olive and olive oil. They are present in the esterified form as secoiridoid derivatives, as well as in the free form, whose amounts increase during olive ripening and olive oil processing as a result of endogenous β-glucosidase hydrolytic activity that release HTy and Ty from the secoiridoids. HTy and Ty display a wide range of biological activities associated to human health. Despite their properties, HTy and Ty show low bioavailability, with fast absorption and elimination in humans, because of their polar character which limits their use as a dietary supplement as well as an additive in foods. Lipophylization of phenolics has been suggested as a useful method to increase their metabolic stability and ability to cross cell membranes. In order to expand the knowledge on the biological activities of Hty and Ty fatty esters as potential ingredients in functional foods with improved quality, the anti-inflammatory properties of a series of Hty and Ty esters with short, medium and long acyl chains by LPS-stimulated murine macrophage cell line were evaluated. The results obtained have demonstrated that, contrary to TyOle, HtyOle has *in vitro* anti-inflammatory properties and can be considered as a booster of the parent HTy. Moreover, HtyOle and TyOle occur in olive oil by-products while they were not detectable in intact olives. Taken together, these findings suggest the potential role of HtyOle and TyOle as markers of quality of olive oil and highlight the value of olive by-products as a source of bio-active compounds to produce medicines, cosmetics, nutraceuticals and functional foods for animal feeding.

BIOGRAPHY

Cinzia Benincasa has completed her PhD in Chemical methodologies for the development of molecules of pharmacological interest from University of Calabria, Italy in 2004. She is a researcher (Scientific disciplinary sector: Food Chemistry) of the Council for Agricultural Research and Economics and works at the Research Centre for Olive, Citrus and Tree Fruit, Italy since 2015. Her area of interest is in applications and determinations of isotopic ratios and trace elements for food traceability; investigation and characterization of phenolic compounds using HPLC, GC-MS/MS and LC/MS techniques; chemical-physical and organoleptic analysis for the characterization of olive oils and chemometric analysis. She has 23 publications that have been cited over 344 times and her publication H-index is 9.

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QUANTITATIVE ANALYSIS OF PHOSPHORUS CONTAINING NUCLEATING AGENT IN POLYMER RESIN BY ICPMS

Birbal Bajia and **Hemant Tyagi**
Indian Oil Corporation Limited, India

Neat polymer materials have poor stability and would result in a commercial failure if they are used virgin. A nucleating agent is used in polypropylene, providing superior mechanical properties, easier dispersion and reduced interaction with metal stearate and to give high degree of crystalline resulting in increased mechanical properties such as hardness, elasticity modulus etc., and improve optical properties such as transparency in different grade of co-polymer polypropylene virgin powder. Nucleating agent and some secondary antioxidants are also used which are phosphorus based. Due to common phosphorus metal in both additives it is difficult to analyse the contribution of individual quantity as per standard test method ASTM D 6247 "Analysis of elemental content in additive in polyolefin by X-Ray fluorescence spectrometry". All components in combination of various additives were also not significantly separated in gas chromatography and high performance liquid chromatography. New method developed for the analysis of nucleating agent in range of 0.01% to 0.1% concentration. Repeatability and validation of method established.

BIOGRAPHY

Birbal Bajia has completed his PhD from MLS University, Rajasthan, India. He is the quality control manager at Indian Oil Corporation limited, Panipat Naphtha cracker- a unit of polymer producer. He has published more than 10 papers in reputed journals and author of three books in the field of engineering chemistry.

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Note:

A STUDY ON THE INFLUENCE OF WATER ON THE L-LEUCINE FRAGMENTATION

Baliulyte L and **Tamuliene J**

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All living organisms are constantly affected by ionizing radiation emitted by natural sources such as cosmic rays and radionuclides contained in rocks from the Earth, food, water and air etc. Moreover, ionizing radiation exposures also occurs during medical procedures. Low-energy electrons are produced due to the interaction of X- and Y rays with organic molecules. These low-energy electrons cause damage of biomolecules, including amino acids, e.g., Leucine. Data on fragmentation of amino acids in water are scarce, although they are relevant to the analysis of processes in living organisms. Hence, the aim of the author's research is to determine whether the appearance energies of fragments differ between conditions with and without the influence of water included. They used density functional theory (DFT) B3LYP method and cc-pVTZ basis set. The polarized continuum model (PCM) method was used to evaluate the presence of water. They applied Gaussian 03 Rev D.01/09 Rev D.01 program. Fragments were selected based on the experimental mass spectrometry data in the NIST database. The strongest peaks in the mass spectrum of L-leucine correspond to m=86 amu, 44 amu and 30 amu. They determined that cation with mass 86 amu is $C_5H_{12}N^+$, cation with mass 44 amu is CO_2^+ and cation with mass 30 amu- CH_4N^+. The results of author's research with and without the influence of water indicate that more energy is needed for the formation of same cations in water.

BIOGRAPHY

Laura Baliulyte is a PhD student at the Institute of Biosciences, Life Sciences Center, Vilnius University, Lithuania. Her area of research mainly focuses on theoretical modelling of amino acids fragmentation, biochemical reactions and biophysical processes. She is the co-author of several articles.

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VIDEO PRESENTATION

DAY 2

SPONTANEOUS ENTROPY DECREASE IN AN ISOLATED MATTER-FIELD SYSTEM

Eliade Stefanescu
Advanced Studies in Physics Center of the Romanian Academy, Romania

The ordered molecular systems, which stand at the basis of our life and activity, are generally believed as being necessarily submitted to a so called Principle II of thermodynamics, asserting their evolution to disorder. In this scientific framework, the appearance of life on Earth, and of so many ordered systems as, for instance, of the fuels, which sustain our civilization, remained as a mystery. However, very recently, a physical system evolving from disorder to order, in this way converting environmental heat into usable energy, has been discovered, in spite of the Principle II of thermodynamics. This is because this principle has been thought and defined for a molecular system, while when a coherent electromagnetic field is present in a resonant cavity it is no more valid. Author invented a semiconductor device which, by heat absorption from the environment, generates a coherent electromagnetic field in the infrared domain ($\lambda \sim 2$ μ). This field is generated in a sequence of n-p-n semiconductor regions, by quantum transitions from the higher states of the n-regions to the lower states of the p-regions, while the heat absorption is undertaken by the electron transfer on the deep-level paths of the p-n Ohmic junctions–when a current is injected in the device, the lower states of the p-regions are enhanced, while the higher states of the n-regions are depleted, which means a temperature decrease of the p-n junctions, and consequently, a heat absorption from the adjacent regions which excites the electrons through these junctions. Since in a structure with N junction, one electron generates N photons, on the account of N processes of energy absorption, in some conditions, the energy consumed for the current injection is much smaller than the radiation energy produced by heat absorption. They studied this phenomenon in detail, in the framework of quantum mechanics.

BIOGRAPHY

Eliade Stefanescu graduated Faculty of Electronics, Section of Physicist Engineers, in 1970, and after a long activity in the field of the research and development of the semiconductor devices, he obtained a PhD in Theoretical Physics in 1990. He discovered a phenomenon of penetrability enhancement of a potential barrier by dissipative coupling. He developed a microscopic theory of open quantum systems, discovered a physical principle and invented a device for heat conversion into usable energy and produced a unitary quantum relativistic theory. He is Member of American Chemical Society and Academy of Romanian Scientists. He received the Prize of Romanian Academy for Physics in 1983 and the Prize "Serban Titeica" in 2014, for his book entitled "OPEN QUANTUM PHYSICS AND ENVIRONMENTAL HEAT CONVERSION INTO USABLE ENERGY". He has been invited to present his results in numerous international conferences, as speaker, keynote speaker and member of the Organizing Committee.

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