

3rd International Conference on

PHARMACEUTICAL CHEMISTRY



October 29-31, 2018 | Brussels, Belgium



Theme: "Recent Advancements, Innovations and future approaches in the fields of Pharmaceutical Chemistry & Drug Discovery process"

****For Available Speaker Slots****

pharmaceuticalchemistry@chemistryconference.org

19+ Interactive Sessions

15+ Keynote Lectures

75+ Plenary Lectures

5+ Workshops

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Email: pharmaceuticalchemistry@pharmaceuticalconferences.org
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<https://pharmaceuticalchemistry.conferenceseries.com/>

Tentative Program

October 29-31, 2018 | Brussels, Belgium

Program at a Glance

Day 1

Day 1		
Morning Sessions	Reception/Registration	08.00-09.00
		TimeGeneral Session
		09.00-09.15Inaugural Address
	Least of 3 Keynote/Plenary Talks	09.15-09.45Keynote/Plenary Talk 1
		09.45-10.15Keynote/Plenary Talk 2
		10.15-10.45Keynote/Plenary Talk 3
	Panel Discussions/Group Photo	
	Coffee/Tea Break 10.45-11.00 (Networking)	
	11.00-12.40	5 Speakers (20 Mins Each)
	Lunch Break 12.40-13.30	
13.30-15.30	6 Speakers (20 Mins Each)	
Coffee/Tea Break 15.30-15.45 (Networking)		
15.45-17.25	5 Speakers (20 Mins Each)	
Evening Sessions		

19 Speakers for Day 1

Day 2

Morning Sessions		Time	Session 1	Session 2
	09.00-10.40		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
	Coffee/Tea Break 10.40-10.55 (Networking)			
	10.55-12.35		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
	Lunch Break 12.35-13.25			
Evening Sessions	13.25-15.05		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
	Poster Sessions			
	Coffee/Tea Break 15.05-15.20 (Networking)			
	15.20-17.00		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)

40 Speakers on Day 2

Day 3

Morning Sessions		Time	Session 1	Session 2
	09.00-10.40		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
	Coffee/Tea Break 10.40-10.55 (Networking)			
	10.55-12.35		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
	Lunch Break 12.35-13.25			
Evening Sessions	13.25-15.05		5 Speakers (20 Mins Each)	5 Speakers (20 Mins Each)
	Poster Sessions			

40 Speakers on Day 3

Coffee/Tea Break 15.05-15.20 (Networking)

15.20-17.00

5 Speakers (20 Mins Each)

5 Speakers (20 Mins Each)

Closing Ceremony

NOTE: Program Schedule is subject to change with final allotment of the speaker slots

For more Details PS: <https://pharmaceuticalchemistry.conferenceseries.com/>
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Note: Workshops and Symposia slots are available. To book slot for Workshop and Symposium send us the proposal.

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Glimpses of Pharmaceutical Chemistry Conferences



Glimpses of Pharmaceutical Chemistry Conferences



Major Scientific Sessions

- **Pharmaceutical Chemistry Novel Aspects**
- **Prospectives of Medicinal Chemistry**
- **Computational Chemistry and Chemical Biology**
- **Biopharmaceutical and Biologic Drugs**
- **Natural Products Chemistry**
- **Protein and Cellular Engineering and Statistical Mechanics**
- **Green Chemistry in Pharma Industry**
- **Drug Designing Methodologies**
- **Drug Delivery techniques**
- **Drug Discovery and Development**
- **Advanced Organic Chemistry and Inorganic Chemistry**
- **Heterocyclic Chemistry**
- **Drug Formulation / Pharmaceutical formulation**
- **Pharmaceutical Analysis**
- **Overview on Pharmaceutical Industry**
- **Research Studies in Pharmacology**
- **Pharmaceutical Biotechnology and Tissue Engineering**
- **Nanomedicine and Nanotechnology**
- **Clinical and Hospital Pharmacy**

Best Poster Award



- You will be given about 5-7 minutes to present your poster including questions and answers. Judges may pose questions during the evaluation of the poster
- Judges will even evaluate the student's enthusiasm towards their study, interest and knowledge in the area of their research
- The winners will be announced at the closing ceremony of the conference. The decision of the winner will be withdrawn if the winner/winners is/are not present at the time of announcement
- Apart from the judging time you may also be present at the poster to share your research with interested delegates



Young Researchers Forum

- Present your research through oral presentations
- Learn about career development and the latest research tools and technologies in your field
- This forum will give pertinent and timely information to those who conduct research and those who use and benefit from research
- Develop a foundation for collaboration among young researchers
- The forum will provide an opportunity for collegial interaction with other young investigators and established senior investigators across the globe
- Interact and share ideas with both peers and mentors

General Queries

pharmaceuticalchemistry@chemistryconference.org

Conference Venue

Brussels, Belgium

Best Tourist Destinations in Brussels



Grand Place



Atomium



St. Michael & St. Gudula Cathedral



Palace of Charles of Lorraine



Parlamentarium



Guildhouses



Autoworld



Mini-Europe



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2nd International Conference on

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Opening Ceremony

Keynote Forum

Introduction

Title: New potent MKLP2 inhibitors in the paprotrain series with high anticancer activity *in vivo*: Design, Synthesis and Structure-Activity relationships

Catherine Guillou, University of Paris-Saclay, France

Title: Mutagenic Impurities in Pharmaceuticals: ICH M7, Purge Factors and the Mirabilis Project

Mark McLaughlin, Merck Sharp & Dohme, USA

Title: From para-aminobenzoic acid to small compounds with multiple biological properties

Gervais Bérubé, Université du Québec à Trois-Rivières, Canada

Group Photo

Networking and Refreshments Break

Sessions: Drug Discovery and Development | Drug Designing Methodologies | Drug Delivery techniques

Session Chair: Catherine Guillou, University of Paris-Saclay, France

Session Co-chair: Zeeshan Ahmad, De Montfort University, UK

Session Introduction

Title: Isolation and Characterization Active Compound From Endophytic Fungi Onion Dayak {Eleutherineamericana (aubl.) Merr} as Antioxidant Activity

Shirly Kumala, Pancasila University Srengseng Sawah, Indonesia

Title: Phosphonate Congeners of Oseltamivir, Zanamivir and Peramivir as Effective Anti-Influenza Drugs

Jim-Min Fang, National Taiwan University, Taiwan

Title: Electrical Encapsulation Drug Delivery Techniques

Zeeshan Ahmad, De Montfort University, UK

Title: E-BABE- Kinetic binding assays for the analysis of protein–ligand interactions

Franz-Josef Meyer-Almes, University of Applied Sciences Darmstadt, Germany

Title: Utilizing eco-friendly nanoparticle techniques in improving drug delivery

Shaaban K Mohamed, Manchester Metropolitan University, UK

Title: Synthesis and biological evaluation of novel antimicrobial cell-penetrating cyclic peptides

Shaima El-Mowafi, National Research Centre, Egypt

Title: α -Methylacyl-CoA racemase (AMACR): Chemical biology approaches to novel prostate cancer drugs

Matthew D Lloyd, University of Bath, UK

Lunch Break

Sessions: Pharmaceutical Chemistry Novel Aspects | Pharmaceutical Analysis | Research Studies in Pharmacology

Session Chair: Xianglin Shi, Chemical Process R&D, Biogen Idec, USA

Session Co-chair: Gervais Bérubé, Université du Québec à Trois-Rivières, Canada

Session Introduction

Title: Peptidomimetic Study on Amyloid Fibril Formation by Alkene-type Dipeptide Isosteres

Tetsuo Narumi, Shizuoka University, Japan

Title: Development of Novel Petasis Reaction Methodologies for Efficient and Scalable Synthesis of Biologically Interesting Compounds

Xianglin Shi, Chemical Process R&D, Biogen Idec, USA

Title: Inclusion of divergent technologies in future point-of-care devices

Johann F. Osmá, Universidad de los Andes, Colombia

Title: Pharmacological Evaluation of Sedative and Hypnotic Activity of Ethyl p-methoxycinnamate and N-hydroxyethyl-p-cinnamamide

Nurmeilis, Syarif Hidayatullah State Islamic University, Indonesia

Title: Analysis of Cathinone and Cathine in Crimson and Green Catha edulis by GC-MS and Determination of The Spermicidal Activity

Azrifitria, Islamic State University (UIN) Syarif Hidayatullah Jakarta, Indonesia

Title: Differentiation of Bovine and Porcine gelatin in vitamin C gummy by High Performance Liquid Chromatography using Principal Component Analysis

Zilhadia, Syarif Hidayatullah Islamic State University, Indonesia

Networking and Refreshments Break

Sessions: Pharmaceutical Chemistry Novel Aspects | Prospectives of Medicinal Chemistry | Heterocyclic Chemistry | Pharmaceutical Analysis

Session Chair: Mark McLaughlin, Merck Sharp & Dohme, USA

Session Co-chair: Piotr Przybylski, Adam Mickiewicz University, Poland

Session Introduction

Title: Spermicidal and Antifertility Activity of Costus Spiralys Leaf Ethanolic Extract in Male Rats

Azrifitria, Islamic State University (UIN) Syarif Hidayatullah Jakarta, Indonesia

Title: Synthesis, antibacterial and anticancer potency of new lactone and lactam macrolide derivatives

Piotr Przybylski, Adam Mickiewicz University, Poland

Title: Hydrogen bonding interactions of tris and bis urea and thioureas with cyanide ligand in an analogue of the sub-site of [FeFe]-hydrogenase

Faizah S Aljohani, Taibah University, Saudi Arabia

Title: Method Development and Validation of Lercanidipine in Human Plasma by Liquid Chromatography Tandem-Mass Spectrometry

Yahdiana Harahap, Universitas Indonesia, Indonesia

Title: Synthesis and Discovery of Highly Potent Agents, Trifluoromethyl Containing Heterocycles Against Influenza Virus

Satoshi Mizuta, Nagasaki University, Japan

Panel Discussion

Day 2 October 03, 2017

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Keynote Forum

Title: Novel sensitive sensors of intracellular viscosity and potential anticancer theranostic agents prepared on the porphyrazine pigments platform for specifically personalized medicine

Larisa Klapshina, Nizhny Novgorod State University, Russia

Title: Synthesis of indole derivatives through transition metals-catalyzed cyclization of 2-alkynylaniline derivatives.

Fabio Marinelli, University of L'Aquila, Italy

Title: Plant molecules affecting female reproductive functions

Alexander V Sirotkin, Constantine the Philosopher University and Research Institute of Animal Production, Slovakia

Networking and Refreshments Break

Sessions: Computational Chemistry and Chemical Biology | Natural Products Chemistry | Pharmaceutical Analysis

Session Chair: Larisa Klapshina, Nizhny Novgorod State University, Russia

Session Co-Chair: Marco Marazzi, University of Lorraine-Nancy & CNRS, France

Session Introduction

Title: Total Synthesis of Tiacumicin B Aglycone, a DFT-Guided Strategy

Emmanuel Roulland, Université Paris Descartes, France

Title: Automated Drug Design of Kinase Inhibitors to treat Chronic Myeloid Leukemia

Aramice Y S Malkhasian, King Abdulaziz University, Saudi Arabia

Title: DNA photosensitization: Irreversible lesions caused by non-covalent binding with organic dyes

Marco Marazzi, University of Lorraine-Nancy & CNRS, France

Title: Patent propensity, R&D and market competition: Dynamic spillovers of innovation leaders and followers

Alvaro Escribano, Universidad Carlos III de Madrid, Spain

Title: An Efficient One Pot Multicomponent synthesis Of Some Novel Substituted Imidazoles using Nano Zirconia Catalyst Under solvent Free Conditions: A Greener “NOSE” approach

Sundaram Singh, Indian Institute of Technology (BHU), India

Title: Towards improving in drug delivery using Silver nano-techniques

Shaaban K. Mohamed, Manchester Metropolitan University, UK

Title: Use of Curcumine, a Pharmaceutically Useful Compound in Organic Reactions

Sangeeta Jagtap, PDEA's Baburaoji Gholap College, India

Lunch Break

Poster Presentations

Poster Judge: Catherine Guillou, University of Paris-Saclay, France

- PC001** **Title: Nitroxide-modified chitosans with enhanced antioxidant potential**
Vasily Sen, P.G. Demidov Yaroslavl State University, Russian Federation
- PC002** **Title: N-Aryl Effects on the Catalyst Reactivity of Imidazolylidene in α 3→ δ 3-Umpolung Addition: Structural Study and Mechanistic Investigation**
Tetsuo Narumi, Shizuoka University, Japan
- PC003** **Title: Analysis of the polar solvents influence on the mechanism of the inhibited oxidation of unsaturated compounds**
Sergey Lednev, P.G. Demidov Yaroslavl State University, Russian Federation
- PC004** **Title: Influence of solvation on the mechanism of the hydroperoxide radicals' addition to the π -bonds of 1,2-and 1,4-diphenylbutadiyne-1,3**
Roman Pliss, P.G. Demidov Yaroslavl State University, Russian Federation
- PC005** **Title: Mathematical Modelling of polychromatic light photokinetics**
Mohammed Alqarni, De Montfort University, UK
- PC006** **Title: High-Throughput Screening to identify novel inhibitors of human α -methylacyl-CoA racemase 1A (AMACR; P504S)**
Matthew D. Lloyd, University of Bath, UK
- PC007** **Title: The secrets and potential of a novel cyclic antimicrobial and cell penetrating peptide**
Margitta Dathe, Leibniz Forschungsinstitute of Molecular Pharmacology, Germany
- PC008** **Title: Nitroxyl radicals as antioxidants against lipid peroxidation: an in vitro study**
Ivan Tikhonov, P.G. Demidov Yaroslavl State university, Russia
- PC009** **Title: Oxidative stress simulation by radical-chain oxidation of vinyl compounds**
Evgeny Pliss, P.G. Demidov Yaroslavl State University, Russian Federation
- PC010** **Title: A novel one pot two-step strategy for regio-chemoselective synthesis of new 3-methyl-6-arylpyridazine-4-carboxamides and 5-oxo-3-aryl-5,6-dihydropyrido[4,3-c]pyridazine-8-carbaldehydes**
Ali Aghaye Lotf va Ata, Urmia University, Iran
- PC011** **Title: Synthesis of some novel 2-(substituted thio)-N-(5-methyl-4-phenylthiazol-2-yl)acetamide and anticancer activity evaluation**
Asaf Evrim EVREN, Anadolu University, Turkey
- PC012** **Title: Synthesis of some novel N-(6-substituted benzothiazole-2-yl)-2-(4-substituted piperazin-1-yl)asetamide derivatives and evaluation their anticancer activity**
Büsra EKSELLI, Anadolu University, Turkey
- PC013** **Title: Conjugated nitroalkenes in reactions with azomethine imines: Synthesis of tetrahydropyrazolo[1,2-a]pyrazolone derivatives**
Nikolay S Zimnitskiy, Ural Federal University, Russia

PC014 Title: An optimized process for supercritical CO₂ extraction of high-value components from *Artemisia annua* L for cosmetic applications

Rosana M Alberici Oliveira, University of Campinas –UNICAMP, Brazil

PC015 Title: Fingernails: Development and validation of a rapid and sensitive method for quantification of cocaine by LC-ESI-MS/MS

Heliara Nascimento, ThoMson Mawss Spectrometry Laboratory-UNICAMP, Brazil

Sessions: Computational Chemistry and Chemical Biology | Heterocyclic Chemistry | Pharmaceutical Analysis

Session Chair: Vladislav Yu Korotaev, Ural Federal University, Russia

Session Co-Chair: Daisuke Yamamoto, Kitasato University, Japan

Session Introduction

Title: Manganese-catalysed hydroperoxidation of carbon–carbon double bonds using molecular oxygen present in air and hydroxylamine under ambient conditions

Daisuke Yamamoto, Kitasato University, Japan

Title: Synthesis And Molecular Docking Of Novel Non-Cytotoxic, Anti-Angiogenic Sulfonyl Coumarin Derivatives Against Hepatocellular Carcinoma Cells *In Vitro*

Eslam EL-SAWY, National Research Centre, Egypt

Title: 3-Nitro-2-(trihalomethyl)-2H-chromenes in Reactions with 1,3-Dipoles: Synthesis and Cytotoxic Activity of D3-Annulated Chromane Derivatives

Vladislav Yu Korotaev, Ural Federal University, Russia

Title: Computational modeling of Cu@furfural imine-decorated Linde sites as the efficient catalyst in regioselective synthesis of triazoles

Tayebeh Hosseinnajad, Alzahra University, Iran

Title: Structural studies of the novel antibacterial target MraY and its interaction with the natural inhibitor compound tunicamycin

Gisela Brändén, University of Gothenburg, Sweden

Title: Synthesis and screening of ursolic acid-benzylidene derivatives as potential anti-cancer agents

Wajaht Amin Shah, University of Kashmir, India

Networking and Refreshments Break

Poster Presentations

Poster Judge: Xianglin Shi, Chemical Process R&D, Biogen Idec, USA

PC016 Title: Rapid and sensitive method for simultaneous determination of first-line anti-tuberculosis drugs in human plasma by HPLC-MS/MS: Application to therapeutic drug monitoring

Shouhong GAO, Shanghai Changzheng Hospital, China

PC017 Title: Homology modeling of different leishmanolysin (gp63) from *leishmania* spp. and molecular docking of flavonoids

Jairo Mercado-Camargo, Universidad de Cartagena, Colombia

PC018 Title: An *in silico* approach to discovering inhibitors of trypanothione reductase from *leishmania* (viannia) *panamensis*

Leonor Cervantes-Ceballos, Universidad de Cartagena, Colombia

PC019 Title: *In vitro* evaluation of cytotoxicity and leishmanicidal activity of terpenes isolated from the leaves of *malachra alceifolia*

Harold Gómez-Estrada, Universidad de Cartagena, Colombia

PC020 Title: Cascade approach to modification of lactone macrolide antibiotics

Krystian Pyta, Adam Mickiewicz University, Poland

PC021 Title: Sizing α , β and γ Cyclodextrins by Capillary Electrophoresis and Indirect UV Detection

Yin Zhou, The University of British Columbia, Canada

PC022 Title: Novel Quinazoline Derivative as RAF Inhibitor

Shih-Chieh Yen, Development Center for Biotechnology, Institute of Pharmaceutics, Taiwan

- PC023** Title: **Determination of heavy metal(PB) content in mineral water produced in IRAN by Flameless Atomic Absorption Spectroscopy (FAAS)**
Rasoul Kazemi, Azad University, Iran
- PC024** Title: **Synthesis of novel Spiro dipyrazolo[3,4-b: 4',3'-e]pyridine**
Bahman Ebrahimi Saatluo, University of Urmia, Iran
- PC025** Title: **DBU/H₂O as an Efficient, Eco-friendly and Inexpensive Catalyst for Transesterification and Transacylation Reactions**
Elaheh Akbarzadeh, Islamic Azad University, Iran
- PC026** Title: **Ab initio and DFT study of energetic, stability, and nuclear magnetic resonance of BN nanotube**
Elham Pournamdari, Islamic Azad University, Iran
- PC027** Title: **In vitro antiproliferative, antioxidant, and apoptosis-inducing activities of dried flower buds of clove extract on human gastric carcinoma**
Ali Karimi, Shahrekord University of Medical Sciences, Iran
- PC028** Title: **Synthesis and cytotoxic properties of new derivatives of dicarboximides**
Mariola Napiórkowska, Medical University of Warsaw, Poland
- PC029** Title: **Discovery of novel aryl hydrocarbon receptor (AhR) antagonists using homology modelling and ligand-based drug design**
Carlos Henrique Tomich de Paula da Silva, University of São Paulo, Brazil

Day 3 October 04, 2017

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Sessions: Pharmaceutical Chemistry Novel Aspects | Prospectives of Medicinal Chemistry | Drug Designing Methodologies | Pharmaceutical Analysis

Session Chair: Francisco Alonso, Universidad de Alicante/ Instituto de Síntesis Orgánica, Spain

Session Co-Chair: Alexander V. Sirotkin, Constantine the Philosopher University and Research Institute of Animal Production, Slovakia

Session Introduction

Title: Copper nanoparticles in organic synthesis

Francisco Alonso, Universidad de Alicante/ Instituto de Síntesis Orgánica, Spain

Title: Rational Design and Synthesis of Innovative RNA Ligands to Target HCV Internal Ribosome Entry Site

Mauro Safir Filho, Universite Côte d'Azur, France

Title: Synthesis of 5,6-Diaryl-1,2,4-triazine derivatives with ethyl acetate moiety as novel neuroprotective agents against H₂O₂ and A β -induced neurotoxicity

Hamid Irannejad, Mazandaran University of Medical Sciences, Iran

Networking and Refreshments Break

Title: PELE Studio: The next generation drug design software

Victor Guallar, Barcelona Supercomputing Center, Spain

Title: Chemical constituents from the rhizomes of Curcuma zedoaria and assessment of their biological activities

Omer Abdalla Ahmed Hamdi, Alneelain University, Sudan

Title: Inorganic Pharmaceuticals: DNA-binding and anticancer activity of new compound

Sartaj Tabassum, King Saud University, Saudi Arabia

Title: Inhibition of immunodeficiency type-1 virus (HIV-1) life cycle by magnetic water

Mandana Behbahani, University of Isfahan, Iran

Title: Synthesis of new series of pyrazolo[3,4-b][1,6]naphthyridine in presence of nano-Al₂O₃

Fatemeh Majidi Arlan, University of Urmia, Iran

Title: Protective effect of green synthesis gold nanoparticles (AuNPs) from *Pulicaria undulata* on the amyloid formation in α -lactalbumin

Arezou Ghahghaei, University of Sistan and Baluchestan, Iran

Title: Determination of Glimepiride in Pharmaceutical Formulations Using HILIC

Yuegang Zuo, University of Massachusetts Dartmouth, USA

Title: Very fast and surprisingly accurate GIAO-mPW1PW91/3-21G//PM7 scaling factor for ^{13}C NMR chemical shifts calculation

Fabio Luiz Paranhos Costa, Federal University of Goiás, Brazil

Lunch Break

Awards & Closing Ceremony



Bookmark your dates

3rd International Conference on

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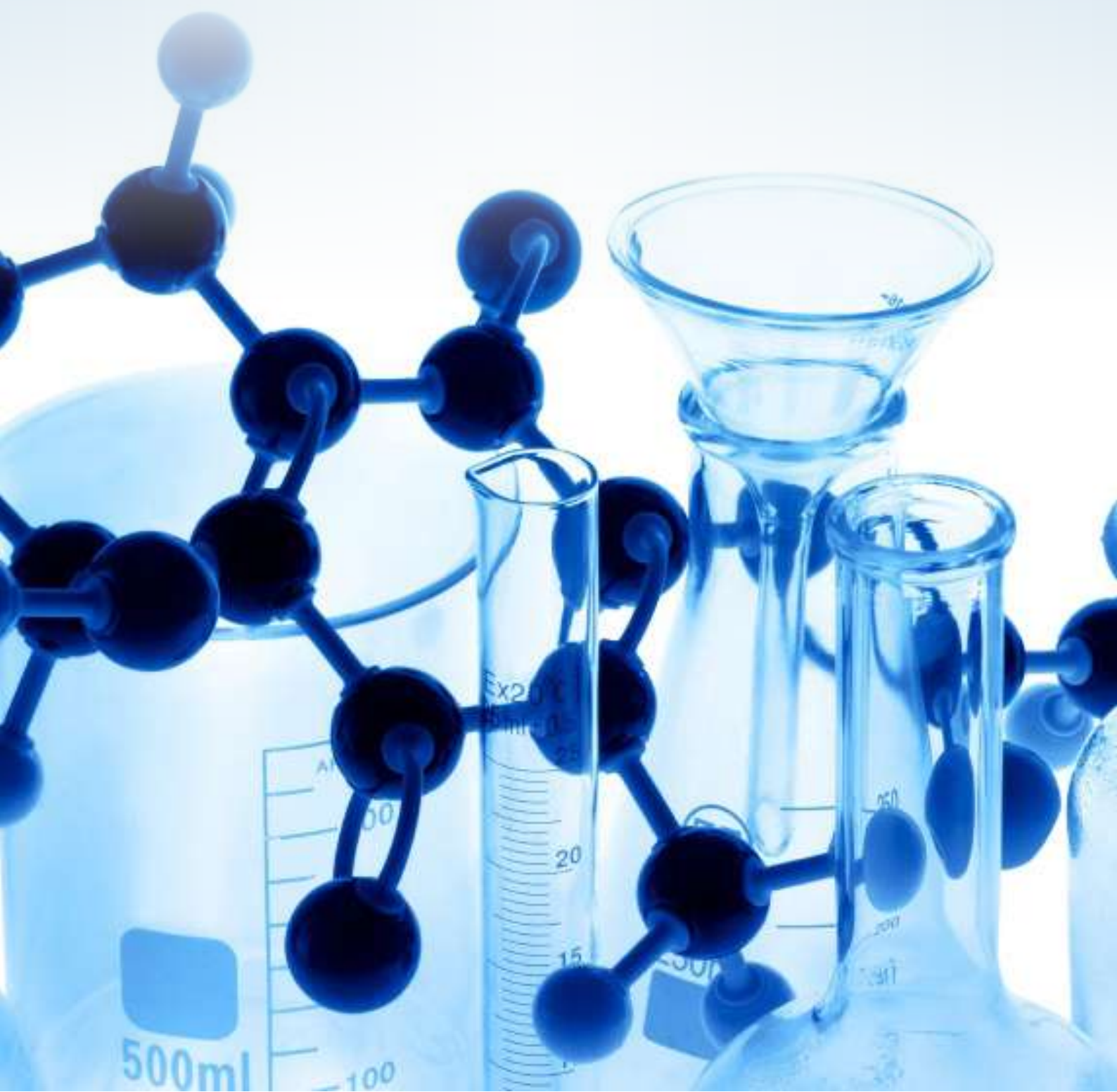
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Scientific Program



Room 8

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Opening Ceremony

Keynote Forum

Title: The enterprise of drug discovery from an academic perspective: from concept to practice

Stephen Hanessian, University of California, USA

Title: A new synthetic methodology for pharmaceutical chemistry

Valery Charushin, Ural Federal University, Russia

Networking and Refreshment Break

Sessions:

Drug Discovery and Therapy | Flow Chemistry

Session Chair: Wei Li, University of Tennessee Health Science Center, USA

Session Co-Chair: Naofumi Hashimoto, Setsunan University, Japan

Session Introduction

Title: Discovery of novel tubulin inhibitors and their synergy with BRAF inhibitors for malignant melanoma

Wei Li, University of Tennessee Health Science Center, USA

Title: Different targeting possibilities using nanoparticles

Sylvia Wagner, Fraunhofer Institute for Biomedical Engineering, Germany

Title: Photodynamic therapy and imaging based on tumor-targeted nanoprobe, pHPMA-conjugated zinc protoporphyrin, and its augmentation

Jun Fang, Sojo University, Japan

Title: Preparation of nanocrystal formulation to improve oral absorption of mebendazole

Naofumi Hashimoto, Setsunan University, Japan

Title: Perspectives of antifungal drug discovery

Josef Jampilek, Comenius University, Slovakia

Title: Effect of Octyl Salicylate with respect to the physical appearance of mono/di capric and caprylic fatty acids Formulations

Siti Salwa Abd Gani, Universiti Putra Malays, Malaysia

Lunch Break

Sessions:

Prospectives of Pharmaceutical Chemistry | Advanced Organic Chemistry | Drug Discovery and Therapy | Molecular Stereochemistry

Session Chair: Alexander Cobb, University of Reading, UK

Session Co-Chair: Vânia André, Universidade de Lisboa, Portugal

Session Introduction

Title: Synthesis of new Indan-1-one-piperazine derivatives as anticholinesterase agents

Yusuf Özkay, Anadolu University, Turkey

Title: New approaches for tyrosinase inhibitors: mannich bases of kojic acid derivatives

Mutlu Dilsiz Aytemi, Hacettepe University, Turkey

Title: From simple chemical building blocks to biological active molecules

Raffaella Mancuso, University of Calabria, Italy

Title: Development of xanthines as adenosine A2A receptor selective antagonists: a systematic approach towards novel nondopaminergic therapy for Parkinson's disease

Ranju Bansal, Panjab University, India

Title: Enzyme-catalyzed reactions

Devrim ÖZDEMIRHAN, Abant İzzet Baysal University, Turkey

Title: New asymmetric organocatalytic methods towards the synthesis of molecules of biological interest

Alexander Cobb, University of Reading, UK

Title: Enantioselective, short and efficient approaches to the synthesis of drugs and biologically active compounds

Satyendra Kumar Pandey, Thapar University, India

Panel Discussion

Day 2 September 06, 2016

Room 8

Keynote Forum

Title: Across the blood-brain barrier: Nanoparticles

Jörg Kreuter, Johann Wolfgang Goethe-University, Frankfurt, Germany

Title: Promising clinical outcome of HPMA-polymer conjugated-pirarubicin (THP)

[P-THP], which exerts three steps for cancer selective delivery

Hiroshi Maeda, Sojo University, Japan

Networking and Refreshment Break

Sessions:

Drug Design and Drug Delivery | Heterocyclic Chemistry Compounds

Session Chair: Paulo Roberto Ribeiro Costa, Universidade Federal do Rio de Janeiro, Brazil

Session Co-Chair: Chunduri Venkata Rao, Sri Venkateswara University, India

Session Introduction

Title: Synthesis and biological activities of 2-chloronicotinaldehyde based novel functionalized heterocyclic compounds

Bhimapaka China Raju, CSIR-Indian Institute of Chemical Technology, India

Title: Discovery of small molecule dna g-quadruplex stabilizing agents: design, synthesis and biological studies

Mrinalkanti Kundu, TCG Lifesciences Pvt. Ltd., INDIA

Title: Development of thienopyrimidines as potential pharmaceuticals

Chunduri Venkata Rao, Sri Venkateswara University, India

Title: Synthesis and biological evaluation of new carbaisoflavonoids with Anti-HCV activity

Paulo Roberto Ribeiro Costa, Universidade Federal do Rio de Janeiro, Brazil

Title: Discovery of novel 2-thio-imidazole derivatives as potent and orally efficacious TGR5 receptor agonists

Sameer Agarwal, Zydus Research Centre, Cadila Healthcare Ltd., India

Title: Design, synthesis and pharmacological evaluation of some novel de-rivatives of 1-{[3-(furan-2-yl)-5-phenyl-4,5-dihydro-1,2-oxazol-4-yl]methyl}-4-methyl piperazine

Gita Chawla, Hamdard University, India

Lunch Break

Sessions:

Heterocyclic Chemistry Compounds | Green Chemistry

Session Chair: Asunción Barbero, University of Valladolid, Spain

Session Co-Chair: Matthias D'hooghe, Ghent University, Belgium

Session Introduction

Title: Development of piperazine derivatives as potential cognition enhancers

Poonam Piplani, Panjab University, India

Title: Synthesis of oxygen and nitrogen heterocycles with potential pharmaceutical properties

Asunción Barbero, University of Valladolid, Spain

Title: Synthesis docking studies and biological evaluation of some novel 1,2,4-triazolo[3,4-b][1,3,4]thiadiazole tagged thieno[2,3-d]pyrimidine derivatives

Settyalli Triloknadh, Sri Venkateswara University, India

Title: One pot condensation reaction of heterocyclic amine, 1, 3- diketone and an aldehydes using in situ generated superoxide ion: a rapid synthesis of structurally diverse drug- like complex heterocycles

Sundaram Singh, Department of chemistry IIT(BHU), India

Title: Application of small-ring azaheterocyclic building blocks for the synthesis of pharmaceutically relevant nitrogen compounds

Matthias D'hooghe, Ghent University, Belgium

Title: BioMOFs – Exploring nalidixic acid metal organic networks envisaging pharmaceutical applications

Vânia André, Universidade de Lisboa, Portugal

Title: Sustainable synthesis via the integration of membranes in chemical reactions

Dominic Ormerod, Flemish Institute for Technological Research (VITO NV), Belgium

Video Presentation by Donna J. Nelson, President of American Chemical Society, USA

Networking and Refreshment Break

Poster Presentations

- PCH001** **Title: Synthesis, molecular docking study and in vitro biological activity of carbohydrate-based peptidomimetics targeting neuropilin-1**
Nadia Pellegrini-Moïse, Université de Lorraine, France
- PCH002** **Title: [18F]Fluoro-C-glycosides to radiolabel peptides for PET imaging**
Sandrine Lamandé-Langle, Université de Lorraine, France
- PCH003** **Title: In vivo and in vitro anti-inflammatory activities of two chromones isolated from Dictyoloma vandellianum**
Luíza C. F. Opretzka, Federal University of Bahia, Brazil
- PCH004** **Title: Dynamic kinetic asymmetric transformations with hard nucleophiles: Cyclopentenones for anti tuberculosis and antibiotics**
Hadia Almahli, University of Oxford, UK
- PCH005** **Title: Synthesis and biological evaluation of novel pyrrolo[2,3-d]pyrimidine derivatives as breast anti cancer**
Khalid Hilmy, Monufya University, Egypt
- PCH006** **Title: The role of circulating serum resistin, serum amyloid A and C-reactive protein as potential risk factors for development of type 2 diabetes mellitus**
Esmat Bauomi Ali Shahin, Al-Azhar University, Egypt
- PCH007** **Title: Water Soluble Platinum(II) Complexes: GLUT mediated cytotoxic properties and selective tumor targeting**
Ran Liu, Tianjin University, P. R. China
- PCH008** **Title: Synthesis of novel disubstituted oxadiazole derivatives and antimicrobial activity**
Serkan Levent, Anadolu University, Turkey
- PCH009** **Title: Synthesis Of new donepezil analogues and evaluation of their cholinesterase inhibitory activity**
Begüm Nürpelin Sağlık, Anadolu University, Turkey
- PCH010** **Title: New Benzimidazole-Hydrazones as MAO Inhibitors**
Ozgur Devrim Can, Anadolu University, Turkey
- PCH011** **Title: Structure, intermolecular and photoinduced intramolecular hydrogen bonding in 2-azolylmethylidene cycloalkanones**
Mark Sigalov, Ben-Gurion University of the Negev, Israel
- PCH012** **Title: Synthesis and anticonvulsant activities of Novel 1-Phenyl/1-(4-chlorophenyl)-2-(1H-triazole-1-yl)ethyl ester derivative compounds**
Irem Bozbey, Inonu University, Turkey
- PCH013** **Title: Synthesis of some new benzalhydrazone derivatives and evaluation of their AChE inhibitory activity in vitro**
Ömer Faruk ÇÖL, Gazi University, Turkey
- PCH014** **Title: Structure-antibacterial activity relationships of N-substituted-(D/L-alaninyl) 1H-1,2,3-triazolyl oxazolidinones**
Oludotun A. Phillips, Kuwait University, Kuwait
- PCH015** **Title: Synthesis and anticholinesterase effects of new 2-substituted benzothiazole derivatives**
Ümide Demir Özkay, Anadolu University, Turkey
- PCH016** **Title: Anticarcinogenic effect of coadministration of α - β unsaturated compounds and quercetin**
Gabriela Carrasco Torres, CINVESTAV, México

Panel Discussion

Day 3

September 07, 2016

Room 8

Keynote Forum

Title: Anticancer agents used in traditional chinese medicine that target prohibitins and the translation initiation factor eIF4a

Laurent Désaubry, CNRS-Strasbourg University, France

Title: Simultaneous extraction and determination of four different groups of pharmaceuticals in compost using optimized ultrasonic extraction and ultrahigh pressure liquid chromatography-mass spectrometry

Miguel Ángel López Zavala, Tecnológico de Monterrey, Mexico

Sessions:

Technologies in Natural Products | Pharmacology Studies | Modern Analytical Techniques

Session Chair: Flavio S P Cardoso, Libbs Pharmaceuticals, Brazil

Session Co-Chair: Anna M Waszkielewicz, Jagiellonian University Medical College, Poland

Session Introduction

Networking and Refreshment Break

Title: Activity of some phenoxyalkyl- and phenoxyethoxyethylamine derivatives on the central nervous system

Anna M Waszkielewicz, Jagiellonian University Medical College, Poland

Title: Design, synthesis, and validation of an in vitro platform peptide -whole cell screening assay using MTT reagent

Sahar Ahmed, Assiut University, Egypt

Title: Application of in situ FTIR for the preparation of 17- α -estradiol via Mitsunobu reaction

Flavio S P Cardoso, Libbs Pharmaceuticals, Brazil

Title: A novel stability-indicating LC method for determination of avanafil

Nafiz Oncu Can, Anadolu University, Turkey

Title: The antimutagenic activity of selected medicinal plants from Jordan

Karem Alzoubi, Jordan University of Science & Technology, Jordan

Title: Drug chimerism as a fusion of two anticancer chemotherapeutics into one entity: Discovery of potent molecular chimera CM358 for treatment of metastatic melanoma

Gary Gellerman, Ariel University, Israel

Title: Phytochemical constituents from garcinia atroviridis

Wen-Nee Tan, Universiti Sains Malaysia, Malaysia

Panel Discussion

Award & Closing ceremony

Lunch Break

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Registrations

Jumeirah Ballroom-3

Opening Ceremony

Keynote Forum

Introduction

R N Saha

BITS Pilani Dubai Campus, UAE

Alex Nivorozhkin

Neo-Advent Technologies LLC., USA

Networking & Refreshments Break

Khaled Mohamed Hosny

King Abdulaziz University, Kingdom of Saudi Arabia

Peter Karpinski

Novartis Pharmaceuticals Corp., USA

Track 3: Recent Technologies in Novel Drug Delivery Systems

Track 4: Nanotechnology in Drug Delivery Systems

Session Chair: **R N Saha**, BITS Pilani Dubai Campus, UAE

Session Co-Chair: **Luisa Fiandra**, Luigi Sacco University Hospital, Italy

Session Introduction

Title: A novel and simple technique for separation of liposomes from unloaded drug molecules

Vignesh Muthuvijayan, Indian Institute of Technology Madras, India

Title: Polymer drug carriers with enhanced penetration into tumor cells

Robert Pola, Institute of Macromolecular Chemistry AS CR, Czech Republic

Title: Delivery of nanoformulated Antiretroviral drugs across the blood brain barrier

Luisa Fiandra, Luigi Sacco University Hospital, Italy

Lunch Break

Title: Block copolymers of poly(N-2-hydroxypropyl methacrylamide) and poly(propylene glycol)—the way to inhibit P-glycoprotein?

Alena Braunova, Institute of Macromolecular Chemistry AS CR, Czech Republic

Title: Early preclinical study of BO-1978 for the treatment of Non-Small Cell Lung Carcinoma (NSCLC), in combination with Gefitinib

Tann-Long Su, Academia Sinica, Taiwan

Title: Improving bioavailability of Resveratrol: Transdermal, transmucosal and nanotechnology strategies

Hudson Caetano Polonini, University of Juiz de Fora, Brazil

Title: Composite Poly(methyl methacrylate)/Poly(ethylene glycol) electrospun nanofibrous mats as a novel wound dressing for controlled release of an Anti-scarring agent

Malihe-Sadat Poormasjedi-Meibod, University of British Columbia, Canada

Title: Silica-based matrixes for drug delivery: Ready for a prime time?

Alex Nivorozhkin, Neo-Advent Technologies LLC., USA

Title: Formulation and evaluation of nutraceutical tablets of lyophilized nanoparticles of Zinc and Asparagus extracts

Sandeep Arora, Chitkara University, India

Networking & Refreshments Break

Title: Development of ligand-mediated drug delivery systems for cancer targeted imaging and therapy

Han-Chung Wu, Academia Sinica, Taiwan

Title: Enteric-coated Alendronate sodium solid lipid nanoparticle; A novel formula to overcome barriers for the treatment of osteoporosis

Khaled Mohamed Hosny, King Abdulaziz University, Kingdom of Saudi Arabia

Title: Exploring the critical stabilizing factors for solid dispersions without drug-polymer interaction: Monitoring and inhibiting amorphous/amorphous phase separation

Min Zhao, University College London School of Pharmacy, UK

Title: Coping with the management of medicine at old age: What older people think? What formulations scientists can do?

Mine Orul Gul, University College London School of Pharmacy, UK

Workshop

Title: Controlled Drug Delivery Systems: Recent Challenges and Opportunities Ahead

Title: Bioactive peptides: Complex structures, synthesis and their controlled drug delivery

Rajiv Dahiya, Association of Pharmacy Professionals and Globus College of Pharmacy, India

Title: Guar gum revisited: Potential carrier for targeted drug delivery systems

Saurabh Dahiya, Apeejay Stya University, India

Panel Discussion

Day 2

March 17, 2015

Keynote Forum

Husam M Younes

Qatar University, Qatar

B B Barik

Jazan University, Kingdom of Saudi Arabia

Networking & Refreshments Break

Track 2: Formulation Aspects for Various Routes of Drug Administration

Track 7: Major Challenges in Drug Delivery System

Session Chair: Naglaa G Ahmed, Dubai Pharmacy College, UAE

Session Chair: B B Barik, Jazan University, Kingdom of Saudi Arabia

Session Introduction

Title: Gloveless robotic technologies in aseptic manufacturing for high potent active pharma ingredients

Sergio Mauri, Fedegari Group, Italy

Title: Oral formulations of Metformin in semi-solid matrices: Design, characterization & in vitro evaluations

Husam M Younes, Qatar University, Qatar

Title: Hepatoprotective and antihepatotoxic drugs from plant sources

Naglaa G Ahmed, Dubai Pharmacy College, UAE

Title: Small animal models of osteoarthritis: Understanding drug bio-distribution, activity, safety, therapeutic effects and mechanisms of action

Mohit Kapoor, University of Toronto, Canada

Title: Mitigating risks associated to auto-injector applications

Robert Schultheis, ZebraSci Inc., USA

Title: Chitosan nanoparticles - Challenges for antibiotic drug delivery using Penicillin as a model drug

B B Barik, Jazan University, Kingdom of Saudi Arabia

Title: Challenges facing liposomal delivery of Vancomycin for combating bacterial biofilm on abiotic surfaces

Nawal Khalafallah, Alexandria University, Egypt

Lunch Break

Title: Hydrogels of solid lipid nanoparticles of curcumin

Ruchi Chawla, Indian Institute of Technology (Banaras Hindu University), India

Title: Ramadan fasting and biological biomarkers: The new opportunities of systems biology and omics sciences

Nicola Luigi Bragazzi, University of Genoa, Italy

Track 1: Pre-formulation Considerations for Conventional Dosage Form Development

Track 10: Advances in Biotherapeutics-Drug Discovery and Development

Session Chair: Mazzucchelli Serena, Luigi Sacco University Hospital, Italy

Session Chair: Maha Aboul-Ela, Beirut Arab University, Lebanon

Title: Phytotherapeutic potentials of selected Middle East natural products

Maha Aboul-Ela, Beirut Arab University, Lebanon

Title: Determination of Ticagrelor chemical stability and characterization of its degradants

Hassane Sadou Yaye, University Paris Sud, France

Title: Evaluation of three chitin metal silicate co-precipitates as a potential multifunctional single excipient in tablet formulations

Faisal Al-Akayleh, Petra University, Jordan

Title: Novel anti-microbial drugs based on mixed ligand zinc(II) complexes with bioactive carboxylates and nitrogen-donor ligands; Synthesis, structure and biological properties

H Abu Ali, Birzeit University, Palestine

Networking & Refreshments Break

Title: Lead to drug candidate: Novel oral kinase inhibitors in cancer therapy

Hsing-Pang Hsieh, National Health Research, Institutes, Taiwan

Title: Considerations in pre-formulation stage of solid and semi-solid dosage forms

Mustafa Hamido, UAE

Poster Presentations PNDDS 01- PNDDS 20

@ Jumeirah Ballroom-3

Poster Presentations PNDDS 21- PNDDS 40

@ Jumeirah Ballroom-3

Day 3 March 18, 2015

Jumeirah Ballroom-3

Track 4: Nanotechnology in Drug Delivery Systems

Track 6: Recent Advances in Targeted Drug Delivery System

Session Chair: Tomas Etrych, Institute of Macromolecular Chemistry AS CR, Czech Republic

Session Chair: Ramesh S Kashi, Merck and Co. Inc., USA

Session Introduction

Title: Polymer based delivery systems for efficient tumor therapy

Tomas Etrych, Institute of Macromolecular Chemistry AS CR, Czech Republic

Title: Nanocages for self-triggered nuclear delivery of Doxorubicin at cancer cells

Mazzucchelli Serena, Luigi Sacco University Hospital, Italy

Title: Development of novel targeted drug delivery systems for the treatment of epilepsy

Sara Ahmadi, Intelligent Polymer Research Institute, Australia

Title: In vivo targeting efficiency of multifunctional nanoconstructs bearing antibody-derived ligands

Marta Truffi, University of Milan, Italy

Networking & Refreshments Break

Title: Pastillation technology based design and development of oral modified release multiparticulate drug delivery system

B Mishra, Indian Institute of Technology (Banaras Hindu University), India

Title: Incidence and predictors of antibiotic prescription errors in an emergency department of a tertiary care facility, central Saudi Arabia

Menyfa Al Anazi, Ministry of National Guard Health Affairs, Kingdom of Saudi Arabia

Title: *In vitro* cytotoxicity and free radical scavenging activity of ethanolic and alkaloidic extracts of *Delphinium staphisagria*

Rachad Alnamer, University of Tamar, Yemen

Title: Enhanced cytotoxic effect of chemically conjugated polymeric sirolimus against ht-29 colon cancer and a-549 lung cancer cell lines

Bonitha Venkata Subrahmanya Lokesh, UCSI University, Malaysia

Title: Synthesis of Benzopyrano[4,3-d]-Pyrimidine derivatives and some of their antimicrobial and cytotoxicity activities

Haya A Abubshait, University of Dammam, Kingdom of Saudi Arabia

Lunch Break

Young Researchers Forum

Title: Mucus permeating SMEDDS containing thiolated compounds

Julia Rohrer, University Innsbruck, Austria

Title: Thiolated silicone oils as novel skin care agents with enhanced adhesiveness and reinforced occlusivity

Alexandra Partenhouse, Leopold-Franzens-University, Austria

Title: Characterisation of nanostructured lipid carriers loaded with Ibuprofen

Blanka Suto, University of Szeged, Hungary

Title: Thiolated poly(aspartic acid) polymers in ophthalmic therapy

Gabriella Horvat, University of Szeged, Hungary

Title: Controlled, delivery of Metronidazole and Doxycycline from polycaprolactone matrices designed for the intravaginal treatment of pelvic inflammatory disease

Meenakshi Pathak, The University of Queensland, Australia

Title: Microscopic evaluation of novel topical formulation for treatment of Arthritis

Mohit Bhagrath, Chitkara University, India

Networking & Refreshments Break

Title: Utility of modified locust bean gum for dissolution improvement of poorly soluble drug

Kanav Midha, Chitkara University, India

Title: pH sensitive Calcium Carbonate-encapsulated Copper bis-(8-hydroxyquinoline) drug delivery system for cancer therapy

Anjala Bulathge, University of Peradeniya, Sri Lanka

Title: Lipid complexed nanocrystals - A safe approach in development of stable nanoparticulates (*in vitro* and *in vivo*) for effective drug delivery

Sajeew Kumar B, Jawaharlal Nehru Technological University, India

Panel Discussion

Award Ceremony

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Keynote Forum

Introduction

Davis L Ford

Texas A&M University, USA

Ashok Kumar Ray

CSIR-National Metallurgical Laboratory, India

Mileva Radonjic

Louisiana State University, USA

S S Amritphale

CSIR-Advanced Materials and Processes Research Institute, India

Group Photo

Coffee Break: @ Atrium

Track 1: Processing Technologies

Track 2: Petroleum Exploration & Field Management

Session Chair: Ildenize Barbosa da Silva Cunha, University of Campinas, Brazil

Session Co-Chair: Bushra Al-Duri, University of Birmingham, UK

Session Introduction

Title: Novel methods for upgrading heavy petroleum products

Russell R Chianelli, University of Texas at El Paso, USA

Title: Mass Spectrometry: A pioneer and renewed tool for petrochemical analysis

Ildenize Barbosa da Silva Cunha, University of Campinas, Brazil

Title: Ethylene-vinyl acetate copolymer-based depressants in marine fuels

Nataliya Kondrasheva, The National Mineral Resources University, Russia

Title: Heterogeneity of fine grained sediment and its hydrocarbon generation and expulsion: An case from Dongying depression

Chen Zhonghong, China University of Petroleum, China

Title: High performance oxygen carriers for chemical looping combustion process by using architectural structure of silica nanoparticles

Yujing Liu, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Title: Further work on energy-return-on-energy-invested

J C Jones, Kazakh-British Technical University, Kazakhstan

Lunch Break @ Atrium

Title: Plasma processing of fossil fuels

Alexandr Ustimenko, Research Institute of Experimental and Theoretical Physics, Kazakhstan

Title: Production of furans (2,5 dimethylfuran) from furfurals (Hydromethoxyfurfural-HMF) as transport fuel molecules

Bushra Al-Duri, University of Birmingham, UK

Title: Highly active nano-dispersed Ruthenium catalyst for efficient oxidation of p-cymene and cumene C-H bond by molecular oxygen

Peter R Makgwane, Council for Scientific Industrial Research, South Africa

Title: The Ural-African transcontinental oil & gas belt

Valentin Stepanov, The National Mineral Resources University, Russia

Title: Surfactants and other factors input for the control of the reservoir interfacial tension (IFT)

M.S Benzagouta, University Larbi Ben Mhidi OEB, Algeria

Title: Pore volume compressibilities and stress sensitivity of low permeability reservoir rocks in China's oilfield development

Sun He, China University of Petroleum, China

Title: Selective propping of high conductivity fractures

David Dogon, Eindhoven University of Technology, Netherlands

Title: Equilibrium calculations in aqueous carbonation of oil shale waste – sulfur compounds

Kadriann Tamm, Tallinn University of Technology, Estonia

Coffee Break @ Atrium

Track 3: Drilling & Well Completions Challenges

Track 4: Piping and vessel engineering & Transport Phenomena

Session Chair: Byoung Yoon Park, Sandia National Laboratories, USA

Session Co-Chair: Arya Shahdi, Islamic Azad University, Iran

Session Introduction

Title: Interbed modeling to predict wellbore damage for big hill strategic petroleum reserve

Byoung Yoon Park, Sandia National Laboratories, USA

Title: Performance investigation of an experimental shale shaker in filtration of low concentration slurry

Saeid Ghaniyari Benis, The University of Akron, USA

Title: A robust modeling approach for frictional pressure loss calculation of three phase flow in inclined eccentric annuli

Arya Shahdi, Islamic Azad University, Iran

Title: Study on gas hydrate blocking mechanism and precaution in wellbore of deep water drilling

Xiangfang Li, China University of Petroleum, China

Title: Inhibitive properties comparison of different polyetheramines in water-based drilling fluid

Hanyi Zhong, China University of Petroleum, China

Title: A new understanding on low permeability oilfield development

Tang Wei, Research Institute of Petroleum Exploration and Development (RIPED) of CNPC, China

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Day 2

October 28, 2014

Tropicana Ball Room

Track 5: Chemical Applications in Producing Oil and Gas

Track 6: Coal & Natural Gas

Track 7: Challenges and Safety in Petrochemical Industry

Track 8: Energy Economics

Session Chair: Ahmed El-Nahas, El-Menoufia University, Egypt

Session Co-Chair: Xi Liu, Cardiff University, UK

Session Introduction

Title: Nanoparticle stabilized emulsions and foams for EOR and LNG spill mitigation

Zhengdong Cheng, Texas A&M University, USA

Title: Development of porous radiant burners for domestic LPG cooking and industrial applications

P Muthukumar, Indian Institute of Technology Guwahati, India

Title: Porous media for improved polymer electrolyte membrane fuel cells

Aimy Bazylak, University of Toronto, Canada

Title: Use of sulfide/phosphate based sorbents for mercury removal from natural gas: A focus on the Hg stabilization

Carla Luciane Manske Camargo, Federal University of Rio de Janeiro, Brazil

Title: Experimental investigation of polymer adsorption-induced permeability reduction in low permeability reservoirs

Hyemin Park, Hanyang University, Korea

Title: First-principles analysis on enzymatic degradation of nylon

Yasuteru Shigeta, University of Tsukuba, Japan

Coffee Break @ Atrium

Title: Effect of miscibility condition for CO₂ flooding on gravity drainage in 2D vertical system

Jinju Han, Hanyang University, Korea

Title: Thermodynamic and kinetic hydrate inhibition performance of MEG solution and its synergistic inhibition with PVCap

Yutaek Seo, Korea Advanced Institute of Science and Technology, Korea

Title: Dearomatization of straight-run diesel fuel by using adsorbents under magnetic field

Irana Safarli Almas, Institute of Petrochemical Processes of Azerbaijan NAS, Azerbaijan

Title: The use of an ultrasonic technology to increase the productivity of oil wells

Anna Abramova, Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Russia

Title: Experimental study of pulverized coal oxycombustion and modelling of devolatilization kinetics

Romain Lemaire, Université Lille Nord de France, France

Title: The investigation of catalytic activity of polyoxide catalysts on the base of fiberglass in the reaction of carbon dioxide conversion of methane

Z A Mansurov, Institute of Combustion Problems, Kazakhstan

Lunch Break @ Atrium

Title: LES and RANS of pulverized coal oxy-combustion in swirl burners

Andrzej Boguslawski, Czestochowa University of Technology, Poland

Title: Applicability of non-exhaustive extraction procedures using Tenax® and HPCD to estimate biodegradable contaminant fractions in soil

Kerstin Derz, Fraunhofer Institute for Molecular Biology and Applied Ecology, Germany

Title: E- Neutron scattering studies of catalyst systems at the ISIS neutron spallation Source

Martin Owen Jones, Oxford University, UK

Title: Avoiding gas hydrate problems in Qatar oil and gas industry: Environmentally friendly solvents for gas hydrate inhibition

Nabila Mohamed, Qatar University, Qatar

Title: Insitu transesterification of wet activated sludge under subcritical conditions

Lan Nguyen Phuong Tran, National Taiwan University of Science and Technology, Taiwan

Title: The development of the methods for processing and using of oil sands as the alternative hydrocarbon feedstock

Sultanov F, Al-Farabi Kazakh National University, Kazakhstan

Track 9: Renewable Energy & Feedstock

Session Chair: Abdallah S Berrouk, The Petroleum Institute, UAE

Session Co-Chair: Stella Bezergianni, Centre for Research & Technology Hellas, Greece

Session Introduction

Title: Fast pyrolysis of lignin

Hilkka Kenttamaa, Purdue University, USA

Title: Photosynthetic bioenergy utilizing CO₂: An approach on flue gases utilization for third generation biofuels

Roberto Parra Saldivir, Monterrey Institute of Technology and Higher Education, Mexico

Coffee Break @ Atrium

Title: Decarbonization of transportation fuels via co-hydroprocessing bio-based feedstocks with petroleum fractions

Stella Bezergianni, Centre for Research & Technology Hellas, Greece

Title: Evaluation of methylic and ethylic biodiesels from Pequi oil (*Caryocar Brasiliense* Camb.) as possible diesel substituents

Marcelo Firmino de Oliveira, Universidade de Sao Paulo, Brazil

Title: Combustion heat release models of biodiesels

Abdullah Abuhabaya, King Abdulaziz University, Saudi Arabia

Title: Biodiesel production from *Acrocomia aculeata* acid oil by (enzyme/enzyme) hydroesterification process: Use of vegetable lipase and fermented solid as low-cost biocatalysts

Erika Cristina G Aguiéiras, Federal University of Rio de Janeiro, Brazil

Title: Drying of energy wood by compression

Tuomas Hakonen, Seinäjoki University of Applied Sciences, Finland

Title: Thermochemistry and kinetics of bioalcohols and bioesters as fossil fuel alternatives. Ab initio and DFT studies

Ahmed El-Nahas, El-Menoufia University, Egypt

Title: Thermogravimetric study of powdered laboratory safety examination gloves

Nasrollah Hamidi, South Carolina State University, USA

Poster Presentations @ Atrium

Title: Fischer-Tropsch synthesis reaction in a novel reactor system of cobalt catalyst coated metallic foam and heat-exchanger type reactor

Jung-Il Yang, Korea Institute of Energy Research, Korea

Title: Study of solvent recovery in solvent deasphalting process

Seonju Ahn, Korea University, South Korea

Title: Reforming of methane with carbon dioxide

Kusman Dossumov, Al-Farabi Kazakh National University, Kazakhstan

Title: Green synthesis of Fe nanoparticles for chromate removal

Christiana Mystrioti, National Technical University of Athens, Greece

Title: Investigation of hexavalent chromium removal from polluted soil using electroremediation

Aikaterini Toli, National Technical University of Athens, Greece

Title: Selective viscosifying for conformance control

Joris van Santvoort, Eindhoven University of Technology, The Netherlands

Title: Fracture flow control

Boaz van der Plas, Eindhoven University of Technology, The Netherlands

Title: Vapor-liquid equilibria of the binary system 2-methylfuran + 1-butanol, present in the production of 2,5-dimethylfuran from biomass

Luis A Follegatti-Romero, University of Campinas, Brazil

Title: Production of a solid enzymatic preparation by *Rhizomucor miehei* from a low-cost agroindustrial residue

Jaqueline Greco Duarte, Federal University of Rio de Janeiro, Brazil

Title: Electrical, optical and structural properties of Ga-Al doped ZnO/Copper/Ga-Al doped ZnO multilayer electrode for thin film solar cells

Kyung Hwan Kim, Gachon University, Republic of Korea

Title: Fracture diagnostics of SRV by well testing and micro-seismic method in tight reservoirs, China

Xiaoliang Zhao, China University of Petroleum, China

Title: Determination of dynamic deliverability equation for fractured horizontal well in tight gas reservoir

Xiangji Dou, China University of Petroleum, China

Title: The mechanisms of gas generation during coal deformation

Rongting Xu, University of Chinese Academy of Sciences, China

Title: The effect of water salinity on silica dissolution rate and subsequent formation damage during chemical EOR process

Khaled A. Elraies, Universiti Teknologi PETRONAS, Malaysia

Title: Influence of crude oil type and production technology on bitumen fractional composition

Audrius Vaitkus, Vilnius Gediminas Technical University, Lithuania

Title: Study on chemical properties of some bituminous materials

Nader Nciri, Korea University of Technology and Education, Republic of Korea

Title: Agricultural machinery problems on fuel consumption, exhaust emissions and their normative assessment

Antanas Juostas, Konekesko Lietuva, Lithuania

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Day 3

October 29, 2014

Tropicana Ball Room

Track 13: Modeling & Simulation

Track 14: Catalysis Concepts

Session Chair: Renbi Bai, National University of Singapore, Singapore

Session Co-Chair: Joseph Zeaiter, American University Beirut, Lebanon

Session Introduction

Title: Determination of boiling point of petrochemicals by gas chromatography-mass spectrometry and multivariate regression analysis of structural activity relationship

Sayo Fakayode, North Carolina A&T State University, USA

Title: Feedback control over the chlorine disinfection process at a wastewater treatment plant using a smith predictor, a method of characteristics and odometric transformation

Feridun Demir, Osmaniye Korkut Ata University, Turkey

Title: CFD and process simulations of air gasification of plastic wastes in a conical spouted bed gasifier

Abdallah S Berrouk, The Petroleum Institute, UAE

Title: Modelling approaches for the estimation of irreducible water saturation and heterogeneities of the commercial Ashtart reservoir from the Gulf of Gabès, Tunisia

Fatma Taktak, UMS University, Dubai

Title: Liquid phase oxidation of cyclohexane using supported novel metals: Catalytic oxidation or autoxidation?

Xi Liu, Cardiff University, UK

Title: Mathematical modelling of the aqueous phase reforming of sorbitol

Joseph Zeaiter, American University Beirut, Lebanon

Coffee Break @ Atrium

Title: Fixed-bed catalytic wet peroxide oxidation of phenol with titania and Au/titania catalysts in dark

Miron Landau, Ben-Gurion University of the Negev, Israel

Title: Process simulation-based optimization of a commercial amine gas sweetening unit

Abdallah S Berrouk, The Petroleum Institute, UAE

Title: The features of structural transformations of asphaltene molecules during hydro conversion of vacuum residue in the presence of nanosized molybdenum disulfide particles

Olga Zaitceva, Gubkin Russian University of Oil and Gas, Russia

Title: New catalysts for biodiesel of 1st and 2nd generation

Wolfgang F Hoelderich, TCHK Holderich-Consultancy, Germany

Title: Foamability and foam stability of several surfactants solutions: The role of salinity and oil presence

Abdulrahman AlQuraishi, King Abdulaziz City for Science and Technology, Saudi Arabia

Title: A four coefficient model for extending the heptanes-plus fraction for gas condensate systems

Raffie Hosein, The University of The West Indies, West Indies

Lunch Break @ Atrium

Track 11: Chemical Reaction Engineering & Applications

Track 12: Processing Technology & Separation Techniques

Track 15: Reservoir Engineering

Session Chair: Romain Lemaire, Université Lille Nord de France, France

Session Co-Chair: Erik Von Harbou, University of Kaiserslautern, Germany

Session Introduction

Title: Operational behavior and reforming kinetics over Ni/YSZ of a planar type pre-reformer for SOFC systems

Van Nhu Nguyen, Forschungszentrum Jülich GmbH, Germany

Title: Analysis of oil sands bitumen pyrolysis based on thermogravimetry and Py-GC/MS

Sangcheol Shin, Korea University, South Korea

Title: Tuning photocatalytic activity of carbon-based assemblies by their morphology and surface functionalization

Grigoriy A Sereda, University of South Dakota, USA

Title: Non-equilibrium modelling of simulated moving bed processes for separation of Xylenes in petrochemical industry

Ahmet R Ozdural, Hacettepe University, Turkey

Title: Morphological analysis and optimisation of heterogeneously catalysed reactive distillation of complex chemical systems

Erik Von Harbou, University of Kaiserslautern, Germany

Title: Experimental investigation of the transport mechanism of several gases during the CVD post-treatment of nanoporous membranes

Anastasios Labropoulos, NCSR Demokritos, Greece

Coffee Break @ Atrium

Title: Novel hydrophilic and oleophobic hollow fiber membrane for effective and low fouling oil/water separation applications

Renbi Bai, National University of Singapore, Singapore

Title: Experimental analysis of the sooting tendency of different oxygenated molecules used as additives in a diesel surrogate

Romain Lemaire, Université Lille Nord de France, France

Title: Coarse-grained simulations of Multiphase distribution in porous media, with application for oil and for gas hydrates

David Wu, Colorado School of Mines, USA

Title: Behavior of oxidative amorphous alloy $\text{Co}_{72}\text{Nb}_{24}\text{B}_4$ on catalytic cracking of methanol to olefin production

Luciano Nascimento, University Pernambuco-UFPE, Brazil

Title: Use alloy quasicrystalline $\text{Al}_{62.2}\text{Cu}_{25.3}\text{Fe}_{12.5}$ for steam reforming of methanol

Lourdes Cristina Lucena Agostinho Jamshidi, University Pernambuco-UFPE, Brazil

Title: Enhanced oil recovery by injection of nanoemulsion systems

Tereza Neuma de Castro Dantas, Federal University of Rio Grande do Norte, Brazil

Title: Multivariable constrained predictive control of main steam temperature in ultra-supercritical coal-fired power unit

Shi-He Chen, Guangdong Electric Power Research Institute, China

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November 30-December 02, 2015 Atlanta, USA



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Scientific Program

2nd International Conference on

Medicinal Chemistry & Computer Aided Drug Designing

October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

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Keynote Forum

Introduction

James K. Bashkin

University of Missouri-St. Louis, USA

Brian S. J. Blagg

The University of Kansas, USA

Coffeebreak: @ Foyer

Xiang-Qun (Sean) Xie

University of Pittsburgh, USA

Tulay Aygan Atesin

The University of Texas-Pan American, USA

Track 1: Rational Drug Designing

Session Chair: Victor J Hruby, University of Arizona, USA

Session Co-Chair: Alexander Heifetz, Evotec (UK) Ltd., UK

Session Introduction

Title: Design and investigation of multivalent ligands for the detection and treatment of diseases

Victor J Hruby, University of Arizona, USA

Title: Structure-based drug discovery for GPCRs: From receptors to ligands

Alexander Heifetz, Evotec (UK) Ltd., UK

Title: DNA-binding polyamides designed against E1, E2 binding sites of HPV DNA show dramatic anti-HPV activity in cell and tissue culture

James K Bashkin, University of Missouri-St. Louis, USA

Title: Structure-guided design, synthesis, and evaluation of guanine-derived inhibitors of the eIF4E mRNA-cap interaction

Xiaoqi Chen, Amgen, USA

Lunch Break @ Carol & Patio

Title: The design and discovery of CXCR4 chemokine receptor antagonists through incorporation of GPCR-MedChem based fragments

Larry Wilson, Emory University and Emory Institute for Drug Development, USA

Title: Understanding the essential requirements for success in structure-based design

Gregory L Warren, OpenEye Scientific Software, USA

Title: Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for the identification and optimization of ligands targeting proteins, RNA and other macromolecules

Alexander D MacKerell, University of Maryland, USA

Title: Computer-aided design of glucokinase activators

Meihua Tu, Pfizer, USA

Title: Non-competitive regulation of the human proteasome by natural products and natural product inspired scaffolds

Jetze J Tepe, Michigan State University, USA

Coffee Break @ Foyer

Title: Rational design approaches to find novel ligands targeting the aryl hydrocarbon receptor: successful applications and mechanistic studies

William H Bisson, Oregon State University, USA

Title: Modulations of protein-protein interactions of EGFRs: Structure, inhibition, dynamics and its implications in breast cancer

Seetharama D. Satyanarayanajois, University of Louisiana at Monroe, USA

Title: Development of new antibiotics by targeting essential enzymes in bacteria: Structure-based design and simulation studies

Concepción González-Bello, Universidad de Santiago de Compostela, Spain

Title: Design and synthesis of novel pyrimidine analogues as HIV-1 integrase inhibitors

Guisen Zhao, Shandong University, China

Title: Synthesis and anti-candida activity evaluation of new [1,2,4] triazolo[3,4-b][1,3,4] thiadiazines

Mashooq Ahmad Bhat, King Saud University, Kingdom of Saudi Arabia

Title: Newer approaches to the discovery of glitazones

Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India

Cocktails Sponsored by Medicinal Chemistry @ Foyer

Tahiti

Track 2: Computer-Aided Drug Design and Structure Determination

Session Chair: Istvan J. Enyedy, Biogen Idec, USA

Session Co-Chair: Nicolas Moitessier, McGill University, Canada

Session Introduction

Title: New approaches to "Hit" optimization

Istvan J. Enyedy, Biogen Idec, USA

Title: Accurate binding site models can be derived from low quality PDB files using an empirical geometry based force field

Colin McMartin, ThistleSoft, USA

Integrating computational approaches into high throughput screening for rational drug discovery

Xin Hu, National Center for Advancing Translational Sciences, National Institutes of Health, USA

Title: Using side-chain models derived from atomic resolution X-ray crystallography to develop force fields which can predict global energy minimum geometries

Regine S Bohacek, BostondeNovo, USA

Lunch Break @ Carol & Patio

Title: Forecaster: A computational tool for drug design and discovery developed by experimentalists for experimentalists

Nicolas Moitessier, McGill University, Canada

Title: Genes to Leads: A rational structure guided lead discovery technology that works for both enzymes and protein-protein interaction targets

Kal Ramnarayan, Sapient Discovery, LLC, USA

Title: Discovery of highly-potent and selective inhibitors for the ABCG2 transporter
Achene Boumedjel, Université Joseph Fourier de Grenoble, France
Title: Predictive application of bioisostere transformations to identify novel high quality compound ideas
Matthew Segall, Optilbrium Ltd., UK
Title: Novel sildenafil analogues: Possible drugs for increased sensitivity to chemotherapeutic agents
Aina Westrheim Ravna, University of Tromsø, Norway

Coffee Break @ Foyer

Title: Structural insights of SIR2 proteins from T. cruzi as promising targets to fight against Chagas disease
Alessandra Nurisso, University of Geneva-University of Lausanne, Switzerland
Title: Stratification of surface lysine residues of bovine testicular hyaluronidase on the base of its 3D structure model: Computer aided drug designing of chondroitin sulphate modified enzyme derivative
Alexander V. Maksimenko, Institute of Experimental Cardiology, Russia
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Day 2 October 16, 2013

Salon B

Track 3: Quantitative Structure-Activity Relationships
 Track 4: Drug Development and Delivery System
 Track 6: Drug Interactions
 Track 8: Pharmacognosy

Session Chair: **Tatsuya TAKAGI**, Osaka University, Japan
 Session Co-Chair: **Cesar M Compadre**, University of Arkansas for Medical Sciences, USA

Session Introduction

Title: In Silico screening for anti-HPV agents using docking studies
Tatsuya TAKAGI, Osaka University, Japan
Title: The development of the tocopherols, a series of novel vitamin E analogues with enhanced bioavailability
Cesar M Compadre, University of Arkansas for Medical Sciences, USA
Title: New polymeric "ruthenium-cyclopentadienyl" complexes for drug delivery in cancer therapy
Andreia Valente, Universidade de Lisboa, Portugal
Title: Unraveling the human multidrug resistance p-glycoprotein poly-specificity
Pierre Falson, Institute of Biology and Chemistry of Proteins, France

Coffee Break @ Foyer

Title: PK modulation of haptenylated peptides via non-covalent antibody complexation
Stefan Dengl, Roche Diagnostics GmbH, Germany
Title: Tumour active plant derived compounds in combination with targeted therapy towards overcoming drug resistance in ovarian cancer
Fazlul Huq, The University of Sydney, Australia
Title: Designed monofunctional platinum found to have significant antitumor activity
Laila Arzuman, The University of Sydney, Australia
Title: A phytochemical and biological investigation of aloe grandidentata salm.-Dyck
Taghreed Abdou Ibrahim, King Saud University, Saudi Arabia
Title: Docking guided QSAR study on a series of N-acetamideindolecarboxylic acid derivatives acting as HCV NS 5B polymerase inhibitors
Vaishali M. Patil, Bharat Institute of Technology, India

Track 5: Drug Discovery

Session Chair: **Gerard Rosse**, Dart Neuroscience, USA
 Session Co-Chair: **Craig M Williams**, University of Queensland, Australia

Session Introduction

Title: Innovative approaches to expand medicinal chemistry space
Gerard Rosse, Dart Neuroscience, USA

Lunch Break @ Carol & Patio

Title: Discovery of a first-in-class topically bioavailable kit inhibitor with clinical activity using computational chemogenomics technology
James Hendrix, nPharmakon LLC, USA
Title: Discovery of a small molecule direct keap1-Nrf2 inhibitor as an anti-oxidant inflammation modulator
Magesh Sadagopan, Otsuka Maryland Medicinal Laboratories, Inc., USA
Title: Can cubane act as a benzene isostere?
Craig M Williams, University of Queensland, Australia
Title: Research and development on novel antitumor agents: Preparation, evaluation, and mechanism of low-molecular-weighted phospho sugar derivatives as IER5/Cdc25B targeted antileukemic agents
Mitsuiji YAMASHITA, Shizuoka University, Japan
Title: Modulators of FGF-FGFR-Heparan sulfate complex: identifications of allosteric antagonists and oligosaccharide agonists as potential novel therapeutics
Gilbert Lassalle, Sanofi Aventis, France
Title: Chemistry, bioactivity, and computational prediction of binding modes for sarsolenane and capnosane diterpenes as PTP1B inhibitors from the hainan soft coral Sarcophyton trocheliophorum marenzeller
Yue-Wei Guo, Shanghai Institute of Materia Medica, China

Coffee Break @ Foyer

Title: On the field of metallodrugs-new ruthenium compounds as anti-tumor agents
Ana Isabel Tomaz, Universidade de Lisboa, Portugal
Title: Design, synthesis and antidiabetic, cardiomyopathy studies of cinnamic acid-amino acid hybrid analogs
Subir Samanta, Birla Institute of Technology, India
Title: Synthesis and screening of newer quinazolin-3(h)-4-One derivatives for anticonvulsant activity
Jayasekhar P Nair, Oman Medical College, Sultanate of Oman
Title: Drug profile matching- drug discovery by polypharmacology-based interaction profiling
Zoltan Simon, Eotvos Lorand University, Hungary
Title: Novel structural elements for drug discovery: Identification, synthesis and application
Pavel Mykhailiuk, Enamine Ltd., Ukraine

Tahiti

Track 12: Recent Research and Developments

Session Chair: **John Spencer**, University of Sussex, UK
 Session Co-Chair: **Carsten Detering**, BioSolveIT Inc, USA

Session Introduction

Title: Synthesis and evaluation of some novel thiazolidinedione derivatives as PPAR- α/γ dual agonist
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India
Title: Unleash the power of the amygdala: How to incorporate MedChem know-how early on in the CADD lead optimization phase
Carsten Detering, BioSolveIT Inc, USA
Title: Drug discovery: Hit to lead, lead to possible clinical candidates-development of androgen receptor down-regulating agents for the treatment of castration resistant prostate cancer
Purushottamachar Puranik, University of Maryland School of Medicine, USA
Title: Synthesis of privileged structure libraries for biological evaluation
John Spencer, University of Sussex, UK

Coffee Break @ Foyer

Title: Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms

Jean Leandro Dos Santos, State University of Sao Paulo, Brazil

Title: Evaluation of serum levels of cadmium and lead in occupationally exposed painters with administration of probiotic (*Lactobacillus pentosus* kca 1) supplemented yogurt: A pilot study

Osadolor H. B., University of Benin, Nigeria

Title: Lipid pattern in serum of patients with type 2 diabetes mellitus

Ashur S Eljamil, Tripoli University, Libya

Title: What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?

Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany

Title: Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer

Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA

Poster Presentations @ Carol & Patio

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Day 3

October 17, 2013

Salon A

Track 10: Receptors and Inhibitors

Session Chair: Prabakaran Narayanasamy, University of Nebraska Medical Center, USA

Session Co-Chair: Xiang-Qun (Sean) Xie, University of Pittsburgh, USA

Session Introduction

Title: The Hsp90 C-terminal binding site, instructions for and ramifications of inhibition

Brian S. J. Blagg, The University of Kansas, USA

Title: Inhibition of prostanoid receptor EP2: A novel anti-inflammatory therapy for chronic neurodegenerative and autoimmune diseases

Thota Ganesh, Emory University School of Medicine, USA

Title: Selective vitamin K2 biosynthesis inhibitors to treat non-replicating *Mycobacterium tuberculosis*

Michio Kurosu, University of Tennessee Health Science Center, USA

Title: Inhibitors of fatty acid amide hydrolase (FAAH): SAR and results in pre-clinical pain models

J. Guy Breitenbucher, Dart Neuroscience LLC, USA

Coffee Break @ Foyer

Title: Discovery of novel bicyclic derivatives to stop the growth of *mycobacterium tuberculosis* by inhibiting MenA

Prabakaran Narayanasamy, University of Nebraska Medical Center, USA

Title: The synthesis of potential inhibitors of panthothenate synthetase

Kellie L Tuck, Monash University, Australia

Title: Design and synthesis of inhibitors of cysteine protease

Debatosh Majumdar, Glycosyn LLC, USA

Title: Inward rectifier potassium channels as emerging drug targets

Jerod S. Denton, Vanderbilt University School of Medicine, USA

Title: Identification of a new class of SUMO specific protease 2 inhibitors utilizing structure based virtual screening approach

Ashutosh Kumar, Zhang Initiative Research Unit, RIKEN, Japan

Title: Are D-neurons and trace amine-associated receptor, Type 1 involved in mesolimbic dopamine hyperactivity of schizophrenia?

Keiko Ikemoto, Fukushima Medical University, Japan

Lunch Break @ Carol & Patio

Title: Harnessing human N-type Ca²⁺ channel receptor by identifying the atomic hotspot regions for its blocker design

C. Gopi Mohan, Amrita Vishwa Vidyapeetham University, India

Title: Discovery of small molecule inhibitors of protein-protein interactions using DNA-encoded chemical libraries

Nils Jakob Vest Hansen, Vipergeren ApS, Denmark

Title: Post-marketing surveillance of active pharmaceutical ingredients in antimalarial drugs used in Malawi

Ibrahim Chikowe, University of Ghana, Ghana

Award Ceremony

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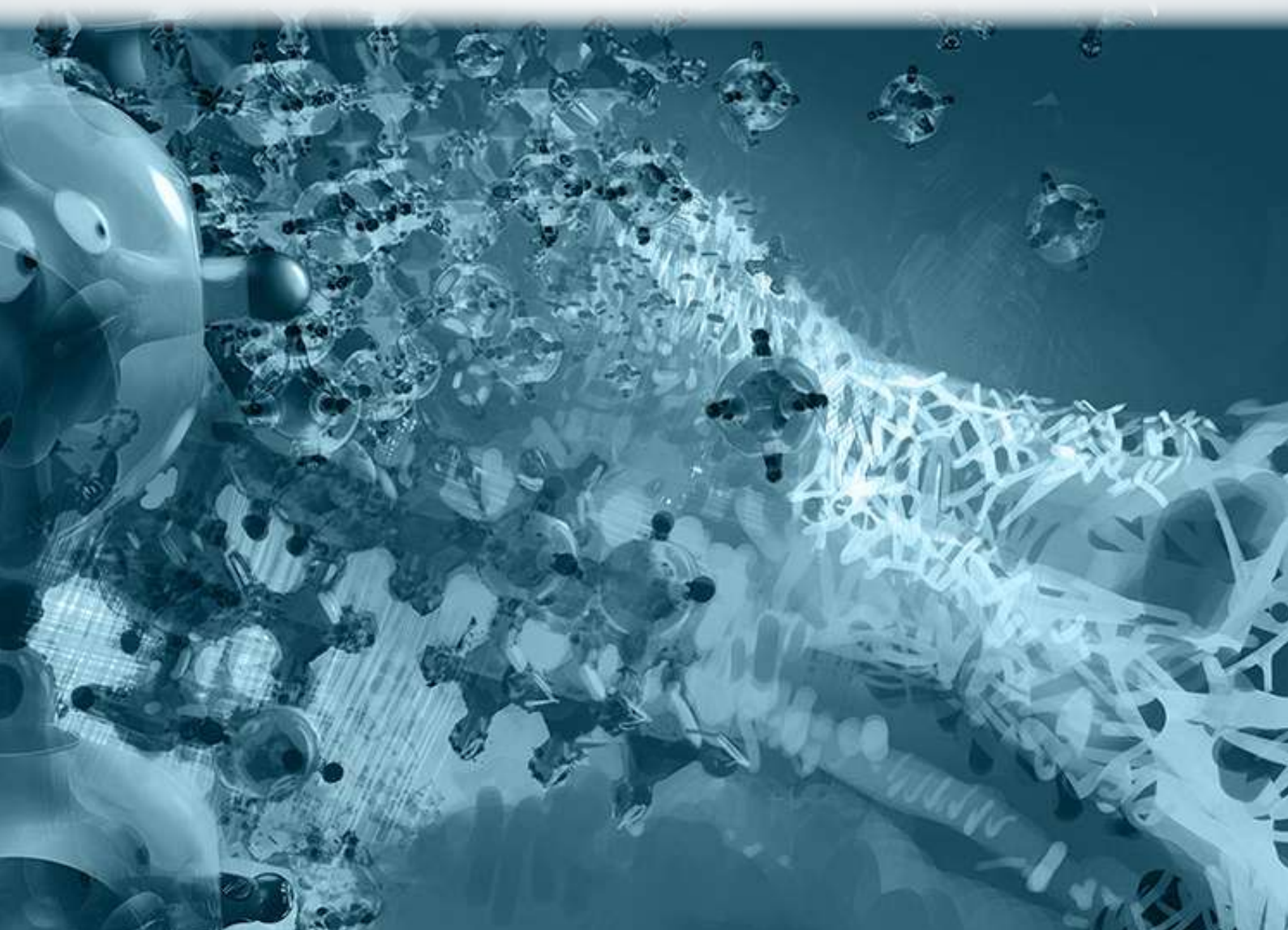
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Versailles B

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Opening Ceremony

Keynote Forum

Introduction

Guy M. Genin

Washington University, USA

Alex V. Vasenkov

CFD Research Corporation, USA

Eugene P. Goldberg

University of Florida, USA

Stephen J Beebe

Old Dominion University, USA

Coffee Break

Track 2: Materials Science & Engineering

Session Introduction

Title: Accelerated material design

Alex V. Vasenkov, CFD Research Corporation, USA

Title: Simple models for plastic deformation and slip avalanches: From crystals to bulk metallic glasses to granular materials

K. A. Dahmen, University of Illinois, USA

Title: Plasticity improvement of Zr-based Bulk Metallic Glasses (BMGs) by laser treatment

P. K. Liaw, The University of Tennessee, USA

Title: Electronic and phonon transport in bulk quantum dot engineered semiconductors

Pierre F. P. Poudeu, University of Michigan, USA

Title: High throughput tribometer for friction, wear, and adhesion measurements

Vivek Kalihari, The Dow Chemical Company, USA

Lunch Break

Title: Energy of slip nucleation and transmission at grain boundaries

Michael D. Sangid, Purdue University, USA

Title: The materials science of powder sorbents for CO₂ capture at high temperatures

Steven J Milne, University of Leeds, UK

Title: Homogeneity measures in functionally graded materials

Jerzy Ratajski, Koszalin University of Technology, Poland

Title: Structural and dielectric characterization of Nickel-Cobalt oxide nanocomposite

Raveendran R, Nanoscience Research Laboratory, India

Title: Determination of the mechanical properties of carbide composites by spherical instrumented indentation

Fjodor Sergejev, Tallinn University of Technology, Estonia

Coffee Break

Title: Thermo-Mechanical large deformation responses of an aluminum alloy processed by Equal Channel Angular Pressing (ECAP)

Muneer Baig, King Saud University, Kingdom of Saudi Arabia

Title: Entrapment of fungus *Rhizomucor tauricus*, removal of Zn (II) from aqueous solution and spectroscopic characterization

A.V.N Swamy, JNTUniversity, India

Title: Potential use of leaf biomass, *Araucaria heterophylla* for removal of Pb⁺²

Ch. V.R. Murthy, Andhra University, India

Title: Effect of bio field treatment on the physical and thermal characteristics of Vanadium pentoxide powders

Shrikant Patil, Trivedi Foundation, USA

Title: Evolution of Nickel Silicide contacts in Silicon nanowires during thermal cycling

Alex Katsman, Israel Institute of Technology, Israel

Title: Fixed-free single walled Boron Nitride nanotube based mass sensor

S. P. Harsha, Indian Institute of Technology Roorkee, India

Track 4: Biophysics & Systems Biology

Track 5: Engineering Physics

Title: Mechanical and electrical interactions between cardiomyocytes and cardiac myofibroblasts in a model of fibrotic remodeling

Guy M. Genin, Washington University, USA

Title: Biophysics models and applications in the study of polysaccharides

Antonio Peramo, University of Michigan, USA

Title: Aerosols hand book

Lev Ruzer, Lawrence Berkeley National Laboratory, USA

Title: Modulation of the mechanical response of biomolecular complexes by the dynamics of applied tension

Ruxandra I. Dima, University of Cincinnati, USA

Title: Ultrashort laser modification of transparent materials: Synergy of excitation/relaxation kinetics, thermodynamics, and mechanics

Nadezhda M. Bulgakova, University of Southampton, UK

Title: Pulse power ablation of melanoma and hepatocellular carcinoma with nanosecond pulsed electric fields

Stephen J Beebe, Old Dominion University, USA

Title: Management of heavy metals in ground water- A case study

Sampath kumar M. C, B.M.S College of Engineering, India

Cocktail: Sponsored by Journal of Material Sciences & Engineering

Day 2

October 23, 2012

Registrations

Versailles B

Track 1: Nanotechnology & Nanoscience

Session Introduction

Title: Atomistic simulations of peptide unfolding and translocation by AAA⁺ biological nanomachines

George Stan, University of Cincinnati, USA

Title: Application of cellulose nanobiocomposite coating in fruits

Kelen Cristina dos Reis, Universidade Federal de Lavras, Brazil

Title: Green-Nanotechnology based smart composite for structural integrity monitoring

Mohamed Saafi, University of Strathclyde, UK

Title: Shape-dependent oriented scaffolding of plasmonic nanoparticles by topological defects for colloidal dimer self-assembly in liquid crystals

Ivan I. Smalyukh, University of Colorado at Boulder, USA

Title: Electric tweezers

Donglei (Emma) Fan, University of Texas at Austin, USA

Coffee Break

Title: Thermosensitive magnetic nanostructured media for hyperthermia and bioimaging

Karen S. Martirosyan, University of Texas at Brownsville, USA

Title: Fabrication and characterization of well-defined organic nanopillar arrays on surfaces

Hai-Feng Frank Ji, Drexel University, USA

Title: Fibronectin adsorption on electronically nanostructured biomaterial surfaces

Andreas Kortge, University of Rostock, Germany

Title: Structural complexity at nanoscale: From single nanoparticle to membrane

Xiao-Min Lin, Center for Nanoscale Materials, USA

Title: Prospects for engineering semiconductor nanowire materials for optoelectronics

Harry E. Ruda, University of Toronto, Canada

Title: Lateral energy transfer in thin film quantum dot induced via plasmonic effects

Seyed M. Sadeghi, University of Alabama, USA

Lunch Break

Title: p-Type conduction in ZnO nanowires from Sb-Decorated Head-to-Head basal plane inversion domain boundaries

Andrew B. Yankovich, University of Wisconsin Madison, USA

Title: Real-Time probing of nanophase evolution in solutions

Yugang sun, Center for Nanoscale Materials, USA

Title: The ionic liquid effect on the preparation of epoxy-silica nanocomposites

Henri S. Schrekker, UFRGS, Brazil

Title: Influence of quality factor on the dynamics of single walled carbon nanotube based mass sensor

Anand Y Joshi, G.H.Patel College of Engineering & Technology, India

Title: High temperature nanophotonics: Controlling the flow of thermal radiation

V. Rinnerbauer, Massachusetts Institute of Technology, USA

Title: Controlled GeSi nanoislands: Fabrication and properties

Zhenyang Zhong, Fudan University, China

Coffee Break

Title: Nanocomposite alternatives to rare-earth permanent magnets

Everett E. Carpenter, Virginia Commonwealth University, USA

Title: Engineered nanopores for protein detection

Liviu Movileanu, Syracuse University, USA

Title: Synthesis and characterization of anti-microbial Ag-TiO₂ nano composite particles and their coatings onto 3-D filters

Cansu Noberi, Yildiz Technical University, Turkey

Title: Natural rubber with gold nanoparticles: Estimation of the amount of nanoparticles in a sample using wavelet transforms

Alexandre Siqueira, Unesp, Brazil

Panel Discussion

Breakout

Track 3: Biomaterials & Biomedical Materials

Track 8: Nonlinear Dynamics and Chaos

Title: Biopolymer-Cell implants and injectable gels for CNS Repair

Eugene P. Goldberg, University of Florida, USA

Title: Use of biomaterials for delivery of chemotrophic proteins in the central nervous system

Elisa Tamariz, Universidad Veracruzana, Mexico

Title: Understanding role of length scale and temperature in indentation induced creep and thermal behavior of Si based materials

VikasTomar, Purdue University, USA

Title: Polyoxometalate (POM) nanocluster- Induced phase transition in phospholipid biomembranes

Y. Elaine Zhu, University of Notre Dame, USA

Title: Next generation polymer nanocomposite electrolytes for lithium ion batteries

Haleh Ardebili, University of Houston, USA

Coffee Break

Title: Radiopaque polymeric microspheres for clinical applications

Ketie Saralidze, Maastricht University, Netherlands

Title: Modal damping as index of structural quality

Sofia Panteliou, University of Patras, Greece

Title: The next generation of controlled drug delivery devices based on Micro-Electro-Mechanical-Systems (MEMS) and novel integration of biomaterials

Noel M. Elman, Massachusetts Institute of Technology, USA

Title: Mora tree (*Maclura tintorea*) leaves as a component in polymer

Svetlana Nikolaeva, Costa Rica's National University, Costa Rica

Title: Sulfonated poly (indene) and PVDF hybrid polyelectrolyte polymer membranes for use in fuel cells

Deysé Elisabeth Ortiz Suman Carpenter, University of Blumenau, Brazil

Panel Discussion

Lunch Break

Poster Presentations

B2B meetings

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Day 3

October 24, 2012

Versailles B

Registrations

Track 6 : Atomic and Nuclear Physics

Track 7 : Optics

Track 9 : Advances in Instrumentation and Techniques

Track 10: Materials Chemistry

Session Introduction

Title: Enhancement and recovery in atomic force microscopy images

Alex Chen, University of North Carolina, USA

Title: Smart materials design in non-linear optics for telecommunications

Jacqueline M. Cole, University of Cambridge, UK

Title: Hollow sphere of copper oxide microparticle prepared by free template and low temperature hydrothermal method

Kanda Wongwailikhit, Rangsit University, Thailand

Coffee Break

Title: Spin polarized current in Graphene pumped by a THz-Signal

Aziz N. Mina, Beni-Suef University, Egypt

Title: Enhancement of washfastness of the Lemongrass oil treated mosquito repellent Nylon nets by air plasma pretreatment

Hasabo A Muhammad Ahamed, Africa City of Technology, Sudan

Title: Structural, optical, photoconductivity and humidity sensing properties of biocomposite doped Cobalt oxide

Udaya Aruldoss, Anna University, India

Panel Discussion

Lunch Break

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