

2nd International Conference on

PHARMACEUTICAL CHEMISTRY

October 02-04, 2017 Barcelona, Spain



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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 Spiralis 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 Linatoyesites 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