

Scientific Program

4th International Conference on

Medicinal Chemistry & Computer Aided Drug Designing

November 02-04, 2015 Atlanta, USA

Sponsor



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Scientific Program

Day 1 November 02, 2015

07:30-09:30 Registrations

Grand Salon-A



09:30-09:55

Opening Ceremony

Keynote Forum

- 09:55-10:00 **Introduction**
- 10:00-10:30 **Concepción González-Bello**
University of Santiago de Compostela, Spain
- 10:30-11:00 **Carsten Detering**
BioSolveIT Inc., USA

Networking & Refreshments Break 11:00-11:20

Group Photo

Track 1: Novel Drug Design

Track 2: Computer Aided Drug Design-CADD

Session Chair: **Concepción González-Bello**, University of Santiago de Compostela, Spain

Session Co-Chair: **Carsten Detering**, BioSolveIT Inc., USA

Session Introduction

- 11:20-11:45 **Novel Multiple Type and Wide Spectral Molecular Targeted Antitumor Agents: Preparation and Preclinical Evaluation of IER5/Cdc25B Targeted Phospha Sugar Derivatives as Well as Attempts of Computer Aided Drug Designing.**
Mitsuji Yamashita, Shizuoka University, Japan
- 11:45-12:10 **In silico design, synthesis and biological evaluation of inhibitors of hypoxia-inducible factor (HIF-1) as antitumor agents**
María Laura Lavaggi, University of the Republic, Uruguay
- 12:10-12:35 **Design of Novel, Selective and Bioavailable Ligands for Closely Related Receptors and Pharmacophores: Conformational and Topographical Considerations.**
Victor J. Hruby, University of Arizona USA
- 12:35-13:00 **"Accelerated and Reliable Lead Discovery: Structure guided drug discovery ideal for collaborative projects"**
Kal Ramnarayan, Sapien Discovery, LLC, USA
- 13:00-13:25 **Investigating the molecular interactions between novel synthetic retinoids and the ligand-binding domains of retinoic acid receptors**
Hesham Haffez, Durham University Durham

Lunch Break 13:25-14:25

Track 3: Fluorination in Medicinal Chemistry

Track 4: Nanomedicine & Fullerene Chemistry

Track 5: Advanced Medicinal Chemistry

Session Chair: **Jonathan Foot**, Pharmaxis Ltd., Australia

Session Co-Chair: **Maria Helena Garcia**, Universidade de Lisboa, Portugal

- 14:25-14:50 **How close are we to predicting binding affinity?**
Carsten Detering, BioSolveIT Inc., USA
- 14:50-15:15 **Ligand-based Screening for anti-Dengue Virus Inhibitor**
Tatsuya Takagi, Osaka University, Japan
- 15:15-15:40 **Nanoparticles with novel methodology to treat infectious diseases**
Prabakaran Narayanasamy, University of Nebraska Medical Center, USA

15:40-16:05 Exploring for bioactive secondary metabolites from the Chinese medicinal mangroves
Yue-Wei Guo, Chinese Academy of Sciences, P R China

Networking & Refreshments Break 16:05-16:25

Day 2 November 03, 2015

Grand Salon-A

Keynote Forum

10:00-10:30 **Thorsten Nowak**
C4X Discovery Manchester United Kingdom

10:30-11:00 **Tatsuya Takagi**
Osaka University, Japan

Networking & Refreshments Break 11:00-11:20 @ Foyer

Track 6: Materialistic Chemistry & Synthetic Chemistry

Track 8: Neurodegenerative Diseases

Session Chair: Thorsten Nowak, C4X Discovery Holdings PLC., United Kingdom

Session Co-Chair: Andreia Valente, Faculdade de Ciências da Universidade de Lisboa Lisboa Portugal

Session Introduction

11:20-11:45 **Identification of sirtuin inhibitors as promising anticancer agents: from screening to activity assays**
Alessandra Nurisso, University of Geneva, Switzerland

11:45-12:10 **Development of new antibiotics targeting shikimate kinase: From concept to practice**
Concepción González-Bello, Universidad de Santiago de Compostela, Spain

12:10-12:35 **Amylin as a Novel Contributor to Alzheimer's Disease and Natural Product Inhibitory Discovery**
Bin Xu, Virginia Tech, USA

12:35-13:00 **Discovery of Novel Orexin-1 Selective Antagonists using NMR Guided Conformational Design**
Thorsten Nowak, C4X Discovery, United Kingdom

13:00-13:25 **2,3-dihydro-1H-isoindoline derivatives as novel drugs for Parkinson's disease: in silico and an in vivo evaluation**
Erik Andrade Jorge, Escuela Superior de Medicina, Mexico

Lunch Break: 13:25-14:25 @ Restaurant

Poster Presentations 14:25-15:25

PME-001 **Computer-aided drug design (CADD): Synthesis and biological evaluation of potential caspase-3 inhibitors as novel Alzheimer's disease therapy**
Lucía Minini, Universidad de la República, Uruguay

PME-002 **Synthesis and biological evaluation of novel 16-dehydropregnenolone acetate derivatives having an ester function at C-3 and triazole ring at C-21 on the 5 α -reductase isoenzymes and on cancer cells lines**
Aylin Viviana Silva Ortiz, Universidad Nacional Autónoma de México, Mexico

PME-003 **Chemogenomic approaches to drug design: Docking-based virtual screening of nematode G-protein coupled receptors for potential anthelmintic agents**
Rabmas Masuka, University of Cape Town, South Africa

PME-004 **New human malaria parasite Plasmodium falciparum dihydroorotate dehydrogenase inhibitors by pharmacophore and structure-based virtual screening**
Elumalai Pavadai, University of Cape Town, South Africa

PME-005 **Poster Presentation by Alessandra Nurisso**
Alessandra Nurisso, University of Geneva, Switzerland

PME-006 **Neuroprotective compounds from Reynoutria sachalinensis**
Jin Bae Weon, Kangwon National University, Korea (1)

PME-007 **Neuroprotective compounds from embryo of Nelumbo nucifera seed**
Jin Bae Weon, Kangwon National University, Korea (2)

PME-008 **Prodrug design and synthesis of oxyresveratrol to improve bioavailability**
Yen Fang Wen, Industrial Technology Research Institute, Taiwan

PME-009 **Computational studies of dipeptidyl peptidase IV inhibitors**
Dhruvi Mahendrabhai Patel, Dharmsinh Desai University, India

- PME-010** **Structure based pharmacophore generation and its applications for identification of dipeptidyl peptidase –IV (DPP-IV) inhibitor**
Khushbu Anilbhai Patel, Dharmsinh Desai University, India
- PME-011** **Oral health quality of life in children with cerebral palsy: Parental perception**
Eman Anwer El Ashiry, King Abdulaziz University, Saudi Arabia
- PME-012** **Evaluation of internal adaptation of some adhesive dental restorative materials using microcomputed tomography (Micro-CT): In vitro randomized blind clinical study**
Najlaa Alamoudi, King Abdulaziz University, Saudi Arabia
- PME-013** **Progesterone receptor (PGR) gene polymorphism is associated with susceptibility to preterm birth**
Immaculate, University of Malaya, Malaysia
- PME-014** **"Antibacterial efficacy of an Unexplored species of Gentianaceae- Exacum pedunculatum on Escherichia coli by a Substantial Computational"**
Lakshmi Huttada, Karnatak University, India
- PME-015** **Novel azetidinone derivatives as antimicrobial agents**
Manal Naser Kadum Hamem, Rajiv Gandhi University Of Health Science, India
- PME-016** **Synthesis, characterization and evaluation of arylamines in a murine model of obesity**
Christian F. Hernández Martínez, Instituto Politécnico Nacional, Mexico
- PME-017** **2,3-dihydro-1H-isoindoline derivatives as novel drugs for Parkinson's disease: In silico and an in vivo evaluation**
Erik Andrade Jorge, Instituto Politécnico Nacional, Mexico (1)
- PME-018** **Poster Presentation by Erik Andrade Jorge**
Erik Andrade Jorge, Instituto Politécnico Nacional, Mexico (2)
- PME-019** **Molecular docking and in vitro assay of isoindolina-1,3-dione amine derivative as novel HDAC8 inhibitor for cancer treatment**
Garcia Gamez Jesus, Escuela Superior de Medicina del Instituto Politécnico Nacional, Mexico
- PME-020** **Screening for inhibitor of recombinant Drosophila melanogaster tyramine-β-hydroxylase**
Md. Nazmul Hasan, Kyushu University, Japan
- PME-021** **Rosmarinic acid potently inhibits amylin-induced neurotoxicity and amyloid formation**
Paul Velander, Virginia Tech, USA
- PME-022** **Irisin as a performed monomer for adipocyte browning**
Lu Zhai, Virginia Tech, USA

Track 7: Drug Design and Chemistry: Cancer Studies

Session Chair: Tatsuya Takagi, Osaka University, Japan

Session Co-Chair: Bin Xu, Virginia Tech, USA

Session Introduction

- 15:00-15:25** **The mode of action of new promising anticancer agents: Multifunctional polymer-ruthenium conjugates**
Andreia Valente, Universidade de Lisboa, Portugal
- 15:25-15:50** **Epi-drug development targeting human G9a H3K9 methyltransferase**
Yong-Hwan Lee, Louisiana State University, USA
- 15:50-16:15** **Nitrones as potential therapeutic agents against Alzheimer's Disease.**
Alicia Merlino, Theoretical and Computational Chemistry Group, Uruguay

Networking & Refreshments Break 16:15-16:35 @ Foyer

- 16:35-17:00** **Small-molecule modulators of thiamine transport in pathogenic bacteria.**
Anna Hirsch, Stratingh Institute for Chemistry University of Groningen The Netherlands
- 17:00-17:25** **Synthesis, Structural Anticancer Activity Relationship, and Docking Study of Novel 5-Deazaflavin Analogs**
Hamed I Ali, Irma Lerma Rangel College of Pharmacy, USA

Day 3 November 04, 2015

Grand Salon-A

Track 9: Drug Discovery and Drug Development

Track 10: Advances in Drug Discovery

Track 11: Hybrid Techniques & Lab-on-a-chip

Track 12: Pharma Market Audit

Session Chair: Concepción González-Bello, Universidad de Santiago de Compostela, Spain

Session Co-Chair: Mitsuji Yamashita, Shizuoka University, Japan

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

Session Introduction

10:00-10:25 **PubChem BioAssay: A public information resource supporting medicinal chemistry and drug discovery research.**

Yanli Wang, National Institutes of Health, USA

Ruthenium drugs for cancer therapy: Small structural changes, different in vivo performances.

10:25-10:50 **Maria Helena Garcia**, Faculdade de Ciências da Universidade de Lisboa Universidade de Lisboa Portugal

Networking & Refreshments Break 10:50-11:10 @ Foyer

11:10-11:35 **Development of selective mechanism-based inhibitors for human Semicarbazide-Sensitive Amine Oxidase (SSAO)**

Jonathan S. Foot, Pharmaxis Ltd., Australia

11:35-12:00 **Targeting the genome of high-risk HPVs with large hairpin polyamides: Promising novel antiviral agents**

Carlos H Castaneda, University of Missouri-St. Louis, USA

12:00-12:25 **A combined in-vitro and in-silico studies of macrocyclic complexes of Tin(II) with potent anti-cancer, anti-inflammatory and anti-microbial properties**

Ekta Rawat, Kurukshetra University, India

12:25-12:50 **Development of a novel class of hyper-multi-targeted computer-aided CREKA/YIGSR**

Ioannis Grigoriadis, Biogenea Pharmaceuticals Ltd, Greece

12:50-13:15 **The prevalence of extra root canals of maxillary first permanent molars among population in Jeddah, Saudi Arabia using Micro-Computed Tomography (Micro-CT)**

Najat Farsi, King Abdulaziz University, KSA

13:15-13:40 **TAAR1 ligands as prospective neuroleptics: From D-neuron research**

Keiko Ikemoto, Iwaki Kyoritsu General Hospital, Japan

Lunch Break: 13:40-14:40 @ Restaurant

Award ceremony

Bookmark your dates

5th International Conference on

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December 01-03, 2016 Chicago, USA



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