07:30-09:30 Registrations

Grand Salon-A

09:30-09:55 Opening Ceremony

Keynote Forum

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

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, Sapient 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
Prabagaran Narayanasamy, University of Nebraska Medical Center, USA
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

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
Lucia Minini, Universidad de la Republica, Uruguay

PME-002  Synthesis and biological evaluation of novel 16-dehydroprogrenolone acetate derivatives having an ester function at C-3 and triazole ring at C-21 on the 5α-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
Dhruti Mahendrabhai Patel, Dharmsinh Desai University, India
tracks 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
andrea 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: prabagaran narayanasamy, university of nebraska medical center, usa

session introduction
10:00-10:25
Yanli Wang, National Institutes of Health, USA

10:25-10:50
Ruthenium drugs for cancer therapy: Small structural changes, different in vivo performances.
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

Medicinal Chemistry & Computer Aided Drug Designing

December 01-03, 2016  Chicago, USA