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Scientific Program

5th International Conference on

Medicinal Chemistry & Computer Aided Drug Designing and Drug Delivery

December 05-07, 2016 Phoenix, USA



Meeting Room A

conference**series.com** 09:00-09:25

Opening Ceremony

Keynote Forum

- 09:25-09:40 Introduction
- 09:40-10:10 **Title: Conformational and dynamic considerations in drug design for g-protein coupled receptors**
Victor J Hruby, University of Arizona, USA
- 10:10-10:40 **Title: Digging in untapped chemical space: how to combine novelty and synthetic access**
Carsten Detering, BioSolveIT Inc., USA

Networking and Refreshment Break 10:40-11:10

- 11:10-11:40 **Title: The use of small molecule proteasome modulation in human diseases**
Jetze J Tepe, Michigan State University, USA

Sessions: Frontiers in Chemistry | Novel Drug Designing & Drug Delivery | Computer Aided Drug Designing-CADD | Hyphenated Chromatographic Techniques for Drug Analysis

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

Session Co-chair: Thorsten Nowak, C4X Discovery Manchester United Kingdom

Session Introduction

- 11:40-12:05 **Title: A set of diagnostic bench tests leads to the development of accurate flexible docking algorithms**
Colin McMartin, ThistleSoft High Meadow, USA
- 12:05-12:30 **Title: Inhibition of amyloid beta peptide oligomerization: Empirical and ab initio studies**
Arvi Rauk, University of Calgary, Canada
- 12:30-12:55 **Title: "Growing" hydrogen bonding waters in molecular complexes!**
Regine Bohacek, Boston De Novo Design, USA

Panel Discussion @ 12:55-13:00

Lunch Break 13:00-14:00 @ Restaurant

Workshop

- 14:00-14:30 **Title: Conformational design in medicinal chemistry - An important under-utilised opportunity**
Thorsten Nowak, C4X Discovery Manchester United Kingdom
- 14:30-14:55 **Title: Design of novel potent and selective agonists at the melanocortin1 receptor**
Minying Cai, Arizona Cancer Center, USA
- 14:55-15:20 **Title: Exploiting unique interactions in the MKK3/6 and ASK1 kinase active sites through computer-aided drug design**
Simone V Bigi, Takeda California, Inc., USA
- 15:20-15:45 **Title: Interaction analysis between cell adhesion factor fimh and its inhibitor by fragment molecular orbital method**
Norihito Kawashita, Osaka University, Japan

Panel Discussion @ 15:45-15:55

Networking and Refreshment Break 15:55-16:10 @ Foyer

Sessions: New Trends in Pharmacology & Drug Development | Analytical & Bioanalytical Techniques | Cancer Studies: Drug Design and Chemistry | Drug Discovery and Drug Delivery: Emerging Diseases

Session Chair: Jetze J Tepe, Michigan State University USA

Session Co-chair: Carsten Detering, BioSolveIT Inc., USA

- 16:10-16:35 **Title: Computer-aided design, efficient synthesis and mechanistic studies of serine protease covalent inhibitors**
Nicolas Moitessier, McGill University, Canada
- 16:35-17:00 **Title: Glycopeptide drugs**
Robin Polt, The University of Arizona, USA
- 17:00-17:25 **Title: Molecular dynamics study of autotaxin with potential allosteric inhibitors**
Eko Aditya, Vrije Universiteit Amsterdam, the Netherlands
- 17:25-17:50 **Title: Boundary-state light emission quantum in biomolecules**
Babak Daneshfard, Shiraz University of Medical Sciences, Iran
- 17:50-18:15 **Title: Dual-function near-infrared (nir) photosensitizer for fluorescence imaging and photodynamic therapy (pdt) of cancer**
Ravindra K Pandey, Roswell Park Cancer Institute, USA

Panel Discussion

Day 2 December 06, 2016

Meeting Room A

Keynote Forum

- 10:00-10:30 **Title: *In Silico* analysis of enantioselective binding of imids to cereblon**
Tatsuya Takagi, Osaka University, Japan
- 10:30-11:00 **Title: Fitted, an evolving docking programs addressing unmet medicinal chemistry needs**
Nicolas Moitessier, McGill University, Canada

Networking & Refreshment Break 11:00-11:20

- 11:20-11:50 **Title: Indeno[1,2-B]indoles: A good scaffold for designing bioactive molecules**
Marc Le Borgne, University Lyon 1, France
- 11:50-12:20 **Title: Innovative and strategic materials for medical technology against tumors: preclinical researches on sugar dendritic GD-DTPA complex MRI contrast agents and IER5/CDC25B targeted novel phospho sugar antitumor agents**
Mitsuji Yamashita, Shizuoka University, Japan

Sessions: ChemBioChem-Antimicrobials and Infectious Agents & Diseases | Neurodegenerative Diseases | Chem-Virology (Zika Virus) | Hematology/Oncology and Stem Cell Therapy | Stereoisomerism & SAR (Structure Activity Relationship) | Chemical Biology | Toxicology and Environmental Chemistry | Clinical Pharmacy Practice

Session Chair: Victor J Hruby, University of Arizona USA

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

- 12:20-12:45 **Title: Targeting the motion of shikimate kinase-opportunities for antibiotic drug development**
Concepción González-Bello, University of Santiago de Compostela, Spain
- 12:45-13:10 **Title: Ligand conformational analysis enabling improved nrf2 activators**
Thorsten Nowak, C4X Discovery Manchester, United Kingdom

Lunch Break 13:10-14:10

Workshop

- 14:10-14:40 **Title: A tale of a low molecular weight inhibitor for bruton's tyrosine kinase, modeled in seesar, the world's best compound ideation software for medicinal chemists**
Carsten Detering, BioSolveIT Inc., USA

14:40-15:05 Title: **Identification of Inhibitors for the Lutheran – Laminin Interaction by molecular modeling techniques to reduce the vaso-occlusive crises of sickle cell disease**

Fabrice Gardebien, Université de la Réunion, France

15:05-15:30 Title: **Differential binding force: A new physicochemical parameter for drug design**

Shoujun Xu, University of Houston, USA

15:30-15:55 Title: **Synthesis of novel agents-effective on leukemia and colon cancer cell lines**

Ilknur Babahan, Adnan Menderes University, Turkey

15:55-16:20 Title: **A Comparative analysis of aspirin from various analgesic formulations using titrimetry, spectroscopic and hyphenated chromatographic techniques**

Ochieng Anthony, Sumait University, Tanzania

16:20-16:45 Title: **First-in-class MCRs coupled with cascade reactions for the generation of molecular complexity**

Christopher Hulme, The University of Arizona, USA

Networking & Refreshment Break 16:45-17:00

Poster Presentations @ 17:00-18:00

CADD 101 Title: **Optimization of the indole-pyrimidine-chrysin hybrid as the lead molecule for anti-inflammatory drugs**

Jagroop Kaur, Guru Nanak Dev University, India

CADD 102 Title: **Rational design, synthesis and working of a tri-ligating receptor: Removal of cyanide from cytochrome c oxidase**

Sukhmeet Kaur, Guru Nanak Dev University, India

CADD 103 Title: **Design, synthesis and biological evaluation of novel 2-phenyl-1-benzopyran-4 one derivatives as potential poly-functional anti-alzheimer's agents**

Majinder Singh, Punjabi University, India

Panel Discussion

Day 3 December 07, 2016

Meeting Room A

Sessions: Nursing in Chemistry | Nanomedicine & Fullerene Chemistry | Chem-Toxicology, Chem-Pharmacology, Chem-Microbiology, Chem-Genomics | Pharmaceutical Industry Overview

Session Chair:

Marc Le Borgne, University Lyon 1, France

Ilknur Babahan, Adnan Menderes University, Turkey

Session Co-chair:

Norihito Kawashita, Osaka University, Japan

Ochieng Anthony, Sumait University, Tanzania

10:00-10:30 Title: **Combined 2D- / 3D-QSAR, molecular docking, accelerated molecular dynamics simulation and QM/Mm calculation studies on pepstatin-a analogues as cathepsin-d inhibitors**

Olayide A. Arodola, University of KwaZulu-Natal, South Africa

10:30-11:00 Title: **Reactive metabolites prediction: What can molecular orbitals tell us?**

Anna Tomberg, McGill University, Canada

Networking & Refreshment Break 11:00-11:20

11:20-11:50 Title: **Virtual flow: A flexible workflow system for virtual screening procedures on high-performance computers**

Christoph Gorgulla, Max Planck Institute for Molecular Genetics, Germany

11:50-12:20 Title: **Evaluating small molecules' potential energy through the long standing chemical principles**

Zhaomin Liu, McGill University, Canada

12:20-12:50 Title: **Current topics in computer-aided drug design technologies: Future aspects**

Reham F. Barghash, National Research Center, Egypt

12:50-13:20 **Title: "SMART" drug based targeted delivery: A new paradigm for nanomedicine strategies**
Sugapriya Dhanasekaran, Prince Sattam Bin Abdullaziz University, KSA

Lunch Break 13:20-14:20

14:20-14:50 **Title: The interaction of metals with alpha-synuclein**
Heather R Lucas, Virginia Commonwealth University, USA

14:50-15:20 **Title: Synthesis of novel anthraquinone anti-cancer drugs: molecular structure, molecular chemical reactivity descriptors and their interactions with DNA**
Tarek M. EL Gogary, Jazan University, KSA

15:20-15:45 **Title: Addressing new targets and cytoprotective compounds against neurodegenerative diseases**
Bruno Andrade, Universidade Estadual do Sudoeste da Bahia, Brazil

Award & Closing Ceremony



Bookmark your dates

6th International Conference on

Medicinal Chemistry & Computer Aided Drug Designing and Drug Delivery

November 06-08, 2017 San Antonio, USA

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