Organize your Events at OMICS Group Conferences

Proposals are invited for organizing Symposia/Workshops at OMICS Group Conferences or OMICS Group will sponsor small events at your universities in related areas under the title of your own. These proposals can be sent to respective conference mail ids or to symposia@omicsonline.org

OMICS Group Conferences
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Phone: +1-650-268-9744, Fax: +1-650-618-1414, Toll free: +1-800-216-6499
Email: medchem2014@omicsgroup.us
Day 1  December 08, 2014

Sierra Ballroom

Opening Ceremony

Keynote Forum

09:55-10:00  Introduction

10:00-10:25  Concepción González-Bello
University of Santiago de Compostela, Spain

10:25-10:50  Patrick Y S Lam
Drexel University, USA

11:05-11:30  Thorsten Nowak
C4X Discovery Holdings PLC., UK

Coffee Break 10:50-11:05 @ Foyer

Track 1: Rational Drug Design
Track 2: Computer-Aided Drug Design and Structure Determination
Session Chair: Patrick Y S Lam, Drexel University, USA
Session Co-Chair: Concepción González-Bello, University of Santiago de Compostela, Spain

Session Introduction

11:30-11:50  Predicting ligand binding affinity: A comparative study on the use of docking vs. Bayesian categorization and random forest recursive partitioning
David C Kombo, Proteostasis Therapeutics, Inc., USA

11:50-12:10  In silico screening for anti-HPV agents using pharmacophore models
Tatsuya Takagi, Osaka University, Japan

12:10-12:30  NMR driven conformational design - A powerful drug design tool
Thorsten Nowak, C4X Discovery Holdings PLC., UK

12:30-12:50  Computer aided design and optimization of kinase and phosphatase inhibitors
Kal Ramnarayan, Sapient Discovery, LLC., USA

12:50-13:10  The use of epitopes against schistosomiasis: The role of molecular modelling
Moacyr Comar Junior, Federal University of São João del Rei, Brazil

13:10-13:30  Structure-based design of covalent inhibitors or protein-protein interactions
Maurizio Pellecchia, Sanford-Burnham Institute for Medical Research, USA

Lunch Break 13:50-14:35 @ Tiburon-Sausalito

Track 3: Quantitative Structure-Activity Relationships
Track 4: Advanced Medicinal Chemistry
Track 8: Drug Interactions and Drug Metabolism
Track 9: Neurodegenerative Diseases
Session Chair: Thorsten Nowak, C4X Discovery Holdings PLC., UK
Session Co-Chair: Istvan J Enyedy, Biogen Idec, USA

Session Introduction

14:35-14:55  Revisiting INH: QSAR-based design of new anti-tubercular compounds
Filomena Martins, Universidade de Lisboa, Portugal

14:55-15:15  In vitro COX inhibitory activity of novel L-α-aminoarylpropionic acid derivatives
A G Zhmakhyan, Yerevan State Medical University, Armenia

15:15-15:35  New developments in docking and scoring
Istvan J Enyedy, Biogen Idec, USA

15:35-15:55  Comparative molecular modeling study between the pre-fusion and post-fusion conformations of newcastle disease virus: Homology modeling, and virtual screening
Mohammed A Khedr, King Faisal University, KSA

Coffee Break 15:55-16:10 @ Foyer

16:10-16:30  Peptide-displaying phage technology in breast cancer diagnosis
Thaise Gonçalves Araújo, Federal University of Uberlandia, Brazil

16:30-16:50  Discovery of small molecule blockers of protein-protein interactions using DNA-encoded small-molecule libraries
Nils Hansen, VipergenApS, Denmark

16:50-17:10  Neuroprotective properties of compound isolated from Dianthus superbus L.
Choong Je Ma, Kangwon National University, Korea

17:10-17:30  Applications of Proteochemometrics - From Species Extrapolation to Cell Line Sensitivity Modelling
Jian Liu, Xi’an Jiaotong-Liverpool University, China

17:30-17:50  Data and Compute Intensive eScience Approaches in Computational Medicinal Chemistry
Scott James Lusher, Netherlands eScience Center, Netherlands

18:10-18:30  Synthesis, Biological Evaluation and 3d Qsar of some Novel Benzimidazole Derivatives as Anti Microbial Compounds
Sonal Dubey, Krupanidhi College of Pharmacy, India

18:30-19:30  Cocktails sponsored by Journal of Medicinal Chemistry @ Tiburon-Sausalito
Day 2  
December 09, 2014  
Sierra Ballroom  
Keynote Forum  

09:30-09:55  
Pierre Falson  
IBCP, France  

Track 5: Cancer Research in Medicinal Chemistry  
Track 6: New Approaches in Drug Discovery  
Session Chair: Andrew B McElroy, Eligochem Ltd., UK  

09:55-10:15  
Mitsuji Yamashita, Shizuoka University, Japan  

10:15-10:35  
Strategies to optimize and use bacterial cytochromes p450 for drug discovery & development  
Nico P E Vermeulen, VU University Amsterdam, Netherlands  

10:35-10:55  
New agonists of the CB2 cannabinoid receptor: Discovery of a new class of analgesic compounds  
Pier Giovanni Baraldi, Università di Ferrara, Italy  

Coffee Break 10:55-11:10 @ Foyer  

11:10-11:30  
Polar drugs  
Andrew B McElroy, Eligochem Ltd., UK  

11:30-11:50  
Drug discovery against category A-C pathogens through MEP pathway  
Prabagaran Narayanasamy, University of Nebraska Medical Center, USA  

11:50-12:10  
Discovery of novel lead compounds by large scale diverse encoded chemical libraries  
Jin Li, HiTiGen Ltd., China  

12:10-12:30  
In silico approach to predict ADME-Tox properties of small organic molecules: Challenges and opportunities for drug discovery  
Maria Miteva, University Paris Diderot, France  

Track 7: Drug Development and Delivery System  
Track 10: Receptors and Inhibitors  
Session Chair: Niren Murthy, University of California, USA  
Session Co-Chair: Peter Teriete, Sanford-Burnham Institute for Medical Research, USA  
Session Co-Chair: Nico P E Vermeulen, VU University Amsterdam, Netherlands  

12:30-12:50  
In vivo delivery of transcription factors with chemically modified oligonucleotides  
Niren Murthy, University of California, USA  

12:50-13:10  
Eradication of asbestos tumors in vivo with histone deacetylase inhibitors-polymer conjugate nanoparticles for acid-responsive drug delivery  
Philippe Bertrand, Institut de Chimie des Milieux et Matériaux de Poitiers, France  

Lunch Break 13:10-14:00 @ Tiburon-Sausalito  

14:00-14:20  
The σ1 receptor as target for novel drugs  
Bernhard Wünsch, Westfalian Wilhelms-University of Münster, Germany  

14:20-14:40  
Using Computer-Aided Drug Design (CADD) techniques to optimize the natural product-derived phenylmethylidene-hydanto in scaffolds as promising antitumor agents  
Mudit Mudit, D’Youville College School of Pharmacy, USA  

14:40-15:00  
Design and development of small peptidomimetics of RXFP1 for the treatment of acute heart failure  
Akhter Hassain, University of Melbourne, Australia  

15:00-15:20  
Exploring pharmacological potential of Brazilian plants: SAM database-A tool for recording and comparison of molecules isolated from plants of the Brazilian semiarid  
Bruno Andrade, State University of Southwest Bahia, Brazil  

Coffee Break 15:20-15:35 @ Foyer  

15:35-15:55  
Novel chemistry-based tools to study epigenetic enzymes in inflammation  
Frank J Dekker, Pharmaceutical Gene Modulation, The Netherlands  

15:55-16:15  
Current SAR on HIV: The flow from phenotypic assays via medicinal chemistry to in silico design  
Peter Teriete, Sanford-Burnham Institute for Medical Research, USA  

16:15-16:35  
Structure guided design and synthesis of SAR107375A, a selective and potent dual thrombin and factor Xa inhibitor  
Jerome Meneyrol, Sanofi-Aventis R&D, France  

16:35-16:55  
Molecular modeling approach to investigate the binding mode of 4-nerolidylcatechol into two subtypes of matrix metalloproteinases  
Kely Medeiros Turra, University of São Paulo, Brazil  

14:30-15:30 Poster Presentations @ Tiburon-Sausalito  
17:30-18:30 Cocktails sponsored by Journal of Drug Designing @ Tiburon-Sausalito  

Day 3  
December 10, 2014  
Sierra Ballroom  

Track 11: Membrane Proteins as Pharmaceutical Targets  
Session Chair: Victor J Hruby, University of Arizona, USA  
Session Co-Chair: Pierre Falson, IBCP, France  

Session Introduction
09:00-09:20 Tracking anti-tumor drugs: Ruthenium(II)-cyclopentadienylcomplexes as promising agents
M Helena Garcia, Universidade de Lisboa, Portugal

09:20-09:40 TAAR1 ligands as prospective neuroleptics: From D-neuron study
Keiko Ikemoto, Iwaki Kyoritsu General Hospital, Japan

09:40-10:00 Small-molecule modulators of thiamine transport in pathogenic bacteria
Anna K H Hirsch, University of Groningen, The Netherlands

10:00-10:20 The behavior of detergents around membrane proteins is more complex than supposed, as revealed by a new method of quantification
Pierre Falson, IBCP, France

10:20-10:40 Design of multivalent ligand for the detection and treatment of disease
Victor J Hruby, University of Arizona, USA

10:40-11:00 Polymer ruthenium-cyclopentadienyl conjugates: A new approach to fight cancer
Andreaia Valente, Universidade de Lisboa, Portugal

Coffee Break 11:00-11:15 @ Foyer

Track 12: Recent Research and Developments
Session Chair: Jetze J Tepe, Michigan State University, USA
Session Co-Chair: Bin Xu, Virginia Tech, USA

11:15-11:35 Design of mechanistically distinct proteasome inhibitors for the treatment of multiple myeloma
Jetze J Tepe, Michigan State University, USA

11:35-11:55 Molecular characterization and design of a key new hormone, irisin
Bin Xu, Virginia Tech, USA

11:55-12:15 Structure-based discovery of new modulators targeting nuclear X receptor alpha for cancer therapy
Ying Su, Sanford-Burnham Medical Research Institute, USA

12:15-12:35 Privileged heterocycles by palladium-catalyzed aerobic oxidative isocyanide insertion
Romano V A Orru, VU University Amsterdam, Netherlands

Lunch Break 12:35-13:20 @ Tiburon-Sausalito

13:20-13:40 Visual binding: A radically new concept to support the medicinal chemist’s quest for innovative NMEs
Carsten Detering, BioSolve IT Inc., USA

13:40-14:00 A G-quadruplex/I-motif switch in the HRAS promoter as target for anthratiophenediones that show a strong anti-proliferative activity in urinary bladder cancer cells
Luigi E Xodo, University of Udine, Italy

14:00-14:20 Multi-target approach to anti-inflammatory drugs - in silico and medicinal chemistry
Eugen Proschak, Goethe-University of Frankfurt, Germany

14:20-14:40 Identification and optimization of tertiary sulfonamides as RORc inverse agonists
Benjamin P Fauber, Genentech, Inc., USA

14:40-15:00 Massive changes to the biophysical properties of DNA upon binding antiviral polyamides
Gaofei He, University of Missouri-St. Louis, USA

Coffee Break 15:00-15:15 @ Foyer

15:15-15:35 The communion of medicinal chemistry and nanotechnology in anticancer therapeutics
Debatosh Majumdar, Glycosyn LLC., USA

15:35-15:55 Evaluation of Satureja hortensis leaves essential oil pharmacological activities
A P Manjikyan, Yerevan State Medical University, Armenia

15:55-16:15 Phytochemicals and antioxidant capacities from Dacryodes rostrata fruits
Prasad K N, Monash University Malaysia, Malaysia

16:15-16:35 Selection and characterization of RNA aptamers targeting the genomic 3’-UTR in the dengue virus
Adriana Freitas Neves, Universidade Federal de Goiás, Brazil

16:35-16:55 SurR9C84A exhibits cardioprotective effects against melphalan induced cardiotoxicity in primary human cardiomyocytes
Ajay Ashok, Deakin University School of Medicine, Australia

Award Ceremony

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4th International Conference on Medicinal Chemistry & Computer Aided Drug Designing
November 02-04, 2015 Atlanta, USA