Scientific Program

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing

December 08-10, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

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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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Day 1 December 08, 2014

07:30-08:30 Registrations

Sierra Ballroom

OMICS Group Conferences
Accelerating Scientific Discovery

09:30-09:55 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

Coffee Break 10:50-11:05 @ Foyer

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

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 schistossomiasis: The role of molecular modelling**
Moacyr Comar Junior, Federal University of São João del Rei, Brazil

13:10-13:30 **Bacterial type II dehydroquinase enzyme: From the reaction mechanism to the structure-based design of inhibitors**
Concepción González-Bello, University of Santiago de Compostela, Spain

13:30-13:50 **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 α-aminoarylpropionic acid derivatives**
A G Zhamharyan, 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 **Investigation of human CA1-induced toxicity in the *Drosophila* model of motor neuron degeneration**
Jian Liu, Xi'an Jiaotong-Liverpool Univeristy, China

17:30-17:50 **Applications of Proteochemometrics - From Species Extrapolation to Cell Line Sensitivity Modelling**
Isidro Cortes-Ciriano, Bioinformatique Structurale Institut Pasteur, France

17:50-18:10 **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

Session Introduction

09:55-10:15 **Research and development for preparation and preclinical evaluation of novel low-molecular-weight phospha sugar antitumor agents targeting IER5/Cdc25B**
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 CB_2 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, HitGen 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

Session Introduction

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 σ_1 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 antimetastatic leads**
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 Hossain, 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, aselective and potent dual thrombinand 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 quantitation**
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**
Andreia 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

Session Introduction

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 anthrathiophenediones 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 5'-UTR in the dengue virus**
Adriana Freitas Neves, Universidade Federal de Goiás, Brazil

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

Award Ceremony

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