144th OMICS Group Conference

Scientific Program

2nd International Conference on

Medicinal Chemistry & Computer Aided Drug Designing

October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

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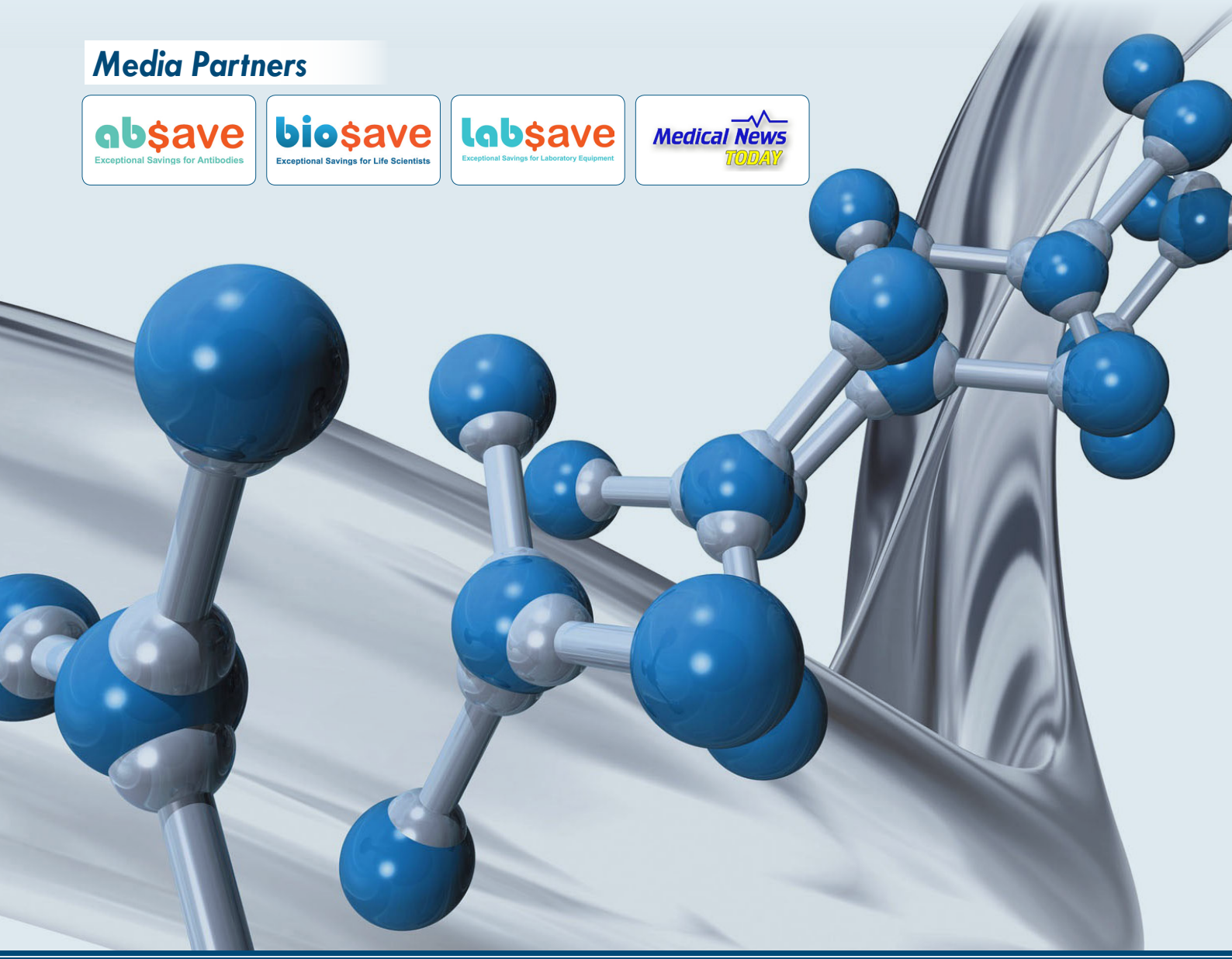

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OMICS Group Conferences
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Day 1 October 15, 2013

08:00-09:00 Registrations

Salon A

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08:30-08:55

Opening Ceremony

Keynote Forum

09:55-10:00 Introduction

10:00-10:25 **James K. Bashkin**
University of Missouri-St. Louis, USA

10:25-10:50 **Brian S. J. Blagg**
The University of Kansas, USA

Coffeebreak: 10:50-11:05 @ Foyer

11:05-11:30 **Xiang-Qun (Sean) Xie**
University of Pittsburgh, USA

11:30-11:55 **Tulay Aygan Atesin**
The University of Texas-Pan American, USA

Track 1: Rational Drug Designing

Session Chair: Victor J Hruby, University of Arizona, USA
Session Co-Chair: Alexander Heifetz, Evotec (UK) Ltd., UK

Session Introduction

11:55-12:15 Design and investigation of multivalent ligands for the detection and treatment of diseases
Victor J Hruby, University of Arizona, USA

12:15-12:35 Structure-based drug discovery for GPCRs: From receptors to ligands
Alexander Heifetz, Evotec (UK) Ltd., UK

12:35-12:55 DNA-binding polyamides designed against E1, E2 binding sites of HPV DNA show dramatic anti-HPV activity in cell and tissue culture
James K Bashkin, University of Missouri-St. Louis, USA

12:55-13:15 Structure-guided design, synthesis, and evaluation of guanine-derived inhibitors of the eIF4E mRNA-cap interaction
Xiaoqi Chen, Amgen, USA

Lunch Break 13:15-14:00 @ Carol & Patio

14:00-14:20 The design and discovery of CXCR4 chemokine receptor antagonists through incorporation of GPCR-MedChem based fragments
Larry Wilson, Emory University and Emory Institute for Drug Development, USA

14:20-14:40 Understanding the essential requirements for success in structure-based design
Gregory L Warren, OpenEye Scientific Software, USA

14:40-15:00 Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for the identification and optimization of ligands targeting proteins, RNA and other macromolecules
Alexander D MacKerell, University of Maryland, USA

15:00-15:20 Computer-aided design of glucokinase activators
Meihua Tu, Pfizer, USA

15:20-15:40 Non-competitive regulation of the human proteasome by natural products and natural product inspired scaffolds
Jetze J Tepe, Michigan State University, USA

Coffee Break 15:40-15:55 @ Foyer

15:55-16:15 Rational design approaches to find novel ligands targeting the aryl hydrocarbon receptor: successful applications and mechanistic studies
William H Bisson, Oregon State University, USA

16:15-16:35 Modulations of protein-protein interactions of EGFRs: Structure, inhibition, dynamics and its implications in breast cancer
Seetharama D. Satyanarayanajois, University of Louisiana at Monroe, USA

16:35-16:55 Development of new antibiotics by targeting essential enzymes in bacteria: Structure-based design and simulation studies
Concepción González-Bello, Universidad de Santiago de Compostela, Spain

16:55-17:15 Design and synthesis of novel pyrimidone analogues as HIV-1 integrase inhibitors
Guisen Zhao, Shandong University, China

17:15-17:35 Synthesis and anti-candida activity evaluation of new [1,2,4] triazolo[3,4-b][1,3,4] thiadiazines
Mashooq Ahmad Bhat, King Saud University, Kingdom of Saudi Arabia

17:35-17:55 Newer approaches to the discovery of glitazones
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India

18:30-19:30 Cocktails Sponsored by **Medicinal Chemistry @ Foyer**

Tahiti

Track 2: Computer-Aided Drug Design and Structure Determination

Session Chair: Istvan J. Enyedy, Biogen Idec, USA
Session Co-Chair: Nicolas Moitessier, McGill University, Canada

Session Introduction

11:55-12:15 New approaches to "Hit" optimization
Istvan J. Enyedy, Biogen Idec, USA

12:15-12:35 Accurate binding site models can be derived from low quality PDB files using an empirical geometry based force field
Colin McMartin, Thistlesoft, USA

12:35-12:55 Integrating computational approaches into high throughput screening for rational drug discovery
Xin Hu, National Center for Advancing Translational Sciences, National Institutes of Health, USA

12:55-13:15 **Using side-chain models derived from atomic resolution X-ray crystallography to develop force fields which can predict global energy minimum geometries**
Regine S Bohacek, BostondeNovo, USA

Lunch Break 13:15-14:00 @ Carol & Patio

14:00-14:20 **Forecaster: A computational tool for drug design and discovery developed by experimentalists for experimentalists**
Nicolas Moitessier, McGill University, Canada

14:20-14:40 **Genes to Leads: A rational structure guided lead discovery technology that works for both enzymes and protein-protein interaction targets**
Kal Ramnarayan, Sapient Discovery, LLC, USA

14:40-15:00 **Discovery of highly-potent and selective inhibitors for the ABCG2 transporter**
Achene Boumedjel, Université Joseph Fourier de Grenoble, France

15:00-15:20 **Predictive application of bioisostere transformations to identify novel high quality compound ideas**
Matthew Segall, Optibrium Ltd., UK

15:20-15:40 **Novel sildenafil analogues: Possible drugs for increased sensitivity to chemotherapeutic agents**
Aina Westrheim Ravna, University of Tromso, Norway

Coffee Break 15:40-15:55 @ Foyer

15:55-16:15 **Structural insights of SIR2 proteins from T. cruzi as promising targets to fight against Chagas disease**
Alessandra Nurisso, University of Geneva-University of Lausanne, Switzerland

16:15-16:35 **Stratification of surface lysine residues of bovine testicular hyaluronidase on the base of its 3D structure model: Computer aided drug designing of chondroitin sulphate modified enzyme derivative**
Alexander V. Maksimenko, Institute of Experimental Cardiology, Russia

18:30-19:30 Cocktails Sponsored by **Medicinal Chemistry @ Foyer**

Day 2 October 16, 2013

Salon B

Track 3: Quantitative Structure-Activity Relationships
Track 4: Drug Development and Delivery System
Track 6: Drug Interactions
Track 8: Pharmacognosy

Session Chair: Tatsuya TAKAGI, Osaka University, Japan
Session Co-Chair: Cesar M Compadre, University of Arkansas for Medical Sciences, USA

Session Introduction

09:00-09:20 **In Silico screening for anti-HPV agents using docking studies**
Tatsuya TAKAGI, Osaka University, Japan

09:20-09:40 **The development of the tocoflexols, a series of novel vitamin E analogues with enhanced bioavailability**
Cesar M Compadre, University of Arkansas for Medical Sciences, USA

09:40-10:00 **New polymeric "ruthenium-cyclopentadienyl" complexes for drug delivery in cancer therapy**
Andreia Valente, Universidade de Lisboa, Portugal

10:00-10:20 **Unraveling the human multidrug resistance p-glycoprotein poly-specificity**
Pierre Falson, Institute of Biology and Chemistry of Proteins, France

Coffee Break 10:20-10:35 @ Foyer

10:35-10:55 **PK modulation of haptenylated peptides via non-covalent antibody complexation**
Stefan Dengl, Roche Diagnostics GmbH, Germany

10:55-11:15 **Tumour active plant derived compounds in combination with targeted therapy towards overcoming drug resistance in ovarian cancer**
Fazlul Huq, The University of Sydney, Australia

11:15-11:35 **Designed monofunctional platinums found to have significant antitumor activity**
Laila Arzuman, The University of Sydney, Australia

11:35-11:55 **A phytochemical and biological investigation of aloe grandidentata salm.-Dyck**
Taghreed Abdou Ibrahim, King Saud University, Saudi Arabia

11:55-12:15 **Docking guided QSAR study on a series of N-acetamideindolecarboxylic acid derivatives acting as HCV NS 5B polymerase inhibitors**
Vaishali M. Patil, Bharat Institute of Technology, India

Track 5: Drug Discovery

Session Chair: Gerard Rosse, Dart Neuroscience, USA
Session Co-Chair: Craig M Williams, University of Queensland, Australia

Session Introduction

12:15-12:35 **Innovative approaches to expand medicinal chemistry space**
Gerard Rosse, Dart Neuroscience, USA

Lunch Break 12:35-13:20 @ Carol & Patio

13:20-13:40 **Discovery of a first-in-class topically bioavailable kit inhibitor with clinical activity using computational chemogenomics technology**
James Hendrix, nPharmakon LLC, USA

13:40-14:00 **Discovery of a small molecule direct keap1-Nrf2 inhibitor as an anti-oxidant inflammation modulator**
Magesh Sadagopan, Otsuka Maryland Medicinal Laboratories, Inc., USA

14:00-14:20 **Can cubane act as a benzene isostere?**
Craig M Williams, University of Queensland, Australia

14:20-14:40 **Research and development on novel antitumor agents: Preparation, evaluation, and mechanism of low-molecular-weighted phospha sugar derivatives as IER5/Cdc25B targeted antileukemic agents**
Mitsuji YAMASHITA, Shizuoka University, Japan

14:40-15:00 **Modulators of FGF-FGFR-Heparan sulfate complex: identifications of allosteric antagonists and oligosaccharide agonists as potential novel therapeutics**
Gilbert Lassalle, Sanofi Aventis, France

15:00-15:20 **Chemistry, bioactivity, and computational prediction of binding modes for sarsolenane and capnosane diterpenes as PTP1B inhibitors from the hainan soft coral Sarcophyton trocheliophorum marenzeller**
Yue-Wei Guo, Shanghai Institute of Materia Medica, China

Coffee Break 15:20-15:35 @ Foyer

15:35-15:55 **On the field of metallodrugs-new ruthenium compounds as anti-tumor agents**
Ana Isabel Tomaz, Universidade de Lisboa, Portugal

15:55-16:15 **Design, synthesis and antidiabetic, cardiomyopathy studies of cinnamic acid-amino acid hybrid analogs**
Subir Samanta, Birla Institute of Technology, India

16:15-16:35 **Synthesis and screening of newer quinazolin-3(h)-4-One derivatives for anticonvulsant activity**
Jayasekhar P Nair, Oman Medical College, Sultanate of Oman

16:35-16:55 **Drug profile matching- drug discovery by polypharmacology-based interaction profiling**
Zoltan Simon, Eotvos Lorand University, Hungary

16:55-17:15 **Novel structural elements for drug discovery: Identification, synthesis and application**
Pavel Mykhailiuk, Enamine Ltd., Ukraine

Tahiti

Track 12: Recent Research and Developments

Session Chair: John Spencer, University of Sussex, UK
Session Co-Chair: Carsten Detering, BioSolveIT Inc, USA

Session Introduction

09:00-09:20 **Synthesis and evaluation of some novel thiazolidinedione derivatives as PPAR-α/γ dual agonist**
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India

09:20-09:40 **Unleash the power of the amygdala: How to incorporate MedChem know-how early on in the CADD lead optimization phase**
Carsten Detering, BioSolveIT Inc., USA

09:40-10:00 **Drug discovery: Hit to lead, lead to possible clinical candidates-development of androgen receptor down-regulating agents for the treatment of castration resistant prostate cancer**
Purushottamachar Puranik, University of Maryland School of Medicine, USA

10:00-10:20 **Synthesis of privileged structure libraries for biological evaluation**
John Spencer, University of Sussex, UK

Coffee Break 10:20-10:35 @ Foyer

10:35-10:55 **Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms**
Jean Leandro Dos Santos, State University of Sao Paulo, Brazil

10:55-11:15 **Evaluation of serum levels of cadmium and lead in occupationally exposed painters with administration of probiotic (Lactobacillus pentosus kca 1) supplemented yogurt: A pilot study**
Osadolor H. B, University of Benin, Nigeria

11:15-11:35 **Lipid pattern in serum of patients with type 2 diabetes mellitus**
Ashur S Eljamil, Tripoli University, Libya

11:35-11:55 **What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?**
Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany

11:55-12:15 **Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer**
Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA

15:30-16:30 **Poster Presentations @ Carol & Patio**
18:30-19:30 Cocktails Sponsored by **Drug Designing: Open Access @ Foyer**

Day 3 October 17, 2013

Salon A

Track 10: Receptors and Inhibitors

Session Chair: Prabagaran Narayanasamy, University of Nebraska Medical Center, USA
Session Co-Chair: Xiang-Qun (Sean) Xie, University of Pittsburgh, USA

Session Introduction

09:00-09:20 **The Hsp90 C-terminal binding site, instructions for and ramifications of inhibition**
Brian S. J. Blagg, The University of Kansas, USA

09:20-09:40 **Inhibition of prostanoid receptor EP2: A novel anti-inflammatory therapy for chronic neurodegenerative and autoimmune diseases**
Thota Ganesh, Emory University School of Medicine, USA

09:40-10:00 **Selective vitamin K2 biosynthesis inhibitors to treat non-replicating Mycobacterium tuberculosis**
Michio Kurosu, University of Tennessee Health Science Center, USA

10:00-10:20 **Inhibitors of fatty acid amide hydrolase (FAAH): SAR and results in pre-clinical pain models**
J. Guy Breitenbucher, Dart Neuroscience LLC, USA

Coffee Break 10:20-10:35 @ Foyer

10:35-10:55 **Discovery of novel bicyclic derivatives to stop the growth of mycobacterium tuberculosis by Inhibiting MenA**
Prabagaran Narayanasamy, University of Nebraska Medical Center, USA

10:55-11:15 **The synthesis of potential inhibitors of panthothenate synthetase**
Kellie L Tuck, Monash University, Australia

11:15-11:35 **Design and synthesis of inhibitors of cysteine protease**
Debatosh Majumdar, Glycosyn LLC, USA

11:35-11:55 **Inward rectifier potassium channels as emerging drug targets**
Jerod S. Denton, Vanderbilt University School of Medicine, USA

11:55-12:15 **Identification of a new class of SUMO specific protease 2 inhibitors utilizing structure based virtual screening approach**
Ashutosh Kumar, Zhang Initiative Research Unit, RIKEN, Japan

12:15-12:35 **Are D-neurons and trace amine-associated receptor, Type 1 involved in mesolimbic dopamine hyperactivity of schizophrenia?**
Keiko Ikemoto, Fukushima Medical University, Japan

Lunch Break 12:35-13:20 @ Carol & Patio

13:20-13:40 **Harnessing human N-type Ca2+ channel receptor by identifying the atomic hotspot regions for its blocker design**
C. Gopi Mohan, Amrita Vishwa Vidyapeetham University, India

13:40-14:00 **Discovery of small molecule inhibitors of protein-protein interactions using DNA-encoded chemical libraries**
Nils Jakob Vest Hansen, Vipergen ApS, Denmark

14:00-14:20 **Post-marketing surveillance of active pharmaceutical ingredients in antimalarial drugs used in Malawi**
Ibrahim Chikowe, University of Ghana, Ghana

Award Ceremony

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