

73<sup>rd</sup> OMICS Group Conference

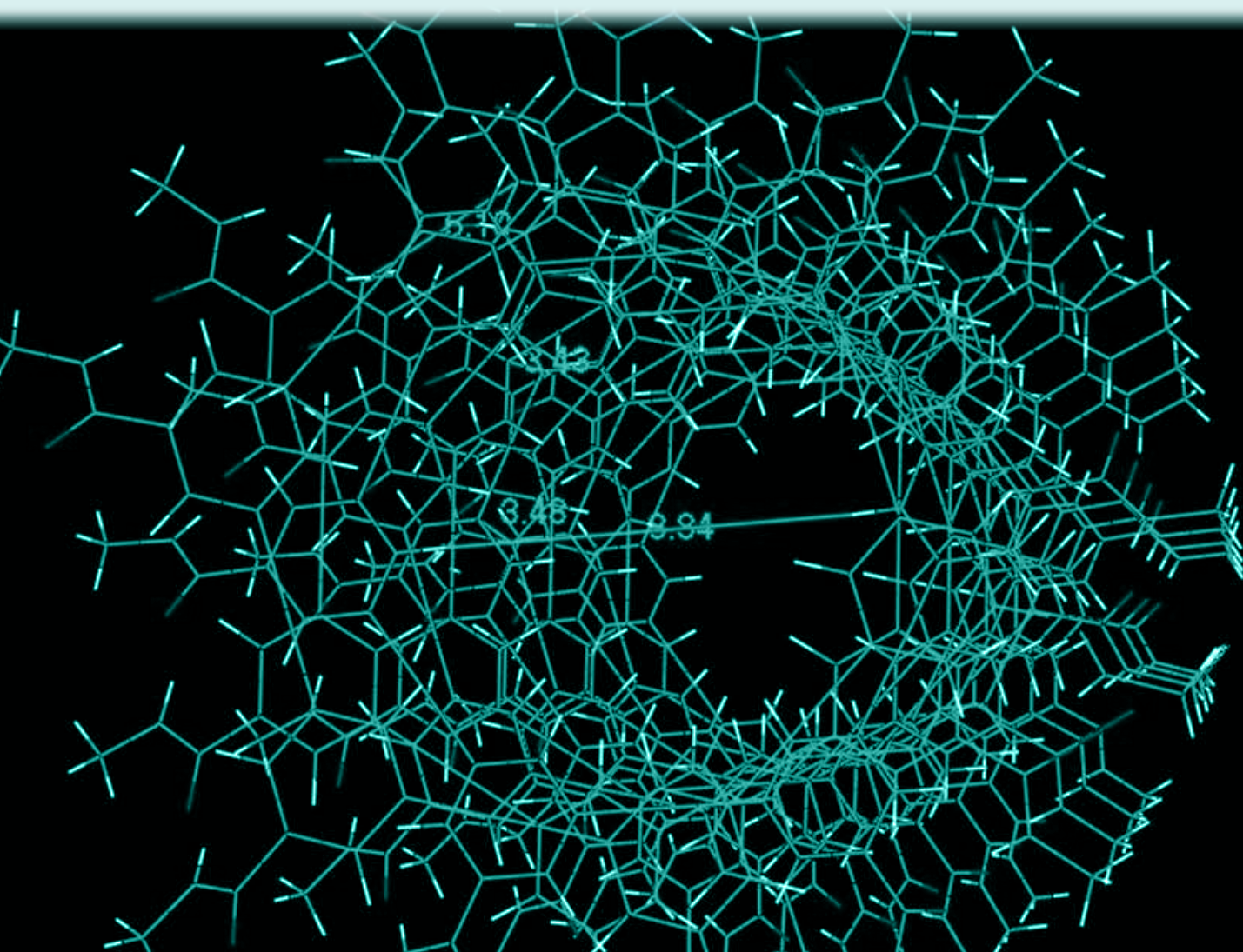
# *Scientific Program*



International Conference and Exhibition on

## **Computer Aided Drug Design & QSAR**

October 29-31, 2012 DoubleTree by Hilton Chicago-North Shore, USA



### **“Organize your Events at OMICS Group Conferences”**

Proposals are invited for organizing Symposia/Workshops at OMICS Group Conferences in related areas under the scheme title of your own. These proposals can be sent to respective conference mail ids or to [symposia@omicsonline.com](mailto:symposia@omicsonline.com)

### **OMICS Group Conferences**

5716 Corsa Ave., Suite 110, Westlake Los Angeles, CA 91362-7354, USA

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## Breakout 1



10:00-10:20

## Opening Ceremony

## Keynote Forum

10:20-10:25 Introduction

10:25-10:50 **Giulio Tarro**

Temple University, USA

10:50-11:15 **Ronan Bureau**

University of Caen Basse-Normandie, France

Coffee Break 11:15-11:30

11:30-11:55 **Li Xing**

Pfizer, USA

Track 1: Molecular Modeling

Track 2: Rational Drug Design

Track 3: Drug Development

Track 4: Structure Prediction

Track 5: Systems Biology

Track 6: Computational Biology

## Session Introduction

11:55-12:15 **Title: Recent technological advancements in ligand-based and structure-based modeling: BCL: Cheminfo and rosetta ligand****Edward W. Lowe Jr.**, Vanderbilt University Center for Structural Biology, USA12:15-12:35 **Title: Specificity of heparin/heparan sulfate binding to proteins****Umesh R. Desai**, Virginia Commonwealth University, USA12:35-12:55 **Title: Discovery of potent, selective and efficacious p38 MAPK inhibitor as clinical drug candidate****Li Xing**, Pfizer, USA

## Lunch Break 12:55-13:55

13:55-14:15 **Title: QSAR model building and analysis of ADME properties: Understanding P-glycoprotein activity****Sookhee Ha**, Merck Research Laboratories, Canada14:15-14:35 **Title: Computer-aided design of inhibitors of DNA methyltransferases****Jose L. Medina-Franco**, Torrey Pines Institute for Molecular Studies, USA14:35-14:55 **Title: Chemoinformatic strategies in the design of new linezolid-like 1,2,4-oxadiazoles active against multidrug resistant Gram-positive pathogens.****Cosimo G. Fortuna**, Università di Catania, Italy

## Coffee Break 14:55-15:10

15:10-15:30 **Title: Screen 3D: A ligand-based 3D similarity search without conformational sampling****Wei Deng (David)**, ChemAxon, USA15:30-15:50 **Title: Pharmacophores vs emerging fragments: Implications in the comprehension of polypharmacological and toxicological properties of chemical derivatives****Ronan Bureau**, University of Caen Basse-Normandie, France15:50-16:10 **Title: Kinome-wide activity models from diverse high-quality datasets****Steven M. Muskal**, Eidogen-Sertanty Inc., USA

16:10-16:30 Panel Discussion

18:00-19:00 Cocktails: Sponsored by Drug Designing: Open Access

Track 7: Structural Bioinformatics

Track 8: Sequence Analysis

Track 9: Data Mining &amp; Data Analysis

Session Introduction

- 10:00-10:20 **Title: Extract chemical information from patents using chemicalize and D2S (Document to Structure)**  
Wei Deng (David), ChemAxon, USA
- 10:20-10:40 **Title: Identifying neuraminidase residues likely to mutate with molecular mechanics free energy**  
Kelly M. Thayer, University of Massachusetts Medical School, USA
- 10:40-11:00 **Title: Chemical targeting of protein methyltransferases**  
Mathieu Schapira, University of Toronto, Canada

Coffee Break 11:00-11:15

- 11:15-11:35 **Title: A simple additive non-parametric regression method and its application to QSAR**  
Tatsuya Takagi, Osaka University, Japan
- 11:35-11:55 **Title: Tumor Liberated Protein (TLP) and human corine in lung cancer cells: Homology or different isoforms in the sequence at the cytoplasmic surface**  
Giulio Tarro, Temple University, USA
- 11:55-12:15 **Title: Screening for novel anti-dengue virus NS3/NS2B inhibitor**  
Norihiro Kawashita, Osaka University, Japan
- 12:15-12:35 **Title: Advanced pharmacophores for accurate virtual screening and identification of opioid lead compounds**  
Sharon D. Bryant, Inte:Ligand GmbH, Austria

Lunch Break 12:35-13:35

- 13:35-13:55 **Title: Human papilloma virus 16 E6 protein as a target for curcuminoids, curcumin conjugates and congeners for chemoprevention of oral and cervical cancers**  
Ajay Kumar Singh, Amity University, India
- 13:55-14:15 **Title: Fuzzy neural network and fuzzy ARTMAP analyses of the affinity of inhibitors for HIV-1 protease**  
Levente Fabry-Asztalos, Central Washington University, USA

14:15-14:35 Panel Discussion

14:35-16:05 Poster Presentations

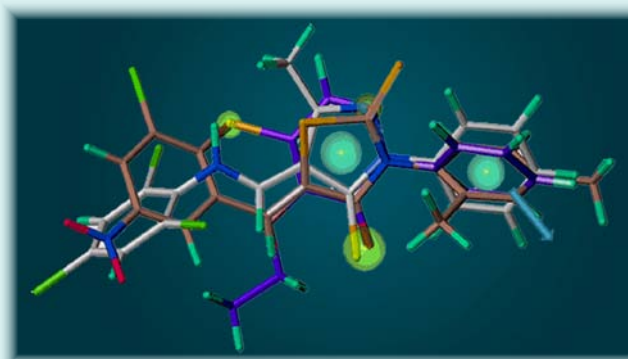
18:00-19:00 Cocktails: Sponsored by Journal of Data Mining in Genomics and Proteomics

Bookmark your dates

2<sup>nd</sup> International Conference and Exhibition on

# In Silico & QSAR

September 4-6, 2013 Orlando-FL, USA



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**Australia:** 1-800-651-097  
**Europe:** 0805-080048

# Upcoming OMICS 2012 Group Conferences

Accelerating Scientific Discovery



International Conference on  
**Regenerative & Functional Medicine**  
November 12-14, 2012  
Hilton San Antonio Airport, USA



2<sup>nd</sup> World Congress on  
**Cell Science & Stem Cell Research**  
November 12-14, 2012  
Hilton San Antonio Airport, USA



International Conference on  
**Clinical Microbiology & Microbial Genomics**  
November 12-14, 2012  
Hilton San Antonio Airport, USA



**Global Biofuels & Bioproduct Summit**  
November 19-21, 2012  
Hilton San Antonio Airport, USA



International Conference and Exhibition on  
**Probiotics**  
November 19-21, 2012  
Hilton San Antonio Airport, USA



International Conference on  
**Genetic Syndromes & Gene Therapy**  
November 19-21, 2012  
Hilton San Antonio Airport, USA



3<sup>rd</sup> International Conference and Exhibition on  
**Analytical & Bioanalytical Techniques**  
November 22-24, 2012  
Hyderabad International Convention Center, India



International Conference and Exhibition on  
**Food Processing and Technology**  
November 22-24, 2012  
Hyderabad International Convention Center, India



2<sup>nd</sup> International Conference and Exhibition on  
**Pharmaceutical Regulatory Affairs**  
November 23-24, 2012  
Hyderabad International Convention Center, India



International Conference and Exhibition on  
**Cosmetology & Cosmetics**  
November 23-24, 2012  
Hyderabad International Convention Center, India



International Conference on  
**Hair Transplantation & Trichology**  
November 26-28, 2012  
Hilton San Antonio Airport, USA



International Conference on  
**Anesthesia & Perioperative Care**  
November 26 - 28, 2012  
Hilton San Antonio Airport, USA



International  
**Toxicology Summit and Expo**  
November 26-28, 2012  
Hilton San Antonio Airport, USA



International Conference and Exhibition on  
**Surgery & Transplantation**  
November 26-28, 2012  
Hilton San Antonio Airport, USA



2<sup>nd</sup> International Conference on  
**Nanotek and Expo**  
December 3-5, 2012  
DoubleTree by Hilton Philadelphia Center City, USA



International Summit on  
**GMP&GCP: USA, Europe, Japan & Asia Pacific**  
December 3-5, 2012  
DoubleTree by Hilton Philadelphia Center City, USA



International Conference on  
**QC, QA and Validation**  
December 3-5, 2012  
DoubleTree by Hilton Philadelphia Center City, USA



International Conference on  
**Obesity & Weight Management**  
December 3-5, 2012  
DoubleTree by Hilton Philadelphia, USA

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