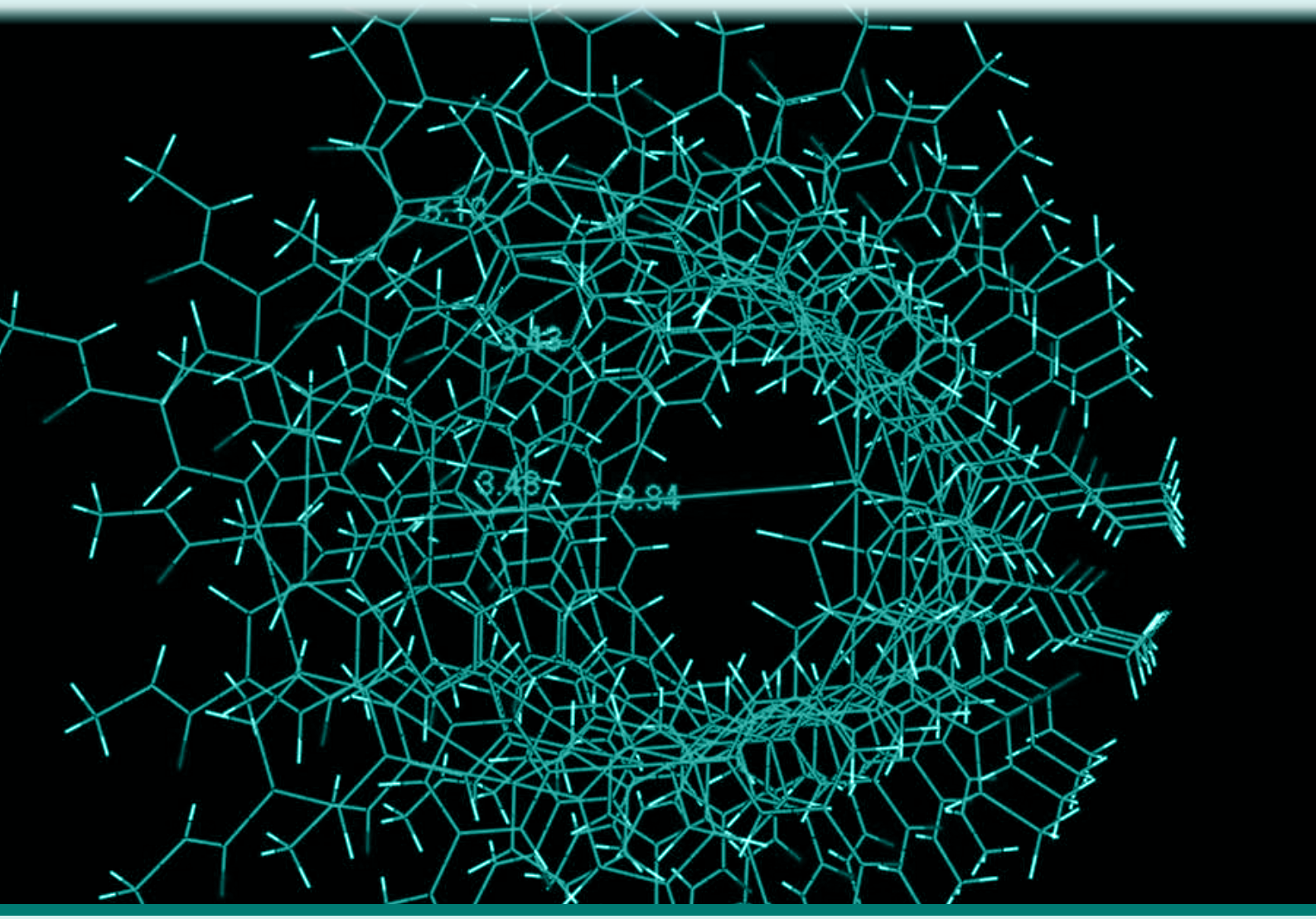
Scientific Program

OMICS Group Conferences
Accelerating Scientific Discovery

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

OMICS Group Conferences
5716 Corsa Ave., Suite 110, Westlake Los Angeles, CA 91362-7354, USA
Phone: +1-650-268-9744, Fax: +1-650-618-1414, Toll free: +1-800-216-6499
Email: cadd2012@omicsgroup.com

18:00-19:00 Registrations

October 28, 2012

Day 1 October 29, 2012

08:00-08:30 Breakfast

09:00-10:00 Registrations

Breakout 1

OMICS Group Conferences
Accelerating Scientific Discovery

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, USA
12:15-12:35	**Title: Specificity of heparin/heparan sulfate binding to proteins** **Umesh R. Desai**, Virginia Commonwealth University, USA
12:35-12:55	**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, Canada
14:15-14:35	**Title: Computer-aided design of inhibitors of DNA methyltransferases** **Jose L. Medina-Franco**, Torrey Pines Institute for Molecular Studies, USA
14:35-14:55	**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, USA
15:30-15:50	**Title: Pharmacophores vs emerging fragments: Implications in the comprehension of polypharmacological and toxicological properties of chemical derivatives** **Ronan Bureau**, University of Caen Basse-Normandie, France
15:50-16:10	**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

Day 2 October 30, 2012

Breakout 1

Track 7: Structural Bioinformatics
Track 8: Sequence Analysis
Track 9: Data Mining & 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** **Matthieu 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** **Norihito 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**

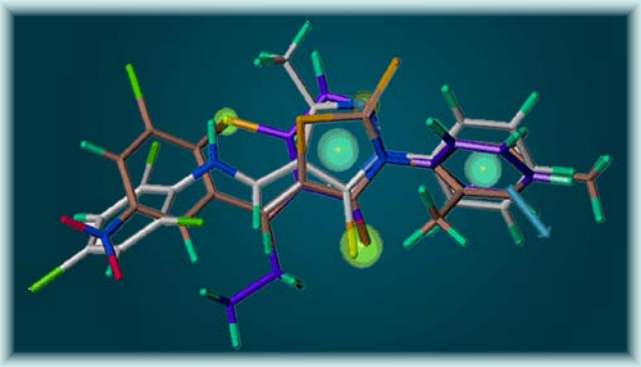
Bookmark your dates

OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference and Exhibition on

In Silico & QSAR

September 4-6, 2013 Orlando-FL, USA



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Europe: 0805-080048

Upcoming OMICS Group Conferences 2012

Accelerating Scientific Discovery



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



2nd 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



3rd 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



2nd 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



2nd 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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