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Scientific Program

5th International Conference on

Medicinal Chemistry & Computer Aided Drug Designing and Drug Delivery

December 05-07, 2016 Phoenix, USA



Day 1 December 05, 2016

07:30-08:30 Registrations

Meeting Room A

conferenceseries.com 09:00-09:25 **Opening Ceremony**

Keynote Forum

09:25-09:40	**Introduction**
09:40-10:10	**Title: Conformational and dynamic considerations in drug design for g-protein coupled receptors** **Victor J Hruby,** University of Arizona, USA
10:10-10:40	**Title: Digging in untapped chemical space: how to combine novelty and synthetic access** **Carsten Detering,** BioSolveIT Inc., USA

Networking and Refreshment Break 10:40-11:10

11:10-11:40	**Title: The use of small molecule proteasome modulation in human diseases** **Jetze J Tepe,** Michigan State University, USA

Sessions: Frontiers in Chemistry | Novel Drug Designing & Drug Delivery | Computer Aided Drug Designing-CADD | Hyphenated Chromatographic Techniques for Drug Analysis

Session Chair: Concepción González-Bello, University of Santiago de Compostela, Spain

Session Co-chair: Thorsten Nowak, C4X Discovery Manchester United Kingdom

Session Introduction

11:40-12:05	**Title: A set of diagnostic bench tests leads to the development of accurate flexible docking algorithms** **Colin McMartin,** ThistleSoft High Meadow, USA
12:05-12:30	**Title: Inhibition of amyloid beta peptide oligomerization: Empirical and ab initio studies** **Arvi Rauk,** University of Calgary, Canada
12:30-12:55	**Title: "Growing" hydrogen bonding waters in molecular complexes!** **Regine Bohacek,** Boston De Novo Design, USA

Panel Discussion @ 12:55-13:00

Lunch Break 13:00-14:00 @ Restaurant

Workshop

14:00-14:30	**Title: Conformational design in medicinal chemistry - An important under-utilised opportunity** **Thorsten Nowak,** C4X Discovery Manchester United Kingdom
14:30-14:55	**Title: Design of novel potent and selective agonists at the melanocortin1 receptor** **Minying Cai,** Arizona Cancer Center, USA
14:55-15:20	**Title: Exploiting unique interactions in the MKK3/6 and ASK1 kinase active sites through computer-aided drug design** **Simone V Bigi,** Takeda California, Inc., USA
15:20-15:45	**Title: Interaction analysis between cell adhesion factor fimh and its inhibitor by fragment molecular orbital method** **Norihito Kawashita,** Osaka University, Japan

Panel Discussion @ 15:45-15:55

Networking and Refreshment Break 15:55-16:10 @ Foyer

Sessions: New Trends in Pharmacology & Drug Development | Analytical & Bioanalytical Techniques | Cancer Studies: Drug Design and Chemistry | Drug Discovery and Drug Delivery: Emerging Diseases

Session Chair: Jetze J Tepe, Michigan State University USA

Session Co-chair: Carsten Detering, BioSolveIT Inc., USA

16:10-16:35	**Title: Computer-aided design, efficient synthesis and mechanistic studies of serine protease covalent inhibitors** **Nicolas Moitessier,** McGill University, Canada
16:35-17:00	**Title: Glycopeptide drugs** **Robin Polt,** The University of Arizona, USA
17:00-17:25	**Title: Molecular dynamics study of autotaxin with potential allosteric inhibitors** **Eko Aditya,** Vrije Universiteit Amsterdam, the Netherlands
17:25-17:50	**Title: Boundary-state light emission quantums in biomolecules** **Babak Daneshfard,** Shiraz University of MedicalSciences, Iran
17:50-18:15	**Title: Dual-function near-infrared (nir) photosensitizer for fluorescence imaging and photodynamic therapy (pdt) of cancer** **Ravindra K Pandey,** Roswell Park Cancer Institute, USA

Panel Discussion

Day 2 December 06, 2016

Meeting Room A

Keynote Forum

10:00-10:30	**Title: *In Silico* analysis of enantioselective binding of imids to cereblon** **Tatsuya Takagi,** Osaka University, Japan
10:30-11:00	**Title: Fitted, an evolving docking programs addressing unmet medicinal chemistry needs** **Nicolas Moitessier,** McGill University, Canada

Networking & Refreshment Break 11:00-11:20

11:20-11:50	**Title: Indeno[1,2-B]indoles: A good scaffold for designing bioactive molecules** **Marc Le Borgne,** University Lyon 1, France
11:50-12:20	**Title: Innovative and strategic materials for medical technology against tumors: preclinical researches on sugar dendritic GD-DTPA complex MRI contrast agents and IER5/CDC25B targeted novel phospha sugar antitumor agents** **Mitsuji Yamashita,** Shizuoka University, Japan

Sessions: ChemBioChem-Antimicrobials and Infectious Agents & Diseases | Neurodegenerative Diseases | Chem-Virology (Zika Virus) | Hematology/Oncology and Stem Cell Therapy | Stereoisomerism & SAR (Structure Activity Relationship) | Chemical Biology | Toxicology and Environmental Chemistry | Clinical Pharmacy Practice

Session Chair: Victor J Hruby, University of Arizona USA

Session Co-chair: Mitsuji Yamashita, Shizuoka University, Japan

12:20-12:45	**Title: Targeting the motion of shikimate kinase-opportunities for antibiotic drug development** **Concepción González-Bello,** University of Santiago de Compostela, Spain
12:45-13:10	**Title: Ligand conformational analysis enabling improved nrf2 activators** **Thorsten Nowak,** C4X Discovery Manchester, United Kingdom

Lunch Break 13:10-14:10

Workshop

14:10-14:40	**Title: A tale of a low molecular weight inhibitor for bruton's tyrosine kinase, modeled in seesar, the world's best compound ideation software for medicinal chemists** **Carsten Detering,** BioSolveIT Inc., USA

14:40-15:05	**Title: Identification of Inhibitors for the Lutheran – Laminin Interaction by molecular modeling techniques to reduce the vaso-occlusive crises of sickle cell disease** **Fabrice Gardebien,** Université de la Réunion, France
15:05-15:30	**Title: Differential binding force: A new physicochemical parameter for drug design** **Shoujun Xu,** University of Houston, USA
15:30-15:55	**Title: Synthesis of novel agents-effective on leukemia and colon cancer cell lines** **Ilknur Babahan,** Adnan Menderes University, Turkey
15:55-16:20	**Title: A Comparative analysis of aspirin from various analgesic formulations using titrimetry, spectroscopic and hyphenated chromatographic techniques** **Ochieng Anthony,** Sumait University, Tanzania
16:20-16:45	**Title: First-in-class MCRs coupled with cascade reactions for the generation of molecular complexity** **Christopher Hulme,** The University of Arizona, USA

Networking & Refreshment Break 16:45-17:00

Poster Presntations @ 17:00-18:00

CADD 101	**Title: Optimization of the indole–pyrimidine–chrysin hybrid as the lead molecule for anti-inflammtory drugs** **Jagroop Kaur,** Guru Nanak Dev University, India
CADD 102	**Title: Rational design, synthesis and working of a tri-ligating receptor: Removal of cyanide from cytochrome c oxidase** **Sukhmeet Kaur,** Guru Nanak Dev University, India
CADD 103	**Title: Design, synthesis and biological evaluation of novel 2-phenyl-1-benzopyran-4 one derivatives as potential poly-functional anti-alzheimer's agents** **Majinder Singh,** Punjabi University, India

Panel Discussion

Day 3 December 07, 2016

Meeting Room A

Sessions: Nursing in Chemistry | Nanomedicine & Fullerene Chemistry | Chem-Toxicology, Chem-Pharmacology, Chem-Microbiology, Chem-Genomics | Pharmaceutical Industry Overview

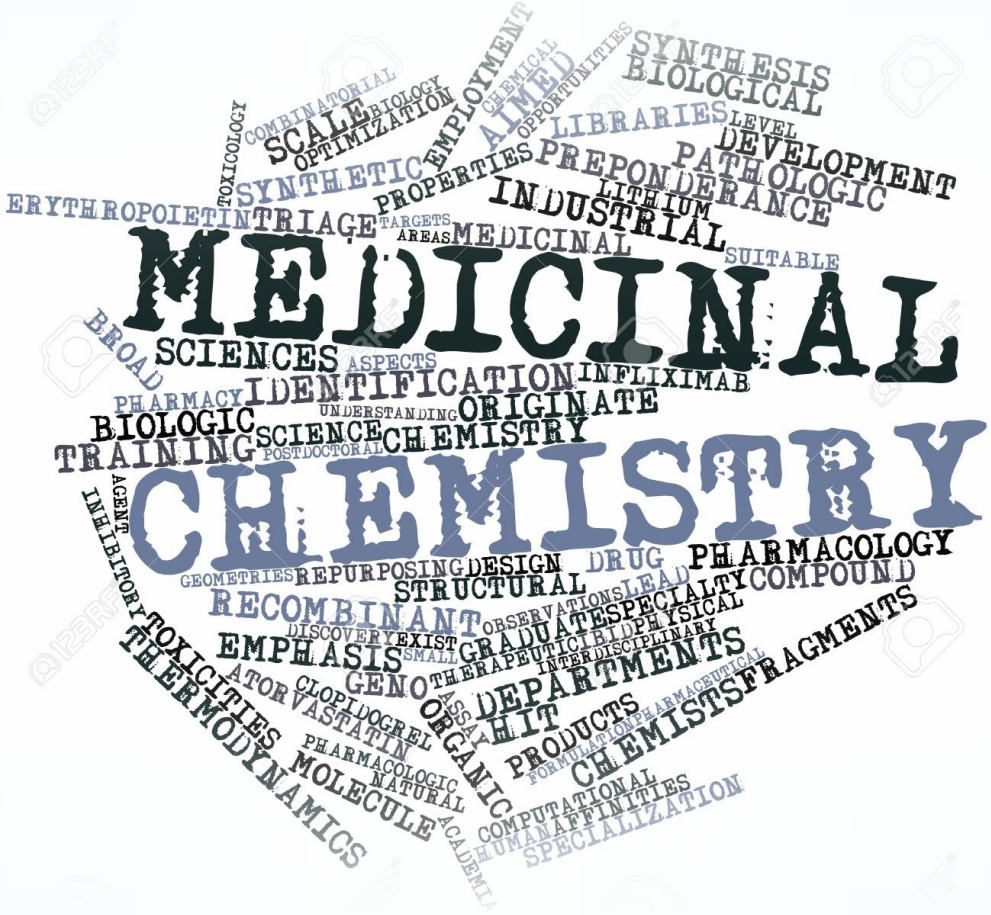
Session Chair:
Marc Le Borgne, University Lyon 1, France
Ilknur Babahan, Adnan Menderes University, Turkey
Session Co-chair:
Norihito Kawashita, Osaka University, Japan
Ochieng Anthony, Sumait University, Tanzania

10:00-10:30	**Title: Combined 2D- / 3D-QSAR, molecular docking, accelerated molecular dynamics simulation and QM/Mm calculation studies on pepstatin-a analogues as cathepsin-d inhibitors** **Olayide A. Arodola,** University of KwaZulu-Natal, South Africa
10:30-11:00	**Title: Reactive metabolites prediction: What can molecular orbitals tell us?** **Anna Tomberg,** McGill University, Canada

Networking & Refreshment Break 11:00-11:20

11:20-11:50	**Title: Virtual flow: A flexible workflow system for virtual screening procedures on high-performance computers** **Christoph Gorgulla,** Max Planck Institute for Molecular Genetics, Germany
11:50-12:20	**Title: Evaluating small molecules' potential energy through the long standing chemical principles** **Zhaomin Liu,** McGill University, Canada
12:20-12:50	**Title: Current topics in computer-aided drug design technologies: Future aspects** **Reham F. Barghash, National Research Center, Egypt**

12:50-13:20	**Title: "SMART" drug based targeted delivery: A new paradigm for nanomedicine strategies** **Sugapriya Dhanasekaran,** Prince Sattam Bin Abdullaziz University, KSA
	Lunch Break 13:20-14:20
14:20-14:50	**Title: The interaction of metals with alpha-synuclein** **Heather R Lucas,** Virginia Commonwealth University, USA
14:50-15:20	**Title: Synthesis of novel anthraquinone anti-cancer drugs: molecular structure, molecular chemical reactivity descriptors and their interactions with DNA** **Tarek M. EL Gogary,** Jazan University, KSA
15:20-15:45	**Title: Addressing new targets and cytoprotective compounds against neurodegenerative diseases** **Bruno Andrade,** Universidade Estadual do Sudoeste da Bahia, Brazil
	Award & Closing Ceremony



Bookmark your dates

6th International Conference on

Medicinal Chemistry & Computer Aided Drug Designing and Drug Delivery

November 06-08, 2017 San Antonio, USA

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