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Pharmaceutical Chemistry

October 02-04, 2017 | Barcelona, Spain

Theme: ***Recent Trends and Advancements in the fields of Pharma and Chemistry***

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Pharmaceutical Chemistry 2017 at Barcelona, Spain

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- Pharmaceutica Analytica Acta

Glimpses of Pharmaceutical Chemistry 2016








About us

Supporting Journals

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Glimpses of Pharmaceutical Chemistry 2016















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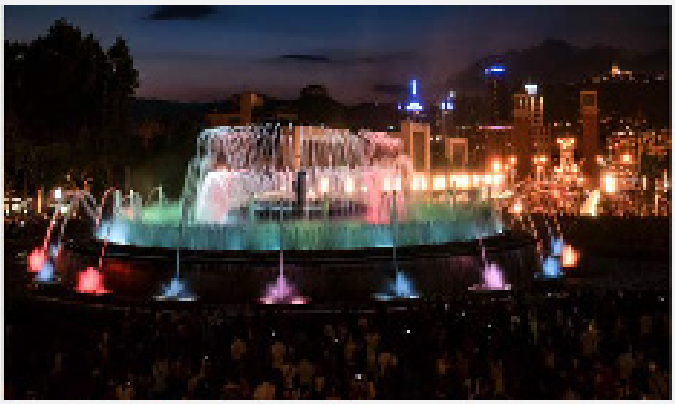
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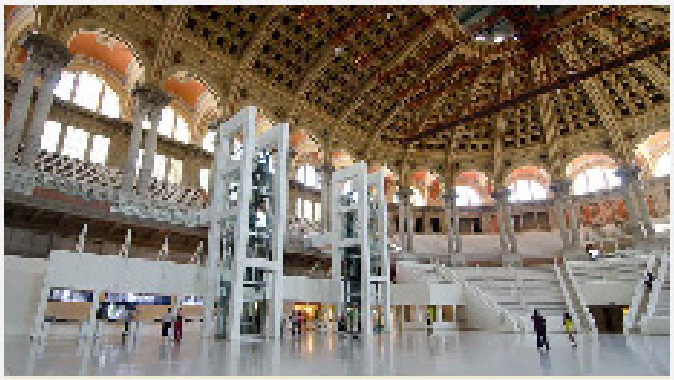
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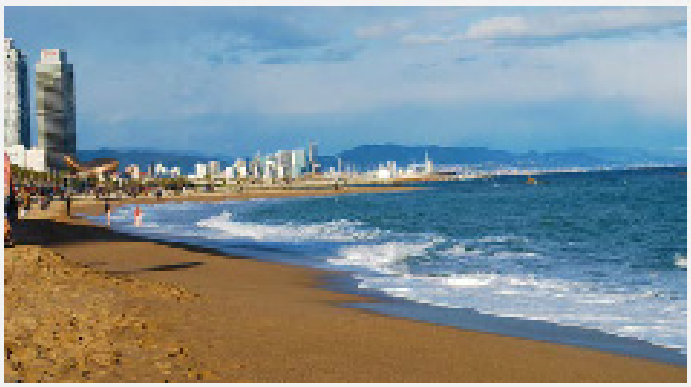
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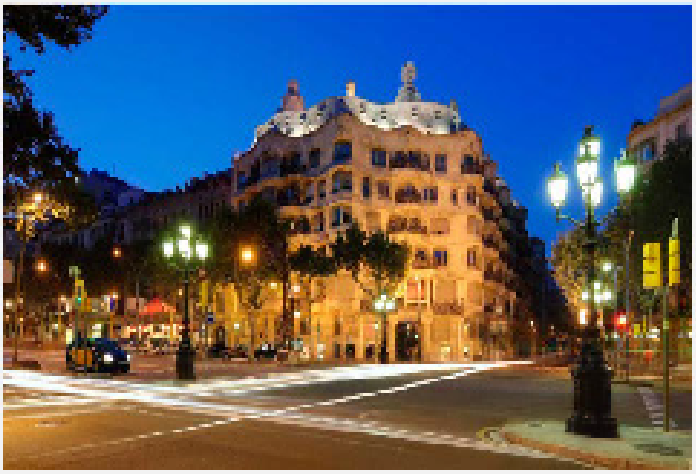
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Important Dates

Abstract Submission Opens: October 02, 2017

Registration Opens: October 15, 2016

Early Bird Registration: April 15, 2017

Mid Registration: May 31, 2017

On Spot Registration: October 02, 2017

Venue

Barcelona, Spain

Contact:

Diana Brigetha | Program Manager | Pharmaceutical Chemistry 2017

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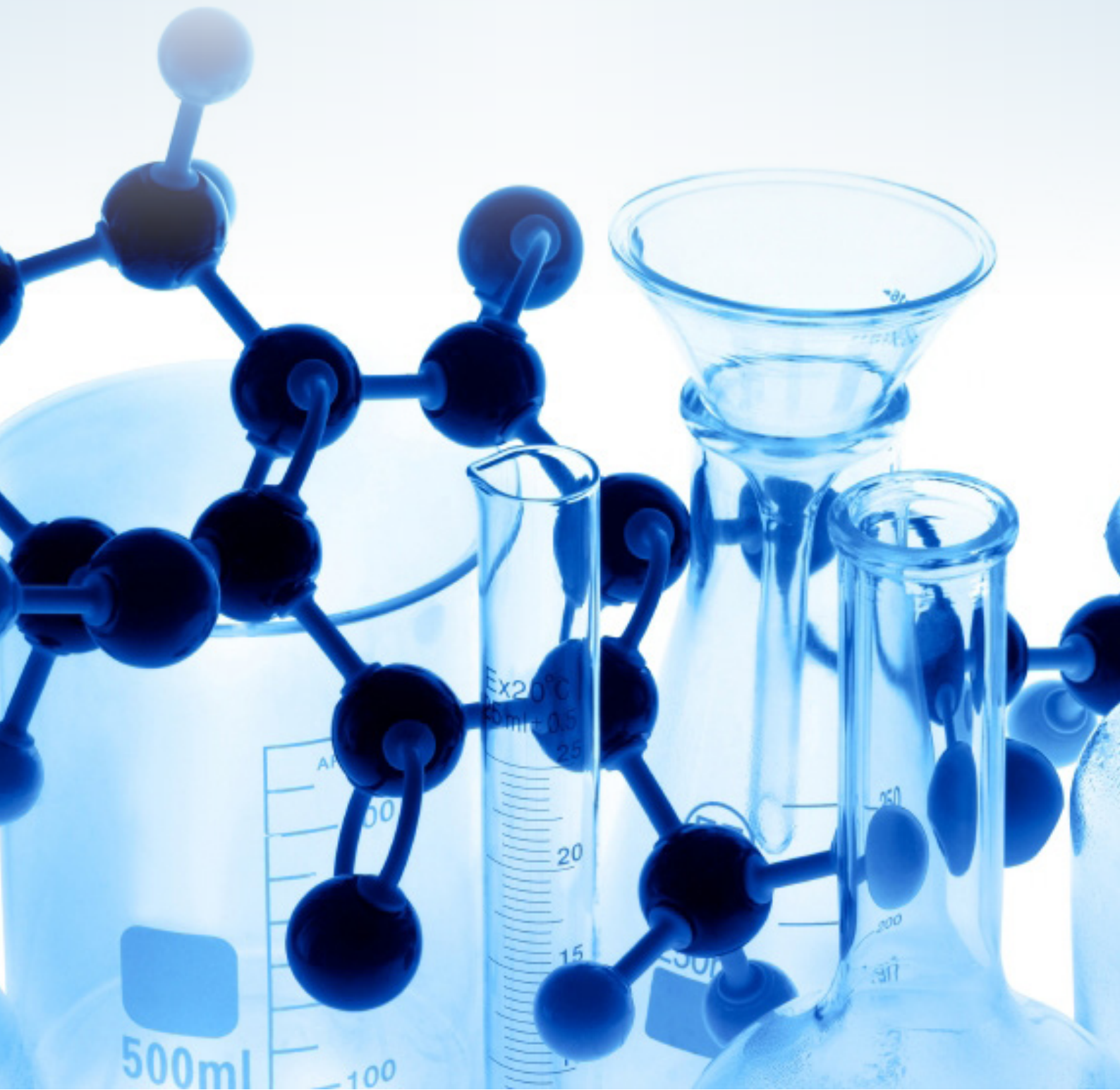
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International Conference on

Pharmaceutical Chemistry

September 05-07, 2016 Frankfurt, Germany

Scientific Program



Opening Ceremony

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Title: The enterprise of drug discovery from an academic perspective: from concept to practice
Stephen Hanessian, University of California, USA

Title: A new synthetic methodology for pharmaceutical chemistry
Valery Charushin, Ural Federal University, Russia

Title: Discovery of novel tubulin inhibitors and their synergy with BRAF inhibitors for malignant melanoma
Wei Li, University of Tennessee Health Science Center, USA

Title: Different targeting possibilities using nanoparticles
Sylvia Wagner, Fraunhofer Institute for Biomedical Engineering, Germany

Title: Photodynamic therapy and imaging based on tumor-targeted nanoprobe, pHPMA-conjugated zinc protoporphyrin, and its augmentation
Jun Fang, Sojo University, Japan

Title: Preparation of nanocrystal formulation to improve oral absorption of mebendazole
Naofumi Hashimoto, Setsunan University, Japan

Title: Perspectives of antifungal drug discovery
Josef Jampilek, Comenius University, Slovakia

Title: Effect of Octyl Salicylate with respect to the physical appearance of mono/di capric and caprylic fatty acids Formulations
Siti Salwa Abd Gani , Universiti Putra Malays, Malaysia

Title: Synthesis of new Indan-1-one-piperazine derivatives as anticholinesterase agents
Yusuf Özkay, Anadolu University, Turkey

Title: New approaches for tyrosinase inhibitors: mannich bases of kojic acid derivatives
Mutlu Dilsiz Aytemi, Hacettepe University, Turkey

Title: From simple chemical building blocks to biological active molecules
Raffaella Mancuso, University of Calabria, Italy

Title: Development of xanthines as adenosine A2A receptor selective antagonists: a systematic approach towards novel nondopaminergic therapy for Parkinson's disease
Ranju Bansal, Panjab University, India

Title: Enzyme-catalyzed reactions
Devrim ÖZDEMIRHAN, Abant Izzet Baysal University, Turkey

Title: New asymmetric organocatalytic methods towards the synthesis of molecules of biological interest
Alexander Cobb, University of Reading, UK

Title: Enantioselective, short and efficient approaches to the synthesis of drugs and biologically active compounds
Satyendra Kumar Pandey, Thapar University, India

Title: Synthesis and biological activities of 2-chloronicotinaldehyde based novel functionalized heterocyclic compounds
Bhimapaka China Raju, CSIR-Indian Institute of Chemical Technology, India

Title: Discovery of small molecule dna g-quadruplex stabilizing agents: design, synthesis and biological studies
Mrinalkanti Kundu, TCG Lifesciences Pvt. Ltd., INDIA

Title: Development of thienopyrimidines as potential pharmaceuticals

Chunduri Venkata Rao, Sri Venkateswara University, India

Title: Synthesis and biological evaluation of new carbaisoflavonoids with Anti-HCV activity

Paulo Roberto Ribeiro Costa, Universidade Federal do Rio de Janeiro, Brazil

Title: Discovery of novel 2-thio-imidazole derivatives as potent and orally efficacious TGR5 receptor agonists

Sameer Agarwal, Zydus Research Centre, Cadila Healthcare Ltd., India

Title: Design, synthesis and pharmacological evaluation of some novel de-rivatives of 1-{[3-(furan-2-yl)-5-phenyl-4,5-dihydro-1,2-oxazol-4-yl]methyl}-4-methyl piperazine

Gita Chawla, Hamdard University, India

Title: Development of piperazine derivatives as potential cognition enhancers

Poonam Piplani, Panjab University, India

Title: Synthesis of oxygen and nitrogen heterocycles with potential pharmaceutical properties

Asunción Barbero, University of Valladolid, Spain

Title: Synthesis docking studies and biological evaluation of some novel 1,2,4-triazolo[3,4-b] [1,3,4]thiadiazole tagged thieno[2,3-d]pyrimidine derivatives

Settypalli Triloknadh, Sri Venkateswara University, India

Title: One pot condensation reaction of heterocyclic amine, 1, 3– diketone and an aldehydes using in situ generated superoxide ion: a rapid synthesis of structurally diverse drug- like complex heterocycles

Sundaram Singh, Department of chemistry IIT(BHU), India

Title: Application of small-ring azaheterocyclic building blocks for the synthesis of pharmaceutically relevant nitrogen compounds

Matthias D'hooghe, Ghent University, Belgium

Title: BioMOFs – Exploring nalidixic acid metal organic networks envisaging pharmaceutical applications

Vânia André, Universidade de Lisboa, Portugal

Title: Sustainable synthesis via the integration of membranes in chemical reactions

Dominic Ormerod , Flemish Institute for Technological Research (VITO NV), Belgium

Video Presentation by Donna J. Nelson, President of American Chemical Society, USA

Title: Synthesis, molecular docking study and in vitro biological activity of carbohydrate-based peptidomimetics targeting neuropilin-1

Nadia Pellegrini-Moïse, Université de Lorraine, France

Title: [18F]Fluoro-C-glycosides to radiolabel peptides for PET imaging

Sandrine Lamandé-Langle, Université de Lorraine, France

Title: In vivo and in vitro anti-inflammatory activities of two chromones isolated from Dictyoloma vandellianum

Luíza C. F. Opretzka, Federal University of Bahia, Brazil

Title: Dynamic kinetic asymmetric transformations with hard nucleophiles: Cyclopentenes for anti tuberculosis and antibiotics

Hadia Almahli, University of Oxford, UK

Title: Synthesis and biological evaluation of novel pyrrolo[2,3-d]pyrimidine derivatives as breast anti cancer

Khalid Hilmy, Monufyia University, Egypt

Title: The role of circulating serum resistin, serum amyloid A and C-reactive protein as potential risk factors for development of type 2 diabetes mellitus

Esmat Bauomi Ali Shahin, Al-Azhar University, Egypt

Title: Water Soluble Platinum(II) Complexes: GLUT mediated cytotoxic properties and selective tumor targeting

Ran Liu, Tianjin University, P. R. China

Title: Synthesis of novel disubstituted oxadiazole derivatives and antimicrobial activity

Serkan Levent, Anadolu University, Turkey

Title: Synthesis Of new donepezil analogues and evaluation of their cholinesterase inhibitory activity

Begüm Nurpelin Saglık, Anadolu University, Turkey

Title: New Benzimidazole-Hydrazones as MAO Inhibitors

Ozgur Devrim Can, Anadolu University, Turkey

Title: Structure, intermolecular and photoinduced intramolecular hydrogen bonding in 2-azolylmethylidene cycloalkanones

Mark Sigalov, Ben-Gurion University of the Negev, Israel

Title: Synthesis and anticonvulsant activities of Novel 1-Phenyl/1-(4-chlorophenyl)-2-(1H-triazole-1-yl)ethyl ester derivative compounds

Irem Bozbey, Inonu University, Turkey

Title: Synthesis of some new benzalhydrazone derivatives and evulation of their AChE inhibitory activity *in vitro*

Ömer Faruk ÇÖL, Gazi University, Turkey

Title: Structure-antibacterial activity relationships of N-substituted-(D/L-alaninyl) 1H-1,2,3-triazolyl oxazolidinones

Oludotun A. Phillips, Kuwait University, Kuwait

Title: Synthesis and anticholinesterase effects of new 2-substituted benzothiazole derivatives

Ümide Demir Özkay , Anadolu University, Turkey

Title: Anticarcinogenic effect of coadministration of α-β unsaturated compounds and quercetin

Gabriela Carrasco Torres , CINVESTAV, México

Title: Activity of some phenoxyalkyl- and phenoxyethoxyethylamine derivatives on the central nervous system

Anna M Waszkielewicz, Jagiellonian University Medical College, Poland

Title: Design, synthesis, and validation of an in vitro platform peptide -whole cell screening assay using MTT reagent

Sahar Ahmed, Assiut University, Egypt

Title: Application of in situ FTIR for the preparation of 17-α-estradiol via Mitsunobu reaction

Flavio S P Cardoso, Libbs Pharmaceuticals, Brazil

Title: A novel stability-indicating LC method for determination of avanafil

Nafiz Oncu Can, Anadolu University, Turkey

Title: The antimutagenic activity of selected medicinal plants from Jordan

Karem Alzoubi, Jordan University of Science & Technology, Jordan

Title: Drug chimerism as a fusion of two anticancer chemotherapeutics into one entity: Discovery of potent molecular chimera CM358 for treatment of metastatic melanoma

Gary Gellerman, Ariel University, Israel

Title: Phytochemical constituents from garcinia atroviridis

Wen-Nee Tan, Universiti Sains Malaysia, Malaysia

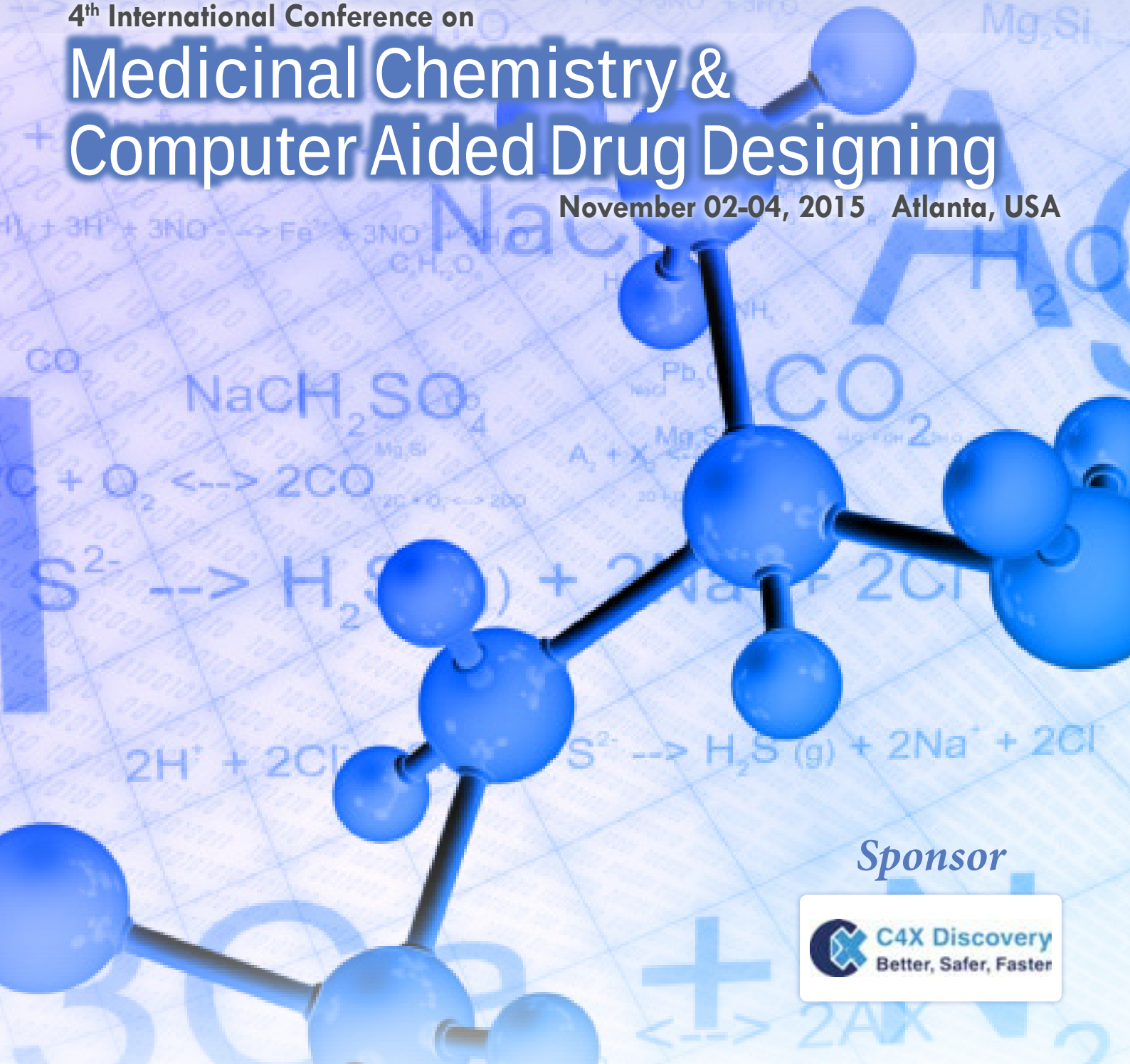
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Opening Ceremony

Introduction

Concepción González-Bello
University of Santiago de Compostela, Spain

Carsten Detering
BioSolveIT Inc., USA

Title: Novel Multiple Type and Wide Spectral Molecular Targeted Antitumor Agents: Preparation and Preclinical Evaluation of IER5/Cdc25B Targeted Phospha Sugar Derivatives as Well as Attempts of Computer Aided Drug Designing.

Mitsuji Yamashita, Shizuoka University, Japan

Title: In silico design, synthesis and biological evaluation of inhibitors of hypoxia-inducible factor (HIF-1) as antitumor agents

María Laura Lavaggi, University of the Republic, Uruguay

Title: Design of Novel, Selective and Bioavailable Ligands for Closely Related Receptors and Pharmacophores: Conformational and Topographical Considerations.

Victor J. Hruby, University of Arizona USA

"Title: Accelerated and Reliable Lead Discovery: Structure guided drug discovery ideal for collaborative projects"

Kal Ramnarayan, Sapient Discovery, LLC, USA

Title: Title: Investigating the molecular interactions between novel synthetic retinoids and the ligand-binding domains of retinoic acid receptors

Hesham Haffez, Durham University Durham

Title: How close are we to predicting binding affinity?

Carsten Detering, BioSolveIT Inc., USA

Title: Ligand-based Screening for anti-Dengue Virus Inhibitor

Tatsuya Takagi, Osaka University, Japan

Title: Nanoparticles with novel methodology to treat infectious diseases

Prabagaran Narayanasamy, University of Nebraska Medical Center, USA

Title: Exploring for bioactive secondary metabolites from the Chinese medicinal mangroves

Yue-Wei Guo, Chinese Academy of Sciences, P R China

Title: Identification of sirtuin inhibitorsas promising anticancer agents: from screening to activity assays

Alessandra Nurisso, University of Geneva, Switzerland

Title: Development of new antibiotics targeting shikimate kinase: From concept to practice

Concepción González-Bello, Universidad de Santiago de Compostela, Spain

Title: Amylin as a Novel Contributor to Alzheimer's Disease and Natural Product Inhibitory Discovery

Bin Xu, Virginia Tech, USA

Title: Discovery of Novel Orexin-1 Selective Antagonists using NMR Guided Conformational Design

Thorsten Nowak, C4X Discovery, United Kingdom

Title: 2,3-dihydro-1H-isoindoline derivatives as novel drugs for Parkinson's disease: in silico and an in vivo evaluation

Erik Andrade Jorge, Escuela Superior de Medicina, Mexico

Title: Computer-aided drug design (CADD): Synthesis and biological evaluation of potential caspase-3 inhibitors as novel Alzheimer's disease therapy

Lucía Minini, Universidad de la República, Uruguay

Title: Synthesis and biological evaluation of novel 16-dehydropregnenolone acetate derivatives having an ester function at C-3 and triazole ring at C-21 on the 5α-reductase isoenzymes and on cancer cells lines

Aylin Viviana Silva Ortiz, Universidad Nacional Autónoma de México, Mexico

Title: Chemogenomic approaches to drug design: Docking-based virtual screening of nematode G-protein coupled receptors for potential anthelmintic agents

Rabmas Masuka, University of Cape Town, South Africa

Title: New human malaria parasite Plasmodium falciparum dihydroorotate dehydrogenase inhibitors by pharmacophore and structure-based virtual screening

Elumalai Pavadai, University of Cape Town, South Africa

Title: Poster Presentation by Alessandra Nurisso

Alessandra Nurisso, University of Geneva, Switzerland

Title: Neuroprotective compounds from Reynoutria sachalinensis

Jin Bae Weon, Kangwon National University, Korea (1)

Title: Neuroprotective compounds from embryo of Nelumbo nucifera seed

Jin Bae Weon, Kangwon National University, Korea (2)

Title: Prodrug design and synthesis of oxyresveratrol to improve bioavailability

Yen Fang Wen, Industrial Technology Research Institute, Taiwan

Title: Computational studies of dipeptidyl peptidase IV inhibitors

Dhruti Mahendrabhai Patel, Dharmsinh Desai University, India

Title: Structure based pharmacophore generation and its applications for identification of dipeptidyl peptidase –IV (DPP-IV) inhibitor

Khushbu Anilbhai Patel, Dharmsinh Desai University, India

Title: Oral health quality of life in children with cerebral palsy: Parental perception

Eman Anwer El Ashiry, King Abdulaziz University, Saudi Arabia

Title: Evaluation of internal adaptation of some adhesive dental resorative materials using microcomputed tomography (Micro-CT): In vitro randomized blind clinical study

Najlaa Alamoudi, King Abdulaziz University, Saudi Arabia

Title: Progesterone receptor (PGR) gene polymorphism is associated with susceptibility to preterm birth

Immaculate, University of Malaya, Malaysia

"Title: Antibacterial efficacy of an Unexplored species of Gentianaceae- Exacum pedunculatum on Escherichia coli by a Substantial Computational"

Lakshmi Huttada, Karnatak University, India

Title: Novel azetidinone derivatives as antimicrobial agents

Manal Naser Kadum Hamem, Rajiv Gandhi Univesity Of Health Science, India

Title: Synthesis, characterization and evaluation of arylamines in a murine model of obesity

Christian F. Hernández Martínez, Instituto Politécnico Nacional, Mexico

Title: 2,3-dihydro-1H-isoindoline derivatives as novel drugs for Parkinson's disease: In silico and an invivo evaluation

Erik Andrade Jorge, Instituto Politécnico Nacional, Mexico (1)

Title: Poster Presentation by Erik Andrade Jorge

Erik Andrade Jorge, Instituto Politécnico Nacional, Mexico (2)

Title: Molecular docking and in vitro assay of isoindolina-1,3-dione amine derivative as novel HDAC8 inhibitor for cancer treatment

Garcia Gamez Jesus, Escuela Superior de Medicina del Instituto Politécnico Nacional, Mexico

Title: Screening for inhibitor of recombinant Drosophila melanogaster tyramine-β-hydroxylase

Md. Nazmul Hasan, Kyushu University, Japan

Title: Rosmarinic acid potently inhibits amylin-induced neurotoxicity and amyloid formation

Paul Velander, Virginia Tech, USA

Title: Irisin as a performed monomer for adipocyte browning

Lu Zhai, Virginia Tech, USA

Title: The mode of action of new promising anticancer agents: Multifunctional polymer-ruthenium conjugates

Andreia Valente, Universidade de Lisboa, Portugal

Title: Epi-drug development targeting human G9a H3K9 methyltransferase

Yong-Hwan Lee, Louisiana State University, USA

Title: Nitrones as potential therapeutic agents against Alzheimer's Disease.

Alicia Merlino, Theoretical and Computational Chemistry Group, Uruguay

Title: Small-molecule modulators of thiamine transport in pathogenic bacteria.

Anna Hirsch, Stratingh Institute for Chemistry University of Groningen The Netherlands

Title: Synthesis, Structural Anticancer Activity Relationship, and Docking Study of Novel 5-Deazaflavin Analogs

Hamed I Ali, Irma Lerma Rangel College of Pharmacy, USA

Title: PubChem BioAssay: A public information resource supporting medicinal chemistry and drug discovery research.

Yanli Wang, National Institutes of Health, USA

Title: Ruthenium drugs for cancer therapy: Small structural changes, different in vivo performances.

Maria Helena Garcia, Faculdade de Ciências da Universidade de Lisboa Universidade de Lisboa Portugal

Title: Development of selective mechanism-based inhibitors for human Semicarbazide-Sensitive Amine Oxidase (SSAO)

Jonathan S. Foot, Pharmaxis Ltd., Australia

Title: Targeting the genome of high-risk HPVs with large hairpin polyamides: Promising novel antiviral agents

Carlos H Castaneda, University of Missouri-St. Louis, USA

Title: A combined in-vitro and in-silico studies of macrocyclic complexes of Tin(II) with potent anti-cancer, anti-inflammatory and anti-microbial properties

Ekta Rawat, Kurukshetra University, India

Title: Development of a novel class of hyper-multi-targeted computer-aided CREKA/YIGSR

Ioannis Grigoriadis, Biogenea Pharmaceuticals Ltd, Greece

Title: The prevalence of extra root canals of maxillary first permanent molars among population in Jeddah, Saudi Arabia using Micro-Computed Tomography (Micro-CT)

Najat Farsi, King Abdulaziz University, KSA

Title: TAAR1 ligands as prospective neuroleptics: From D-neuron research

Keiko Ikemoto, Iwaki Kyoritsu General Hospital, Japan

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Registrations

Opening Ceremony

Introduction

Concepción González-Bello
University of Santiago de Compostela, Spain

Patrick Y S Lam
Drexel University, USA

Thorsten Nowak
C4X Discovery Holdings PLC., UK

Title: 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
Title: *In silico* screening for anti-HPV agents using pharmacophore models
Tatsuya Takagi, Osaka University, Japan
Title: NMR driven conformational design - A powerful drug design tool
Thorsten Nowak, C4X Discovery Holdings PLC., UK
Title: Computer aided design and optimization of kinase and phosphatase inhibitors
Kal Ramnarayan, Sapient Discovery, LLC., USA
Title: The use of epitopes against schistossomiasis: The role of molecular modelling
Moacyr Comar Junior, Federal University of São João del Rei, Brazil
Title: 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
Title: Structure-based design of covalent inhibitors or protein-protein interactions
Maurizio Pellecchia, Sanford-Burnham Institute for Medical Research, USA
Title: Revisiting INH: QSAR-based design of new anti-tubercular compounds
Filomena Martins, Universidade de Lisboa, Portugal
Title: *In vitro* COX inhibitory activity of novel α-aminoarylpropionic acid derivatives
A G Zhamharyan, Yerevan State Medical University, Armenia
Title: New developments in docking and scoring
Istvan J Enyedy, Biogen Idec, USA
Title: 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
Title: Peptide-displaying phage technology in breast cancer diagnosis
Thaise Gonçalves Araújo, Federal University of Uberlandia, Brazil
Title: Discovery of small molecule blockers of protein-protein interactions using DNA-encoded small-molecule libraries
Nils Hansen, VipergenApS, Denmark
Title: Neuroprotective properties of compound isolated from *Dianthus superbus L.*
Choong Je Ma, Kangwon National University, Korea
Title: Investigation of human CA1-induced toxicity in the *Drosophila* model of motor neuron degeneration
Jian Liu, Xi'an Jiaotong-Liverpool Univeristy, China
Title: Applications of Proteochemometrics - From Species Extrapolation to Cell Line Sensitivity Modelling
Isidro Cortes-Ciriano, Bioinformatique Structurale Institut Pasteur, France
Title: Data and Compute Intensive eScience Approaches in Computational Medicinal Chemistry
Scott James Lusher, Netherlands eScience Center, Netherlands
Title: Synthesis, Biological Evaluation and 3d Qsar of some Novel Benzimidazole Derivatives as Anti Microbial Compounds
Sonal Dubey, Krupanidhi College of Pharmacy, India
Title: 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
Title: Strategies to optimize and use bacterial cytochromes p450 for drug discovery & development
Nico P E Vermeulen, VU University Amsterdam, Netherlands
Title: New agonists of the CB_2 cannabinoid receptor: Discovery of a new class of analgesic compounds
Pier Giovanni Baraldi, Università di Ferrara, Italy
Title: Polar drugs
Andrew B McElroy, Eligochem Ltd., UK
Title: Drug discovery against category A-C pathogens through MEP pathway
Prabagaran Narayanasamy, University of Nebraska Medical Center, USA
Title: Discovery of novel lead compounds by large scale diverse encoded chemical libraries
Jin Li, HitGen Ltd., China
Title: *In silico* approach to predict ADME-Tox properties of small organic molecules: Challenges and opportunities for drug discovery

Maria Miteva, University Paris Diderot, France
Title: *In vivo* delivery of transcription factors with chemically modified oligonucleotides
Niren Murthy, University of California, USA
Title: 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
Title: The σ_1 receptor as target for novel drugs
Bernhard Wünsch, Westfalian Wilhelms-University of Münster, Germany
Title: 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
Title: Design and development of small peptidomimetics of RXFP1 for the treatment of acute heart failure
Akhter Hossain, University of Melbourne, Australia
Title: 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
Title: Novel chemistry-based tools to study epigenetic enzymes in inflammation
Frank J Dekker, Pharmaceutical Gene Modulation, The Netherlands
Title: 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
Title: Structure guided design and synthesis of SAR107375A, aselective and potent dual thrombinand factor Xa inhibitor
Jerome Meneyrol, Sanofi-Aventis R&D, France
Title: 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
Title: Tracking anti-tumor drugs: Ruthenium(II)-cyclopentadienylcomplexes as promising agents
M Helena Garcia, Universidade de Lisboa, Portugal
Title: TAAR1 ligands as prospective neuroleptics: From D-neuron study
Keiko Ikemoto, Iwaki Kyoritsu General Hospital, Japan
Title: Small-molecule modulators of thiamine transport in pathogenic bacteria
Anna K H Hirsch, University of Groningen, The Netherlands
Title: The behavior of detergents around membrane proteins is more complex than supposed, as revealed by a new method of quantitation
Pierre Falson, IBCP, France
Title: Design of multivalent ligand for the detection and treatment of disease
Victor J Hruby, University of Arizona, USA
Title: Polymer 'ruthenium-cyclopentadienyl' conjugates: A new approach to fight cancer
Andreia Valente, Universidade de Lisboa, Portugal
Title: Design of mechanistically distinct proteasome inhibitors for the treatment of multiple myeloma
Jetze J Tepe, Michigan State University, USA
Title: Molecular characterization and design of a key new hormone, irisin
Bin Xu, Virginia Tech, USA
Title: Structure-based discovery of new modulators targeting nuclear X receptor alpha for cancer therapy
Ying Su, Sanford-Burnham Medical Research Institute, USA
Title: Privileged heterocycles by palladium-catalyzed aerobic oxidative isocyanide insertion
Romano V A Orru, VU University Amsterdam, Netherlands
Title: Visual binding: A radically new concept to support the medicinal chemist's quest for innovative NMEs
Carsten Detering, BioSolve IT Inc., USA
Title: 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
Title: Multi-target approach to anti-inflammatory drugs - *in silico* and medicinal chemistry
Eugen Proschak, Goethe-University of Frankfurt, Germany
Title: Identification and optimization of tertiary sulfonamides as RORc inverse agonists
Benjamin P Fauber, Genentech, Inc., USA
Title: Massive changes to the biophysical properties of DNA upon binding antiviral polyamides
Gaofei He, University of Missouri-St. Louis, USA
Title: The communion of medicinal chemistry and nanotechnology in anticancer therapeutics
Debatosh Majumdar, Glycosyn LLC., USA
Title: Evaluation of *Satureja hortensis* leaves essential oil pharmacological activities
A P Manjikyan, Yerevan State Medical University, Armenia
Title: Phytochemicals and antioxidant capacities from *Dacryodes rostrata* fruits
Prasad K N, Monash University Malaysia, Malaysia
Title: Selection and characterization of RNA aptamers targeting the genomic 5'-UTR in the dengue virus
Adriana Freitas Neves, Universidade Federal de Goiás, Brazil
Title: SurR9C84A exhibits cardioprotective effects against melphalan induced cardiotoxicityin primary human cardiomyocytes
Ajay Ashok, Deakin University School of Medicine, Australia

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Day 1 October 15, 2013

Registrations

Opening Ceremony

Introduction

James K. Bashkin
University of Missouri-St. Louis, USA

Brian S. J. Blagg
The University of Kansas, USA

Xiang-Qun (Sean) Xie
University of Pittsburgh, USA

Tulay Aygan Atesin
The University of Texas-Pan American, USA

Title: Design and investigation of multivalent ligands for the detection and treatment of diseases
Victor J Hruby, University of Arizona, USA

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

Title: 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

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

Title: 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

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

Title: 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

Title: Computer-aided design of glucokinase activators
Meihua Tu, Pfizer, USA

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

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

Title: 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

Title: 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

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

Title: 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

Title: Newer approaches to the discovery of glitazones
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India

Title: New approaches to "Hit" optimization
Istvan J. Enyedy, Biogen Idec, USA

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

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

Title: 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

Title: Forecaster: A computational tool for drug design and discovery developed by experimentalists for experimentalists
Nicolas Moitessier, McGill University, Canada

Title: 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

Title: Discovery of highly-potent and selective inhibitors for the ABCG2 transporter
Achene Boumedjel, Université Joseph Fourier de Grenoble, France

Title: Predictive application of bioisostere transformations to identify novel high quality compound ideas
Matthew Segall, Optibrium Ltd., UK

Title: Novel sildenafil analogues: Possible drugs for increased sensitivity to chemotherapeutic agents
Aina Westrheim Ravna, University of Tromso, Norway
Title: 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
Title: 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
Title: In Silico screening for anti-HPV agents using docking studies
Tatsuya TAKAGI, Osaka University, Japan
Title: 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
Title: New polymeric "ruthenium-cyclopentadienyl" complexes for drug delivery in cancer therapy
Andreia Valente, Universidade de Lisboa, Portugal
Title: Unraveling the human multidrug resistance p-glycoprotein poly-specificity
Pierre Falson, Institute of Biology and Chemistry of Proteins, France
Title: PK modulation of haptenylated peptides via non-covalent antibody complexation
Stefan Dengl, Roche Diagnostics GmbH, Germany
Title: Tumour active plant derived compounds in combination with targeted therapy towards overcoming drug resistance in ovarian cancer
Fazlul Huq, The University of Sydney, Australia
Title: Designed monofunctional platinums found to have significant antitumor activity
Laila Arzuman, The University of Sydney, Australia
Title: A phytochemical and biological investigation of aloe grandidentata salm.-Dyck
Taghreed Abdou Ibrahim, King Saud University, Saudi Arabia
Title: 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
Title: Innovative approaches to expand medicinal chemistry space
Gerard Rosse, Dart Neuroscience, USA
Title: Discovery of a first-in-class topically bioavailable kit inhibitor with clinical activity using computational chemogenomics technology
James Hendrix, nPharmakon LLC, USA
Title: Discovery of a small molecule direct keap1-Nrf2 inhibitor as an anti-oxidant inflammation modulator
Magesh Sadagopan, Otsuka Maryland Medicinal Laboratories, Inc., USA
Title: Can cubane act as a benzene isostere?
Craig M Williams, University of Queensland, Australia
Title: 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
Title: Modulators of FGF-FGFR-Heparan sulfate complex: identifications of allosteric antagonists and oligosaccharide agonists as potential novel therapeutics
Gilbert Lassalle, Sanofi Aventis, France
Title: 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
Title: On the field of metallodrugs-new ruthenium compounds as anti-tumor agents
Ana Isabel Tomaz, Universidade de Lisboa, Portugal
Title: Design, synthesis and antidiabetic, cardiomyopathy studies of cinnamic acid-amino acid hybrid analogs
Subir Samanta, Birla Institute of Technology, India
Title: Synthesis and screening of newer quinazolin-3(h)-4-0ne derivatives for anticonvulsant activity
Jayasekhar P Nair, Oman Medical College, Sultanate of Oman
Title: Drug profile matching- drug discovery by polypharmacology-based interaction profiling
Zoltan Simon, Eotvos Lorand University, Hungary
Title: Novel structural elements for drug discovery: Identification, synthesis and application
Pavel Mykhailiuk, Enamine Ltd., Ukraine
Title: Synthesis and evaluation of some novel thiazolidinedione derivatives as PPAR-α/γ dual agonist
Praveen Thaggikuppe Krishnamurthy, JSS College of Pharmacy, India
Title: 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
Title: 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
Title: Synthesis of privileged structure libraries for biological evaluation
John Spencer, University of Sussex, UK
Title: 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
Title: 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
Title: Lipid pattern in serum of patients with type 2 diabetes mellitus

Ashur S Eljamil, Tripoli University, Libya
Title: 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
Title: 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
Title: The Hsp90 C-terminal binding site, instructions for and ramifications of inhibition
Brian S. J. Blagg, The University of Kansas, USA
Title: Inhibition of prostanoid receptor EP2: A novel anti-inflammatory therapy for chronic neurodegenerative and autoimmune diseases
Thota Ganesh, Emory University School of Medicine, USA
Title: Selective vitamin K2 biosynthesis inhibitors to treat non-replicating Mycobacterium tuberculosis
Michio Kurosu, University of Tennessee Health Science Center, USA
Title: Inhibitors of fatty acid amide hydrolase (FAAH): SAR and results in pre-clinical pain models
J. Guy Breitenbucher, Dart Neuroscience LLC, USA
Title: Discovery of novel bicyclic derivatives to stop the growth of mycobacterium tuberculosis by Inhibiting MenA
Prabagaran Narayanasamy, University of Nebraska Medical Center, USA
Title: The synthesis of potential inhibitors of panthothenate synthetase
Kellie L Tuck, Monash University, Australia
Title: Design and synthesis of inhibitors of cysteine protease
Debatosh Majumdar, Glycosyn LLC, USA
Title: Inward rectifier potassium channels as emerging drug targets
Jerod S. Denton, Vanderbilt University School of Medicine, USA
Title: 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
Title: Are D-neurons and trace amine-associated receptor, Type 1 involved in mesolimbic dopamine hyperactivity of schizophrenia?
Keiko Ikemoto, Fukushima Medical University, Japan
Title: 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
Title: Discovery of small molecule inhibitors of protein-protein interactions using DNA-encoded chemical libraries
Nils Jakob Vest Hansen, Vipergen ApS, Denmark
Title: Post-marketing surveillance of active pharmaceutical ingredients in antimalarial drugs used in Malawi
Ibrahim Chikowe, University of Ghana, Ghana