# Tentative Program

## 6th World Congress on

# Medicinal Chemistry

## Milan, Italy June 7-8 2017



medicinalchemistry@chemistryconference.org

## Speakers Slots Available

| | | | |
|---|---|---|---|
| 19+ Interactive Sessions | 15+ Keynote Lectures | 75+ Plenary Lectures | 5+ Workshops |

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Email: medicinalchemistry@chemistryconference.org

# Keynotes @ Medicinal Chemistry 2017



**Mario Ciampolini**

*University of Florence, Italy*

***Title : Physiology versus Pharmacology***

*Strategic Solutions Leader, GE Healthcare, USA*

***Title : Digital Biomanufacturing and Advanced Bioinks Enable 3D Bioprinting***



**William Whitford**



**Ahmed Radwan**

*CEO of PIONEERA HealthCare Group,Uk*

***Biosimilars - Pharmaceutical Industry Trends - Generic Drugs - Strategic Pharmaceutical Management***

*University of Florence,Italy*

***Title : A Reproducible, subjective limit in intake***



**Gaia Cecchi**



**Alexander Heifetz**

*Evotec Ltd, Uk*

***Title : Accurate Assessment of Protein-Ligand Interaction Energy in Seconds with Quantum Mechanics***

*Institute of Chemical Biology and Fundamental Medicine, Russia*

***Title : Synthesis and Biological Evaluation of Novel Classes of Tyrosyl-DNA Phosphodiesterase 1 Inhibitors***



**Olga Lavrik**

# Renowned Speakers @ Medicinal Chemistry 2017


Mario-Ciampolini


Bill Whitford


Ahmed M. Radwan


Alexander Heifetz


Matyus peter


Concepción González-Bello


Gaia Cecchi


John WM Yuen


Olga Lavrik


Yun Lu


Fabiola Porta


Giovanna Bergamini


Maia Merlani


Malkhaz Getia


L Amiranashvili


Nana Gorgaslidze


Hilal Kılınç


N.Nadaraia


n himon Ben-Shabat


Yoko Matsumoto


Jane Otado


Michele Tonelli


Kasatkin A, Urakov A


Neeraj tandon


Hamid Irannejad


Hasnah Osman


Szu-Han Chen


Wei-Hsin Hsu

# Tentative Program

## 6th World Congress on

# Medicinal Chemistry

## Milan, Italy June 7-8 2017

**Program at a Glance**

### Day 1

**Morning Sessions**

| | | |
|---|---|---|
| **Reception/Registration** | **08.00-09.00** | |
| | **Time** | **General Session** |
| Least of 3 Keynote/Plenary Talks | 09.00-09.15 | Inaugural Address |
| | 09.15-09.45 | Keynote/Plenary Talk 1 |
| | 09.45-10.15 | Keynote/Plenary Talk 2 |
| | 10.15-10.45 | Keynote/Plenary Talk 3 |
| Panel Discussions/Group Photo | | |
| **Coffee/Tea Break 10.45-11.00 (Networking)** | | |
| 11.00-12.40 | 5 Speakers (20 Mins Each) | |

**Evening Sessions**

| | |
|---|---|
| **Lunch Break 12.40-13.30** | |
| 13.30-15.30 | 6 Speakers (20 Mins Each) |
| **Coffee/Tea Break 15.30-15.45 (Networking)** | |
| 15.45-17.25 | 5 Speakers (20 Mins Each) |

**Day 1**

19 Speakers for

### Day 2

**Morning Sessions**

| | | | |
|---|---|---|---|
| | **Time** | **Session 1** | **Session 2** |
| 09.00-10.40 | | 5 Speakers (20 Mins Each) | 5 Speakers (20 Mins Each) |
| **Coffee/Tea Break 10.40-10.55 (Networking)** | | | |
| 10.55-12.35 | | 5 Speakers (20 Mins Each) | 5 Speakers (20 Mins Each) |

**Evening Sessions**

| | | |
|---|---|---|
| **Lunch Break 12.35-13.25** | | |
| **13.25-15.05** | **5 Speakers (20 Mins Each)** | **5 Speakers (20 Mins Each)** |
| Poster Sessions | | |
| **Coffee/Tea Break 15.05-15.20 (Networking)** | | |
| **15.20-17.00** | **5 Speakers (20 Mins Each)** | **5 Speakers (20 Mins Each)** |

**Day 2**

40 Speakers on

**NOTE: Program Shedule is subject to change with final allotment of the speaker slots**

## Note:

**Keynote Slots, Speaker, Workshops and Symposia slots are available. To book slot for Workshop and Symposium send us the proposal.**

**Call for Abstract:**
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Medicinal Chemistry 2017
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6th World Congress on
Medicinal Chemistry & Drug Design
June 07-08, 2017 Milan, Italy

# Tentative Scientific Program

***KEYNOTE Presentation Slots Available***

June 07-08, 2017

**Registrations**

**Opening Ceremony**

**Title : Digital Biomanufacturing and Advanced Bioinks Enable 3D Bioprinting**
William Whitford, Strategic Solutions Leader, GE Healthcare, USA

**Title : Mapping the Vibrational Transition-State Conformational Change in Enzymes for Drug Design**
Yun Lu, University Edwardsville Edwardsville, USA

**Title : Phenotypes of a Novel Series of 3-Phosphoglycerate Dehydrogenase Inhibitors**
Nello Mainolfi, Cambridge, USA

**Title : Drug Design via a Scaffold Hopping Strategy: Case Studies on Discovery of Clinical Candidates H3 Receptor Antagonist and β-Tryptase Inhibitor**
Zhongli Gao, Principal Scientist at Sanofi, USA

**Title : Successful strategies for recruitment of african americans into clinical and translational studies**
Jane Otado, Howard University Washington, USA

**Title : Drug Hunting Vs Drug Fishing**
Youssef Bennani,Vertex Pharmaceuticals, Canada

**Title : Physiology versus Pharmacology**
Mario Ciampolini, University of Florence, Italy

**Title : A Reproducible, subjective limit in intake**
Gaia Cecchi, University of Florence,Italy

**Title : Host DHFR-directed cycloguanil analogues endowed with promising activity against influenza virus and respiratory syncytial virus**
Michele Tonelli, University of Genoa, Italy

**Title : CZ415, a highly selective mTOR inhibitor showing in vivo efficacy in a collagen induced arthritis (CIA) model**
Giovanna Bergamini, Cellzome, a GSK company, Germany

**Title : Bioactive natural products from Symphytum (Boraginaceae)**
Maia Merlani, Tbilisi State Medical University, Georgia

**Title : 5-Steroidal hydrazones: synthesis and biological activity**
Lela Amiranashvili, Tbilisi State Medical University, Georgia

**Title : Development of Analytical Procedure for the standardization of bromelain from the pineapple (Ananas comosus L. Merr)**
Nana Gorgaslidze, Tbilisi State Medical University, Georgia

**Title : 5-Steroidal amines: synthesis and biologicaly activity**
Nanuli Nadaraia, Tbilisi State Medical University, Georgia

**Title : Quantification of some medical preparations of the plant origin**
Malkhaz Getia, Tbilisi State Medical University, Georgia

**Title : Synthesis and Biological Evaluation of Novel Classes of Tyrosyl-DNA Phosphodiesterase 1 Inhibitors**
Olga Lavrik, Institute of Chemical Biology and Fundamental Medicine, Russia

**Title : Biosimilars; expanding the scope of biologic therapy through wider patient access**
Ahmed Radwan, CEO of PIONEERA HealthCare Group, Uk

**Title : Ganoderma lucidum-Cytotoxic effects and Cytokine gene induction as compared with the immunobladder® BCG in murine MB49 cells**
John Yuen, School of Nursing, Hong Kong

**Title : Therapeutic effects of trehalose liposomes against carcinoma along with apoptosis in vitro and in vivo**
Yoko Matsumoto, Sojo University, Department of Life Sciences, JAPAN

**Title : Disabling Essential Enzyme Motion for Catalysis: An Efficient Approach for Shikimate Kinase Inhibition**
Concepción González-Bello, Universidade de Santiago de Compostela, Spain

**Title : In the pursuit of ideal hits for antifungal research**
Jeanmart Stephane, Syngenta Crop Protection AG, Stein Switzerland

**Title : Design of new drugs: Challenges for the rational development of novel ligands with affinity for G-protein-coupled receptors**
José Raúl Bahena , ESM - Instituto Politécnico Nacional , Mexico

**Title : Structure-based design of subtype selective antagonists for the ionotropic glutamate receptors: Successes and failures**
Lennart Bunch, University of Copenhagen, Denmark

**Title : Cyclopentenes for anti tuberculosis and antibiotics**
Hadia Almahli, University of Oxford, United Kingdom

**Title : Early findings in the development of an enzymatically triggered nanoformulation**
Daniel Ehrsam, University of Basel, Switzerland

**Title : Elaboration and grafting of gold nanoparticles functionalized for a better sensibility of the biosensors of cancer with multiple detection**

Ali H. Adabo-kako, CNRS-University of Franche-Comté, France

**Title : The New Steroids From Silene Montbretiana**

Hilal Kılınç, Dokuz Eylül University, Turkey

**Title : Accurate Assessment of Protein-Ligand Interaction Energy in Seconds with Quantum Mechanics**

Alexander Heifetz , Evotec Ltd, Uk

**Title : Pathogenesis of alimentary diabetes: recovery by loss of 20% body weight, and by attainment of initial hunger as well as of low bg before meals**

Gaia Cecchi , University of Florence, Italy

**Title : Anticancer activity of some [1,2,4]triazepino[2,3-a] quinazoline derivatives: monolayer and multicellular spheroids in vitro models**

Hanem awad, National Research Centre, Egypt

**Title : Why the drug solutions may cause inflammation at the injection site**

Anton Kasatkin, Izhevsk State Medical Academy, Russia

**Title : Branched amphiphilic cationic oligo-peptides for delivery of HPV-16 DNA vaccines**

Adriana Avila Flores , Auburn University,USA

**Title : β-Strand Mimicry: Exploring Oligothienylpyridine Foldamers**

Jana Sopkova-de Oliveira Santos, University of Caen Normandy, France

**Title : Synthesis of New Naturally Furanocoumarins Derivatives and Difuranocoumarin Using Phenyl Acetylene as Starting Material for Increasing its Antiproliferative Activity**

Yasser Selim, Zagazig University, Egypt

**Title : The role of technologies of nonlinear stimulation in the treatment of brain diseases and potential of their applications in healthy individuals**

Marina, Moscow Helmholtz Research Institute of Eye Diseases, Russian

**Title : α,β-unsaturated compounds derived from arylamines as possible new treatment against Leukemia**

Luis Angel, Instituto Politécnico Nacional, México

**Title : Identification of Thiadiazinyl-coumarin derivatives as dengue virus-2 NS2B/NS3 protease inhibitors**

Hasnah Osman, Universiti Sains Malaysia, Malaysia

**Title : The Study on Serum Protein Spectrum Expression Changes for Patients with Gastrointestinal Disease Before and After Acupuncture**

Yanhong, Chinese PLA General Hospital, China

**Title : Study of protector effect of chemlal olive leaves extract on nephropathy induced by mercury in mouse**

Nadia Dekdouk, Université des Frères Mentouri Constantine, Algérie

**Title : Ezyme triggered nanomaterial for cancer therapy**
Fabiola Porta, University of Basel,Basel, Switzerland

**Title : Pyrroles-a novel synthetic method for pyrrole derivatives from nitrodienes**
Mohamed elatawy,University of Milan, egypt

**Title : Isoconvertional approach for non-isothermal decomposition of un-irradiated and photon-irradiated 5-fluorouracil**
Refaat Mhfouz, Assiut University, Egypt

**Title : Synthesis of new peptidomimetics as HIV-1 protease inhibitors through simple and cost-effective synthetic routes**
Jean-Pierre Kayembe, Rhodes University, Grahamstown, South Africa.

**Title : The great potential of phenolic copounds isolated from Limonium densiflorum to quench and protect human cell against free radicals**
Faten Medini, University of Quebec in Chicoutimi, Tunisia

**Title : Passiflora incarnata l. Of endophytic fungi rooted flavone chrysin (5,7-dihydroxy flavone) and gold nanoparticles towards anticancer activity**
sivaramakrishnan, Bharathidasan University, India

**Title : Design and Synthesis of Sugar Phosphates for Inhibition of Tuberculosis Maltosytransferase**
Wei-Hsin Hsu, National Taiwan University, Taiwan

**Title : Synthesis of Oseltamvir Using Diels–Alder Reaction of 1,3-Butadiene Bearing 2-Carboxy and 4-Alkoxy Substituenes**
Szu-Han Chen, National Taiwan University, Taiwan

**Title : Phospholipid-based prodrugs for the treatment of IBD: Drug targeting strategy**
Shimon Ben-Shabat, Ben-Gurion University of the Negev, Israel

**Title : Synthesis and Characterization of 2-((4R,4aR,5aS,6S)-1,3-dioxo3m3a,4,4a,5,5a6,6a-octahydro-4,6-ethenocyclopropa[f]isoindol-2(1H)-yl)-N-(substituted phenyl) acetamides anticepted to have HIV-1 activity**
Abdulmajeed AlSamarrai, University of Samarra, Iraq

**Title : Investigation of the Biochemical Mechanism of Action of Antioxidants in the Prevention of Cancer**
Kissi Mudie, Ethiopian Public Health Institute, Ethiopia

**Title : Therapeutic Important Medicinal Plants and Way Forward**
Neeraj Tondan, Indian Council of Medical Research,India

**Title : Synthesis and anticancer activity of 6-aryl-2-napthyl-imidazo[2,1-b][1,3,4]thiadiazole**
Subhas S, KLE University's College of Pharmacy, India

**Title : The great potential of phenolic copounds isolated from Limonium densiflorum to quench and protect human cell against free radicals**
Faten Medini, Laboratoire des Plantes Aromatiques et Médicinales, Tunisia

**Title : Anticonvulsant activity of 1,2-Diarylethylidene hydrazinecarboximidamides: synthesis, biological, and computational study**

Hamid, Faculty of Pharmacy, Mazandaran University of Medical Sciences, IRAN

**Title : Synthesis of 7-(2-substituted-phenylthiazolidinyl)-benzopyran-2-one derivatives**

Anil.K, Indian Institute of Integrative Medicine (CSIR),INDIA

**Title : Isobutylbromide-Pyrimidine Hybrids: Potential Anticancer Agents.**

Mohammad Shaquiquzzaman, Drug Design and Medicinal Chemistry, India

**Title : Protective effect of the standardized extract of Holmskioldia sanguinea on tumor bearing mice**

Mahesh Pal, CSIR-National Botanical Research Institute, India

**Title : Benzimidazole-Pyrimidine Hybrids: Potential Anticancer Agents.**

Wasim, Drug Design and Medicinal Chemistry Lab,India

**Title : Pharmacophore Modeling, 3D-QSAR and Docking Study of Dibenzepinones, Dibenzoxepines, and Benzosuberones as p38α MAP Kinase Inhibitors**

Mohemmed Faraz, Drug Design and Medicinal Chemistry Lab, India

**Title : Proficient gem-dichlorination, oxidation and nitrile oxide cyclisation: synthesis of a Novel fluxional 4-chromanone derivatives**

Anil. K, Indian Institute of Integrative Medicine (CSIR), Jammu-INDIA

**Title : 1,3,4-Oxadiazle Tailored Compounds: Synthesis and Assessment of In Vitro Antimalarial Activity**

Garima, Drug Design and Medicinal Chemistry Lab, India

**Title : Drug Design, Synthesis and Evaluation: Identification of Drug-like Gquadruplex DNA Stabilizing Agents As Potential Anti-cancer Therapeutics**

Mrinalkanti Kundu, TSMU Iovel Kutateladze Institute of Pharmacochemistry,India

**Title : Pyranochromene triones: Synthesis of new series of Anti-tubercular agent**

Denish Karia, TCG Lifesciences Pvt. Ltd, INDIA

**Title : Synthesis and solubilization of Flurbiprofen derivatives and investigation of their biological activities.**

Muhammad Mustaqeem, University of Sargodha, Pakistan

**Title : Morphological and structural features of adenovirus particles by reacting with bacterial**
A.V. Golovan, Zabolotny Institute of Microbiology and Virology of NASU, Ukraine

**Title : Investigation of effect of medium on volumetric and ultrasonic studies of pharmaceutical excipients**
Bushra Naseem, Lahore College for Women University, Pakistan

**Title : Enhancing the solubility of Flurbiprofen and its derivatives and investigation of their biological activities.**
Muhammad Mustaqeem, University of Sargodha, Pakistan

**Title : Determination of heavy metal(PB) content in mineral water produced in IRAN by Flameless Atomic Absorption Spectroscopy (FAAS)**
Rasoul Kazemi, Azad University, IRAN

**Title : Transition metal complexes/organometallic compounds as anticancer/anti HIV drugs or in pharmaceutical industry**
Prakash Kinthada, JNTU University, India

**Title : Design and development of ureas and amides as p38 kinase inhibitors**
Ravindra Kulkarni,Kakatiya University, India

**Title : Effect of intermittent feeding on learning and spatial memory and metabolic symptoms of chronic stress in male mice**
Ghassem Attarzadeh Yazdi, Hormozgan University of Medical Science, Iran

**Title : Targeted anti-bacterial and anti-fungal drug carrying nanomedicines**
Itai Benhar,Tel-Aviv University, Israel

***ORAL/POSTER Presentation Slots Available***

**Workshop/Symposium Slots Available**

Note: This is only tentative scientific program, the final allotment of slots may subject to change

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## Glimpses of Medicinal Chemistry Conferences













# Tentative Program

## Glimpses of Medicinal Chemistry Conferences










## Major Scientific Sessions

- Medicinal Chemistry
- Pharmaceutical Sciences
- Bioorganic and Medicinal Chemistry
- Drug Design and Drug Development
- CADD (Computer Aided Drug Design)
- Pharmacology and toxicology
- Synthetic Organic Chemistry
- BioInorganic Chemistry
- Chemical Biology
- Organometallic Chemistry
- Anticancer agents in Medicinal Chemistry
- Radiopharmaceuticals
- Pharmaceutical Industry
- Clinical Pharmacology
- Bioisostere
- Analytical Chemistry
- Nanomedicine
- Stereochemistry
- Pharmacovigilance

### Best Poster Award



- You will be given about 5-7 minutes to present your poster including questions and answers. Judges may pose questions during the evaluation of the poster
- Judges will even evaluate the student's enthusiasm towards their study, interest and knowledge in the area of their research
- The winners will be announced at the closing ceremony of the conference. The decision of the winner will be withdrawn if the winner/winners is/are not present at the time of announcement
- Apart from the judging time you may also be present at the poster to share your research with interested delegates



### Young Researchers Forum

- Present your research through oral presentations
- Learn about career development and the latest research tools and technologies in your field
- This forum will give pertinent and timely information to those who conduct research and those who use and benefit from research
- Develop a foundation for collaboration among young researchers
- The forum will provide an opportunity for collegial interaction with other young investigators and established senior investigators across the globe
- Interact and share ideas with both peers and mentors

General Queries
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## Conference Venue

Milan, Italy


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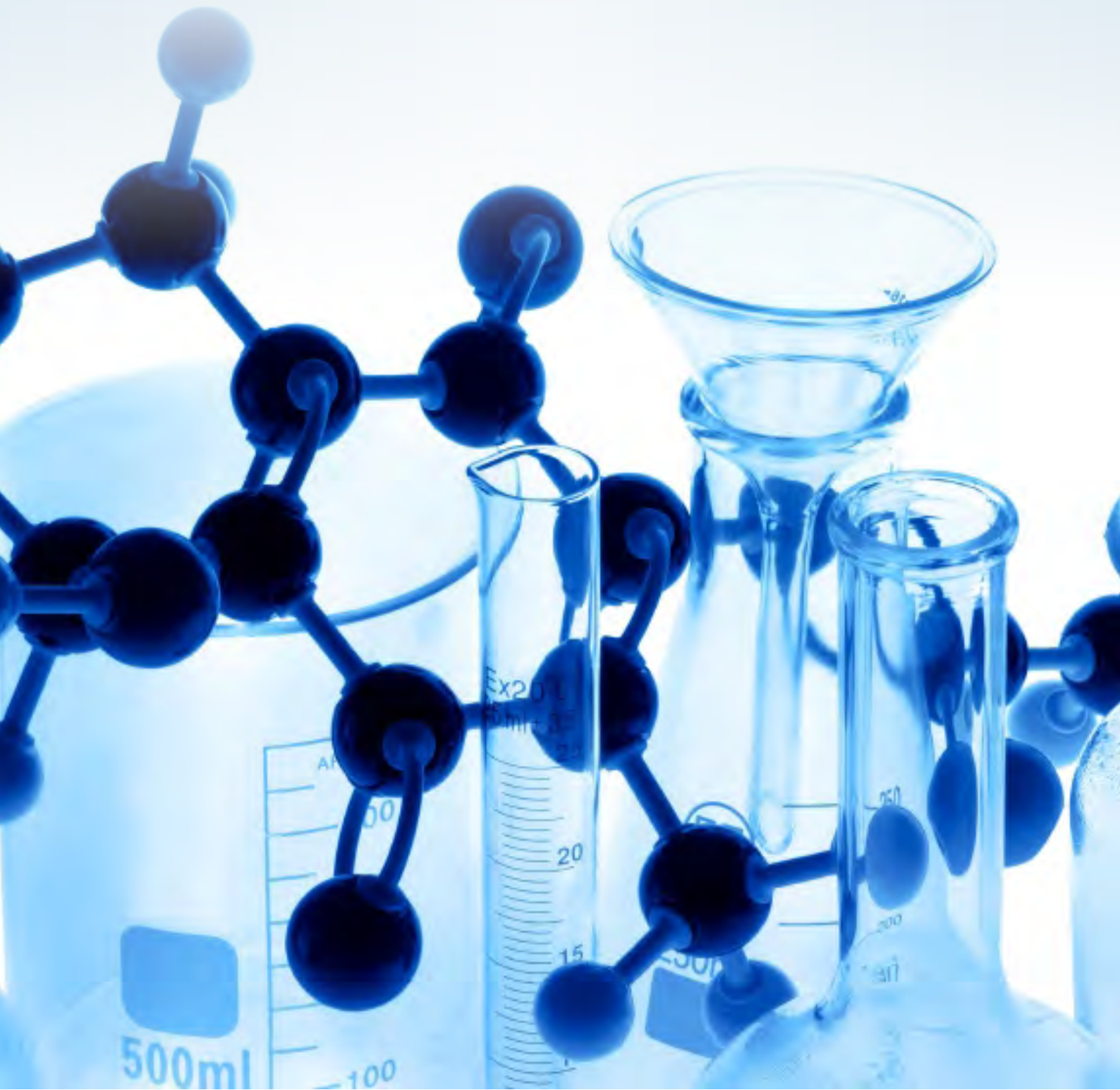
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International Conference on

# 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

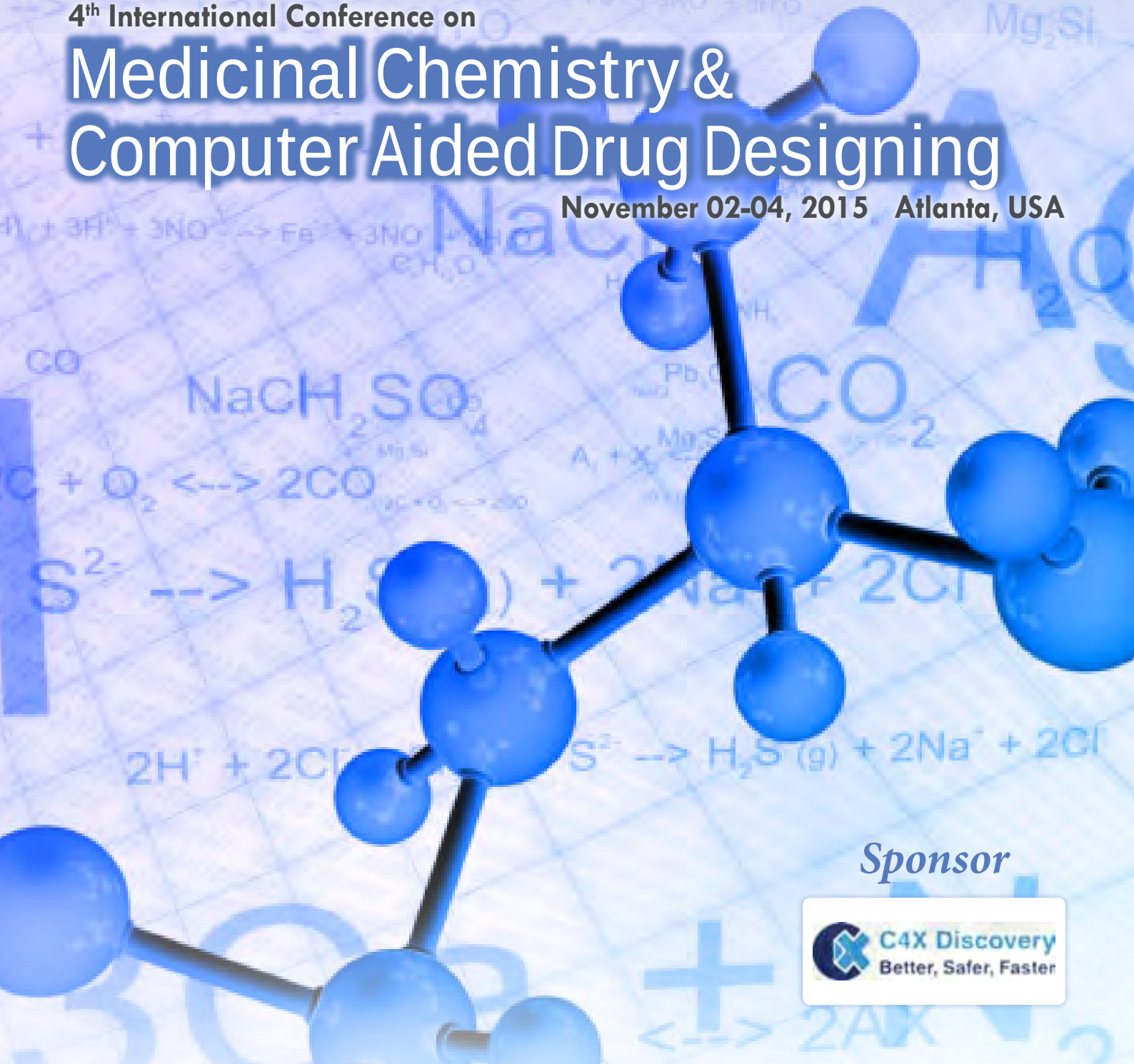
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# Scientific Program

4th International Conference on

# Medicinal Chemistry & Computer Aided Drug Designing

November 02-04, 2015 Atlanta, USA



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Registrations

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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

# Medicinal Chemistry & Computer Aided Drug Designing

December 08-10, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA



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Day 1 December 08, 2014

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 $\sigma_1$ 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

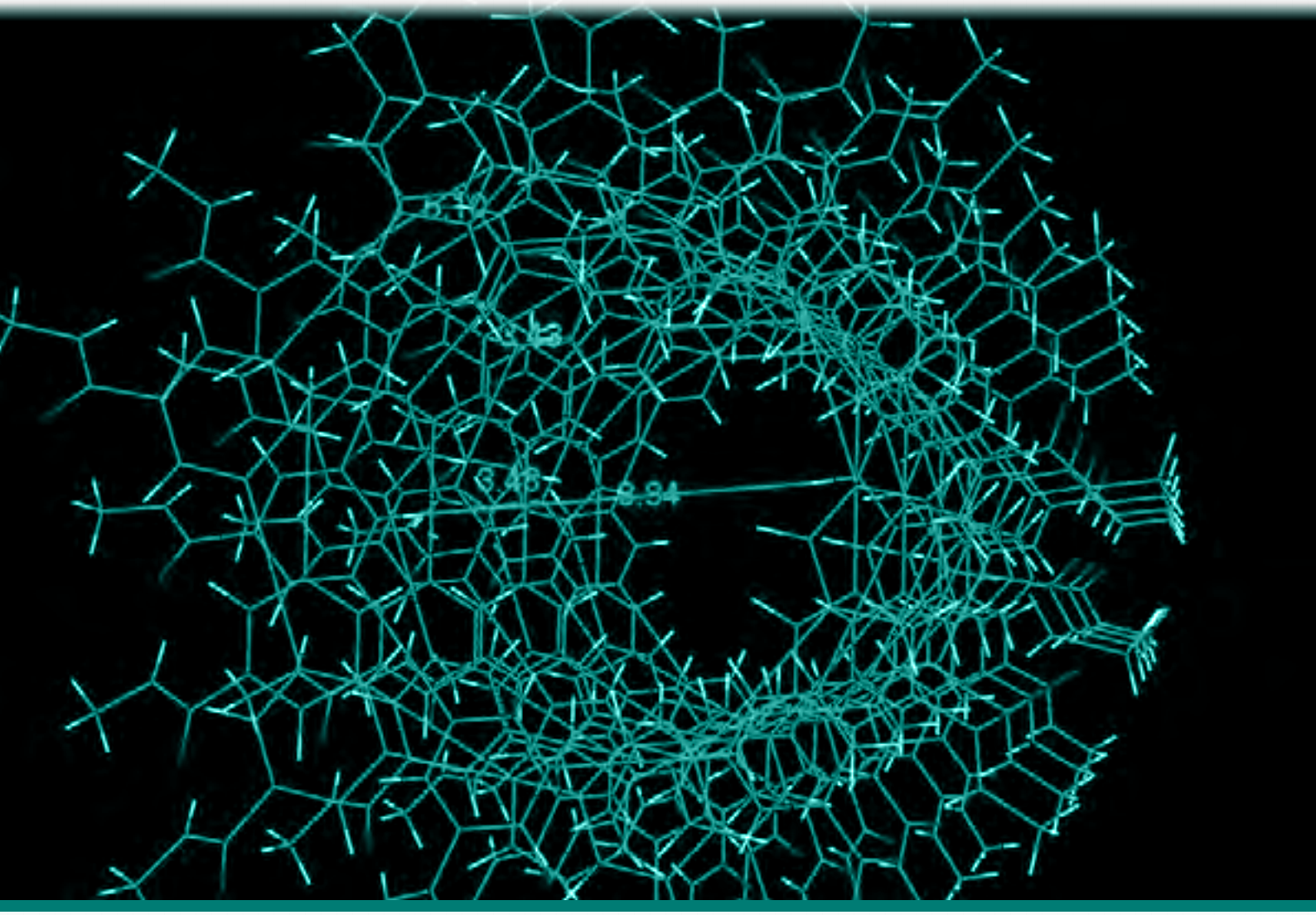
73rd OMICS Group Conference

# Scientific Program

## International Conference and Exhibition on

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Registrations October 28, 2012

Day 1 October 29, 2012

Breakfast
Registrations

# Opening Ceremony

Introduction

**Giulio Tarro**
Temple University, USA

**Ronan Bureau**
University of Caen Basse-Normandie, France

**Li Xing**
Pfizer, USA

**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

**Title: Specificity of heparin/heparan sulfate binding to proteins**

**Umesh R. Desai,** Virginia Commonwealth University, USA

**Title: Discovery of potent, selective and efficacious p38 MAPK inhibitor as clinical drug candidate**

**Li Xing,** Pfizer, USA

**Title: QSAR model building and analysis of ADME properties: Understanding P-glycoprotein activity**

**Sookhee Ha,** Merck Research Laboratories, Canada

**Title: Computer-aided design of inhibitors of DNA methyltransferases**

**Jose L. Medina-Franco,** Torrey Pines Institute for Molecular Studies, USA

**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

**Title: Screen 3D: A ligand-based 3D similarity search without conformational sampling**

**Wei Deng (David),** ChemAxon, USA

**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

**Title: Kinome-wide activity models from diverse high-quality datasets**

**Steven M. Muskal,** Eidogen-Sertanty Inc., USA

**Title: Extract chemical information from patents using chemicalize and D2S (Document to Structure)**

**Wei Deng (David),** ChemAxon, USA

**Title: Identifying neuraminidase residues likely to mutate with molecular mechanics free energy**

**Kelly M. Thayer,** University of Massachusetts Medical School, USA

**Title: Chemical targeting of protein methyltransferases**

**Matthieu Schapira,** University of Toronto, Canada

**Title: A simple additive non-parametric regression method and its application to QSAR**

**Tatsuya Takagi,** Osaka University, Japan

**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

**Title: Screening for novel anti-dengue virus NS3/NS2B inhibitor**

**Norihito Kawashita,** Osaka University, Japan

**Title: Advanced pharmacophores for accurate virtual screening and identification of opioid lead compounds**

**Sharon D. Bryant,** Inte:Ligand GmbH, Austria

**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

**Title: Fuzzy neural network and fuzzy ARTMAP analyses of the affinity of inhibitors for HIV-1 protease**

**Levente Fabry-Asztalos,** Central Washington University, USA

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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Email: *medchem2013@omicsonline.net*

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-$\alpha/\gamma$ 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

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## Medicinal Chemistry 2017

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