“Organize your Events at OMICS Group Conferences”

Proposals are invited for organizing Symposia/Workshops at OMICS Group Conferences or OMICS Group will sponsor small events at your universities in related areas under the title of your own. These proposals can be sent to respective conference mail ids or to symposia@omicsonline.org

OMICS Group Conferences
5716 Corsa Ave., Suite 110, Westlake Los Angeles, CA 91362-7354, USA
Phone: +1-650-268-9744, Fax: +1-650-618-1414, Toll free: +1-800-216-6499
Email: medchem2013@omicsonline.net
**Keynote Forum**

**09:55-10:00**  
*Introduction*  
**James K. Bashkin**  
University of Missouri-St. Louis, USA

**10:00-10:25**  
**Brian S. J. Blagg**  
The University of Kansas, USA

**10:25-10:50**  
**Xiang-Qun (Sean) Xie**  
University of Pittsburgh, USA

**11:05-11:30**  
**Tulay Aygan Atesin**  
The University of Texas-Pan American, USA

**Coffeebreak: 10:50-11:05 @ Foyer**

**Track 1: Rational Drug Designing**

**Session Chair:** Victor J Hruby, University of Arizona, USA  
**Session Co-Chair:** Alexander Heifetz, Evotec (UK) Ltd., UK

**11:55-12:15**  
**Design and investigation of multivalent ligands for the detection and treatment of diseases**  
**Victor J Hruby**, University of Arizona, USA

**12:15-12:35**  
**Structure-based drug discovery for GPCRs: From receptors to ligands**  
**Alexander Heifetz**, Evotec (UK) Ltd., UK

**12:35-12:55**  
**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

**12:55-13:15**  
**Structure-guided design, synthesis, and evaluation of guanine-derived inhibitors of the eIF4E mRNA-cap interaction**  
**Xiaoqi Chen**, Amgen, USA

**Lunch Break 13:15-14:00 @ Carol & Patio**

**14:00-14:20**  
**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

**14:20-14:40**  
**Understanding the essential requirements for success in structure-based design**  
**Gregory L Warren**, OpenEye Scientific Software, USA

**14:40-15:00**  
**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

**15:00-15:20**  
**Computer-aided design of glucokinase activators**  
**Meihua Tu**, Pfizer, USA

**15:20-15:40**  
**Non-competitive regulation of the human proteasome by natural products and natural product inspired scaffolds**  
**Jetze J Tepe**, Michigan State University, USA

**Coffee Break 15:40-15:55 @ Foyer**

**15:55-16:15**  
**Rational design approaches to find novel ligands targeting the aryl hydrocarbon receptor: successful applications and mechanistic studies**  
**William H Bisson**, Oregon State University, USA

**16:15-16:35**  
**Modulations of protein-protein interactions of EGFRs: Structure, inhibition, dynamics and its implications in breast cancer**  
**Seetharama D. Satyanarayanaojis**, University of Louisiana at Monroe, USA

**16:35-16:55**  
**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

**16:55-17:15**  
**Design and synthesis of novel pyrimidine analogues as HIV-1 integrase inhibitors**  
**Guisen Zhao**, Shandong University, China

**17:15-17:35**  
**Synthesis and anti-candida activity evaluation of new [1,2,4] triazolo[3,4-b][1,3,4] thiadiazines**  
**Mashoos Ahmad Bhat**, King Saud University, Kingdom of Saudi Arabia

**17:35-17:55**  
**Newer approaches to the discovery of glitazones**  
**Praveen Thaggikkupure Krishnamurthy**, JSS College of Pharmacy, India

**18:30-19:30**  
**Cocktails Sponsored by Medicinal Chemistry @ Foyer**

**Track 2: Computer-Aided Drug Design and Structure Determination**

**Session Chair:** Istvan J. Enyedy, Biogen Idec, USA  
**Session Co-Chair:** Nicolas Moitessier, McGill University, Canada

**11:55-12:15**  
**New approaches to “Hit” optimization**  
**Istvan J. Enyedy**, Biogen Idec, USA

**12:15-12:35**  
**Accurate binding site models can be derived from low quality PDB files using an empirical geometry based force field**  
**Colin McMartin**, Thistlesoft, USA

**12:35-12:55**  
**Integrating computational approaches into high throughput screening for rational drug discovery**  
**Xin Hu**, National Center for Advancing Translational Sciences, National Institutes of Health, USA
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, BostondNovo, USA

12:55-13:15

Lunch Break 13:15-14:00 @ Carol & Patio

14:00-14:20

Forecasting: A computational tool for drug design and discovery developed by experimentalists for experimentalists

Nicolas Moisessi, McGill University, Canada

14:20-14:40

Genes to Leads: A rational structure guided lead discovery technology that works for both enzymes and protein-protein interaction targets

Kal Ramnarayan, Sopient Discovery, LLC, USA

14:40-15:00

Discovery of highly-potent and selective inhibitors for the ABCG2 transporter

Achme Boumedjel, Université Joseph Fourier de Grenoble, France

15:00-15:20

Predictive application of bioisostere transformations to identify novel high quality compound ideas

Matthew Segall, Optibrium Ltd., UK

15:20-15:40

Novel sildenafil analogues: Possible drugs for increased sensitivity to chemotherapeutic agents

Aina Westheim Ravna, University of Tromso, Norway

15:55-16:15

Structural insights of SIR2 proteins from T. cruzi as promising targets to fight against Chagas disease

Alessandra Nurizzo, University of Geneva-University of Lausanne, Switzerland

16:15-16:35

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. Makisimenko, Institute of Experimental Cardiology, Russia

18:30-19:30 Cocktails Sponsored by Medicinal Chemistry @ Foyer
**Track 12: Recent Research and Developments**

**Session Chair:** John Spencer, University of Sussex, UK

**Session Co-Chair:** Carsten Detering, BioSolveIT Inc, USA

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Introduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>16:55-17:15</td>
<td>Pavel Mykhailiuk, Enamine Ltd, Ukraine</td>
</tr>
</tbody>
</table>

**Session Tracks**

<table>
<thead>
<tr>
<th>Track</th>
<th>Session</th>
<th>Speaker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms</td>
<td>Jean Leandro Dos Santos, State University of Sao Paolo, Brazil</td>
</tr>
<tr>
<td></td>
<td>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</td>
<td>Osadolor H. B, University of Benin, Nigeria</td>
</tr>
<tr>
<td></td>
<td>Lipid pattern in serum of patients with type 2 diabetes mellitus</td>
<td>Ashur S Eljemili, Tripoli University, Libya</td>
</tr>
<tr>
<td></td>
<td>What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?</td>
<td>Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany</td>
</tr>
<tr>
<td></td>
<td>Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer</td>
<td>Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA</td>
</tr>
<tr>
<td>10:35-15:55</td>
<td>Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms</td>
<td>Jean Leandro Dos Santos, State University of Sao Paolo, Brazil</td>
</tr>
<tr>
<td>10:55-11:15</td>
<td>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</td>
<td>Osadolor H. B, University of Benin, Nigeria</td>
</tr>
<tr>
<td>11:15-11:35</td>
<td>Lipid pattern in serum of patients with type 2 diabetes mellitus</td>
<td>Ashur S Eljemili, Tripoli University, Libya</td>
</tr>
<tr>
<td>11:35-11:55</td>
<td>What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?</td>
<td>Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany</td>
</tr>
<tr>
<td>11:55-12:15</td>
<td>Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer</td>
<td>Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA</td>
</tr>
</tbody>
</table>

**Coffee Break 10:20-10:35 @ Foyer**

**Poster Presentations @ Carol & Patio**

**Coffee Break 10:20-10:35 @ Foyer**

**Day 3 October 17, 2013**

**Track 10: Receptors and Inhibitors**

**Session Chair:** Probaragan Narayanasamy, University of Nebraska Medical Center, USA

**Session Co-Chair:** Xiang-Qun (Sean) Xie, University of Pittsburgh, USA

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Introduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00-09:20</td>
<td>The Hsp90 C-terminal binding site, instructions for and ramifications of inhibition</td>
</tr>
<tr>
<td>09:20-09:40</td>
<td>Inhibition of prostaglandin receptor EP2: A novel anti-inflammatory therapy for chronic neurodegenerative and autoimmune diseases</td>
</tr>
<tr>
<td>09:40-10:00</td>
<td>Selective vitamin K2 biosynthesis inhibitors to treat non-replicating Mycobacterium tuberculosis</td>
</tr>
<tr>
<td>10:00-10:20</td>
<td>Inhibitors of fatty acid amide hydrolase (FAAH): SAR and results in pre-clinical pain models</td>
</tr>
</tbody>
</table>

**Coffee Break 10:20-10:35 @ Foyer**

**Session Tracks**

<table>
<thead>
<tr>
<th>Track</th>
<th>Session</th>
<th>Speaker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms</td>
<td>Jean Leandro Dos Santos, State University of Sao Paolo, Brazil</td>
</tr>
<tr>
<td></td>
<td>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</td>
<td>Osadolor H. B, University of Benin, Nigeria</td>
</tr>
<tr>
<td></td>
<td>Lipid pattern in serum of patients with type 2 diabetes mellitus</td>
<td>Ashur S Eljemili, Tripoli University, Libya</td>
</tr>
<tr>
<td></td>
<td>What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?</td>
<td>Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany</td>
</tr>
<tr>
<td></td>
<td>Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer</td>
<td>Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA</td>
</tr>
<tr>
<td>10:35-10:55</td>
<td>Design, synthesis and pharmacological evaluation of novel hybrid compounds to treat sickle cell disease symptoms</td>
<td>Jean Leandro Dos Santos, State University of Sao Paolo, Brazil</td>
</tr>
<tr>
<td>10:55-11:15</td>
<td>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</td>
<td>Osadolor H. B, University of Benin, Nigeria</td>
</tr>
<tr>
<td>11:15-11:35</td>
<td>Lipid pattern in serum of patients with type 2 diabetes mellitus</td>
<td>Ashur S Eljemili, Tripoli University, Libya</td>
</tr>
<tr>
<td>11:35-11:55</td>
<td>What can we expect from new therapeutic strategies in nano-pharmacology and nano-medicine?</td>
<td>Hans-Christian Siebert, Research Institute for Bioinformatics and Nanotechnology (RI-B-NT), Germany</td>
</tr>
<tr>
<td>11:55-12:15</td>
<td>Mitochondria specific antioxidants and their derivatives in the context of the drug development for neuro degeneration and cancer</td>
<td>Gjumrakch Aliev, GALLY International Biomedical Research Consulting LLC, USA</td>
</tr>
<tr>
<td>10:00-10:20</td>
<td>Inhibitors of fatty acid amide hydrolase (FAAH): SAR and results in pre-clinical pain models</td>
<td>J. Guy Breitenbucher, Dart Neuroscience LLC, USA</td>
</tr>
</tbody>
</table>

**Lunch Break 12:35-13:20 @ Carol & Patio**

**Book your dates**

**3rd International Conference on Medicinal Chemistry & Computer Aided Drug Designing**

**August 18-20, 2014**  **Beijing, China**

**OMICS Group Inc.**
2360 Corporate Circle, Suite 400
Henderson, NV 89074-7722, USA
Ph: +1-888-843-8169
Fax: +1-650-618-1417
omicsonline@omicsonline.com

**OMICS Publishing Group**
5716 Corsa Ave., Suite 110, Westlake
Los Angeles, CA 91362-7354, USA
Ph: +1-650-268-9744
Fax: +1-650-618-1414
omicsonline@omicsonline.org

**OMICS Group**
SEZ Unit, Building No. 20, 9th Floor
APIIC Layout, HITEC City
Hyderabad-500081, AP, INDIA
Ph: 040-40131923, 040-47482222
omicsgroup@omicsgroup.org