

# ASMC'09 Kiev

## Program

---

**Sunday August 23, 2009**

**Registration**

**Welcome reception**

### Monday August 24, 2009

#### Opening

#### Morning Session

##### Session Chair

Dr Scott A. BILLER  
(AGIOS PHARMACEUTICALS, Cambridge, United States)

##### The Metalated Flatland Conduit to New Synthetic Aromatics and Heteroaromatic Chemistry

Prof. Victor SNIECKUS  
(QUEEN'S UNIVERSITY, Ontario, Canada)

##### C-H Activation: Direct Arylation and Alkenylation of Oxazoles

Dr. Florence MAHUTEAU  
(INSTITUT CURIE, ORSAY, France)

#### Coffee-break

##### Orally Active, Brain Penetrant Beta-Secretase (BACE) Inhibitors: Consolidating Property-Based and Structure-Based Drug Design

Dr. Stephen HITCHCOCK  
(AMGEN INC, Thousand Oaks, United States)

##### From Structures to Systems: Structure Based Design of Therapeutics and Imaging Probes

Dr. Ulrich WENDT  
(SANOFI AVENTIS, Frankfurt, Germany)

##### Structure-Activity Relationships and Cancer-Cell Selective Toxicity Of Novel Inhibitors of Glioma-Associated Oncogene Homolog 1 (Gli1)-Mediated Transcription

Dr Naoaki FUJII  
(ST.JUDE CHILDREN'S RESEARCH HOSPITAL, Memphis, United States)

##### Molecular Recognition at the Active Site of Catechol-O-Methyl Transferase (COMT): Energetically Favorable Expulsion of a Single Water Molecule with Novel Bisubstrate Inhibitors.

Mr Manuel ELLERMANN  
(ETH ZURICH, Zurich, Switzerland)

#### Lunch and Poster Session 1

#### Afternoon Session

##### Session Chair

Prof. Victor SNIECKUS  
(QUEEN'S UNIVERSITY, Ontario, Canada)

##### Bio-Inspired Organocatalysis: From Concepts to Applications in Heterocycle Synthesis

Prof. Magnus RUEPING  
(RWTH AACHEN, Aachen, Germany)

## Program

---

### **Discovery of Ixempratm (ixabepilone), an Epothilone Analogue for Treatment of Metastatic Breast Cancer**

Dr. Gregory VITE  
(BMS, Princeton, United States)

### **Design and Synthesis of Novel Polyketide Molecular Frameworks to Access Natural Product-Like Protein-Protein Interaction Inhibitors as Novel Chemotherapeutic Agents**

Dr Giovanna ZINZALLA  
(LONDON SCHOOL OF PHARMACY, London, United Kingdom)

### **Coffee-break and Poster Session 1**

### **Compound Collection Enhancement (CCE): Increasing Quality and Size of the AZ Compound Collection**

Dr. Kay BRICKMANN  
(ASTRA ZENECA, Mölndal, Sweden)

### **Approach to the Synthesis of Pycnanthuquinone C by Gold(I)-Catalyzed Cyclization of 1,5-Enynes**

Ms NURIA HUGUET  
(INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA, Tarragona, Spain)

### **C-H: A New Functional Group for Streamlining Synthesis**

Prof. Christina WHITE  
(UNIVERSITY OF ILLINOIS, Urbana, United States)

### **Closing of the day**

**Tuesday August 25, 2009**

### **Morning Session**

#### **Session Chair**

Dr Edmond DIFFERDING  
(UCB, Braine-l'Alleud, Belgium)

#### **Development and Applications of New Metal-Catalyzed Carbon-Carbon Bond Forming Reactions**

Prof. Jonathan A. ELLMAN  
(UNIVERSITY OF CALIFORNIA, Berkeley, United States)

#### **Case Histories of Fragment Based Discovery: from Crystal to Clinic**

Dr David REES  
(ASTEX THERAPEUTICS, Cambridge, United Kingdom)

#### **Design and synthesis of polyfluoroalkyl-containing purine isosters and phospho-purines as a potential Adenosine Deaminase (ADA) and Inosine 5'-monophosphate dehydrogenase (IMPDH) inhibitors**

Dr Dmytro VOLOCHNYUK  
(ENAMINE, Kyiv, Ukraine)

### **Coffee-break and Poster Session 1**

#### **The Fight against AIDS. The "Old" Reverse Transcriptase (RT) and the "New" DDX3**

Prof. Maurizio BOTTA  
(UNIVERSITY OF SIENA, Siena, Italy)

#### **Targeting Protein-Protein Interactions: Bcl-2 Family Protein Inhibitors to Treat Cancer**

Dr. Steve ELMORE  
(ABBOTT LABORATORIES, Abbott Park, United States)

#### **Discovery Biology Fueled with Synthetic Chemicals**

Prof. Patrick G. HARRAN  
(UNIVERSITY OF CALIFORNIA, Los Angeles, United States)

### **Lunch & Poster session 1**

### **Afternoon Session: Business Mini-Symposium**

#### **Session Chair**

Dr Gene VAISBERG  
(CHEMBRIDGE CORPORATION, San Diego, United States)

#### **Compound Screenings in Model Plants to Identify New Agrochemicals: Strengths and Limitations**

Dr. Dominique AUDENAERT  
(GHENT UNIVERSITY, GHENT, Belgium)

#### **Creating a medicinal chemistry created screening library**

Dr. Peter BEAN  
(CYTOKINETICS, South San Francisco, United States)

## Program

---

### **Optimization of a Small Molecule Screening Library to support HTS Campaigns Across Diverse Therapeutic Areas and Target Classes**

Dr. Andrew.J. GARTON  
(OSI PHARMACEUTICALS, Framingdale, United States)

### **Strategies Toward The Establishment and Evolution of a CNS Focused Small Molecule Screening Collection**

Dr. Kevin HODGETTS  
(GALENEA, CAMBRIDGE, United States)

### **Small Molecule Screening Libraries in Drug Discovery: Today & Tomorrow**

Dr. Duncan JUDD  
(GLAXOSMITHKLINE, Essex, United Kingdom)

### **JHCC - When Vast Chemical Diversity Meets Ion Channel Targets**

Dr Min LI  
(JOHNS HOPKINS MEDICAL SCHOOL, Baltimore, United States)

### **Coffee-break**

### **Navigating the NIH Roadmap - Building a Screening Collection for Discovery of Biological Probes**

Dr. Victor PANCHENKO  
(BIOFOCUS, San Francisco, United States)

### **Kinase Inhibitors in Compound Collection of Life Chemicals**

Dr. Alexander POKHOLENKO  
(LIFE CHEMICALS, Ukraine)

### **Chemically Validated Combinatorial Approach to Large Libraries of Individual Drug Like Compounds**

Dr. Aleksandr SHIVANYUK  
(MACROCHEM, Kiev, Ukraine)

### **Scaffold-based Libraries: It's design and applications**

Dr. Bernd WENDT  
(EMBL HEIDELBERG, Heidelberg, Germany)

### **Out-Sourcing Of Small Molecule Screening Libraries: Lessons From The Past, View Into The Future**

Dr Gene VAISBERG  
(CHEMBRIDGE CORPORATION, San Diego, United States)

### **Q & A**

### **Closing of the day**

**Wednesday August 26, 2009**

### Morning Session

#### Session Chair

Prof. Valery P. KUKHAR  
(INSTITUTE OF BIOORGANIC CHEMISTRY AND PETROCHEMISTRY, Kyiv, Ukraine)

#### The Chemistry of DNA Repair and DNA Lesion Tolerance

Prof. Thomas CARELL  
(LUDWIG-MAXIMILIANS-UNIVERSITY MUNICH, München, Germany)

#### Design of BCR-Abl Kinase Inhibitors to Treat Imatinib-Resistant Leukaemia

Dr Paul W. MANLEY  
(NOVARTIS PHARMA, Basel, Switzerland)

#### SQUIRREL<sub>nov</sub>: De Novo Design of a PPAR $\alpha$ Agonist by Bioisosteric Replacement

Dr Ewgenij PROSCHAK  
(UNIVERSITÄT FRANKFURT, Frankfurt a. M., Germany)

### Coffee-break

#### Discovery of PF-610355: An Inhaled Once-daily Beta-2 Adrenoceptor Agonist for Asthma & COPD

Mr. Paul GLOSSOP  
(PFIZER GLOBAL R&D, Sandwich Kent, United Kingdom)

#### Discovery of NVP-BEZ235, a New Anti-Cancer Drug Candidate Targeting the PI3K/Akt/mTOR Pathway

Dr. Frédéric STAUFFER  
(NOVARTIS INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

#### Conformational Restriction as a Design Concept for Unnatural Amino Acids

Prof. Igor KOMAROV  
(KIEV TARAS SHEVCHENKO UNIVERSITY, Kiev, Ukraine)

#### Directed Evolution of Enzymes: New Biocatalysts for Organic Synthesis'

Prof. Nicholas John TURNER  
(UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

### Lunch and Poster Session 2

### Free afternoon

**Thursday August 27, 2009**

### Morning Session

#### Session Chair

Prof. Gerhard ECKER  
(UNIVERSITY OF VIENNA, Vienna, Austria)

#### A Small Molecule with a Big Impact: Inspirations from Proline Catalysis

Prof. Benjamin LIST  
(MAX PLANCK INSTITUTE, Muelheim an der Ruhr, Germany)

#### The Structure Based Design of Potent, Selective BACE1 Inhibitors as Potential Disease Modifying Treatments for Alzheimer's Disease

Dr AI ROBICHAUD  
(SAGE, Princeton, United States)

#### Chiral Imidates: A New Class of Nitrogen-Based Chiral Ligands.

Prof. Johan VAN DER EYCKEN  
(UGENT, Ghent, Belgium)

### Coffee-break and Poster Session 2

#### Orexin Receptor Antagonists – A New Therapeutic Principle in CNS Disorders?

Dr Christoph BOSS  
(ACTELION PHARMACEUTICALS LTD, Allschwil, Switzerland)

#### Guanidinium Toxins: Unique Natural Products in both Form and Function

Prof. Justin DU BOIS  
(STANFORD UNIVERSITY, Stanford, United States)

#### Cation–Pi Interactions in the S4 Pocket of Factor Xa: Dramatic Enhancement upon N-Alkylation of Ammonium Ions

Ms Laura Maria SALONEN  
(ETH ZURICH, Zurich, Switzerland)

### Lunch and Poster Session 2

### Afternoon Session

#### Session Chair

Prof. Erick M. CARREIRA  
(ETH ZÜRICH, Zürich, Switzerland)

#### Small Molecule Drug Discovery in the Modern World

Dr Michael VARNEY  
(GENENTECH, South San Francisco, United States)

#### Synthesis of Fluorine Containing Amino Acids with Biological Interest

Prof. Valery P. KUKHAR  
(INSTITUTE OF BIOORGANIC CHEMISTRY AND PETROCHEMISTRY, Kyiv, Ukraine)

## Program

---

### **Building Molecular Complexity via Gold Catalysis**

Prof. Antonio M. ECHAVARREN  
(INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA (ICIQ), Tarragona, Spain)

### **Coffee-break**

### **The Discovery of the Oral Antifungal Agent Albaconazole: a Case History**

Dr. Xavi BARTROLI  
(PALAU PHARMA, Palau de Plegamans, Spain)

### **New Catalytic Strategies for Chemical Synthesis**

Prof. Matthew GAUNT  
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

### **Closing Remarks**

### **Symposium banquet**