### **Plenary Lectures**

Plenary Lecture
Umpolung and the Art of Innovation



Youssef BENNANI (VERTEX PHARMACEUTICALS, Laval (Quebec), Canada)

Plenary Lecture
The Future of Medicinal Chemistry



Hans-Joachim BÖHM (HOFFMANN-LA ROCHE, Basel, Switzerland)

### Berlin: The Dynamic Science Metropole Responds to Challenges and Opportunities of the 21st Century



Günter STOCK (HEALTH CAPITAL BERLIN BRANDENBURG, Berlin, Germany)

Opening Lecture
Can Structure Lead to Better Antibiotics?



Ada YONATH (WEIZMANN INSTITUTE OF SCIENCE, Rehovot, Israel)

#### **EFMC Award Lectures**

The Prous Institute-Overton & Meyer Award for New Technologies in Drug Discovery Lecture Fragment-Based Drug Discovery - a Decade of Thinking Small



Harren JHOTI (ASTEX THERAPEUTICS, Cambridge, United Kingdom)

# The UCB-Ehrlich Award for Excellence in Medicinal Chemistry Lecture New Derivatives and Stereoisomers of Fenoterol: a Versatile Tool to Stimulate The B2 Adrenergic Receptor with Novel Therapeutical Perspectives



Krzysztof JOZWIAK (MEDICAL UNIVERSITY OF LUBLIN, Lublin, Poland)

## Nauta Award for Pharmacochemistry Lecture Targeting IRS1/2 and Targeting the Immune System to Eradicate Metastatic Tumors as New Modalities of Cancer Therapy



Alexander LEVITZKI (HEBREW UNIVERSITY OF JERUSALEM, Jerusalem, Israel)

#### **Prize Lectures**

http://www.ismc2012.org Page 1/14

EFMC Prize for a Young Medicinal Chemist in Industry
Minimising CNS Side Effects: DMPK Considerations in the design of Drugs with Limited Brain Penetration



Sharan BAGAL (PFIZER NEUSENTIS, Cambridge, United Kingdom)

#### EFMC Prize for a Young Medicinal Chemist in Academia Developing Inhibitors of the Bromodomain-acetyl-lysine Interaction



Stuart CONWAY (UNIVERSITY OF OXFORD, Los Angeles, United States)

IUPAC Richter Prize Lecture
Design and Synthesis of Drug Prototypes Inspired by Natural Products



Stephen HANESSIAN (UNIVERSITY OF MONTREAL, MONTREAL, QC, Canada)

#### Young Investigator Prize by DPhG and GDCh



Christian OTTMANN (MAX-PLANCK SOCIETY, Eindhoven, The Netherlands)

## **Invited Speakers**

#### New Phase I Enzymes Involved in Drug Metabolism and Prodrug Activation

#### The Discovery and Development of Anacetrapib



Amjad ALI (MERCK & CO. INC., Kenilworth, United States)

### Fragment-based Discovery of Modulators for PPI and Allosteric Enzymes



Michelle ARKIN (UNIVERSITY OF CALIFORNIA, San Francisco, CA, United States)

## Discovery of BAY 94-8862: A non-Steroidal Antagonist of the Mineralocorticoid Receptor for the Treatment of Cardiorenal Diseases



Lars BARFACKER (BAYER HEALTHCARE, WUPPERTAL, Germany)

Computer-assisted Lead Generation: Fact or Fiction

http://www.ismc2012.org Page 2/14



Karl-Heinz BARINGHAUS (SANOFI, Frankfurt, Germany)

#### Computational Approaches to Polypharmacology and Mode-of-Action Analysis



Andreas BENDER (UNIVERSITY OF CAMBRIDGE, United Kingdom)

## Identification of a New Chemical Class of Potent Antimycobacterial Compounds Derived from BM 212: Design, Synthesis, Biological Evaluation and Study of their Mode of Action



Mariangela BIAVA (LA SAPIENZA UNIVERSITY OF ROMA, Roma, Italy)

## Working with Medicinal Chemistry Experts in Academia and Industry to Generate Novel Inhibitors ("probes") for Novel Epigenetic Proteins



Paul BRENNAN (UNIVERSITY OF OXFORD, Oxford, United Kingdom)

## The Discovery of UCB5857 a Novel and Selective PI3K delta Inhibitor for the Treatment of Inflammatory Disease



Dan BROOKINGS (UCB, Slough, United Kingdom)

### GPCR Structure Based Drug Design Using Stabilised Receptors (StaRs)



Giles BROWN (HEPTARES, Hertfordshire, United Kingdom)

### **Chemical Probes for Epigenetics**



Mark BUNNAGE (PFIZER, Boston, United States)

## Strategies For The Design and Discovery of Compounds with Directed Against Challenging Targets of HIV-1 Life Cycle



Maria Jose CAMARASA (CSIC, Madrid, Spain)

#### Frontloading Toxicity Detection in order to Lower Costs and Attrition



Bruce D. CAR (BMS, Princeton, United States)

http://www.ismc2012.org Page 3/14

## Discovery of a Novel 2-aminothiazole Derivative (NVP-BYL719) with Potent and Selective PI3Kalpha Inhibitory Activity



Giorgio CARAVATTI (NOVARTIS, Basel, Switzerland)

#### Realizing the Potential of Antibody-Drug Conjugates for the Treatment of Cancer



Ravi CHARI (IMMUNOGEN, Waltham, United States)

#### **Small Molecule Control of Intracellular Protein Levels**



Craig CREWS (YALE UNIVERSITY, New Haven, CT, United States)

#### Industrialization of QSAR Model Generation-a Paradigm Shift in Predictive Modeling?



Andy DAVIS (ASTRAZENECA, Mölndal, Sweden)



Iwan DE ESCH (VU AMSTERDAM, Amsterdam, The Netherlands)

### Structure-Based Design of Novel Antibiotics for Treating Multidrug-resistant Bacterial Infections



Erin DUFFY (RIB-X PHARMACEUTICALS, Boston, United States)

#### **Drug Discovery in Neglected Diseases: Challenges and Opportunities**



Rich ELLIOTT (BILL AND MELINDA GATES FOUNDATION, Seattle, United States)

#### Transforming Pharmaceutical Manufacturing: Continuous - The Ultra Lean Way of Manufacturing



James EVANS (NOVARTIS/MIT CENTER FOR CONTINUOUS MANUFACTURING, Cambridge, United States)

### Downsizing Proteins: Peptidomimetics Beyond the Rule of Five



David FAIRLIE (UNIVERSITY OF QUEENSLAND, Brisbane, Australia)

## From Determinants of Binding to Modulators of Protein-Protein-Interactions

http://www.ismc2012.org Page 4/14

Holger GOHLKE (HEINRICH HEINE UNIVERSITY DÜSSELDORF, Düsseldorf, Germany)

## Discovery and Optimization of New Benzimidazole and Benzoxazole Pyrimidone PI3KB Inhibitors for the Treatment of PTEN-deficient Cancers



Frank HALLEY (SANOFI, Vitry-sur-Seine, France)

### Isoform Selective PDE4B Inhibitors: Testing a Hypothesis for Improved Therapeutic Index



Nicole HAMBLIN (GLAXO WELLCOME, Stevenage, United Kingdom)

#### From Chromatin Modulation to Drug Discovery: BET Bromodomain and EZH2 Inhibition



Jean-Christophe HARMANGE (CONSTELLATION PHARMACEUTICALS, Cambridge, United States)

### The Interface between Academia and Industry – Opportunities for Medicinal Chemists



Torsten HOFFMANN (F. HOFFMANN-LA ROCHE, Basel, Switzerland)

#### Stem Cells and Small Molecules



Lilian HOOK (PLASTICELL LTD., London, United Kingdom)

#### **Discovery of Chemical Probes for Histone Methyltransferases**



Jian JIN (UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

### **Antitubercular Nitroimidazoles**



Takushi KANEKO (TB ALLIANCE, New York, United States)



Danijel KIKELJ (UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**Session Chair** 

http://www.ismc2012.org Page 5/14



Gerhard KLEBE (PHILIPPS-UNIVERSITY MARBURG, Marburg, Germany)

#### API Bioavailability Hurdles - What Formulation Can Do



Peter LANGGUTH (JOHANNES GUTENBERG UNIVERSITY MAINZ, Mainz, Germany)

#### **Ligand Efficiency Metrics: A Cure for Molecular Inflation?**



Paul LEESON (GLAXOSMITHKLINE, Nuneaton, United Kingdom)

#### The Role of Passive Diffusion and Carrier-Mediated Transport in the Intestinal Drug Absorption Process



Hans LENNERNAS (UPPSALA UNIVERSITY, Uppsala, Sweden)



Alessio LODOLA (UNIVERSITY OF PARMA, Parma, Italy)

#### Selective Ion Channel Blockers for the Treatment of Atrial Fibrillation



David MADGE (XENTION, London, United Kingdom)

#### Maximizing Efficacy: How to win the Quest for Highly Potent Drugs



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

### Inhibiting Glucose Transport via SGLT Inhibitors - the Next New Diabetes Drug Family?



Michael MARK (BOEHRINGER INGELHEIM, Biberach, Germany)

### The Central Valine Concept revealed Indolyl-Imidazole Scaffold as p53-Hdm2 PPI Inhibitors



Keiichi MASUYA (NOVARTIS, Basel, Switzerland)

Development of M1 Allosteric Modulators for the Treatment of CNS Disorders and Improving Cognition

http://www.ismc2012.org Page 6/14



Bruce MELANCON (VANDERBILT CENTER FOR NEUROSCIENCE DRUG DISCOVERY, Nashville, United States)

#### **Predicting the Safety Profile of Bioactive Small Molecules**



Jordi MESTRES (IMIM AND UNIVERSITY POMPEU FABRA, Girona, Spain)

## In vitro – in vivo Extrapolation: Application of in vitro Approaches for Reaction Phenotyping and the Prediction of Metabolic Drug Clearance and Drug-Drug Interaction Potential



John MINERS (FLINDERS UNIVERSITY SCHOOL OF MEDICINE, Bedford Park, Australia)

### **Medicinal Chemistry Challenges for Kinetoplastid Diseases**



Charlie MOWBRAY (DRUGS FOR NEGLECTED DISEASES INITIATIVE (DNDI), Geneva, Switzerland)

#### Kinase Inhibitors with Pre-engineered Binding Kinetic Signatures



Gerhard MUELLER (MERCACHEM, Basel, Germany)

#### Arming Antibodies with Drugs and other Payloads: from the Bench to the Clinic



Dario NERI (ETH ZÜRICH, Zürich, Switzerland)

## PF-4958242: A Novel AMPA Positive Allosteric Modulator (PAM) for the Treatment of Cognitive Deficits Associated with Schizophrenia



Christopher O'DONNELL (PFIZER, New York, United States)

#### Small-Molecule Stabilization of 14-3-3 Protein-Protein Interactions: a Feasible Approach in Drug Discovery?



Christian OTTMANN (MAX-PLANCK SOCIETY, Eindhoven, The Netherlands)

### The Resurgence of Covalent Drugs



Russell PETTER (CELGENE AVILOMICS RESEARCH, Bedford, United States)

http://www.ismc2012.org Page 7/14

## **Nanomedicinal Chemistry and Nanotechnology**



Maurizio PRATO (UNIVERSITY OF TRIESTE, Trieste, Italy)

## Fragment-based Chemical Tools Targeting Proteases and Tyrosine Phosphatases Developed by Dynamic Ligation and Design



Jörg RADEMANN (UNIVERSTITÄT LEIPZIG, Leipzig, Germany)

#### Importance of Particle Size Control for Poorly Soluble Drugs



Thomas RAMMELOO (JANSSEN R&D, BEERSE, Belgium)

LE, LLE and FBDD



David REES (ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

#### **Biologics: Future Medicines for Metabolic Diseases?**



Cristina RONDINONE (MEDIMMUNE, Gaithersburg, United States)

#### Stem Cell Chemistry and its Impact in Drug Discovery



Angela RUSSELL (UNIVERSITY OF OXFORD, Oxford, United Kingdom)

#### **Novel Paradigms for GPCR Allosteric Modulator Identification**



Stephan SCHANN (DOMAIN THERAPEUTICS, Strasbourg, France)

## Structures of Active and Inactive G Protein Coupled Receptors: Implications for the Activation Mechanism and Pharmacology



Gebhard F.X. SCHERTLER (PAUL SCHERRER INSTITUTE, Villigen, Switzerland)

The Discovery and Optimization of a Novel Series of LPA Receptor Antagonists with Efficacy in Multiple Mouse Models of Fibrosis

http://www.ismc2012.org Page 8/14



Jon SEIDERS (BMS, San Diego, United States)

#### **Empowered Antibodies for Cancer Therapy**



Peter SENTER (SEATTLE GENETICS, Bothell, United States)

#### A Major Leap into the Chemical Space of Protein-Protein Interaction Inhibitors



Olivier SPERANDIO (INSERM, Paris, France)

#### **RaPID Discovery of Non-Traditional Peptide Drug Leads**



Hiroaki SUGA (UNIVERSITY OF TOKYO, Tokyo, Japan)

#### Improved Prediction of in vivo Effects by Combining Cheminformatics and Short-term Assay Data

Alexander TROPSHA (UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

#### **Experiences of Fragment-based Drug Discovery**

Marcel VERDONK (ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

## Translational Strategies for Identifying Chemically Reactive Metabolites as Cause for Adverse Drug Reactions



Nico VERMEULEN (VU UNIVERSITY, Amsterdam, The Netherlands)

### Polymer-conjugates as Nano-sized Medicines



Maria VICENT (RESEARCH CENTRE PRÍNCIPE FELIPE, Valencia, Spain)

### **Antimalarial Medicinal Chemistry "Opportunities and Challenges"**



David WATERSON (MEDICINES FOR MALARIA VENTURE, Geneva, Switzerland)

## A Novel Asymmetric Propargylation Reaction and its Application to the Large Scale Synthesis of Drug Candidates

http://www.ismc2012.org



Nathan YEE (BOEHRINGER INGELHEIM PHARMACEUTICALS, Ridgefield, United States)

#### Ligand Efficiency and Physical Properties Control, the Keys to Successful Drug Discovery?



Rob YOUNG (GLAXOSMITHKLINE, Hertfordshire, United Kingdom)

## Innovation Needs New Ways of Thinking: Talk to a Chemical Biologist in Academia



Giovanna ZINZALLA (KAROLINSKA INSTITUTET, Cambridge, United Kingdom)

### **Oral Communications**

Development of Small Molecule Embryonic Stem Cell Stimulators of Cardiogenesis: Case Study of a Medicinal Chemistry Approach

#### Targeting Protein-Protein Interactions in the Brain



Kristian STROMGAARD (UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

## Discovery and SARs of Novel Benzimidazole Derivatives as Potential Flap Inhibitors Based on a Combined Ligand- and Structure-Based Virtual Screening



Erden BANOGLU (GAZI UNIVERSITY, Ankara, Turkey)

## Structure-Activity-Relationship Study of (2S,3R)-3-(3-Carboxy-phenyl)-pyrrolidine-2-carboxylic Acid: Towards First Selective Kainate Receptor Subtype 3 (GluK3) Antagonist



Lennart BUNCH (UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

#### Towards a Differential Antimalarial Drug Through the Tres Cantos Antimalarial Set (TCAMS)



Félix CALDERÓN (GLAXOSMITHKLINE, Madrid, Spain)

#### Discovery of JNJ-18038683, a Selective 5-HT7 Receptor Antagonist: Preclinical and Clinical Evaluation



Nicholas CARRUTHERS (JOHNSON & JOHNSON R&D, San Diego, United States)

Fragments, Fits, Fingerprints: Structure-Based Virtual Screening for Fragment-Like GPCR Ligands

http://www.ismc2012.org Page 10/14

Chris DE GRAAF (VU UNIVERSITY AMSTERDAM, Amsterdam, The Netherlands)

#### New Selective Androgen Receptor Modulators (SARM) for the Treatment of Cachexia



Pierre DEPREZ (GALAPAGOS, Romainville, France)

### Optimization of Novel Alkylpyrazoles as Potent Antimalarial Agents



Beatriz DÍAZ HERNÁNDEZ (GLAXOSMITHKLINE R&D SPAIN, Tres Cantos, Spain)

#### **Targeting Oncogenic microRNAs: Toward New Chemotherapies**



Maria DUCA (UNIVERSITY OF NICE SOPHIA ANTIPOLIS, Nice, France)

### **Anti-Adhesion Therapy for the Treatment of Infective Diseases**



Beat ERNST (UNIVERSITY OF BASEL, Basel, Switzerland)

## Boosting Ethionamide as a New Strategy to Fight Tuberculosis: in vitro and in vivo Validation of 1,2,4-Oxadiazole EthR Inhibitors



Marion FLIPO (U761 BIOSTRUCTURE AND DRUG DISCOVERY, Lille, France)

## Total Synthesis of New Functionalized Epothilone Analogs for Prodrug Design and Tumor Targeting



Fabienne GAUGAZ (ETH ZÜRICH, Zürich, Switzerland)

## The Discovery and Early Clinical Development of CNV1014802: A Novel, NAV1.7 Selective, State-Dependent Sodium Channel Blocker for the Treatment of Neuropathic Pain



Gerard GIBLIN (CONVERGENCE PHARMACEUTICALS, Cambridge, United Kingdom)

#### A Chemical Biology Tool Developed in Yeast for Direct Targets Identification of a Bioactive Compound



Marie-Edith GOURDEL (HYBRIGENICS SAS, Paris, France)

#### Targeted, Polymer-Based Nanoparticles for Delivery of Camptothecin

http://www.ismc2012.org Page 11/14



Han HAN (CALIFORNIA INSTITUTE OF TECHNOLOGY, Pasadena, United States)

## Aldehyde Oxidase Metabolism - An Emerging but Surmountable Problem in Modern Drug Discovery



Peter JONES (PFIZER, Cambridge, United States)

## 4-Phenyl Imidazoles: A Novel Class of Phosphodiesterase 10A (PDE10A) Inhibitors as a Potential New Generation of Antipsychotics



Jan KEHLER (H. LUNDBECK A/S, Valby, Denmark)

### Disrupting the Amyloid Cascade- BACE 1 Inhibition for the Treatment of Alzheimer's Disease



Daniel LA (AMGEN, Cambridge, United States)

## From the Clinic to the Lab and Back -Discovery of PAN-CDK Inhibitors



Ulrich LÜCKING (BAYER HEALTHCARE, Basel, Switzerland)

## Novel Triazolopyridine Compounds as Selective JAK1 Kinase Inhibitors: From Target Discovery to the Clinical Candidate GLPG0634



Christel MENET (GALAPAGOS, Brussels, Belgium)

## Multi-Criteria Decision Making Methods: A Paradigm Applied to the Discovery of the First SV2C Selective Chemical Series



Joël MERCIER (UCB, BRAINE-L'ALLEUD, Belgium)

#### **Endoperoxide-Vinyl Sulfone Hybrids as Dual Acting Antimalarials**



Rudi OLIVEIRA (IMED.UL, Lisboa, Portugal)

## Developments of an Integrated in Silico Prediction System of Drug Toxicity Endpoints



Manuel PASTOR (UNIVERSITAT POMPEU FABRA, Barcelona, Spain)

http://www.ismc2012.org Page 12/14

#### Discovery and Profiling of Potent and Selective mTOR Inhibitor GDC-0349



Zhonghua PEI (GENENTECH, INC, South San Francisco, United States)

### The Power of Molecular Matched-Pair Analysis in Drug Design: Case Study of Oxadiazoles



Alleyn T. PLOWRIGHT (ASTRAZENECA, Cambridge, United Kingdom)

## Tetrahydroquinoline Derivatives as Potent and Selective Factor XIA Inhibitors



Mimi QUAN (BMS, Pennington, United States)

## 4,4-Dioxo-5,6-Dihydro-[1,4,3]Oxathiazines as a Novel Class of 11ß-HSD1 Inhibitors for the Treatment of Diabetes



Kurt RITTER (SANOFI, Frankfurt, Germany)

#### New Inhibitors of Cathepsin A for the Treatment of Cardiovasuclar Diseases



Sven RUF (SANOFI, Frankfurt, Germany)

#### Potent and Selective Autotaxin (ATX) Inhibitors



Kai SCHIEMANN (MERCK KGAA, DARMSTADT, Germany)

### Novel Potent and Selective NAM'S of the GABAA 5 Receptor Sub-Type



Andrew THOMAS (F. HOFFMANN-LA ROCHE LTD, Basel, Switzerland)

## Discovery of the Clinical Candidate TMC647055, a non Nucleoside Inhibitor of the Hepatitis C Virus NS5B Polymerase



Sandrine VENDEVILLE (JANSSEN INFECTIOUS DISEASES, Beerse, Belgium)

Towards Modulators of GABA Transporters: Screening of "Pseudo-static" Dynamic Combinatorial Libraries by ms Binding Assays

http://www.ismc2012.org Page 13/14

## EFMC-ISMC 2012

## **Confirmed Speakers**



Klaus T. WANNER (LUDWIG - MAXIMILIANS-UNIVERSITÄT MÜNCHEN, Munich, Germany)

## **WORKSHOPS**

### **WORKSHOP NOVALIX**

BIOPHYSICAL TECHNIQUES IN DRUG DISCOVERY

#### **WORKSHOP ACCELRYS**

NEW COMPUTATIONAL METHODS FOR FRAGMENT BASED LEAD DESIGN

http://www.ismc2012.org Page 14/14