

## Confirmed Speakers

### 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 Pharmacochimistry 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

## Confirmed Speakers

### 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 HANESEAN  
(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

## Confirmed Speakers



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)

## Confirmed Speakers

### Discovery of a Novel 2-aminothiazole Derivative (NVP-BYL719) with Potent and Selective PI3K $\alpha$ 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

## Confirmed Speakers

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

## Confirmed Speakers



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

## Confirmed Speakers



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 AVIOMICS RESEARCH, Bedford, United States)

## Confirmed Speakers

### 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  
(UNIVERSITÄT 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



## Confirmed Speakers



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

## Confirmed Speakers



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-HT<sub>7</sub> 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

## Confirmed Speakers

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**

## Confirmed Speakers



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)

## Confirmed Speakers

### 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 11 $\beta$ -HSD1 Inhibitors for the Treatment of Diabetes



Kurt RITTER  
(SANOFI, Frankfurt, Germany)

### New Inhibitors of Cathepsin A for the Treatment of Cardiovascular 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

## Confirmed Speakers

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

## WORKSHOPS

### WORKSHOP NOVALIX

BIOPHYSICAL TECHNIQUES IN DRUG DISCOVERY

### WORKSHOP ACCELRYX

NEW COMPUTATIONAL METHODS FOR FRAGMENT BASED LEAD DESIGN