

Programme

Sunday September 2, 2012

16:30 Opening Ceremony

16:50 Berlin: The Dynamic Science Metropole Responds to Challenges and Opportunities of the 21st Century

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

Chair

Eckhard OTTOW
(BAYER HEALTHCARE, Berlin, Germany)

17:15 EFMC Award Ceremony

**17:40 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)

Chair

Henk TIMMERMAN
(VU UNIVERSITY AMSTERDAM, Oegstgeest, The Netherlands)

**18:25 Opening Lecture
Can Structure Lead to Better Antibiotics?**

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

New Phase I Enzymes Involved in Drug Metabolism and Prodrug Activation

Bernd CLEMENT
(UNIVERSITY OF KIEL, Kiel, Germany)

19:15 Welcome Reception

Programme

Monday September 3, 2012

- 08:30 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 Therapeutic Perspectives**
Krzysztof JOZWIAK
(MEDICAL UNIVERSITY OF LUBLIN, Lublin, Poland)

Chair

Christophe GENICOT
(UCB BIOPHARMA, Brussels, Belgium)

- 09:15 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)

Chair

Josep Jr. PROUS
(PROUS INSTITUTE FOR BIOMEDICAL RESEARCH, Barcelona, Spain)

- 10:00 Exhibition & Coffee**

Session 1.1 New Small Molecule Approaches for Neglected Diseases

Session Chair

Jeremy BURROWS
(MEDICINES FOR MALARIA VENTURE (MMV), Geneva, Switzerland)

- 10:35 Drug Discovery in Neglected Diseases: Challenges and Opportunities**

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

- 11:15 Medicinal Chemistry Challenges for Kinetoplastid Diseases**

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

- 11:35 Antimalarial Medicinal Chemistry "Opportunities and Challenges"**

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

- 11:55 Antitubercular Nitroimidazoles**

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

Session 1.2 Intractable Targets: Is Bigger Better?

Session Chair

Herbert WALDMANN
(MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)

- 10:35 RaPID Discovery of Non-Traditional Peptide Drug Leads**

Hiroaki SUGA
(UNIVERSITY OF TOKYO, Tokyo, Japan)

- 11:15 Downsizing Proteins: Peptidomimetics Beyond the Rule of Five**

David FAIRLIE
(UNIVERSITY OF QUEENSLAND, Brisbane, Australia)

- 11:55 Small-Molecule Stabilization of 14-3-3 Protein-Protein Interactions: a Feasible Approach in Drug Discovery?**

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

Programme

Session 1.3 Chemistry and Stem-cell Research - Small Molecule Modulation of Stem Cells for Regenerative Medicines

Session Chair

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

10:35 Stem Cell Chemistry and its Impact in Drug Discovery

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

11:15 Stem Cells and Small Molecules

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

11:55 Development of Small Molecule Embryonic Stem Cell Stimulators of Cardiogenesis: Case Study of a Medicinal Chemistry Approach

12:15 WORKSHOPS

12:15 Poster Session 1 - Lunch

12:15 WORKSHOP ACCELRY'S

NEW COMPUTATIONAL METHODS FOR FRAGMENT BASED LEAD DESIGN

Session 2.4 Antibody-Drug Conjugates - Finally Ready for Prime Time? (ACS SESSION I)

Session Chair

Gene DUBOWCHIK
(BMS, Wallingford, United States)

13:50 Empowered Antibodies for Cancer Therapy

Peter SENTER
(SEATTLE GENETICS, Bothell, United States)

14:30 Realizing the Potential of Antibody-Drug Conjugates for the Treatment of Cancer

Ravi CHARI
(IMMUNOGEN, Waltham, United States)

15:10 Arming Antibodies with Drugs and other Payloads: from the Bench to the Clinic

Dario NERI
(ETH ZÜRICH, Zürich, Switzerland)

Session 2.5 Metabolic Disorders

Session Chair

Peter MOHR
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

13:50 Biologics: Future Medicines for Metabolic Diseases?

Cristina RONDINONE
(MEDIMMUNE, Gaithersburg, United States)

14:30 Inhibiting Glucose Transport via SGLT Inhibitors - the Next New Diabetes Drug Family?

Michael MARK
(BOEHRINGER INGELHEIM, Biberach, Germany)

15:10 4,4-Dioxo-5,6-Dihydro-[1,4,3]Oxathiazines as a Novel Class of 11 β -HSD1 Inhibitors for the Treatment of Diabetes

Kurt RITTER
(SANOFI, Frankfurt, Germany)

Session 2.6 Anti-Infectives and the Resistance Problem

Session Chair

Programme

Maurizio BOTTA
(UNIVERSITY OF SIENA, Siena, Italy)

13:50 Structure-Based Design of Novel Antibiotics for Treating Multidrug-resistant Bacterial Infections

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

14:30 Strategies For The Design and Discovery of Compounds with Directed Against Challenging Targets of HIV-1 Life Cycle

Maria Jose CAMARASA
(CSIC, Madrid, Spain)

14:50 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)

15:10 Endoperoxide-Vinyl Sulfone Hybrids as Dual Acting Antimalarials

Rudi OLIVEIRA
(IMED.UL, Lisboa, Portugal)

15:30 Exhibition & Coffee

Session 3.7 Chemical Biology Approaches in Drug Discovery

Session Chair

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

16:20 Small Molecule Control of Intracellular Protein Levels

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

17:00 Fragment-based Chemical Tools Targeting Proteases and Tyrosine Phosphatases Developed by Dynamic Ligation and Design

Jörg RADEMANN
(UNIVERSITÄT LEIPZIG, Leipzig, Germany)

17:40 A Chemical Biology Tool Developed in Yeast for Direct Targets Identification of a Bioactive Compound

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

Session 3.8 Fighting Cancer: Kinases and Beyond

Session Chair

Carlos GARCIA-ECHEVERRIA
(SANOFI, Vitry sur Seine, France)

16:20 The Resurgence of Covalent Drugs

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

17:00 Discovery of a Novel 2-aminothiazole Derivative (NVP-BYL719) with Potent and Selective PI3Kalpha Inhibitory Activity

Giorgio CARAVATTI
(NOVARTIS, Basel, Switzerland)

17:20 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)

17:40 Discovery and Profiling of Potent and Selective mTOR Inhibitor GDC-0349

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

Session 3.9 Designing Better Drugs: Ligand Efficiency Guided Optimization in Drug Discovery (ACS Session II)

Session Chair

Programme

Kap-Sun YEUNG
(BMS, Cambridge, United States)

16:20 Ligand Efficiency Metrics: A Cure for Molecular Inflation?

Paul LEESON
(GLAXOSMITHKLINE, Nuneaton, United Kingdom)

16:55 LE, LLE and FBDD

David REES
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

17:30 Ligand Efficiency and Physical Properties Control, the Keys to Successful Drug Discovery?

Rob YOUNG
(GLAXOSMITHKLINE, Hertfordshire, United Kingdom)

Session 3.10 Sunset Session: How the Industrial/Academic Interface is Changing Medicinal Chemistry

Chair

Alan BROWN
(PFIZER NEUSENTIS, Deal, United Kingdom)

18:05 The Interface between Academia and Industry – Opportunities for Medicinal Chemists

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

18:20 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)

18:35 Innovation Needs New Ways of Thinking: Talk to a Chemical Biologist in Academia

Giovanna ZINZALLA
(KAROLINSKA INSTITUTET, Cambridge, United Kingdom)

20:30 Concert

Programme

Tuesday September 4, 2012

08:30 Plenary Lecture
The Future of Medicinal Chemistry
Hans-Joachim BÖHM
(HOFFMANN-LA ROCHE, Basel, Switzerland)

Chair
Edmond DIFFERDING
(DIFFERDING CONSULTING, Louvain-la-Neuve, Belgium)

09:15 IUPAC Richter Prize Lecture
Design and Synthesis of Drug Prototypes Inspired by Natural Products
Stephen HANESSIAN
(UNIVERSITY OF MONTREAL, MONTREAL, QC, Canada)

Chair
Robin GANELLIN
(UNIVERSITY COLLEGE LONDON, London, United Kingdom)

10:00 Exhibition & Coffee

Session 4.11 Strategies to Tackle Challenging Targets in Oncology

Session Chair
Martin MISSBACH
(NOVARTIS, Basel, Switzerland)

10:35 Maximizing Efficacy: How to win the Quest for Highly Potent Drugs
Paul W. MANLEY
(NOVARTIS PHARMA, Basel, Switzerland)

11:15 Kinase Inhibitors with Pre-engineered Binding Kinetic Signatures
Gerhard MUELLER
(MERCACHEM, Basel, Germany)

11:35 The Central Valine Concept revealed Indolyl-Imidazole Scaffold as p53-Hdm2 PPI Inhibitors
Keiichi MASUYA
(NOVARTIS, Basel, Switzerland)

11:55 Total Synthesis of New Functionalized Epothilone Analogs for Prodrug Design and Tumor Targeting
Fabienne GAUGAZ
(ETH ZÜRICH, Zürich, Switzerland)

Session 4.12 Recent Highlights in Medicinal Chemistry

Session Chair
Maria Luz LOPEZ-RODRIGUEZ
(COMPLUTENSE UNIVERSITY OF MADRID, Madrid, Spain)

10:35 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)

11:00 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)

11:25 Potent and Selective Autotaxin (ATX) Inhibitors
Kai SCHIEMANN
(MERCK KGAA, DARMSTADT, Germany)

Programme

- 11:50 Discovery of the Clinical Candidate TMC647055, a non Nucleoside Inhibitor of the Hepatitis C Virus NS5B Polymerase**

Sandrine VENDEVILLE
(JANSSEN INFECTIOUS DISEASES, Beerse, Belgium)

Session 4.13 New Opportunities in Lead Discovery

Session Chair

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

- 10:35 Computer-assisted Lead Generation: Fact or Fiction**

Karl-Heinz BARINGHAUS
(SANOFI, Frankfurt, Germany)

- 11:15 Computational Approaches to Polypharmacology and Mode-of-Action Analysis**

Andreas BENDER
(UNIVERSITY OF CAMBRIDGE, United Kingdom)

- 11:35 Experiences of Fragment-based Drug Discovery**

Marcel VERDONK
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

- 11:55 From Determinants of Binding to Modulators of Protein-Protein-Interactions**

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

- 12:15 Poster Session 2 - Lunch**

- 12:15 WORKSHOP NOVALIX**

BIOPHYSICAL TECHNIQUES IN DRUG DISCOVERY

Session 5.14 Epigenetics - An Area Offering Formidable Challenges and Opportunities for Medicinal Chemists

Session Chair

Dashyant DHANAK
(GLAXOSMITHKLINE, United States)

- 13:50 Chemical Probes for Epigenetics**

Mark BUNNAGE
(PFIZER, Boston, United States)

- 14:30 From Chromatin Modulation to Drug Discovery : BET Bromodomain and EZH2 Inhibition**

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

- 14:50 Discovery of Chemical Probes for Histone Methyltransferases**

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

- 15:10 Targeting Oncogenic microRNAs: Toward New Chemotherapies**

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

Session 5.15 New Developments in CNS Drug Research

Session Chair

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

- 13:50 Development of M1 Allosteric Modulators for the Treatment of CNS Disorders and Improving Cognition**

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

- 14:30 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)

Programme

15:10 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)

Session 5.16 Targeting Protein-Protein Interactions

Session Chair

Kristian STROMGAARD
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

13:50 Fragment-based Discovery of Modulators for PPI and Allosteric Enzymes

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

14:30 A Major Leap into the Chemical Space of Protein-Protein Interaction Inhibitors

Olivier SPERANDIO
(INSERM, Paris, France)

15:10 Targeting Protein-Protein Interactions in the Brain

Kristian STROMGAARD (UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

15:30 Exhibition & Coffee

Session 6.17 What's New in GPCR Research?

Session Chair

Ad P. IJZERMAN
(LEIDEN UNIVERSITY, Leiden, The Netherlands)

16:20 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)

17:00 GPCR Structure Based Drug Design Using Stabilised Receptors (StaRs)

Giles BROWN
(HEPTARES, Hertfordshire, United Kingdom)

17:20 Novel Paradigms for GPCR Allosteric Modulator Identification

Stephan SCHANN
(DOMAIN THERAPEUTICS, Strasbourg, France)

17:40 Fragments, Fits, Fingerprints: Structure-Based Virtual Screening for Fragment-Like GPCR Ligands

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

Session 6.18 Next Generation of Cardiovascular Drugs

Session Chair

Hanno WILD
(BAYER HEALTHCARE, Wuppertal, Germany)

16:20 The Discovery and Development of Anacetrapib

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

17:00 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)

17:20 Selective Ion Channel Blockers for the Treatment of Atrial Fibrillation

David MADGE
(XENTION, London, United Kingdom)

17:40 Tetrahydroquinoline Derivatives as Potent and Selective Factor XIA Inhibitors

Mimi QUAN
(BMS, Pennington, United States)

Programme

Session 6.19 Hot Trends in Process Chemistry

Session Chair

Vittorio FARINA
(JANSSEN R&D, Beerse, Belgium)

16:20 Transforming Pharmaceutical Manufacturing: Continuous - The Ultra Lean Way of Manufacturing

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

17:00 Importance of Particle Size Control for Poorly Soluble Drugs

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

17:40 A Novel Asymmetric Propargylation Reaction and its Application to the Large Scale Synthesis of Drug Candidates

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

Session 7.20 Sunset Session: Productivity vs. Development of Independent and Creative Thinking During the PhD Period

18:00 Chair

Silvia ORTEGA GUTIERREZ
(COMPLUTENSE UNIVERSITY OF MADRID, Madrid, Spain)

Danijel KIKELJ
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

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

Alessio LODOLA
(UNIVERSITY OF PARMA, Parma, Italy)

Freya KLEPSCH
(UNIVERSITY OF VIENNA, Vienna, Austria)

Programme

Wednesday September 5, 2012

08:30 Prize ceremony

**08:45 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)

Chair

Janet ROBERTSON
(TES PHARMA S.R.L., Corciano , Italy)

**09:05 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)

Chair

Hein COOLEN
(3V-LSI, Utrecht, The Netherlands)

09:25 Young Investigator Prize by DPhG and GDCh
Christian OTTMANN
(MAX-PLANCK SOCIETY, Eindhoven, The Netherlands)

Chair

Peter GMEINER
(FRIEDRICH ALEXANDER UNIVERSITY, Erlangen, Germany)

09:45 Exhibition & Coffee

Session 8.21 Predictive Tools, Virtual Screening and Cheminformatics

Session Chair

Andy DAVIS
(ASTRAZENECA, Mölndal, Sweden)

10:35 Industrialization of QSAR Model Generation-a Paradigm Shift in Predictive Modeling ?
Andy DAVIS
(ASTRAZENECA, Mölndal, Sweden)

11:15 Improved Prediction of in vivo Effects by Combining Cheminformatics and Short-term Assay Data
Alexander TROPSHA
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

11:55 The Power of Molecular Matched-Pair Analysis in Drug Design: Case Study of Oxadiazoles
Alley T. PLOWRIGHT
(ASTRAZENECA, Cambridge, United Kingdom)

Session 8.22 New Promising Developments

Session Chair

Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)

10:35 Anti-Adhesion Therapy for the Treatment of Infective Diseases
Beat ERNST
(UNIVERSITY OF BASEL, Basel, Switzerland)

11:00 Disrupting the Amyloid Cascade- BACE 1 Inhibition for the Treatment of Alzheimer's Disease

Programme

Daniel LA
(AMGEN, Cambridge, United States)

11:25 New Selective Androgen Receptor Modulators (SARM) for the Treatment of Cachexia

Pierre DEPREZ
(GALAPAGOS, Romainville, France)

11:50 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)

Session 8.23 Drug Safety: What Toxic Effects can be Reasonably Predicted?

Session Chair

Thomas STEGER-HARTMANN
(BAYER HEALTHCARE, Berlin, Germany)

10:35 Frontloading Toxicity Detection in order to Lower Costs and Attrition

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

11:15 Translational Strategies for Identifying Chemically Reactive Metabolites as Cause for Adverse Drug Reactions

Nico VERMEULEN
(VU UNIVERSITY, Amsterdam, The Netherlands)

11:35 Predicting the Safety Profile of Bioactive Small Molecules

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

11:55 Developments of an Integrated in Silico Prediction System of Drug Toxicity Endpoints

Manuel PASTOR
(UNIVERSITAT POMPEU FABRA, Barcelona, Spain)

12:15 Poster Session 3 - Lunch

15:00 Excursions

20:00 Gala Dinner

Thursday September 6, 2012

Session 9.24 Molecular Therapies for Inflammatory and Autoimmune Diseases

Session Chair

Graham WARRELOW
(UCB, Slough, United Kingdom)

- 08:35 The Discovery of UCB5857 a Novel and Selective PI3K delta Inhibitor for the Treatment of Inflammatory Disease**
Dan BROOKINGS
(UCB, Slough, United Kingdom)
- 09:00 The Discovery and Optimization of a Novel Series of LPA Receptor Antagonists with Efficacy in Multiple Mouse Models of Fibrosis**
Jon SEIDERS
(BMS, San Diego, United States)
- 09:25 Isoform Selective PDE4B Inhibitors: Testing a Hypothesis for Improved Therapeutic Index**
Nicole HAMBLIN
(GLAXO WELLCOME, Stevenage, United Kingdom)
- 09:50 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)

Session 9.25 First Time Disclosures

Session Chair

Katarzyna KIEC-KONONOWICZ
(JAGIELLONIAN UNIVERSITY, Krakow, Poland)

- 08:35 Towards a Differential Antimalarial Drug Through the Tres Cantos Antimalarial Set (TCAMS)**
Félix CALDERÓN
(GLAXOSMITHKLINE, Madrid, Spain)
- 09:00 Optimization of Novel Alkylpyrazoles as Potent Antimalarial Agents**
Beatriz DÍAZ HERNÁNDEZ
(GLAXOSMITHKLINE R&D SPAIN, Tres Cantos, Spain)
- 09:25 From the Clinic to the Lab and Back -Discovery of PAN-CDK Inhibitors**
Ulrich LÜCKING
(BAYER HEALTHCARE, Basel, Switzerland)
- 09:50 New Inhibitors of Cathepsin A for the Treatment of Cardiovascular Diseases**
Sven RUF
(SANOFI, Frankfurt, Germany)

Session 9.26 Challenges and Opportunities for Drug Metabolism in Drug Discovery and Preclinical Drug Development (AFMC Session)

Session Chair

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

- 08:35 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)
- 09:15 New Phase I Enzymes Involved in Drug Metabolism and Prodrug Activation**
- 09:55 Aldehyde Oxidase Metabolism - An Emerging but Surmountable Problem in Modern Drug Discovery**
Peter JONES
(PFIZER, Cambridge, United States)
- 10:15 Exhibition & Coffee**

Programme

Session 10.27 From Nano to Macro (EUCHEMS Session)

Session Chair

Péter MÁTYUS
(SEMMEIWEIS UNIVERSITY, Budapest, Hungary)

10:50 Polymer-conjugates as Nano-sized Medicines

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

11:30 Nanomedicinal Chemistry and Nanotechnology

Maurizio PRATO
(UNIVERSITY OF TRIESTE, Trieste, Italy)

12:10 Targeted, Polymer-Based Nanoparticles for Delivery of Camptothecin

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

Session 10.28 Late Breaking News

Session Chair

Pascal GEORGE
(SCT & INDEPENDENT SCIENTIFIC EXPERT & ADVISER, Longvilliers, France)

10:50 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)

11:15 Discovery of JNJ-18038683, a Selective 5-HT₇ Receptor Antagonist: Preclinical and Clinical Evaluation

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

11:40 Novel Triazolopyridine Compounds as Selective JAK1 Kinase Inhibitors: From Target Discovery to the Clinical Candidate GLPG0634

Christel MENET
(GALAPAGOS, Brussels, Belgium)

12:05 Novel Potent and Selective NAM'S of the GABAA 5 Receptor Sub-Type

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

Session 10.29 The Impact of Transporters in Drug Discovery and Oral Bioavailability Enhancement (EUFEPS Session)

Session Chair

Andreas LINK
(UNIVERSITY OF GREIFSWALD, Germany)

10:50 The Role of Passive Diffusion and Carrier-Mediated Transport in the Intestinal Drug Absorption Process

Hans LENNERNAS
(UPPSALA UNIVERSITY, Uppsala, Sweden)

11:30 API Bioavailability Hurdles - What Formulation Can Do

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

12:10 Towards Modulators of GABA Transporters: Screening of "Pseudo-static" Dynamic Combinatorial Libraries by ms Binding Assays

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

12:30 Plenary Lecture Umpolung and the Art of Innovation

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

Chair

Programme

Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)

13:15 **Poster Prizes, Closing Remarks & Welcome to ISM 2014**