

### Sunday September 7, 2014

- 16:15**      **Opening Ceremony**
- 16:35**      **Portugal: the Right Place to build Partnerships in Health**  
Dr Joaquim CUNHA  
(HEALTH CLUSTER PORTUGAL, Maia, Portugal)
- 16:50**      **Partnership between Public and Private Sources: Pharma and IMI Perspective**  
Dr Paul Peter TAK  
(EFPIA, Brentford, United Kingdom)
- 17:10**      **EFMC Award Ceremony**
- 17:35**      **The Nauta Award for Pharmacochemistry  
Pursuing Compound Quality**  
Dr Paul LEESON  
(GLAXOSMITHKLINE, United Kingdom)
- 18:20**      **High Resolution Mass Spectrometry in Clinical Proteomics**  
Prof. Dr Matthias MANN  
(MAX PLANCK INSTITUTE OF BIOCHEMISTRY, Martinsried, Germany)
- 19:10**      **Welcome Reception**

## Programme Schedule

### Monday September 8, 2014

- 08:30 The UCB-Ehrlich Award for Excellence in Medicinal Chemistry  
Small Molecule Control Of Intracellular Protein Levels**  
Prof. Craig CREWS  
(YALE UNIVERSITY, New Haven, United States)
- 09:15 The Prous Institute-Overton and Meyer Award for New Technologies i Drug Discovery  
Thermodynamics Assisted Drug Discovery**  
Dr György G. FERENCZY (HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)  
Prof. Gyorgy KESERU (HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)
- 10:00 Exhibition & Coffee**

#### Session 1.1 Inflammation: the Common Link in Multifactorial Disorders?

- 10:30 Session Chair**  
Dr Angeliki KOUROUNAKIS  
(UNIVERSITY OF ATHENS, Athens, Greece)
- 10:35 Inflammation, Obesity and Metabolic Disease**  
Dr Ajay CHAWLA  
(UNIVERSITY OF CALIFORNIA, San Francisco, United States)
- 11:15 CB2 Agonists Protect from Inflammation Related Kidney Damage and Fibrosis**  
Dr Uwe GREETHER  
(F. HOFFMANN-LA-ROCHE, Basel, Switzerland)
- 11:35 The Discovery of APD334, a Selective S1P1 Functional Antagonist**  
Dr Robert JONES  
(ARENA PHARM, SAN DIEGO, United States)
- 11:55 Discovery of Small Molecule Ror? Modulators for the Treatment of Autoimmune Diseases**  
Dr Frank NARJES  
(ASTRAZENECA, Mölndal, Sweden)

#### Session 1.2 Computational Approaches To Guide Medicinal Chemistry

- 10:30 Session Chair**  
Prof. Helmut GRUBMÜLLER  
(MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)
- 10:35 Mechanoenzymatics of Biomolecular Machines: Free Energies, Dynamics, Function**  
Prof. Helmut GRUBMÜLLER  
(MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)
- 11:15 Efficient Determination Of Protein-Ligand Standard Binding Free Energies And Permeabilities With A  
Computational Microcalorimeter**  
Dr Chris CHIPOT  
(UNIVERSITY OF ILLINOIS, Urbana, United States)
- 11:35 Binding Affinity Prediction from Molecular Simulation – Soon a Standard Method in Structure-Based Drug  
Design?**  
Dr Clara CHRIST  
(BAYER PHARMA, Berlin, Germany)
- 11:55 P-Glycoprotein/Membrane Role on Multidrug Resistance: Insights from In Silico Studies**  
Mr Ricardo FERREIRA  
(FACULTY OF PHARMACY, UNIVERSITY OF LISBON, Lisbon, Portugal)

#### Session 1.3 Organic Synthesis that Changed Medicinal Chemistry

- 10:30 Session Chair**  
Dr Morten JORGENSEN  
(H. LUNDBECK A/S, Valby, Denmark)
- 10:35 Recent Advances In Asymmetric Catalysis**

## Programme Schedule

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

**11:15 New Stereoselective Organocatalytic Reactions for the Synthesis of Isoquinoline Alkaloids**

Prof. Pier Giorgio COZZI  
(UNIVERSITY OF BOLOGNA, Bologna, Italy)

**11:35 Metalation of Polyfunctional Heterocyclic Compounds: Applications in Agrochemistry**

Dr Marc MOSRIN  
(BAYER CROPSOURCE AG, Frankfurt am Main, Germany)

**11:55 Development of Novel Building Blocks to Accelerate Drug Discovery**

Dr Pavel MYKHAILIUK  
(ENAMINE, Kyiv, Ukraine)

**12:15 Exhibition & Lunch**

### Session 2.4 Combating Antibiotic Resistance

**13:15 Session Chair**

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

**13:20 Aminoglycoside Mechanisms of Action, Resistance and Toxicity – Prospects for Antibiotic Drug Development**

Prof. Erik BOETTGER  
(UNIVERSITY OF ZÜRICH, Zürich, Switzerland)

**14:00 Visualising Novel Macrolide Antibiotics Bound to Their Ribosomal Target**

Prof. Stephen DOUTHWAITE  
(UNIVERSITY OF SOUTHERN DENMARK, Odense, Denmark)

**14:20 The Ribosome as a Drug Target: Insights from Structural Investigations - Towards Rational Drug Design**

Dr Moran SHALEV BEN AMI  
(WEIZMANN INSTITUTE, Rehovot, Israel)

**14:40 Antagonists of the Pseudomonas Quinolone Signal Receptor (PQSR) as Promising Anti-Virulence Agents**

Dr Martin EMPTING  
(HELMHOLTZ-INSTITUTE F. PHARMACEUTICAL RESEARCH SAARLAND, Saarbrücken, Germany)

### Session 2.5 Taming Natural Products: Novel Natural Products, Complex Synthesis, Mutasynthesis

**13:15 Session Chair**

Prof. Anake KIJJOA  
(UNIVERSITY OF PORTO, Porto, Portugal)

**13:20 Natural Products as Driving Force for Innovation in Pharmaceutical Research and Development**

Dr Esther SCHMITT  
(NOVARTIS, Basel, Switzerland)

**14:00 Sponging Off Nature for New Drug Leads**

Prof. Raymond ANDERSEN  
(UNIVERSITY OF BRITISH COLUMBIA, Vancouver, Canada)

**14:20 Bioactive Secondary Metabolites From The Soil And Marine-Derived Fungi Of The Genus Neosartorya**

Prof. Anake KIJJOA  
(UNIVERSITY OF PORTO, Porto, Portugal)

**14:40 From Malaysian Biodiversity to the Total Synthesis of Dual Inhibitors of BCL-XL and MCL-1 Anti-Apoptotic Protein**

Dr Fanny ROUSSI  
(ICSN - CNRS, Gif sur Yvette, France)

### Session 2.6 Mechanism-Based Prediction of Drug-Induced Liver Injury (Eufeps Session)

**13:15 Session Chair**

Prof. Nico VERMEULEN  
(VU UNIVERSITY, Amsterdam, The Netherlands)

**13:20 Mechanism-Based Prediction of Drug-Induced Liver Injury**

## Programme Schedule

Dr Christopher GOLDRING  
(UNIVERSITY OF LIVERPOOL, Liverpool, United Kingdom)

**14:00 Strategies to Identify and Manage the Risks of Chemically Reactive Drug Metabolites**

Prof. Nico VERMEULEN  
(VU UNIVERSITY, Amsterdam, The Netherlands)

**14:20 Being More Certain About Uncertainty In Computational Toxicology Modeling**

Dr Scott BOYER  
(KAROLINSKA INSTITUTET, Södertälje, Sweden)

**14:40 Covalent Modification of Histones by Nevirapine - A Plausible Pathway to Nevirapine-Induced Cancers?**

Dr Alexandra ANTUNES  
(INSTITUTO SUPERIOR TÉCNICO, Lisbon, Portugal)

**15:00 Exhibition & Coffee**

**15:30 MedChemComm Prize Winner : Phage Selection Of Bicyclic Peptides For Therapeutic Application**

Prof. Christian HEINIS  
(ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL), Lausanne, Switzerland)

### Session 3.7 EFMC Session

**15:55 Session Chair**

Dr Phil JONES  
(UNIVERSITY OF DUNDEE, Lanarkshire, United Kingdom)

**16:00 The Open Phacts Discovery Platform - Semantic Data Integration For Medicinal Chemists**

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

**16:30 European Lead Factory - Game Changing For Innovative Medicines**

Dr Dimitrios TZALIS  
(TAROS CHEMICALS, Dortmund, Germany)

**17:00 Funding Opportunities with the Innovative Medicines Initiative 2**

Dr Colm CARROLL  
(INNOVATIVE MEDICINES INITIATIVE, Brussels, Belgium)

**17:30 Poster Session I and Networking**

**19:30 End of the day**

**20:30 Concert (free of charge, but subject to registration)**

## Programme Schedule

### Tuesday September 9, 2014

- 08:30 Prize Ceremony**
- 08:35 EFMC Prize for a Young Medicinal Chemist in Industry  
Design, Synthesis and Properties of Potent Inhibitors of Pseudomonas Aeruginosa Deacetylase LpxC**  
Dr Grazia PIZZI  
(NOVARTIS PHARMA, Basel, Switzerland)
- 08:55 EFMC Prize for a Young Medicinal Chemist in Academia  
Inhibitors and Substrates of the Human Lysine Deacylase Enzymes**  
Prof. Christian A. OLSEN  
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)
- 09:15 Plenary Lecture**  
Dr Sabine HADIDA  
(VERTEX PHARMACEUTICALS, San Diego, United States)
- 10:00 Exhibition & Coffee**

### Session 4.8 Applications of Positron Emission Tomography in Drug Discovery (ACS Session I)

- 10:30 Session Chair**  
Dr Sam BONACORSI  
(BRISTOL-MYERS SQUIBB, Princeton, United States)
- 10:35 PET Imaging: Synthesis of Radiopharmaceuticals and their Application in Personalized Medicine and Drug Discovery**  
Dr Peter J.H. SCOTT  
(UNIVERSITY OF MICHIGAN, Ann Arbor, United States)
- 11:15 A Rational Approach to the Development of Radioligands and PET Ligands for Drug Development**  
Dr Chad ELMORE  
(ASTRAZENECA PHARMACEUTICALS, Mölndal, Sweden)
- 11:35 Design, Synthesis and Development of Lysophosphatidic Acid Receptor 1 (LPA1) PET Radioligands for Lung Receptor Occupancy Imaging**  
Dr Sam BONACORSI  
(BRISTOL-MYERS SQUIBB, Princeton, United States)
- 11:55 Quantitative Imaging of Mglu5 Allosteric Binding Site and its Occupancy by Positron Emission Tomography with The Novel Fluorine-18 Labelled Probe [<sup>18</sup>f]Pss232**  
Dr Stefanie KRAMER  
(ETH ZÜRICH, Zürich, Switzerland)

### Session 4.9 Decoding Disease: Liganding and Drugging Bromodomain Epigenetic Readers

- 10:30 Session Chair**  
Prof. Stuart CONWAY  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)
- 10:35 BETting on Bromodomains: Developing Inhibitors of the Bromodomain-Acetyl-Lysine Interaction**  
Prof. Stuart CONWAY  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)
- 11:15 A First In Class Chemical Probe For Family VIII Bromodomains**  
Dr Dafydd OWEN  
(PFIZER, Cambridge, United States)
- 11:35 Epigenetic Drug Discovery: Small Molecule Inhibitors of Class IV Bromodomain Proteins**  
Prof. Paul FISH  
(UCL SCHOOL OF PHARMACY, London, United Kingdom)

## Programme Schedule

**11:55 Interrogation the Bromodomain Family through Chemical Biology**

Dr Steve BELLON  
(CONSTELLATION PHARMACEUTICALS, Cambridge, United States)

**Session 4.10 Organic Synthesis: New Developments  
(EuChemS Session)**

**10:30 Session Chair**

Prof. Péter MÁTYUS (SEMMELWEIS UNIVERSITY, Budapest, Hungary)  
(THERMO FISHER SCIENTIFIC)

**10:35 Experiences with Natural Product Total Synthesis**

Prof. Alois FÜRSTNER  
(MAX PLANCK INSTITUT FÜR KOHLENFORSCHUNG, Muelheim an der Ruhr, Germany)

**11:15 New Synthetic Routes of Nitrogen and Oxygen Heterocycles and Related Compounds**

Prof. Artur M.S. SILVA  
(UNIVERSITY OF AVEIRO, Aveiro, Portugal)

**11:35 Fast and Safe Synthesis of Pharmaceutically Relevant Molecules**

Prof. Thomas WIRTH  
(UNIVERSITY OF CARDIFF, Cardiff, United Kingdom)

**11:55 Metal Assisted Synthetic Approaches to Heterocyclic Small Molecules for the Treatment of Cardiovascular Diseases**

Prof. Marko D. MIHOVILOVIC  
(VIENNA UNIVERSITY OF TECHNOLOGY, Vienna, Austria)

**12:15 Exhibition & Lunch**

**Session 5.11 Oncology: Kinases and Beyond**

**13:15 Session Chair**

Dr Mario VARASI  
(EUROPEAN INSTITUTE OF ONCOLOGY, Milano, Italy)

**13:20 Therapeutic Opportunities Offered by the Excessive Lactate Production in Cancer**

Prof. Filippo MINUTOLO  
(UNIVERSITY OF PISA, Pisa, Italy)

**14:00 Novel Anti-Cancer Treatment Targeting Vps34**

Dr Jessica MARTINSSON  
(SPRINT BIOSCIENCE, Stockholm, Sweden)

**14:20 Exploiting Tumor Metabolic Vulnerabilities with Novel OxPhos Inhibitors**

Dr Maria Emilia DI FRANCESCO  
(UTMD ANDERSON CANCER CENTER, Houston, United States)

**14:40 Discovery and Characterization of A-366, a Novel, Potent and Highly Selective Inhibitor of Histone Methyltransferase G9a**

Dr Michael MICHAELIDES  
(ABBVIE, North Chicago, United States)

**Session 5.12 Recent Advances in Anti-infective Agents  
(AFMC Session)**

**13:15 Session Chair**

Dr Ming-Hua HSU  
(NATIONAL TSING HUA UNIVERSITY, Hsinchu, Taiwan)

**13:20 Development of New Anti-Infective Agents and a Novel Delivery Strategy**

Prof. Reuben JIH-RU HWU  
(NATIONAL TSING HUA UNIVERSITY, Hsinchu, Taiwan)

**14:00 Synthesis of Anti-infective Cyclic Natural Products and Natural Product-like Compounds**

Prof. Han-Young KANG  
(CHUNGBUK NATIONAL UNIVERSITY, Cheongju, Korea, South)

**14:20 Novel Boron-containing Anti-infective Agents**

## Programme Schedule

Dr Jacob PLATTNER  
(ANACOR PHARMACEUTICALS, Palo Alto, United States)

**14:40 Lectins as Targets in Antiadhesion Therapy - Example of DC-SIGN And FimH Antagonists**

Assoc. Prof. Marko ANDERLUH  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

### Session 5.13 New Strategies for Lead Generation

**13:15 Session Chair**

Dr Maria BLANCO-PILLADO  
(ELI LILLY AND COMPANY, Indianapolis, United States)

**13:20 Integration of New Chemical Diversity and Design Approaches in Lead Generation**

Dr Timothy GRESE  
(ELI LILLY AND COMPANY, Indianapolis, United States)

**14:00 The Impact of Polypharmacology on Lead Generation**

Prof. Jordi MESTRES  
(IMIM AND UNIVERSITY POMPEU FABRA, Barcelona, Spain)

**14:20 Starting Small, Thinking Big: The Application of Fragment Based Drug Discovery to Lead Generation**

Dr Steve WOODHEAD  
(TAKEDA CALIFORNIA, San Diego, United States)

**14:40 Discovery of the First and Only Small Molecule II-17 Blockers**

Dr Nils HANSEN  
(VIPERGEN, Copenhagen, Denmark)

**15:00 Exhibition & Coffee**

**15:30 Medicinal Chemistry Experts in Pharma are Helping us to Generate Freely Available Novel Probes in Order to Facilitate Target Discovery**

Prof. Chas BOUNTRA  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

**16:30 Poster Session II and Networking**

**18:30 End of the day**

### Wednesday September 10, 2014

- 08:30 IUPAC Richter Prize Lecture  
Medicinal Chemistry, Quo Vadis? - The Changing Climate In R&D**  
Dr Helmut BUSCHMANN  
(PHARMA CONSULTING AACHEN, Aachen, Germany)
- 09:15 Innovation Through Chemistry at the Interfaces of the Scientific Disciplines**  
Dr Martin MISSBACH  
(NOVARTIS, Basel, Switzerland)
- 10:00 Exhibition & Coffee**

#### Session 6.14 New Chemical Entities: Beyond Small Molecules

- 10:30 Session Chair**  
Prof. Stan VAN BOECKEL  
(LEIDEN INSTITUTE OF CHEMISTRY, Leiden, The Netherlands)
- 10:35 Cyclic Peptides from the nature to the synthetic ones**  
Prof. Fernando ALBERICIO  
(UNIVERSITY OF BARCELONA, Barcelona, Spain)
- 11:15 Successful Drug Discovery And Development Case Studies Of Protein Epitope Mimetics**  
Dr Daniel OBRECHT  
(POLYPHOR, Allschwil, Switzerland)
- 11:35 Cell-Permeable Peptide Therapeutics to Effectively Access Intracellular Targets in Cancer Stem Cells**  
Dr Jörg VOLLMER  
(NEXIGEN, Cologne, Germany)
- 11:55 Novel Inhibitors of Alzheimer's Associated Beta-Secretase-Clusters of Heparan Sulfate**  
Dr Olga ZUBKOVA  
(VICTORIA UNIVERSITY OF WELLINGTON, Lower Hutt , New Zealand)

#### Session 6.15 Novel Agents for the Treatment of C. Difficile (ACS Session II)

- 10:30 Session Chair**  
Prof. Steven FIRESTINE  
(WAYNE STATE UNIVERSITY, Detroit, United States)
- 10:35 Discovery and Development of Surotomycin for the Treatment of C. difficile**  
Dr Jared SILVERMAN  
(CUBIST PHARMACEUTICALS, Lexington, United States)
- 11:15 Invited Lecture**  
Dr Terry BOWLIN  
(MICROBIOTIX, Worcester, United States)
- 11:35 Targeting Spore Germination to Prevent Clostridium Difficile Infections**  
Dr Ernesto ABEL-SANTOS  
(UNIVERSITY OF NEVADA, LAS VEGAS, Nevada, Las Vegas, United States)
- 11:55 Cadazolid: A New Antibiotic in Development for the Treatment of Clostridium Difficile-Associated Diarrhea (CDAD)**  
Dr Philippe PANCHAUD  
(ACTELION PHARMACEUTICALS LTD, Allschwil, Switzerland)

#### Session 6.16 Kinetic and Thermodynamic Aspects of Ligand Binding

- 10:30 Session Chair**  
Prof. Gyorgy KESERU  
(HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)
- 10:35 Exploring the Dynamics of Ligand-Protein Interactions using SPR Biosensors**



## Programme Schedule

Prof. Helena DANIELSON  
(UPPSALA UNIVERSITY, Uppsala, Sweden)

**11:15 Breaking The Equilibrium Dissociation Constant Into Fragments: The Use Of Binding Kinetics And Thermodynamics In The Development Of Selective Ligands.**

Prof. Iwan DE ESCH  
(VU UNIVERSITY AMSTERDAM, Amsterdam, The Netherlands)

**11:35 Medicinal Chemistry Optimisation Of Binding Kinetics**

Prof. Mike WARING  
(ASTRAZENECA, Newcastle upon Tyne, United Kingdom)

**11:55 CRTH2: Can Residence Time Help?**

Dr Elena GOMEZ  
(ALMIRALL, BARCELONA, Spain)

**12:15 Exhibition & Lunch**

### Session 7.17 Recent Highlights in Medicinal Chemistry

**13:15 Session Chair**

Prof. Carlos MONTANARI  
(UNIVERSITY OF SAO PAULO, Sao Paulo, Brazil)

**13:20 Cebranopadol, a Novel, Potent Analgesic**

Dr Henning STEINHAGEN  
(GRÜNENTHAL, Verona, Italy)

**13:40 Discovery of BAY 1002670 - A Highly Potent and Selective Progesterone Receptor Modulator for Gynecological Therapies**

Dr Wolfgang SCHWEDE  
(BAYER, Berlin, Germany)

**14:00 Design, Synthesis and Biological Evaluation of Potent and Selective Class IIA Histone Deacetylase Inhibitors as a Potential Therapy for Huntington's Disease**

Dr Christopher LUCKHURST  
(BIOFOCUS, Saffron Walden, United Kingdom)

**14:20 Structure-Guided Design of Potent, Selective, Orally Bioavailable Tankyrase Inhibitors**

Dr Erin DIMAURO  
(AMGEN, Cambridge, United States)

**14:40 Novel Potent Inhibitors of the Histone Demethylase KDM1A**

Dr Paola VIANELLO  
(EUROPEAN INSTITUTE OF ONCOLOGY, Milan, Italy)

### Session 7.18 Hot Topics in Ion Channels

**13:15 Session Chair**

Prof. Brian COX  
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Brighton, United Kingdom)

**13:20 An Introduction To Ion Channels As Drug Targets**

Prof. Morten GRUNNET  
(LUNDBECK, Valby, Denmark)

**14:00 CNV1014802, a Novel Nav1.7 Selective State-Dependent Sodium Channel Blocker for the Treatment of Chronic Pain: From Discovery to Phase 2 Clinical Study**

Dr Gerard GIBLIN  
(CONVERGENCE PHARMACEUTICALS, Cambridge, United Kingdom)

**14:20 Pain-relieving Peptides Targeting Acid-Sensing Ion Channels**

Dr Eric LINGUEGLIA  
(CNRS-UNIVERSITY OF NICE SOPHIA ANTIPOLIS, Valbonne, France)

**14:40 Discovery of Ivacaftor (Vx-770), a Cfr Potentiator for the Treatment of Cystic Fibrosis in G551d Patients**

Dr Sabine HADIDA  
(VERTEX PHARMACEUTICALS, San Diego, United States)

### Session 7.19 Allosteric Modulators for CNS Diseases

## Programme Schedule

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**13:15 Session Chair**

Dr Wolfgang FROESTL  
(AC IMMUNE, Lausanne, Switzerland)

**13:20 Functional and Structural Insights into GPCR Allostery**

Prof. Arthur CHRISTOPOULOS  
(MONASH UNIVERSITY, Parkville, Australia)

**14:00 Discovery of the mGlu5 Negative Allosteric Modulator RO4917523**

Dr Georg JAESCHKE  
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

**14:20 Allosteric Protein Kinases Inhibitors for Neurodegenerative Diseases Therapies**

Prof. Ana MARTINEZ  
(INSTITUTO DE QUIMICA MEDICA-CSIC, Madrid, Spain)

**14:40 Antibodies as Tools to Enable Small Molecule Drug Discovery**

Dr Marta WESTWOOD  
(UCB, Slough, United Kingdom)

**15:00 Excursions**

**20:00 Banquet**

### Thursday September 11, 2014

#### Session 8.20 GPCR Structural Biology: New Therapeutic Opportunities?

**08:30 Session Chair**

Prof. Jan STEYAERT  
(VUB, Brussels, Belgium)

**08:35 High End Design for GPCRs: Combining Protein Structure, Biophysical Data and Computational Water Network Energies**

Dr. Jonathan MASON  
(HEPTARES THERAPEUTICS, Welwyn Garden City, United Kingdom)

**09:15 Nanobody-Enabled Fragment Screening On Active-State Constrained GPCRs**

Prof. Jan STEYAERT  
(VUB, Brussels, Belgium)

**09:35 Covalent Agonists Facilitating Crystallisation of GPCRs**

Prof. Peter GMEINER  
(FRIEDRICH ALEXANDER UNIVERSITY, Erlangen, Germany)

**09:55 Crystallographic Structures Enable the Discovery of Selective 5-Ht1b Receptor Ligands through Virtual Screening**

Dr David RODRIGUEZ DIAZ  
(STOCKHOLM UNIVERSITY, Solna, Sweden)

#### Session 8.21 Neglected Tropical Diseases: Shaping Future Trends

**08:30 Session Chair**

Prof. Kelly CHIBALE  
(UNIVERSITY OF CAPE TOWN, Cape Town, South Africa)

**08:35 Update on Chemotherapy of Tropical Diseases Caused by Protozoan Parasites**

Prof. Reto BRUN  
(SWISS TROPICAL AND PUBLIC HEALTH INSTITUTE, Basel, Switzerland)

**09:15 Antimalarial Trioxolanes - Exploiting Peroxide Reduction For Parasite-Selective Drug Delivery**

Dr Adam RENSLO  
(UNIVERSITY OF CALIFORNIA, San Francisco, United States)

**09:35 Antimalarial Lead Discovery from phenotypic screening: Unraveling the Black Box**

Dr Francisco-Javier GAMO  
(GLAXOSMITHKLINE, Madrid, Spain)

**09:55 Improving Physicochemical Properties of a Lapatinib-Based Lead Compound that Targets Trypanosoma Brucei**

Prof. Jennifer WOODRING  
(NORTHEASTERN UNIVERSITY, Boston, United States)

#### Session 8.22 New Therapies for Metabolic Disorders

**08:30 Session Chair**

Dr Jürgen MACK  
(BOEHRINGER INGELHEIM, Biberach an der Riss, Germany)

**08:35 Pharmaceutical Protein & Peptide Engineering: From Once Daily To Once Weekly GLP-1 Dosing**

Dr Jesper LAU  
(NOVO NORDISK, Maaloev, Denmark)

**09:15 1,1'-Spiro-Substituted Hexahydrofuroquinoline Derivatives As Potent And Polar Cholesteryl Ester Transfer Protein (CETP) Inhibitors**

Dr Thomas TRIESELMANN  
(BOEHRINGER INGELHEIM PHARMA GMBH & CO. KG, Biberach an der Riss, Germany)

**09:35 Omarigliptin: A Once-weekly Oral Antidiabetic Agent**

Dr Tesfaye BIFTU  
(MERCK, Rahway, United States)

**09:55 Discovery of GPR103 Ligands Demonstrating the Anorexigenic Effect in vivo of GPR103 Antagonism**

Dr Anneli NORDQVIST  
(ASTRAZENECA, Mölndal, Sweden)

## Programme Schedule

10:15 **Exhibition & Coffee & Snacks**

### Session 9.23 Late Breaking News

10:45 **Session Chair**

Dr Laurence LAFANECHERE  
(CNRS, Grenoble, France)

10:50 **CHF-6001, an Inhaled PDE4 Inhibitor for Asthma and COPD: Synthesis, In Vitro and In Vivo Characterization**

Dr Maurizio DELCANALE  
(CHIESI, Parma, Italy)

11:10 **The Discovery of AZD5069; a CXCR2 Antagonist In Phase II Clinical Trials for the Treatment of Asthma**

Dr Rhona COX  
(ASTRAZENECA, Mölndal, Sweden)

11:30 **Discovery of BAY 85-8501, a Novel and Highly Potent Induced-Fit Binder of Human Neutrophil Elastase for Pulmonary Diseases**

Dr Franz VON NUSSBAUM  
(BAYER PHARMA, Lyon, France)

11:50 **Discovery of TD-5959 (Batefenterol/GSK-961081): A First-in-Class Dual Pharmacology Multivalent Muscarinic Antagonist and Beta-2 Agonist (MABA) for the Treatment of COPD**

Dr Adam HUGHES  
(THERAVANCE INC., South San Francisco, United States)

12:10 **Identifying Selective Inhibitors of FGFR4 Kinase**

Dr Kurt PIKE  
(ASTRAZENECA, Cambridge, United Kingdom)

### Session 9.24 Neurodegeneration: Deeper Understanding of Disease Biology and Emerging Therapeutic Options

10:45 **Session Chair**

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

10:50 **CaV1.3-Selective L-Type Calcium Channel Negative Allosteric Modulators. Novel Therapeutics to Slow the Progression of Parkinson's Disease**

Prof. Rick SILVERMAN  
(NORTHWESTERN UNIVERSITY, Evanston, United States)

11:30 **Restoration of Muscle Mass and Lifespan in a Mouse Model of Spinal Muscular Atrophy by Molecular Correction of SMN2 Splicing Defect**

Dr Hasane RATNI  
(F. HOFFMANN-LA ROCHE LTD, Basel, Switzerland)

11:50 **Fragment-Based Discovery of BACE Inhibitors for Alzheimer's Disease**

Dr Andrew STAMFORD  
(MERCK RESEARCH LABORATORIES, Rahway, United States)

12:10 **The Evolution of an in vivo Efficacious Bace1 Inhibitor**

Dr Daniel OEHLRICH  
(JOHNSON & JOHNSON PHARMACEUTICAL RESEARCH AND DEVELOPMENT, Beerse, Belgium)

### Session 9.25 Translational Medicine: Case Studies with Biomarkers and PKPD Modeling

10:45 **Session Chair**

Dr Yves P. AUBERSON  
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

10:50 **Translational Modeling in Support to Discovery and Early Development**

Dr Thierry LAVE  
(F.HOFFMANN-LA ROCHE LTD, Basel, Switzerland)

11:30 **Non-Clinical Characterization And Clinical Translation Of LY2811376 And LY2886721**

Dr Dustin James MERGOTT  
(ELI LILLY, Indianapolis, United States)

11:50 **A HTS Assay Predicting Both Passive Intestinal Absorption and Affinity Constant Towards Human Serum Albumin in a Two End-Point Measurement**

## Programme Schedule

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Mr Alban BUJARD  
(UNIVERSITY OF GENEVA, Geneva, Switzerland)

**12:10 Biomarkers after Bacteriochlorin Based Photodynamic Therapy against Cancer**

Dr Martyna KRZYKAWSKA-SERDA  
(FACULTY OF BIOCHEMISTRY, BIOPHYSICS AND BIOTECHNOLOGY, JAGIELLONIAN UNIVERSITY, Krakow, Poland)

**12:30 Closing Lecture  
Personalised Medicinal Systems Chemistry**

Prof. Hans WESTERHOFF  
(VU UNIVERSITY AMSTERDAM, Amsterdam, The Netherlands)

**13:15 Closing Remarks, Poster Prizes and Welcome to EFMC-ISMIC 2016**