

### Sunday August 28, 2016

#### Registration

#### Opening Ceremony

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

#### Science, Art and Drug Discovery, a Personal Perspective

Sir Simon CAMPBELL  
(SCIENTIFIC CONSULTANT, Poole, United Kingdom)

#### Chair

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

#### The European Research Council (ERC) and its Support for Medicinal Chemistry

Prof. Klaus BOCK  
(UNIVERSITY OF COPENHAGEN , Copenhagen, Denmark)

#### Chair

Prof. Rebecca DEPRez-POULAIN  
(UNIVERSITY OF LILLE, Lille, France)

#### Award Ceremony

Prof. Koen AUGUSTYNS  
(UNIVERSITY OF ANTWERP, Antwerp, Belgium)

#### NAUTA AWARD FOR PHARMACOCHEMISTRY

#### Molecular Recognition Studies with Chemical and Biological Systems: A Multi-Dimensional Approach to Support Structure-Based Drug Design

Prof. François DIEDERICH  
(ETH ZURICH, Zürich, Switzerland)

#### Chair

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

#### Late-Stage Fluorination

Prof. Tobias RITTER  
(MAX-PLANCK-INSTITUT FÜR KOHLENFORSCHUNG, Mulheim, Germany)

#### Chair

Dr Anette GRAVEN SAMS  
(H. LUNDBECK, Valby, Denmark)

#### Welcome Reception Sponsored by Concept Life Sciences

### Monday August 29, 2016

#### **UCB-EHRLICH AWARD FOR EXCELLENCE IN MEDICINAL CHEMISTRY Traversing the Valley of Death in Anticancer Drug Discovery**

Prof. Paul J. HERGENROTHER  
(UNIVERSITY OF ILLINOIS, Urbana, United States)

#### **Chair**

Dr Laurent PROVINS  
(UCB, Braine-l'Alleud, Belgium)

#### **Cross-Coupling Approaches to Saturated N-Heterocycles**

Prof. Jeffrey BODE  
(ETH ZURICH, Zürich, Switzerland)

#### **Chair**

Karin BRINER  
(NOVARTIS, South San Francisco, United States)

#### **Exhibition & Coffee**

### **Session 1.1 Intramolecular Hydrogen Bonding and its Impact in Drug Design and Discovery (ACSMEDI Session)**

#### **10:30 Session Chairs**

Dr Amjad ALI (MERCK & CO. INC., Kenilworth, United States)  
Dr Tanweer KHAN (MERCK, SHARP & DOHME, Kenilworth, United States)

#### **10:35 The Need of Implementing Intramolecular Hydrogen Bonding (IMHB) Considerations in Drug Discovery and How to do it**

Prof. Giulia CARON  
(UNIVERSITY OF TORINO, Torino, Italy)

#### **11:15 Intramolecular Hydrogen Bond Expectations in Medicinal Chemistry**

Dr Fabrizio GIORDANETTO  
(D.E. SHAW RESEARCH LLC, New York, United States)

#### **11:35 Intramolecular Hydrogen Bonding as a Design Element in Medicinal Chemistry**

Dr Bernd KUHN  
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

#### **11:55 Intramolecular Hydrogen Bonds in the Design of CREBBP Bromodomain Ligands**

Prof. Stuart CONWAY  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

### **Session 1.2 Drug Discovery Approaches Toward Targeting Ras**

#### **10:30 Session Chair**

Dr Joachim RUDOLPH  
(GENENTECH, South San Francisco, United States)

#### **10:35 Studying Ciliary Trafficking and How it Leads to RAS Drug Candidates**

Prof. Alfred WITTINGHOFER  
(MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)

#### **11:15 Chemical Biological Modulation of KRas-Signaling**

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

#### **11:35 Inhibition of Prenylated KRAS: Tools to Discover and Characterize RAS Ligands**

Dr Johanna JANSEN  
(NOVARTIS, Emeryville, United States)

#### **11:55 Small Molecule Binding Sites on the RAS: SOS Complex Can Be Exploited for Inhibition of RAS Activation**

Dr. Jon WINTER-HOLT  
(ASTRAZENECA, Macclesfield, United Kingdom)

## Programme Schedule

### Session 1.3 New Antibacterials. An Update

**10:30 Session Chair**

Prof. Malcolm PAGE  
(JACOBS UNIVERSITY, Bremen, Germany)

**10:35 New Antibacterial Agents in the Pipeline**

Dr Eric DESARBRE  
(BASILEA PHARMACEUTICA, Basel, Switzerland)

**11:15 Mechanistic and Inhibition Studies on Metallo-Beta-Lactamases**

Prof. Christopher J. SCHOFIELD  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

**11:35 Enterobactin-Dependent Iron Uptake Pathway as a Gate for Antibiotic Trojan Horse Strategies Against Pseudomonas Aeruginosa**

Dr Gaëtan MISLIN  
(UNIVERSITY OF STRASBOURG, Illkirch-Graffenstaden, France)

**11:55 Exploring Hit-Identification Strategies for Energy-Coupling Factor Transporters, a Novel Target for the Development of Antibiotics**

Ms Leticia MONJAS GOMEZ  
(UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)

### Exhibition & Lunch

### Flash Poster Presentations (12:30-13:10)

#### Session Chair

Prof. Stuart CONWAY  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

### Session 2.1 Peptides: Pushing Permeability and Bioavailability Beyond the Rule of 5 (ACSMEDI Session)

**13:15 Session Chairs**

Dr Peter CHENG (BRISTOL-MYERS SQUIBB, Hopewell, United States)  
Dr Claudio MAPELLI (BRISTOL-MYERS SQUIBB, United States)

**13:20 Peptides and Peptidomimetics: Overcoming Problems of Activity, Selectivity and Bioavailability of Integrin Ligands**

Dr Horst KESSLER  
(TECHNISCHE UNIVERSITÄT MÜNCHEN, Garching, Germany)

**14:00 Discovery & Optimization of Clips-Constrained Bicyclic Peptides (2clips) Using Pepscan Peptide Arrays**

Prof. Peter TIMMERMAN  
(PEPSCAN THERAPEUTICS, Lelystad, The Netherlands)

**14:20 Phage-Encoded Combinatorial Chemical Libraries Based on Bicyclic Peptides**

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

**14:40 Attempts at Oral Delivery of a Series of Short Unnatural Peptides: Still Like Pushing a Camel Through the Eye of a Needle?**

Dr Claudio MAPELLI  
(BRISTOL-MYERS SQUIBB, United States)

### Session 2.2 Recent Progress in the Treatment of Ophthalmological Diseases

**13:15 Session Chair**

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

**13:20 Molecular Pharmacodynamics of Visual Cycle Modulators in Protection Against Retinal Degeneration**

Prof. Krzysztof PALCZEWSKI  
(CASE WESTERN RESERVE UNIVERSITY, Cleveland, United States)

**14:00 The Back of The Eye: Treatment Challenges and Opportunities**

## Programme Schedule

Dr Muneto MOGI  
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)

**14:20 Regorafenib Eye Drops for Wet AMD – Challenges in Translatability of Preclinical Data Into Clinical Efficacy**

Dr Michael BÖTTGER  
(BAYER PHARMA, Wuppertal, Germany)

**14:40 Systemic Administration of an Allosteric GSK-3 Inhibitor Delays Photoreceptor Cell Death and Preserves Visual Function in a Retinitis Pigmentosa Mouse Model**

Prof. Ana MARTINEZ  
(CSIC, Madrid, Spain)

### Session 2.3 Molecular Tissue Targeting

**13:15 Session Chair**

Dr Malin LEMURELL  
(ASTRAZENECA, Gothenburg, Sweden)

**13:20 Ligand-Targeted Therapeutic and Imaging Agents for Multiple Human Diseases**

Prof. Philip S. LOW  
(PURDUE UNIVERSITY, West Lafayette, United States)

**14:00 Peptide Drugs to Target GPCR - State of the Art and Innovative Applications**

**14:20 The Development of Pyrrolobenzodiazepine in Antibody Drug Conjugates**

Dr Philip HOWARD  
(SPIROGEN LTD, London, United Kingdom)

**14:40 Photoisomerisable Allosteric Modulators Allow a Fine Control of mGlu Receptors with Light in Vivo (EFMC-YMCS Presentation Prize)**

Mr Xavier GÓMEZ-SANTACANA  
(VRIJE UNIVERSITEIT AMSTERDAM, Amsterdam, The Netherlands)

**Exhibition & Coffee**

### Session 3. First Time Disclosures

**15:30 Session Chair**

Dr David WITTY  
(CONVERGENCE PHARMACEUTICALS, United Kingdom)

**15:35 Discovery and Development of the Highly Potent, Highly Selective Cathepsin S Inhibitor RG7625 for the Treatment of Autoimmune Diseases**

Dr Wolfgang HAAP  
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

**16:05 First Time Disclosure of a Development Candidate to Treat Severe Acute Pancreatitis through a Drug Discovery Partnership Between GSK and the University of Edinburgh**

Dr John LIDDLE  
(GLAXOSMITHKLINE, Mölndal, Sweden)

**16:35 Discovery of AZD3241 is a Potent and Selective Myeloperoxidase Inhibitor for the Treatment of Neurodegenerative Disorders**

Dr Jörg HOLENZ  
(ASTRAZENECA NEUROSCIENCE, Collegeville, United States)

**17:05 Discovery of the HCV NS5A Inhibitor MK-8408 (RUZASVIR)**

Dr Joe KOZLOWSKI  
(MERCK, SHARP & DOHME, Rahway, United States)

**Poster Session (even numbers) with drinks**

**End of the day**

### Tuesday August 30, 2016

#### **PROUS INSTITUTE-OVERTON AND MEYER AWARD FOR NEW TECHNOLOGIES IN DRUG DISCOVERY Nanobody-Enabled HTS for the Discovery of GPCR Agonists**

Prof. Jan STEYAERT  
(VUB, Brussels, Belgium)

#### **Chair**

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

#### **EFMC Prize Ceremony**

Prof. Rui MOREIRA  
(UNIVERSITY OF LISBON, Lisbon, Portugal)

#### **EFMC Prize for a Young Medicinal Chemist in Industry Inhibition of the COP9 Signalosome as a Novel Approach to Treat Cancer"**

Dr Jean QUANCARD  
(NOVARTIS, Basel, Switzerland)

#### **EFMC Prize for a Young Medicinal Chemist in Academia Sigma Hole Bonding in Kinase Drug Discovery**

Prof. Frank BÖCKLER  
(EBERHARD-KARLS UNIVERSITY TUEBINGEN, Tübingen, Germany)

#### **Exhibition & Coffee**

### **Session 4.1 Making Small Molecule Synthesis Simpler, General, and Automatic**

#### **10:30 Session Chair**

Prof. Martin D. BURKE  
(UNIVERSITY OF ILLINOIS, Urbana, United States)

#### **10:35 Towards a More Generalized and Automated Approach for Small Molecule Synthesis**

Prof. Martin D. BURKE  
(UNIVERSITY OF ILLINOIS, Urbana, United States)

#### **11:15 Robot Scientists, the Replication Crisis, and Cancer**

Prof. Ross KING  
(UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

#### **11:35 Identifying Synthetic Opportunities Using Chemplanner - How Computers Assist Chemists in Covering a Greater Synthetic Space**

Dr Orr RAVITZ  
(WILEY, Chichester, United Kingdom)

#### **11:55 The evoSpace - A Synthesis-Driven Environment that Finds Accessible, Well-Behaved Compounds by Design**

Dr Marcus GASTREICH  
(BIOSOLVEIT, St. Augustin, Germany)

### **Session 4.2 Hot Topics in Cardiovascular Diseases Research**

#### **10:30 Session Chair**

Dr Susanne ROEHRIG  
(BAYER HEALTHCARE, Wuppertal, Germany)

#### **10:35 Discovery of a First-in-Class PAR4 Antagonist as a Novel Antithrombotic**

Dr Scott PRIESTLEY  
(BRISTOL-MYERS SQUIBB, Hopewell, United States)

#### **11:15 Discovery of Novel LPA1 Antagonist: Design and SAR Studies**

## Programme Schedule

Dr Masahiko TERAKADO  
(ONO PHARMACEUTICAL, Osaka, Japan)

- 11:35 Discovery of Clinical Candidate Ribuvaptan, a Dual Acting Vasopressin V1a/V2 Receptor Antagonist for the Treatment of Heart Failure**

Dr Carsten SCHMECK  
(BAYER, Wuppertal, Germany)

- 11:55 Classification of Adams Binding Sites: the First Step Toward Selective ADAMTS7 Inhibitors**

Mrs Michaela MÜLLER  
(UNIVERSITÄT ZU LÜBECK, Lübeck, Germany)

### Session 4.3 Neglected Diseases

- 10:30 Session Chair**

Dr Timothy MILES  
(GSK, Madrid, Spain)

- 10:35 Utilization of Novel Benzoxaboroles as Drug Candidates to Treat Neglected Tropical Diseases**

Dr Robert T. JACOBS  
(ANACOR PHARMACEUTICALS, California, United States)

- 11:15 The Development of DDD853651; a Potential Candidate for the Treatment of Visceral Leishmaniasis**

Dr Michael THOMAS  
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

- 11:35 Pharmacological Reversion of Antibiotic Resistance in Mycobacterium Tuberculosis : Design of SMART Trojan Molecules to Reprogram The Bacteria**

Prof. Benoit DEPPEZ  
(INSTITUT PASTEUR OF LILLE, Lille, France)

- 11:55 The Discovery and Development of Novel Macrophilicidal Agents for the Treatment of Onchocerciasis and Lymphatic Filariasis**

Dr Thomas VON GELDERN  
(ABBVIE, Chicago, United States)

### Exhibition & Lunch

**Advion Lunch Workshop: Compact Mass Spectrometry - The User's Perspective (12:15-13:45)**

**Flash Poster Presentations (12:30-13:10)**

### Session Chair

Dr Sharan BAGAL  
(ASTRAZENECA, Cambridge, United Kingdom)

### Session 5.1 Synthesis Driven Innovation

- 13:15 Session Chair**

Dr Jesus EZQUERRA  
(LABORATORIOS LILLY, Alcobendas, Spain)

- 13:20 Expanding the Macrocyclic Chemical Space**

Prof. Alexander DÖMLING  
(UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)

- 14:00 Potent and Highly Selective Bromodomain Ligands... a Platform for Reaction Discovery**

Prof. Cristina NEVADO  
(UNIVERSITY OF ZURICH, Zurich, Switzerland)

- 14:20 Nucleophilic Boron for the Preparation of Highly Functionalized Small Rings**

Prof. Mariola TORTOSA  
(AUTONOMOUS UNIVERSITY OF MADRID, Madrid, Spain)

- 14:40 Rapid Composition of Tricyclic Spiranoind Lactones: Access to Natural Frames and Application in Selective Silencing of the Pain Receptor TRPV1**

## Programme Schedule

Prof. Dmitry TSVELIKHOVSKY  
(THE HEBREW UNIVERSITY OF JERUSALEM, Jerusalem, Israel)

### Session 5.2 Modulation of Protein-Protein Interactions - Novel Opportunities for Drug Discovery

**13:15 Session Chair**

Dr Christian OTTMANN  
(EINDHOVEN UNIVERSITY OF TECHNOLOGY, Eindhoven, The Netherlands)

**13:20 Validating New Epigenetic Targets by Selective Protein Interaction Inhibitors of Bromodomains**

Prof. Stefan KNAPP  
(GOETHE UNIVERSITY FRANKFURT, Frankfurt am Main, Germany)

**14:00 Releasing the Brake on Apoptosis. Discovery of Bcl-2 Family Protein Inhibitors**

Dr Steven ELMORE  
(ABBVIE, North Chicago, United States)

**14:20 DNA-Encoded Chemical Library for Protein-Protein Interactions**

Dr Jin LI  
(HITGEN LTD, Chengdu, Sichuan, China)

**14:40 From Fragment to in vivo Activity for a Challenging PPI Target: the Discovery of Potent Inhibitors of the KEAP1-NRF2 Interaction**

Dr David NORTON  
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

### Session 5.3 Current Advances and Future Opportunities for the Treatment of Neurodegenerative Disorders

**13:15 Session Chair**

Dr Theodora CALOGEROPOULOU  
(NATIONAL HELLENIC RESEARCH FOUNDATION, Athens, Greece)

**13:20 Possibilities and Pitfalls: Disease Modifying Drugs for Alzheimer's Disease**

Dr Eric KARRAN  
(FOUNDATIONAL NEUROSCIENCE CENTER, ABBVIE, Cambridge, United States)

**14:00 Tackling Neurodegenerative Diseases Through Multi-Target and Theranostic Small Molecules**

Prof. Maria Laura BOLOGNESI  
(UNIVERSITY OF BOLOGNA, Bologna, Italy)

**14:20 Discovery of Brain-Penetrable LpPLA2 Inhibitor for Alzheimer's Disease**

Dr Xiaomin ZHANG  
(GLAXOSMITHKLINE, Shanghai, China)

**14:40 Modulation of RS67,333: from a 5-HT4R Partial Agonist to the Identification of Several Promising Multi-Target Directed Ligands for Alzheimer's Disease**

Prof. Christophe ROCHAIS  
(UNIVERSITY OF CAEN, Caen, France)

#### Exhibition & Coffee

#### Robotics, Artificial Intelligence, and Medicinal Chemistry: A Look Into the Future

Dr Derek LOWE  
(VERTEX PHARMACEUTICALS, Cambridge, United States)

#### Chair

Dr Matthew TOZER  
(CONSULTANT, Bognor Regis, United Kingdom)

#### Poster Session (odd numbers) with drinks

#### Close Poster Session

#### Public Lecture

End of the day



### Wednesday August 31, 2016

#### **IUPAC-RICHTER PRIZE**

##### **The Discovery of Sofosbuvir: A Breakthrough Curative Therapy for Hepatitis C**

Dr Michael SOFIA  
(ARBUS BIOPHARMA, Doylestown, United States)

#### **Chair**

Dr Janos FISCHER  
(RICHTER PLC, Budapest, Hungary)

#### **DNA-Encoded Chemical Libraries**

Prof. Dario NERI  
(ETH ZÜRICH, Zürich, Switzerland)

#### **Chair**

#### **Exhibition & Coffee**

### **Session 6.1 Big Data in Medicinal Chemistry**

#### **10:30 Session Chair**

Prof. Andrew HOPKINS  
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

#### **10:35 Big Data in Medicinal Chemistry?**

Prof. Gisbert SCHNEIDER  
(ETH ZÜRICH, Zürich, Switzerland)

#### **11:15 Exploiting Linked Open Data - Transporter Profiling and Beyond**

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

#### **11:35 Mining Structural Protein-Ligand Interactions to Navigate Medicinal Chemistry Space**

Dr Chris DE GRAAF  
(VU UNIVERSITY AMSTERDAM, Cambridge, United Kingdom)

#### **11:55 Non Coding RNA as a Small Molecule Druggable Target**

Dr Graham SMITH  
(MERCK, SHARP & DOHME, Boston, United States)

### **Session 6.2 New Horizons in GPCR-targeted Medicinal Chemistry**

#### **10:30 Session Chair**

Prof. Christa MÜLLER  
(UNIVERSITY OF BONN, Bonn, Germany)

#### **10:35 Identification of Allosteric Inhibitors of GPCRs Using SBDD**

Dr Miles CONGREVE  
(HEPTARES, Welwyn Garden City, United Kingdom)

#### **11:15 Medicinal Chemistry of Purinergic Signalling: Targets and Drugs for the Immunotherapy of Cancer**

Prof. Christa MÜLLER  
(UNIVERSITY OF BONN, Bonn, Germany)

#### **11:35 Targeting Long-Chain Fatty Acid Receptors FFA1 and FFA4 for Treatment of Metabolic Diseases**

Prof. Trond ULVEN  
(UNIVERSITY OF SOUTHERN DENMARK, København Ø, Denmark)

#### **11:55 Optimising Membrane Interactions to Achieve Duration of Action for Inhaled Drug Candidates**

Dr Mark HEALY  
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)

## Programme Schedule

### Session 6.3 Novel Approaches to the Treatment of Cancer

**10:30 Session Chair**

Dr Jonathan BENNETT  
(MERCK, SHARP & DOHME, Boston, United States)

**10:35 Small Molecule Approaches to Immune-Modulation in Cancer**

Dr Ronan O'HAGAN  
(MERCK, SHARP & DOHME, Boston, United States)

**11:15 The Identification of GSK2879552, a Mechanism Based Irreversible Inhibitor of the Histone Lysine Demethylase LSD1**

Dr Neil W. JOHNSON  
(GLAXOSMITHKLINE, Collegeville, United States)

**11:35 Discovery of AG-120 – A First-in-class Inhibitor of IDH1 Mutant Enzymes for the Treatment of Cancers Harboring IDH1 Mutations**

Dr Janeta POPOVICI-MULLER  
(AGIOS PHARMACEUTICALS, United States)

**11:55 Targeting the Janus-Faced Nature of IDO1 in Immuno-Oncology**

Prof. Antonio MACCHIARULO  
(UNIVERSITY OF PERUGIA, Perugia, Italy)

**Exhibition & Lunch**

**Chemical Computing Group Lunch Workshop: Structure-Based Drug Design and Ligand Modification (12:15-13:45)**

### Session 7.1 Emerging Topics

**13:15 Session Chair**

Prof. Antonello MAI  
(SAPIENZA UNIVERSITY OF ROME, Rome, Italy)

**13:20 Phenotypic Screening for the Discovery of Novel Molecules for Therapeutic Heart Regeneration**

Dr Allyn T. PLOWRIGHT  
(ASTRAZENECA, Cambridge, United Kingdom)

**13:45 How can Advances in Cryo-Electron Microscopy Revolutionize Medicinal Chemistry?**

Dr Neil RANSON  
(UNIVERSITY OF LEEDS, Leeds, United Kingdom)

**14:10 Interaction of 4,5,6,7-Tetrahydrobenzo[1,2-D]Thiazoles with the Cellular Chaperone HSP90 as a Potential Pathway to Inhibit Hepatitis C Virus Replication**

Prof. Tihomir TOMASIC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**14:35 RSC Prize Lecture: Advanced Chemical Genetics for Epigenetics: Bump and Hole and PROTACs (2016 MedChemComm Emerging Investigator Lectureship)**

Prof. Alessio CIULLI  
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

### Session 7.2 Innovation in Kinase Drug Discovery

**13:15 Session Chair**

Dr Christel MENET  
(CONFO THERAPEUTICS, Brussels, Belgium)

**13:20 Broad Multiparametric Profiling of Kinase Inhibitors**

Dr Herman VAN VLIJMEN  
(JANSSEN, Beerse, Belgium)

**14:00 New Pseudokinase Drug Targets in the Human Kinome**

Prof. Patrick EYERS  
(UNIVERSITY OF LIVERPOOL, Liverpool, United Kingdom)

**14:20 Switch Control Inhibitors: an Advance in Type II Kinase Inhibition**

## Programme Schedule

Dr Daniel FLYNN  
(DECIPHERA PHARMACEUTICALS, Lawrence, United States)

**14:40 First Disclosure of CDZ173 - Discovery of a New Generation of Potent and Selective PI3K Delta Inhibitors for Autoimmune and Inflammatory Diseases**

Dr Nicolas SOLDERMANN  
(NOVARTIS, Basel, Switzerland)

### Session 7.3 The Importance of Solute Carrier Transporters in Drug Discovery (MedChemComm Session)

**13:15 Session Chair**

Dr David HEPWORTH  
(PFIZER MEDICINES DESIGN, Cambridge, United States)

**13:20 Solute Carriers, Metabolism and Drug Response: a Magic Triangle**

Prof. Giulio SUPERTI-FURGA  
(RESEARCH CENTER FOR MOLECULAR MEDICINE (CEMM), Vienna, Austria)

**14:00 The Design and Evaluation of URAT1 Inhibitors for the Treatment of Hyperuricemia and Gout**

Dr David HEPWORTH  
(PFIZER MEDICINES DESIGN, Cambridge, United States)

**14:20 The Cellular Uptake of Pharmaceutical Drugs is Transporter-Mediated - A Problem not of Biophysics but of Systems Biology**

Prof. Douglas KELL  
(UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

**14:40 Drug Targets in the Solute Carrier Classification (SLC)**

Dr Daniela DIGLES  
(UNIVERSITY OF VIENNA, Vienna, Austria)

**Excursions**

**Banquet**

### Thursday September 1, 2016

#### Session 8.1 Covalent Drugs Revisited (AFMC Session)

- 08:30 Session Chair**  
Prof. Zhengying PAN  
(PEKING UNIVERSITY, Shenzhen, China)
- 08:35 Targeted Covalent Inhibitors of Bruton's Tyrosine Kinases - Design, Evaluation and Follow-up**  
Prof. Zhengying PAN  
(PEKING UNIVERSITY, Shenzhen, China)
- 09:15 Chemical Biology Efforts in Cancer Drug Discovery**  
Prof. Huchen ZHOU  
(SHANGHAI JIAO TONG UNIVERSITY, Shanghai, China)
- 09:35 Advances in the Development of Covalent EGFR Inhibitors: from Early Hits to Osimertinib**  
Dr Gail WRIGLEY  
(ASTRAZENECA, Cambridge, United Kingdom)
- 09:55 Rapid Discovery of Potent and Selective Covalent Inhibitors via Covalent Docking**  
Dr Nir LONDON  
(THE WEIZMANN INSTITUTE OF SCIENCE, Rehovot, Israel)

#### Session 8.2 Novel Molecular Probes for in Vivo Chemistry

- 08:30 Session Chair**  
Dr Marc ROBILLARD  
(TAGWORKS PHARMACEUTICALS, Eindhoven, The Netherlands)
- 08:35 Antibody Imaging and Therapy Using in Vivo Click and Click-to-Release Strategies**  
Dr Marc ROBILLARD  
(TAGWORKS PHARMACEUTICALS, Eindhoven, The Netherlands)
- 09:15 Novel Antibody-Tetrazine Conjugate for Breast Cancer Imaging**  
Mr Eduardo RUIVO  
(UNIVERSITY OF ANTWERP, Antwerp, Belgium)
- 09:35 Atypical Bile Acids as Chemical Probes for Diagnosis and Therapy Monitoring of Progressive Cholestatic Liver Disease in HSD3B7 Patients**  
Prof. Antimo GIOIELLO  
(UNIVERSITY OF PERUGIA, Perugia, Italy)
- 09:55 RSC Prize Lecture:  
Chemical Pharmacology of Protein Conjugates and Natural Products (2016 Chem Soc Rev Emerging Investigator Lectureship)**  
Prof. Gonçalo BERNARDES  
(INSTITUTO DE MEDICINA MOLECULAR, PORTUGAL & UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

#### Session 8.3 Recent Advances on Approaches to Treat Pain

- 08:30 Session Chair**  
Dr Alan BROWN  
(STRATIFIED MEDICAL, Deal, United Kingdom)
- 08:35 The Painful Reality of Drug Discovery and Development**  
Dr Paul BESWICK  
(UNIVERSITY OF SUSSEX, Brighton, United Kingdom)
- 09:15 Challenges in the Discovery of Sigma-1 Receptor Antagonists for the Treatment of Pain**  
Dr Carmen ALMANSA  
(ESTEVE, Barcelone, Spain)
- 09:35 Functionally Irreversible Non-Covalent Inhibitors of FAAH: a Safer Approach?**  
Dr Philippe NANTERMET  
(MERCK & CO. INC (MSD), West Point, United States)
- 09:55 Towards Low-Risk Painkillers: Human Dipeptidyl Peptidase III (hDPPIII) as a Novel Target for Therapeutic Pain Intervention**

## Programme Schedule

Ms Shalinee JHA  
(GRAZ UNIVERSITY OF TECHNOLOGY, Graz, Austria)

### Exhibition & Coffee

#### Session 9.1 High Throughput Screening Strategies to Obtain High Quality Leads

**10:45 Session Chair**

Prof. Jonathan BAELL  
(MONASH UNIVERSITY, Parkville, Australia)

**10:50 Histone Acetyltransferase Inhibitors, from Screening to Optimization - a Tricky Track**

Prof. Jonathan BAELL  
(MONASH UNIVERSITY, Parkville, Australia)

**11:30 Direct and Synergistic Inhibition of The HCV NS5A Protein**

Dr Makonen BELEMA  
(BRISTOL-MYERS SQUIBB, Wallingford, United States)

**11:50 Discovery of In Vivo Active and Selective Diacylglycerol Lipase-Alpha Inhibitors**

Dr Mario VAN DER STELT  
(LEIDEN UNIVERSITY, Leiden, The Netherlands)

**12:10 Anti-Wolbachia (A-WOL) Drug Discovery: Novel Hit Finding Via Ligand Based Virtual Screening Combined With HTS**

Dr Neil G BERRY  
(UNIVERSITY OF LIVERPOOL, Liverpool, United Kingdom)

#### Session 9.2 Late Breaking News

**10:45 Session Chair**

Dr Luc VAN HIJFTE  
(SCT & NOVALIX, Nijmegen, The Netherlands)

**10:50 Discovery of PF-06840003, a Novel IDO1 Inhibitor for Cancer Immunotherapy**

Dr Stefano CROSIGNANI  
(ITEOS THERAPEUTICS SA, Gosselies, Belgium)

**11:15 Driving Tumors into Mitotic Catastrophe - Lead Generation of MPS1 Inhibitors Leading to Two Clinical Candidates BAY 1161909 and BAY 1217389**

Dr Volker K. SCHULZE  
(BAYER PHARMA AG, Berlin, Germany)

**11:40 Delivering First-in-Class In Vitro Chemical Probes Against Poly (ADP Ribose) Glycohydrolase (PARG)**

Dr Allan JORDAN  
(CANCER RESEARCH UK MANCHESTER INSTITUTE, Manchester, United Kingdom)

**12:05 Discovery of Ubrogepant (MK-1602): a Potent, Selective and Orally Bioavailable CGRP Receptor Antagonist for the Acute Treatment of Migraine**

Dr Mark FRALEY  
(MERCK, SHARP & DOHME, West Point, United States)

#### Session 9.3 Showcase Brazil

**10:45 Session Chair**

Prof. Andrei LEITÃO  
(UNIVERSITY OF SAO PAULO, São Carlos, Brazil)

**10:50 Molecular Design, Synthesis and Trypanocidal Activity of Dipeptidyl Nitriles as Cruzain Inhibitors**

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

**11:30 Research, Development & Innovation at Aché Laboratórios Farmacêuticos**

Dr Cristiano GUIMARAES  
(ACHÉ PHARMACEUTICAL, Brazil)

**11:50 Effects of Novel Acylhydrazones Derived From 4-Quinolone on the Acetylcholinesterase Activity and A $\beta$ 2 Peptide Fibrils Formation**

Mrs Gisele SILVESTRE DA SILVA  
(UNICAMP, São Paulo, Brazil)

## Programme Schedule

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**12:10 Antiplatelet and Antithrombotic Activity of 1,2,5-Oxadiazole-2-N-Oxide Derivatives**

Mr Luiz Antonio DUTRA  
(STATE UNIVERSITY OF SAO PAULO - UNESP, Araraquara, Brazil)

**Heterocycles and Medicinal Chemistry: The Importance of Innovative Synthesis**

Dr Anthony WOOD  
(PFIZER, Waltham, United States)

**Chair**

Dr Franz VON NUSSBAUM  
(BAYER PHARMA, Berlin, Germany)

**Closing Remarks, Poster Prizes and Welcome to EFMC-ISMIC 2018**

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