

Sunday August 28, 2016

13:30 Registration

16:00 Opening Ceremony

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

16:20 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)

17:05 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)

17:30 Award Ceremony

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

**17:50 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)

18:40 Late-Stage Fluorination

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

Chair

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

19:25 Welcome Reception Sponsored by Concept Life Sciences

Monday August 29, 2016

**08:30 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)

09:15 Cross-Coupling Approaches to Saturated N-Heterocycles

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

Chair

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

10:00 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)

12:15 Exhibition & Lunch

12:30 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)

15:00 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)

17:35 Poster Session (even numbers) with drinks

19:30 End of the day

Programme Schedule

Tuesday August 30, 2016

**08:30 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)

09:15 EFMC Prize Ceremony
Prof. Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)

**09:20 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)

**09:40 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)

10:00 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 Adamts 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)

12:15 Exhibition & Lunch

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

12:30 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)

15:00 Exhibition & Coffee

15:30 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)

16:15 Poster Session (odd numbers) with drinks

18:15 Close Poster Session

19:00 Public Lecture

21:30 End of the day

Wednesday August 31, 2016

08:30 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)

09:15 DNA-Encoded Chemical Libraries
Prof. Dario NERI
(ETH ZÜRICH, Zürich, Switzerland)

Chair

10:00 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 Dada 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)
- 12:15 Exhibition & Lunch**
- 12:15 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**
Dr 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)

15:00 Excursions

20:00 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)

10:15 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 β 2 Peptide Fibrils Formation

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

Programme Schedule

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)

12:30 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)

13:15 Closing Remarks, Poster Prizes and Welcome to EFMC-ISMIC 2018

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