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

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Speaker</th>
<th>Institution/Location</th>
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<tbody>
<tr>
<td>08:30</td>
<td>UCB-EHRlich Award for Excellence in Medicinal Chemistry: Traversing the Valley of Death in Anticancer Drug Discovery</td>
<td>Prof. Paul J. HERGENROTHER (UNIVERSITY OF ILLINOIS, Urbana, United States)</td>
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<td></td>
<td>Chair</td>
<td>Dr. Laurent PROVINS (UCB, Braine-l'Alleud, Belgium)</td>
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<tr>
<td>09:15</td>
<td>Cross-Coupling Approaches to Saturated N-Heterocycles</td>
<td>Prof. Jeffrey BODE (ETH ZÜRICH, Zürich, Switzerland)</td>
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<td></td>
<td>Chair</td>
<td>Dr. Karin BRINER (NOVARTIS, Cambridge, United States)</td>
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<tr>
<td>10:00</td>
<td>Exhibition &amp; Coffee</td>
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#### Session 1.1 Intramolecular Hydrogen Bonding and its Impact in Drug Design and Discovery (ACSMEDI Session)

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<th>Time</th>
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<tr>
<td>10:30</td>
<td>Session Chairs</td>
<td>Dr. Amjad ALI (MERCK &amp; CO. INC., Kenilworth, United States)</td>
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<td>Dr. Tanweer KHAN (MERCK, SHARP &amp; DOHME, Kenilworth, United States)</td>
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<tr>
<td>10:35</td>
<td>The Need of Implementing Intramolecular Hydrogen Bonding (IMHB) Considerations in Drug Discovery and How to do it</td>
<td>Prof. Giulia CARON (UNIVERSITY OF TORINO, Torino, Italy)</td>
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<tr>
<td>11:15</td>
<td>Intramolecular Hydrogen Bond Expectations in Medicinal Chemistry</td>
<td>Dr. Fabrizio GIORDANETTO (DE. SHAW RESEARCH LLC, New York, United States)</td>
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<tr>
<td>11:35</td>
<td>Intramolecular Hydrogen Bonding as a Design Element in Medicinal Chemistry</td>
<td>Dr. Bernd KUHN (F. HOFFMANN-LA ROCHE, Basel, Switzerland)</td>
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<tr>
<td>11:55</td>
<td>Intramolecular Hydrogen Bonds in the Design of CREBBP Bromodomain Ligands</td>
<td>Prof. Stuart CONWAY (UNIVERSITY OF OXFORD, Oxford, United Kingdom)</td>
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#### Session 1.2 Drug Discovery Approaches Toward Targeting Ras

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<th>Time</th>
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<tr>
<td>10:30</td>
<td>Session Chair</td>
<td>Dr. Joachim RUDOLPH (GENENTECH, South San Francisco, United States)</td>
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<tr>
<td>10:35</td>
<td>Studying Ciliary Trafficking and How it Leads to RAS Drug Candidates</td>
<td>Prof. Alfred WITTINGHOFER (MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)</td>
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<tr>
<td>11:15</td>
<td>Chemical Biological Modulation of KRas-Signaling</td>
<td>Prof. Herbert WALDMANN (MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)</td>
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<td>11:35</td>
<td>Inhibition of Prenylated KRAS: Tools to Discover and Characterize RAS Ligands</td>
<td>Dr. Johanna JANSEN (NOVARTIS, Emeryville, United States)</td>
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<tr>
<td>11:55</td>
<td>Small Molecule Binding Sites on the RAS: SOS Complex Can Be Exploited for Inhibition of RAS Activation</td>
<td>Dr. Jon WINTER-HOLT (ASTRAZENECA, Macclesfield, United Kingdom)</td>
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### Session 1.3 New Antibacterials. An Update

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<thead>
<tr>
<th>Time</th>
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<tr>
<td>10:30</td>
<td>Session Chair</td>
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<td>Prof. Malcolm PAGE</td>
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<td>(JACOBS UNIVERSITY, Bremen, Germany)</td>
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<td>10:35</td>
<td>New Antibacterial Agents in the Pipeline</td>
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<td>Dr Eric DESARBRE</td>
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<td>(BASILEA PHARMACEUTICA, Basel, Switzerland)</td>
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<td>11:15</td>
<td>Mechanistic and Inhibition Studies on Metallo-Beta-Lactamases</td>
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<td>Prof. Christopher J. SCHOFIELD</td>
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<td></td>
<td>(UNIVERSITY OF OXFORD, Oxford, United Kingdom)</td>
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<td>11:35</td>
<td>Enterobactin-Dependent Iron Uptake Pathway as a Gate for Antibiotic Trojan Horse Strategies Against Pseudomonas Aeruginosa</td>
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<td>Dr Gaëtan MISLIN</td>
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<td>(UNIVERSITY OF STRASBOURG, Illkirch-Graffenstaden, France)</td>
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<td>11:55</td>
<td>Exploring Hit-Identification Strategies for Energy-Coupling Factor Transporters, a Novel Target for the Development of Antibiotics</td>
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<td>Ms Leticia MONJAS GOMEZ</td>
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<td>(UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)</td>
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#### 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)

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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>13:15</td>
<td>Session Chairs</td>
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<td></td>
<td>Dr Peter CHENG (BRISTOL-MYERS SQUIBB, Hopewell, United States)</td>
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<td>Dr Claudio MAPELLI (BRISTOL-MYERS SQUIBB, United States)</td>
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<tr>
<td>13:20</td>
<td>Peptides and Peptidomimetics: Overcoming Problems of Activity, Selectivity and Bioavailability of Integrin Ligands</td>
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<td>Dr Horst KESSLER</td>
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<td>(TECHNISCHE UNIVERSITÄT MÜNCHEN, Garching, Germany)</td>
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<td>14:00</td>
<td>Discovery &amp; Optimization of Clips-Constrained Bicyclic Peptides (2clips) Using Pepscan Peptide Arrays</td>
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<td>Prof. Peter TIMMERMAN</td>
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<td>(PEPSCAN THERAPEUTICS, Lelystad, The Netherlands)</td>
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<tr>
<td>14:20</td>
<td>Phage-Encoded Combinatorial Chemical Libraries Based on Bicyclic Peptides</td>
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<td>Prof. Christian HEINIS</td>
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<td></td>
<td>(ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL), Lausanne, Switzerland)</td>
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<tr>
<td>14:40</td>
<td>Attempts at Oral Delivery of a Series of Short Unnatural Peptides: Still Like Pushing a Camel Through the Eye of a Needle?</td>
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<td>Dr Claudio MAPELLI</td>
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<td>(BRISTOL-MYERS SQUIBB, United States)</td>
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### Session 2.2 Recent Progress in the Treatment of Ophthalmological Diseases

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<tr>
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<tr>
<td>13:15</td>
<td>Session Chair</td>
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<td>Dr Yves P. AUBERSON</td>
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<td>(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)</td>
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<tr>
<td>13:20</td>
<td>Molecular Pharmacodynamics of Visual Cycle Modulators in Protection Against Retinal Degeneration</td>
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<td>Prof. Krzysztof PALCZEWSKI</td>
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<td>(CASE WESTERN RESERVE UNIVERSITY, Cleveland, United States)</td>
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<tr>
<td>14:00</td>
<td>The Back of The Eye: Treatment Challenges and Opportunities</td>
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Programme Schedule

Dr Muneto MOGI  
(NOVAARTIS 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, Stevenage, United Kingdom)  
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
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 ROEHRRIG
        (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
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)

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**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, Palo Alto, California, United States)

**11:15**  
**The Development of DDD853851; 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 DEPREZ  
(UNIVERSITY OF LILLE 2, Lille, France)

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

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

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**12:15**  
**Exhibition & Lunch**

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**12:15**  

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

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**Session Chair**

Dr Sharan BAGAL  
(ASTRAZENECA, Cambridge, United Kingdom)

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**Session 5.1 Synthesis Driven Innovation**

**13:15**  
**Session Chair**

Dr Jesus EZQUERRA  
(LABORATORIOS LILLY, Alcobendas, Spain)

**13:20**  
**Expanding the Macrocycle 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 Spiranoid Lactones: Access to Natural Frames and Application in Selective Silencing of the Pain Receptor TRPV1**
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
(GOE THE 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 EKARRAN
(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)

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
(ARIBUTUS BIOPHARMA, Doylestown, PA, 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 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
(NOVAARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)
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


Session 7.1 Emerging Topics

13:15  Session Chair
Prof. Antonello MAI
(UNIVERSITY OF ROME, Rome, Italy)

13:20  Phenotypic Screening for the Discovery of Novel Molecules for Therapeutic Heart Regeneration
Dr Alleyn T. PLOWRIGHT
(ASTRAZENECA, Frankfurt-Am-Main, Germany)

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
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, Macclesfield, 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)
Dr Goncalo 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, Barcelona, 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
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 GUISMARAES  
(ACHE PHARMACEUTICAL, Brazil)

11:50 Effects of Novel Acyhydrazones Derived From 4-Quinolone on the Acetylcholinesterase Activity and A?42 Peptide Fibrils Formation  
Mrs Gisele SILVESTRE DA SILVA  
(UNICAMP, São Paulo, Brazil)
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-ISMC 2018  
Prof. Marko ANDERLUH  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)