

### Sunday September 2, 2018

**13:30 Registration**

**16:00 Opening Ceremony**

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

**16:20 Chair**

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

**Zika Virus: An Old Virus with a New Face**

Prof. Tatjana AVSIC-ZUPANC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**16:50 Chair**

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

**It's a Small-Molecule World: Medicinal Chemistry Challenges and Opportunities for the Next Decade**

Dr Bayard HUCK  
(MERCK BIOPHARMA, Darmstadt, Germany)

**17:20 Award Ceremony**

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

**17:40 Chair**

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

**NAUTA AWARD FOR PHARMACOCHEMISTRY**

**Tools and Drugs for Purine Targets - Important Players in Inflammation and Cancer**

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

**18:25 Chair**

Prof. Hans Ulrich STILZ  
(NOVO NORDISK, Malov, Denmark)

**Synthetic Glycoconjugate Vaccines against Bacterial Infections**

Prof. Peter H. SEEBERGER  
(MAX PLANCK INSTITUTE OF COLLOIDS AND INTERFACES, Berlin, Germany)

**19:10 Welcome Reception**

**20:30 End of the Day**

## Programme Schedule

### Monday September 3, 2018

**08:30 Chair**

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

**UCB-EHRLICH AWARD FOR EXCELLENCE IN MEDICINAL CHEMISTRY  
How Best to Discover Bioactive Small Molecules?**

Prof. Adam NELSON  
(UNIVERSITY OF LEEDS, Leeds, United Kingdom)

**09:15 Chair**

Prof. Roberto DI SANTO  
(SAPIENZA UNIVERSITY OF ROME, Rome, Italy)

**The Therapeutic Challenge of the New Era: Developing and Making Available Life Changing Treatment to Patients with Rare Diseases**

Dr Diego ARDIGO  
(CHIESI GROUP, PARMA, Italy)

**10:00 Exhibition & Coffee**

#### Session *Session 1 'Technologies'*

##### Artificial Intelligence Applications in Medicinal Chemistry

**10:30 Session Chair**

Dr Jonas BOSTRÖM  
(ASTRAZENECA, Mölndal, Sweden)

**10:35 Artificial Intelligence. Not Just Another Name for in Silico Design**

Dr David E. LEAHY  
(THE DISCOVERY BUS LTD, Macclesfield, United Kingdom)

**11:15 Re-Energising Small Molecule Drug Discovery**

Dr Willem VAN HOORN  
(EXSCIENTIA, Dundee, United Kingdom)

**11:35 Computer-Aided Synthesis Planning**

Mr Marwin SEGLER  
(BENEVOLENTAI, London, United Kingdom)

**11:55 Potency and Patents, New Arenas for Matched Molecular Pair Analysis in the AI World**

Dr AI DOSSETTER  
(MEDCHEMICA LIMITED, Macclesfield, United Kingdom)

#### Session *Session 2 'Therapeutic Areas'*

##### Immuno-Oncology: Novel Therapeutic Opportunities

**10:30 Session Chair**

Dr Luc VAN HIJFTE  
(SCT & MERCACHEM-SYNCOM, Nijmegen, The Netherlands)

**10:35 Small Molecule Immune Checkpoint Antagonists for Cancer Therapy**

Dr Murali RAMACHANDRA  
(AURIGENE DISCOVERY TECHNOLOGIES LTD, Bangalore, India)

**11:15 Tankyrase Inhibitor Development: Evidence for Potential in Cancer Immune Therapy**

Prof. Stefan KRAUSS  
(UNIVERSITY OF OSLO, Oslo, Norway)

**11:35 Small Molecules Inhibiting PD1-PDL1 Immune Checkpoint**

Dr Shabnam SHAABANI  
(UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)

## Programme Schedule

### 11:55 **New Small-Molecule Immune Checkpoint Inhibitors: A Step Forward in Cancer Immunotherapy**

Ms Ana Rita DE CARVALHO ACURCIO  
(UNIVERSITY OF LISBON, Lisbon, Portugal)

### Session *Session 3 'Chemical Biology'*

#### **Glycans in Medicinal Chemistry: Carbohydrate-Based Vaccines (EuChemS Session)**

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

Dr Sonsoles MARTIN-SANTAMARIA  
(BIOLOGICAL RESEARCH CENTER, Madrid, Spain)

### 10:35 **Breaking the Limits in Analyzing Carbohydrate Recognition by NMR**

Dr Jesus JIMENEZ-BARBERO  
(CIC BIOGUNE, Derio, Spain)

### 11:15 **Targeting of Cancer Specific Glycopeptide Epitopes**

Prof. Hans WANDALL  
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

### 11:35 **A Multidisciplinary Strategy to Synthetic Carbohydrate-Based Conjugates for Vaccination against Shigella: from Concept to First-in-Human Study**

Dr Laurence MULARD  
(PASTEUR INSTITUTE, Paris, France)

### 11:55 **Glycoside Antagonists of Bacterial Lectins: New Treatment Options for Recurrent and Antibiotic Resistant UTI**

Prof. James JANETKA  
(WASHINGTON UNIVERSITY IN SAINT LOUIS, Saint Louis, United States)

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

### Session *Session 4 'Technologies'*

#### **Timing is Everything: Target Binding Kinetics and Pharmacokinetics**

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

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

### 13:20 **"Micro-Pharmacokinetics": How Local Drug Concentration Influences Observed Binding Kinetics**

Prof. Steven CHARLTON  
(UNIVERSITY OF NOTTINGHAM, Nottingham, United Kingdom)

### 14:00 **Allosteric Modulation of the mGlu2 Receptor: from Structure-Kinetic Relationships to in vivo Efficacy (2017 MedChemComm Emerging Investigator Lectureship)**

Dr Laura HEITMAN  
(UNIVERSITY OF LEIDEN, Leiden, The Netherlands)

### 14:20 **Target Binding Kinetics and its Relevance in the in vivo Context**

Dr Liesbeth DE LANGE  
(UNIVERSITY OF LEIDEN, Leiden, The Netherlands)

### 14:40 **Large-Scale Analysis of Kinase Inhibitors' Target Binding Kinetics and its Implications for Drug Discovery**

Ms Victoria GEORGI  
(BAYER AG, Berlin, Germany)

### Session *Session 5 'Therapeutic Areas'*

#### **Life Science at the Interface of Agro and Pharma**

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

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

### 13:20 **A New Target in Fungal Protein Biosynthesis: Shared Learnings for AgChem and MedChem**

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

## Programme Schedule

- 14:00 Natural Products as Leads in Agrochemistry**  
Dr Joachim RHEINHEIMER  
(BASF, Ludwigshafen am Rhein, Germany)
- 14:20 Synthesis and Fungicidal Activity of a New Family of Oxysterol Binding Protein Inhibitors**  
Dr Laura QUARANTA  
(SYNGENTA AG, Basel, Switzerland)
- 14:40 Targeting Non Essential Bacterial Targets as a Novel Route to Counteract Bacterial Resistance**  
Prof. Gabriele COSTANTINO  
(UNIVERSITY OF PARMA, Parma, Italy)

### Session *Session 6 'Chemical Biology'*

#### Recent Advances in Targeted Protein Degradation

- 13:15 Session Chair**  
Dr Gregory HOLLINGWORTH  
(NOVARTIS PHARMA AG, Basel, Switzerland)
- 13:20 Recent Advances in Bifunctional Degradable Molecules (e.g. SNIPER) for Targeted Protein Degradation via the Ubiquitin Proteasome System; Status and Outlook**  
Dr Mikihiro NAITO  
(NATIONAL INSTITUTE OF HEALTH SCIENCES, Tokyo, Japan)
- 14:00 Targeting 'Undruggable' Transcription and Translation Factors for Degradation with Low Molecular Weight Cereblon Modulators**  
Dr Philip CHAMBERLAIN  
(CELGENE, Alameda, United States)
- 14:20 The Zinc-Degrome**  
Dr Nicolas THOMÄ  
(FRIEDRICH MIESCHER INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)
- 14:40 Drugging the Fbw7 E3 Ligase with a Combined Computational and Biophysical Approach**  
Dr Carles GALDEANO  
(UNIVERSITY OF BARCELONA, Barcelona, Spain)
- 15:00 Exhibition & Coffee**

### Session *Session 7*

#### First Time Disclosures

- 15:30 Session Chair**  
Dr Emmanuel PINARD  
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)
- 15:35 Discovery of RG7916, a Selective SMN2 Splicing Modifier for the Treatment of Spinal Muscular Atrophy**  
Dr Hasane RATNI  
(F. HOFFMANN-LA ROCHE LTD, Basel, Switzerland)
- 16:05 Discovery of LOU064, a Covalent BTK Inhibitor with Best in Class Selectivity**  
Dr Robert PULZ  
(NOVARTIS PHARMA, Basel, Switzerland)
- 16:35 Discovery of a Novel Oral NO- and Heme-Independent sGC Activator BAY 1101042**  
Dr Michael G. HAHN  
(BAYER HEALTHCARE, Wuppertal, Germany)
- 17:05 First Time Disclosure of BI 409306, a First in Class PDE9 Inhibitor for the Treatment of CNS Diseases**  
Dr Riccardo GIOVANNINI  
(BOEHRINGER INGELHEIM, Biberach, Germany)
- 17:35 Poster Session 1 (even numbers) & Networking**
- 19:30 End of the Day**



### Tuesday September 4, 2018

**08:30 Chair**

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

**PROUS INSTITUTE-OVERTON AND MEYER AWARD FOR NEW TECHNOLOGIES IN DRUG DISCOVERY  
Activity-Based Proteomics - Protein and Ligand Discovery on a Global Scale**

Prof. Benjamin CRAVATT  
(THE SCRIPPS RESEARCH INSTITUTE, La Jolla, United States)

**09:15 Chair**

Dr Phil JONES  
(BIOASCENT, Glasgow, United Kingdom)

**Sugars & Proteins: Glycomimetics to Target Infectious Disease**

Prof. Benjamin DAVIS  
(OXFORD UNIVERSITY, Oxford, United Kingdom)

**10:00 Exhibition & Coffee**

### Session *Session 8 'Technologies'*

#### New Chemical Modalities in Medicinal Chemistry

**10:30 Session Chair**

Dr Eric VALEUR  
(ASTRAZENECA, IMED BIOTECH UNIT, Cambridge, United States)

**10:35 New Modalities for Complex and Unprecedented Biological Targets**

Dr Eric VALEUR  
(ASTRAZENECA, IMED BIOTECH UNIT, Cambridge, United States)

**11:15 Cell Permeability with Beyond 'Rule of 5' Modalities – Do We Understand How This Works?**

Dr Nick TERRETT  
(MERCK SHARP & DOHME RESEARCH GMBH (MSD), Kriens, Switzerland)

**11:35 Novel Hybrid Macrocyclic Modalities for Structure-Based Protein Mimetics**

Dr Stephanie GUERET  
(ASTRAZENECA-MAX PLANCK INSTITUTE SATELLITE UNIT, Dortmund, Germany)

**11:55 Small-Molecule Stabilization of Protein-Protein Interactions by Natural Products, Supramolecular Ligands, Fragments and Macrocycles**

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

### Session *Session 9 'Therapeutic Areas'*

#### Targeting Aggregated Proteins in Neurodegenerative Diseases with Small Molecules

**10:30 Session Chair**

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

**10:35 Understanding Aggregation Inhibition of Alpha-Synuclein and Tau by Small Molecules**

Prof. Markus ZWECKSTETTER  
(MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)

**11:15 Discovery of Peptidomimetics Targeting Protein-Protein Interactions of Alpha-Synuclein**

Dr Wolfgang WRASIDLO  
(UNIVERSITY OF CALIFORNIA SAN DIEGO, La Jolla, United States)

**11:35 Targeting the Monomeric Intrinsically Disordered Structural State of Tau and Alpha-Synuclein by Small Molecules as a Potential Therapeutic Strategy for Alzheimer's and Parkinson's Disease**

## Programme Schedule

Dr Gergely TOTH  
(CANTABIO PHARMACEUTICALS INC., Sunnyvale, United States)

**11:55 Brain-Penetrant Autophagy Modulators for Treating Neurodegenerative Diseases**

Dr Steve ANDREWS  
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

### Session Sessions 10 'Chemical Biology'

#### Targeting the STING Pathway (Stimulator of Interferon Genes)

**10:30 Session Chair**

Dr Thorsten OOST  
(BOEHRINGER INGELHEIM, Biberach, Germany)

**10:35 Intracellular DNA Sensing in Health and Disease**

Prof. Andrea ABLASSER  
(EPFL, Lausanne, Switzerland)

**11:15 Modification of Cyclic Dinucleotides to Enhance Modulation of the Innate Immune Response**

Dr Diane COE  
(GLAXOSMITHKLINE, Stevenage, United Kingdom)

**11:35 Use of Cyclic Dinucleotides (CDNs) to Induce Stimulator of Interferon Genes (STING)-Dependent Antitumor Immunity**

Dr Cedric BOULARAN  
(INVIVOGEN, Toulouse, France)

**11:55 In vivo Anti-Viral and -Tumor Effect Of 3'3'-cAIMP STING Activation**

Dr Martin K. THOMSEN  
(AARHUS UNIVERSITY, Aarhus C, Denmark)

**12:15 Exhibition & Lunch**

**12:15 Chemical Computing Group Workshop**

**MOEsaic: The application of Matched Molecular Pair Analysis to SAR Exploration**

#### Session Flash Posters 1

**Chair**

Prof. Lucija PETERLIN MASIC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**13:15 Opportunity for 10 young scientists to present a summary of their poster**

Discover the presenters [here](#)

#### Session Flash Posters 2

**Chair**

Dr Ziga JAKOPIN  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**13:15 Opportunity for 10 young scientists to present a summary of their poster**

Discover the presenters [here](#)

#### Session Flash Posters 3

**Chair**

Dr Tihomir TOMASIC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

## Programme Schedule

13:15 **Opportunity for 10 young scientists to present a summary of their poster**

Discover the presenters [here](#)

### Session *Session 11 'Technologies'*

#### Expanding Medicinal Chemists' Synthetic Toolbox

13:45 **Session Chair**

Prof. Gyorgy KESERU  
(HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)

13:50 **Capturing Biological Activity in Natural Product Fragments by Chemical Synthesis**

Prof. Karl GADEMANN  
(UNIVERSITY OF ZÜRICH, Zürich, Switzerland)

14:30 **Stuck in a Rut with Old Chemistry**

Dr Jonas BOSTRÖM  
(ASTRAZENECA, Mölndal, Sweden)

14:50 **New Chemical Libraries in Exploration of Chemical Space**

Prof. Jurij SVETE  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

15:10 **Integrated System for the Expedited Generation and Characterization of Drug-Like Libraries for Hit-to-Lead Explorations**

Prof. Antimo GIOIELLO  
(UNIVERSITY OF PERUGIA, Perugia, Italy)

### Session *Session 12 'Therapeutic Areas'*

#### Breakthroughs in Polypharmacology Towards Neurological Disorders (ACS Session)

13:45 **Session Chair**

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

13:50 **Multi-Functional Treatments for Multi-Factorial Neurodegenerative Disorders: the Challenge of Alzheimer's Disease**

Dr Mark J. MILLAN  
(INSTITUT DE RECHERCHES SERVIER, Croissy-sur-Seine, France)

14:30 **Beyond Single-Target Activities: Using Polypharmacology and Systems Readouts for Compound Selection and Mode-of-Action Analysis**

Prof. Andreas BENDER  
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

14:50 **In silico Polypolarmacology**

Dr Giovanni BOTTEGONI  
(HEPTARES THERAPEUTICS, Welwyn Garden City, United Kingdom)

15:10 **Metabotropic Glutamate Receptor Type 2 Positive Allosteric Modulators (mGlu2 Receptor PAMS) as a Transformational Epilepsy Treatment**

Dr Jose CID  
(JANSSEN R&D, Toledo, Spain)

### Session *Session 13 'Chemical Biology'*

#### Chemical Biology Approaches to Target Identification

13:45 **Session Chair**

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

13:50 **Activity-Based Glycosidase Profiling in Biomedicine and Biotechnology**

Prof. Hermen OVERKLEEF  
(LEIDEN UNIVERSITY, Leiden, The Netherlands)

14:30 **An Iron Hand over Cancer Stem Cells**



## Programme Schedule

Dr Raphaël RODRIGUEZ  
(INSTITUT CURIE, Paris, France)

**14:50 Charting the Structure-Resistance Landscape of Novel Antibiotics**

Mr Tamas REVESZ  
(BIOLOGICAL RESEARCH CENTRE, HUNGARIAN ACADEMY OF SCIENCES, Szeged, Hungary)

**15:10 Buruli Ulcer and the mTOR Pathway: Total Synthesis, Structure-Activity and Target Elucidation Studies of Mycolactones**

Dr Matthias GEHRINGER  
(UNIVERSITY OF TUEBINGEN, Tuebingen, Germany)

**15:30 Exhibition & Coffee**

### Session Flash Posters 4

#### Chair

Prof. Danijel KIKELJ  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**16:00 Opportunity for 15 young scientists to present a summary of their poster**

Discover the presenters [here](#)

### Session Flash Posters 5

#### Chair

Prof. Jurij SVETE  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**16:00 Opportunity for 15 young scientists to present a summary of their poster**

Discover the presenters [here](#)

### Session Flash Posters 6

#### Chair

Prof. Janez ILAS  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**16:00 Opportunity for 15 young scientists to present a summary of their poster**

Discover the presenters [here](#)

**16:45 Poster Session 2 (odd numbers) & Networking**

**18:45 End of Poster Session**

**20:00 Concert**

### Wednesday September 5, 2018

- 08:30 Chair**  
Dr Jürgen MACK  
(BOEHRINGER INGELHEIM, Biberach an der Riss, Germany)
- Development of Non-Nucleosidic Compounds against DNA Viruses of the Herpes Group. The Era After Nucleosides: Letemovir and Pritelivir**  
Dr Helga RÜBSAMEN-SCHAEFF  
(AICURIS GMBH & CO. KG, Wuppertal, Germany)
- 09:15 EFMC Prize Ceremony**  
Dr Matthew TOZER (CONSULTANT, Cambridge, United Kingdom)  
Prof. Rui MOREIRA (UNIVERSITY OF LISBON, Lisbon, Portugal)
- 09:20 EFMC Prize for a Young Medicinal Chemist in Industry**  
**The Challenges of Restoring Programmed Cell Death Through MCL1 Inhibition**  
Dr Marton CSEKEI  
(SERVIER RESEARCH INSTITUTE OF MEDICINAL CHEMISTRY, Budapest, Hungary)
- 09:40 EFMC Prize for a Young Medicinal Chemist in Academia**  
**Carbohydrate-binding Proteins as Targets for Anti-Infectives and Diagnostics: ESKAPE pathogen Pseudomonas aeruginosa and its Lectins**  
Dr Alexander TITZ  
(HELMHOLTZ INSTITUTE FOR PHARMACEUTICAL SCIENCES, Saarbrücken, Germany)
- 10:00 Exhibition & Coffee**

### Session *Session 14 'Technologies'*

#### Development of New Synthetic Methodologies for Drug Discovery (CPA Session)

- 10:30 Session Chair**  
Dr Ming-Qiang ZHANG  
(AMGEN, Shanghai City, China)
- 10:35 Tricyclic Peptides via Templated Tandem CLIPS/CUAAC Cyclizations**  
Prof. Peter TIMMERMAN  
(PEPSCAN THERAPEUTICS, Lelystad, The Netherlands)
- 11:15 Asymmetric Synthesis of Statin API as the Hypolipidemic Agents: The Evolution from the Chemical Kinetic Resolution to the Asymmetric Catalytic Technology (An Odyssey)**  
Prof. Fener CHEN  
(FUDAN UNIVERSITY, Shanghai Shi, China)
- 11:35 Practical Asymmetric Hydrogenation**  
Prof. Xumu ZHANG  
(SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY, Guangdong, China)
- 11:55 Synthesis of MedChem-Relevant Gem-Difluorocycloalkane Building Blocks**  
Prof. Dmytro VOLOCHNYUK  
(ENAMINE LTD, Kyiv, Ukraine)

### Session *Session 15 'Therapeutic Areas'*

#### Upcoming Treatments for NASH and Other Fibrotic Diseases

- 10:30 Session Chair**  
Prof. Roberto PELLICCIARI  
(TES PHARMA SRL, Corciano, Italy)
- 10:35 Obeticholic Acid, Leading in the NASH Race. History and Perspectives**

## Programme Schedule

Prof. Roberto PELLICCIARI  
(TES PHARMA SRL, Corciano, Italy)

- 11:15 Discovery of LUN452 (Tropifexor), a Highly Potent, Non-Bile Acid FXR Agonist for the Treatment of Cholestatic Liver Diseases and NASH**

Dr David TULLY  
(NOVARTIS, Emeryville, United States)

- 11:35 The First Class of Orally Available Mono-Saccharide Galectin-3 Inhibitors for Treatment of Fibrosis (NASH) and Cancer**

Dr Fredrik ZETTERBERG  
(GALECTO BIOTECH, Gothenburg, Sweden)

- 11:55 Development of Small-Molecule Inhibitors of Adipose Triglyceride Lipase (ATGL)**

Ms Anna MIGGLAUTSCH  
(TU GRAZ, Graz, Austria)

### Session *Session 16 'Chemical Biology'*

#### Recent Developments in Kinase Inhibitors

- 10:30 Session chair**

Prof. Stefan LAUFER  
(UNIVERSITY OF TÜBINGEN, Tübingen, Germany)

- 10:35 EGFR Triple Mutant L858R\_T790M\_C797S Recent Set-Backs and New Hope in Fighting Mutant Non-Small Cell Lung Cancer**

Prof. Stefan LAUFER  
(UNIVERSITY OF TÜBINGEN, Tübingen, Germany)

- 11:15 Design and Rationale for Exquisite Selectivity of Preclinical and Clinical Kinase Inhibitors**

Dr Laurent SCHIO  
(SANOFI, Vitry sur Seine, France)

- 11:35 Chemical Probes for New Therapeutic Concept Discovery**

Dr Peter ETTMAYER  
(BOEHRINGER-INGELHEIM, Vienna, Austria)

- 11:55 Discovery of the TYK2 Selective Inhibitor PF-6826647 for the Treatment of Crohn's Disease, and Other Autoimmune Conditions**

Dr Brian GERSTENBERGER  
(PFIZER, Cambridge, United States)

- 12:15 Exhibition & Lunch**

- 12:15 Schrödinger Workshop  
Data Driven Drug Design – Using LiveDesign**

### Session *Session 17*

#### Emerging Topics

- 13:15 Session Chair**

Prof. Gabriele COSTANTINO  
(UNIVERSITY OF PARMA, Parma, Italy)

- 13:20 Development of Potent, Selective, CNS Penetrant Small Molecule Inhibitors of Notum to Potentiate Wnt Signaling for the Maintenance of Synaptic Function in Alzheimer's Disease**

Prof. Paul FISH  
(ARUK UCL DRUG DISCOVERY INSTITUTE, London, United Kingdom)

- 13:40 Synthetic Small-Molecule RNA Ligands: Scope and Therapeutic Applications**

Dr Maria DUÇA  
(UNIVERSITÉ CÔTE D'AZUR, Nice, France)

- 14:00 Discovery of First-in Class, Selective and Noncovalent Small Molecule Inhibitors of DNMT1**

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

## Programme Schedule

**14:20 ASTX660, the First Fragment-Derived IAP Antagonist in the Clinic**

Dr Steven HOWARD  
(ASTEX THERAPEUTICS, Cambridge, United Kingdom)

**14:40 IUPAC-Richter Prize Lecture  
Discovery of CFTR Modulators For The Treatment of Cystic Fibrosis**

Dr Peter GROOTENHUIS  
(VERTEX PHARMACEUTICALS, San Diego, United States)

### Session *Session 18 'Therapeutic Areas'*

#### Addressing Infectious Diseases in the Developing Countries (AFMC Session)

**13:15 Session Chair**

Dr Renate GRIFFITH  
(UNIVERSITY OF NEW SOUTH WALES, UNSW Sydney, Australia)

**13:20 All Bugs are Shallow: Open Source Drug Discovery**

Prof. Matthew TODD  
(UNIVERSITY COLLEGE LONDON, London, United Kingdom)

**14:00 Towards the Development of Novel Inhibitors for Chikungunya Virus Infection: Approaches in Structure-Activity-Metabolism Relationship (SAMR) Studies**

Prof. Christina CHAI  
(NATIONAL UNIVERSITY OF SINGAPORE, Singapore, Singapore)

**14:20 Identification of New Antimalarial GSK607: An Example of Adaptive and Differentiated Early Drug Development**

Dr Esther FERNANDEZ  
(GLAXOSMITHKLINE, Tres Cantos, Spain)

**14:40 Mechanisms of HIV-1 Nucleocapsid Protein Inhibition by Small Molecules Targeting RNA**

Dr Alice SOSIC  
(UNIVERSITY OF PADOVA, Padova, Italy)

### Session *Session 19 'Chemical Biology'*

#### The Sphingosine-1-Phosphate Axis: Therapeutic Potential in Inflammation, Cancer, and More (ACS Session)

**13:15 Session Chair**

Dr Tony LEE  
(GILEAD SCIENCES, Seattle, United States)

**13:20 Unravelling the Mysteries of the Sphinx: Novel Targets and Small-Molecule Therapeutics from the Sphingolipid Synthesis and Signaling Pathway**

Prof. Bernard FLYNN  
(MONASH UNIVERSITY, Parkville, Australia)

**14:00 Active Site Inhibitors of Sphingosine 1-Phosphate Lyase - Exploring Novel Biology with Tool Compounds**

Dr Sven WEILER  
(BASILEA PHARMACEUTICA INTERNATIONAL LTD., Basel, Switzerland)

**14:20 Controlling Sphingosine-1-Phosphate Levels as a Therapeutic Strategy**

Dr Webster L. SANTOS  
(VIRGINIA TECH, Blacksburg, United States)

**15:00 End of the Day**

**15:30 Excursions**

**20:00 Banquet**

### Thursday September 6, 2018

#### Session *Session 20 'Technologies'*

##### Recent Developments in Nucleoside Medicinal Chemistry

**08:30 Session Chair**

Dr Jared CUMMING  
(MSD, Boston, United States)

**08:35 Cyclic Dinucleotide STING Agonists as Anti-Tumor Agents**

Dr Wes TROTTER  
(MSD, Boston, United States)

**09:15 Discovery of JNJ-64619178 as a Potent and Selective PRMT5 Inhibitor for the Treatment of Lung and Hematologic Cancers**

Dr Jan Willem THURING  
(JANSSEN PHARMACEUTICA NV, Beerse, Belgium)

**09:35 Design and Synthesis of Congeners of Cyclic ADP-Ribose, a Ca<sup>2+</sup>-Mobilizing Second Messenger, Toward Identification of the Target Protein**

Prof. Satoshi SHUTO  
(HOKKAIDO UNIVERSITY, Sapporo, Japan)

**09:55 Development of Novel Sialyltransferase Inhibitors via Computer Aided Drug Design**

Mr Andrew MONTGOMERY  
(UNIVERSITY OF WOLLONGONG, Wollongong, Australia)

#### Session *Session 21 'Therapeutic Areas'*

##### Inflammatory and Autoimmune Diseases

**08:30 Session Chair**

Prof. Stanislav GOBEC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**08:35 Nonpeptidic Selective Inhibitors of Immunoproteasome**

Prof. Stanislav GOBEC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

**09:15 Small Molecule Immunomodulators that Target Toll-Like Receptors**

Prof. Hang YIN  
(TSINGHUA UNIVERSITY, Beijing, China)

**09:35 A Dual Modulator of Farnesoid X Receptor and Soluble Epoxide Hydrolase to Treat Non-Alcoholic Steatohepatitis (EFMC-YMCS Presentation Prize)**

Dr Daniel MERK  
(ETH ZÜRICH, Zürich, Switzerland)

**09:55 Discovery of SPL-707: A Potent, Selective, and Orally Bioavailable SPPL2a Inhibitor**

Dr Juraj VELCICKY  
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

#### Session *Session 22 'Chemical Biology'*

##### Enzyme Activators and Positive Allosteric Modulators

**08:30 Session Chair**

Prof. Joachim MITTENDORF  
(BAYER AG, Wuppertal, Germany)

**08:35 Design, Synthesis, and Mechanism of  $\beta$ -Glucocerebrosidase Activators for Gaucher's and Parkinson's Diseases**

Prof. Richard B. SILVERMAN  
(NORTHWESTERN UNIVERSITY, Evanston, United States)

**09:15 Positive Allosteric Modulators of the GABA-B Receptor**

Dr Sean C. TURNER  
(ABBVIE, Ludwigshafen am Rhein, Germany)

## Programme Schedule

**09:35 The Value of Orthogonal Techniques for Elucidating Binding Site(s) of GPCR Allosteric Modulators: a Case Study With Positive Allosteric Modulators of Dopamine Receptors**

Dr Anne VALADE  
(UCB, Braine-l'Alleud, Belgium)

**09:55 AMPA Receptor Positive Allosteric Modulators Based on New Scaffolds: Design, Synthesis, and Studies**

Dr Vladimir A. PALYULIN  
(LOMONOSOV MOSCOW STATE UNIVERSITY, Moscow, Russia)

**10:15 Exhibition & Coffee (brunch)**

### Session *Session 23 'Technologies'*

#### **PET Imaging as a Tool for in vivo Drug Evaluation and Development (EANM Session)**

**10:45 Session Chair**

Prof. Antony GEE  
(KING'S COLLEGE LONDON, London, United Kingdom)

**10:50 PET Molecular Imaging – an Overview**

Prof. Antony GEE  
(KING'S COLLEGE LONDON, London, United Kingdom)

**11:30 PET in Neuroscience Drug Discovery and Development**

Dr Magnus SCHOU  
(KAROLINSKA INSTITUTE, Stockholm, Sweden)

**11:50 PET for Oncology Drug Discovery and Development**

Prof. Bert WINDHORST  
(VU UNIVERSITY MEDICAL CENTER, Amsterdam, The Netherlands)

**12:10 Discovery of Candidates for PET Molecular Imaging of Pathological TDP-43 Aggregates in Frontotemporal Dementia and Amyotrophic Lateral Sclerosis Patients**

Dr Vincent DARMENCY  
(AC IMMUNE SA, Lausanne, Switzerland)

### Session *Session 24*

#### **Late Breaking News**

**10:45 Session Chair**

Dr Anna KARAWAJCZYK  
(SELVITA, Krakow, Poland)

**10:50 First Disclosure of the Clinical Candidate BAY-840, a Potent And Selective hBradykinin B1 Antagonist for the Treatment of Chronic Inflammatory Diseases, Generated within the Bayer-Evotec Strategic Alliance**

Dr Stefan BÄURLE  
(BAYER AG, Berlin, Germany)

**11:10 Discovery of GDC-0077: A Highly Selective Inhibitor and Degradator of Mutant PI3K-Alpha**

Dr Jamie KNIGHT  
(CHARLES RIVER, Harlow, United Kingdom)

**11:30 Anti-HBV Drug Discovery Enabled by Structure-Based Drug Design and Phenotypic Screening**

Dr Hong SHEN  
(ROCHE INNOVATION CENTER, Shanghai, China)

**11:50 Discovery of AZD4573, a Potent and Selective Inhibitor of CDK9 that Enables Transient Target Engagement for the Treatment of Haematological Malignancies**

Dr Bernard BARLAAM  
(ASTRAZENECA, Cambridge, United Kingdom)

**12:10 The Discovery of CNP520, an Amino-1,4-Oxazine BACE Inhibitor in Prevention Studies**

Dr Rainer MACHAUER  
(NOVARTIS PHARMA AG, Basel, Switzerland)

## Programme Schedule

### Session *Session 25 'Therapeutic Areas'*

#### Cardiometabolic Diseases

**10:45 Session Chair**

Dr Jesper LAU  
(NOVO NORDISK, Maaloev, Denmark)

**10:50 C-Natruiretic Peptide Agonists for Cardiovascular Disease**

Prof. David SELWOOD  
(UNIVERSITY COLLEGE LONDON, London, United Kingdom)

**11:30 The Discovery of Semaglutide - A Journey from Ala Scan to Structural Design of GLP-1 Analogues**

Dr Jesper LAU  
(NOVO NORDISK, Maaloev, Denmark)

**11:50 Discovery and Optimization of Non-Covalent, Selective, and Bioavailable Small Molecule Inhibitors of the KEAP1-Nrf2 Pathway**

Dr Hauke SZILLAT  
(SANOFI, Frankfurt, Germany)

**12:10 Discovery and Clinical Evaluation of MK-8150, a Novel Nitric Oxide Donor with a Unique Mechanism of Nitric Oxide Release**

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

**12:30 Chair**

Dr Cornelia ZUMBRUNN  
(IDORSIA PHARMACEUTICALS, Allschwil, Switzerland)

**Smart Chemical Probes: from Bromodomain Ligands to Natural Products**

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

**13:15 Closing Remarks, Poster Prizes and Welcome to EFMC-ISMIC 2020**

Prof. Marko ANDERLUH (UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)  
Dr Yves P. AUBERSON (NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)