

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

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

Dr 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, Monheim, Germany)

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

Dr Franz VON NUSSBAUM
(BAYER, Monheim, 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-Degrade**
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, Gothenburg, Sweden)

10:35 New Modalities for Complex and Unprecedented Biological Targets

Dr Eric VALEUR
(ASTRAZENECA, IMED BIOTECH UNIT, Gothenburg, Sweden)

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
(RESEARCH CENTRE FOR NATURAL SCIENCES, 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: Letermovir 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 LJN452 (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**

Prof. Maria DUCA
(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 Ca²⁺-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 β -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-Natriuretic 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, SHARP & DOHME, 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)