

Sunday September 2, 2018

Registration

Steklena Hall

Opening Ceremony

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

Kocka Hall

Chair

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

Kocka Hall

Zika Virus: An Old Virus with a New Face

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

Kocka Hall

Chair

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

Kocka Hall

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

Dr Bayard HUCK
(MERCK BIOPHARMA, Darmstadt, Germany)

Kocka Hall

Award Ceremony

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

Kocka Hall

Chair

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

Kocka Hall

NAUTA AWARD FOR PHARMACOCHEMISTRY

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

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

Kocka Hall

Chair

Prof. Hans Ulrich STILZ
(NOVO NORDISK, Cambridge, United States)

Kocka Hall

Synthetic Glycoconjugate Vaccines against Bacterial Infections

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

Programme Schedule

Kocka Hall

Welcome Reception

Steklena & Kupola Hall

End of the Day

Programme Schedule

Monday September 3, 2018

Chair

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

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

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

Chair

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

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)
Kocka Hall

Exhibition & Coffee

Steklana & Kupola Hall

Session Session 1 'Technologies'

Artificial Intelligence Applications in Medicinal Chemistry

Marmorna Hall 1

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
(EXSCIENCIA, Dundee, United Kingdom)

11:35 Computer-Aided Synthesis Planning

Dr Marwin SEGLER
(BENEVOLENTAI, Cambridge, 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

Kocka Hall

10:30 Session Chair

Dr Luc VAN HIJFTE
(MERCACHEMSYNCOM, Nijmegen, The Netherlands)

10:35 Small Molecule Immune Checkpoint Antagonists for Cancer Therapy

Programme Schedule

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)

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)

Marmorna Hall 2

10:30 Session Chair

Dr Sonsoles MARTIN-SANTAMARIA
(CIB-CSIC, 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)

Exhibition & Lunch

Steklana & Kupola Hall

Session Session 4 'Technologies'

Timing is Everything: Target Binding Kinetics and Pharmacokinetics

Marmorna Hall 1

13:15 Session Chair

Prof. Ad P. IJZERMAN
(LEIDEN UNIVERSITY, 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)

Prof. 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

Programme Schedule

Ms Victoria GEORGI
(BAYER AG, Berlin, Germany)

Session Session 5 'Therapeutic Areas'

Life Science at the Interface of Agro and Pharma

Kocka Hall

- 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)
- 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

Marmorna Hall 2

- 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, San Diego, 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)

Exhibition & Coffee

Steklana & Kupola Hall

Session Session 7

First Time Disclosures

Kocka Hall

- 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**

Programme Schedule

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)

Poster Session 1 (even numbers) & Networking

Steklena & Kupola Hall

End of the Day

Programme Schedule

Tuesday September 4, 2018

Chair

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

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)
Kocka Hall

Chair

Dr Phil JONES
(BIOASCENT, Glasgow, United Kingdom)
Kocka Hall

Sugars & Proteins: Glycomimetics to Target Infectious Disease

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

Exhibition & Coffee

Steklana & Kupola Hall

Session Session 8 'Technologies'

New Chemical Modalities in Medicinal Chemistry

Marmorna Hall 1

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 Stéphanie GUERET
(ASTRAZENECA-MAX PLANCK INSTITUTE SATELLITE UNIT, Mölndal, Sweden)

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

Kocka Hall

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

Programme Schedule

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

Dr Gergely TOTH

(CANTABIO PHARMACEUTICALS INC., Palo Alto, 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)

Marmorna Hall 2

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)

Exhibition & Lunch

Steklana & Kupola Hall

Chemical Computing Group Workshop

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

Povodni Mož Hall 3

Session Flash Posters 1

Marmorna Hall 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

Kocka Hall

Chair

Programme Schedule

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

Marmorna Hall 2

Chair

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

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

Marmorna Hall 1

13:45 Session Chair

Prof. György 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)

Kocka Hall

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, United Kingdom)

14:50 In silico Polypolarmacology

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

Programme Schedule

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

Marmorna Hall 2

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

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

Prof. Matthias GEHRINGER
(UNIVERSITY OF TUEBINGEN, Tuebingen, Germany)

Exhibition & Coffee

Steklana & Kupola Hall

Session Flash Posters 4

Marmorna Hall 1

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

Kocka Hall

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

Marmorna Hall 2

Chair

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

Programme Schedule

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

Discover the presenters [here](#)

Poster Session 2 (odd numbers) & Networking

Steklena & Kupola Hall

End of Poster Session

Concert

Cankarjem dom - Linhart Hall

Programme Schedule

Wednesday September 5, 2018

Chair

Dr Jürgen MACK
(BOEHRINGER INGELHEIM, Biberach an der Riss, Germany)
Kocka Hall

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)
Kocka Hall

EFMC Prize Ceremony

Dr Matthew TOZER (CONSULTANT, Bognor Regis, United Kingdom)
Prof. Rui MOREIRA (UNIVERSITY OF LISBON, Lisbon, Portugal)
Kocka Hall

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)
Kocka Hall

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)
Kocka Hall

Exhibition & Coffee

Steklana & Kupola Hall

Session Session 14 'Technologies'

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

Marmorna Hall 1

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)

Programme Schedule

Session Session 15 'Therapeutic Areas'

Upcoming Treatments for NASH and Other Fibrotic Diseases

Kocka Hall

10:30 Session Chair

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

10:35 Obeticholic Acid, Leading in the NASH Race. History and Perspectives

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

11:15 Discovery of LNJ452 (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

Marmorna Hall 2

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)

Exhibition & Lunch

Steklana & Kupola Hall

Schrödinger Workshop Data Driven Drug Design – Using LiveDesign

Povodni Mož Hall 3

Session Session 17

Emerging Topics

13:15 Session Chair

Programme Schedule

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 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)

- 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)

Kocka Hall

- 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)

Marmorna Hall 2

- 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)

Programme Schedule

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

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

End of the Day

Excursions

Banquet

Cankarjev dom - Grand Reception Hall

Programme Schedule

Thursday September 6, 2018

Session Session 20 'Technologies'

Recent Developments in Nucleoside Medicinal Chemistry

Marmorna Hall 1

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

Kocka Hall

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

Marmorna Hall 2

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, IL, United States)

Programme Schedule

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

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

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)

Exhibition & Coffee (brunch)

Steklana & Kupola Hall

Session Session 23 'Technologies'

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

Marmorna Hall 1

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

Kocka Hall

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)

Programme Schedule

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

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

Session Session 25 'Therapeutic Areas'

Cardiometabolic Diseases

Marmorna Hall 2

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 & CO. INC., Kenilworth, United States)

Chair

Dr Cornelia ZUMBRUNN
(IDORSIA PHARMACEUTICALS, Allschwil, Switzerland)

Kocka Hall

Smart Chemical Probes: from Bromodomain Ligands to Natural Products

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

Kocka Hall

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)

Kocka Hall