

Programme

Thursday September 6, 2018

13:45 **Registration**

14:30 **Welcome and opening**

Session Chair

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

14:35 **KL01 - From Hits, to Leads to Chemical Probes: An Exciting Journey**

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

YMCS competition presentation session I

Session Chair

Dr Daniel MERK
(ETH ZÜRICH, Zürich, Switzerland)

15:05 **OC01 - Impact and Prediction of Binding Kinetics on in Vivo Drug Efficacy
Winner of the young medicinal chemist meeting in France**

Dr Abdenmour BRAKA
(IRIM, Gif-sur-Yvette, France)

15:25 **OC02 - Prospective Applications of Artificial Intelligence in de Novo Molecular Design for Drug Discovery**

Mr Lukas FRIEDRICH
(ETH ZURICH, Zurich, Switzerland)

15:45 **OC03 - Targeted Metabolomics Profiling as a Basis for Predictive Models in Multiple Sclerosis Research
Winner of the young medicinal chemist meeting in Russia**

Mr Marat KASAKIN
(INSTITUTE OF CHEMICAL BIOLOGY AND FUNDAMENTAL MEDICINE, Novosibirsk, Russia)

16:05 **Flash poster presentations (0-10)**

**FP01 - Targeting Basic Defect in Cystic Fibrosis: Discovery and Development of Novel Nanomolar F508-Del
CFTR Correctors**

Dr Alejandra RODRIGUEZ-GIMENO
(ISTITUTO ITALIANO DI TECNOLOGIA, Genova, Italy)

**FP02 - Buruli Ulcer and The mTOR Pathway: Total Synthesis, Structure-Activity and Target Elucidation
Studies of Mycolactones**

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

FP03 - The Development of New Treatments for Multi-Drug Resistant Tuberculosis

Ms Lisa BARBARO
(MONASH UNIVERSITY, Reservoir, Australia)

**FP04 - Synthesis and Characterisation of Psoralen Derivates as Inhibitors of The 25i Subunit of the
Immunoproteasome**

Programme

Ms Eva Shannon SCHIFFRER
(UNIVERSITY OF LJUBLJANA, FACULTY OF PHARMACY, Zirovnica, Slovenia)

FP05 - Fragment-Based Approach Applied to The Discovery of Protein-Protein Interaction Stabilisers

Mr Dario VALENTI
(TAROS CHEMICALS GMBH & CO. KG, Dortmund, Germany)

FP06 - The Use of Irreversible Ligands in the Quest to Obtain the First Ligand-Bound X-Ray Structures of The Adenosine A1 Receptor

Dr Manuela JORG
(MONASH UNIVERSITY, Parkville, Australia)

FP07 - Inhibitors of Human Sialyltransferases as Novel Anti-Metastatic Agents

Mr Chris DOBIE
(UNIVERSITY OF WOLLONGONG, Gwynneville, Australia)

FP08 - 3-Oxabicyclo[4.1.0]Heptane: A Bioisostere for Morpholine as a Kinase Hinge Binding Moiety

Mr Declan SUMMERS
(GLAXOSMITHKLINE, Stevenage, United Kingdom)

FP09 - Development of Small-Molecule Inhibitors of Adipose Triglyceride Lipase (ATGL)

Ms Anna MIGGLAUTSCH
(TU GRAZ, Graz, Austria)

FP10 - Covalent Fragment-Based Discovery of New Mura Inhibitors

Dr Martina HRAST
(FAKULTETA ZA FARMACIJO, Ljubljana, Slovenia)

16:25 Coffee Break

YMCS competition presentation session II

Session Chair

Dr Kristina GONCHARENKO
(SPIROCHEM AG, Basel, Switzerland)

16:40 OC04 - The Design and Synthesis of Bromodomain Photoaffinity Probes
Winner of the young medicinal chemist meeting in the United Kingdom

Mr David FALLON
(GLAXOSMITHKLINE, Stevenage, United Kingdom)

17:00 OC05 - Gemini-Type Protacs: a Small Molecule-Based Strategy for Self-directed Inactivation of Cereblon

Dr Christian STEINEBACH
(UNIVERSITY OF BONN, Bonn, Germany)

17:20 OC06 - Investigation of Direct Effect of Psychoactive Compounds on Invertebrate Neurons in Real Time
Winner of the young medicinal chemist meeting in Hungary

Dr Gabor MAASZ
(HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)

17:40 OC07 - Hydrogen peroxide sensitive prodrugs of methotrexate and aminopterin for the treatment of rheumatoid arthritis
Winner of the young medicinal chemist meeting in Denmark

Dr Jorge PEIRO CADAHIA
(NUEVOLUTION A/S, Copenhagen, Denmark)

18:00 Flash poster presentations (10-20)

Programme

FP11 - Rational Design of Optimized Allosteric Effectors of Cathepsins K and S Based on Succinimide-Glycinate Scaffold

Ms Tjasa GORICAN
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

FP12 - Covalent Inhibition with Terminal Alkyne As 'Inert' Electrophile

Mrs Elma MONS
(LEIDEN UNIVERSITY MEDICAL CENTER, Leiden, The Netherlands)

FP13 - Exploration of Chemical Space of Two Classes of INHA Inhibitors

Dr Izidor SOSIC
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

FP14 - Late-Stage Functionalization of Peptides: Novel Site-Selective Modification & Bioconjugation

Dr Anaïs NOISIER
(ASTRAZENECA, Mölndal, Sweden)

FP15 - Identification of A GSK-3 β /CK-1 γ Inhibitor: Dual Target and Dual Mechanisms of Action as Possible Strategy for The Treatment of Parkinson's Disease.

Prof. Stephanie FEDERICO
(UNIVERSITY OF TRIESTE, Trieste, Italy)

FP16 - Discovery of Benzothiazole-Based DNA Gyrase and Topoisomerase IV Inhibitors with Broad Spectrum Antibacterial Activity

Ms Martina DURCIK
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

FP17 - Development of Peptides as Therapeutics for Pharmacological Intervention in Vital Protein Cascades

Dr Christina LAMERS
(UNIVERSITY OF BASEL, Leipzig, Germany)

FP18 - Deep Learning Applications in The Design and Identification of Antibacterial Compounds

Dr Marko JUKIC
(FAKULTETA ZA FARMACIJO, UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

FP19 - The Design and Synthesis of Novel Inhibitors of the Notch Activation Complex Kinase for Notch Mediated Tumorigenesis

Ms Tanya KELLEY
(UNIVERSITY OF MIAMI, miami, United States)

18:20 **Poster presentation session 1 (Odd numbers) & Networking drink**

20:00 **End of the day**

20:15 **Optional Networking Event (until 21:30)**

Programme

Friday September 7, 2018

YMCS competition presentation session III

Session Chair

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

- 08:30** **OC08 - Fosmidomycin Analogs as Antimalarial and Antitubercular Agents - a Prodrug Approach**
Winner of the young medicinal chemist meeting in Belgium (KVCV)
Ms Charlotte COURTENS
(UGENT, Gent, Belgium)
- 08:50** **OC09 - Metal-Chelating Acetohydroxamic Acids against Hepatitis C Virus and Flaviviruses**
Winner of the young medicinal chemist meeting in Greece
Ms Erofilis GIANNAKOPOULOU
(NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS, Athens, Greece)
- 09:10** **OC10 - Elucidation of the Antifungal Mechanism of Action of Bis-Guanyldrazones**
Winner of the young medicinal chemist meeting in Serbia
Ms Jelena LAZIC
(UNIVERSITY OF BELGRADE, FACULTY OF CHEMISTRY, Belgrade, Serbia)
- 09:30** **OC11 - Discovery and Optimisation of N-Phenylpyrrolamides as DNA Gyrase B Inhibitors**
Winner of the young medicinal chemist meeting in Slovenia
Dr Nace ZIDAR
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)
- 09:50** **OC12 - The Effect of Singlet Oxygen Production and Lipophilicity of the Photosensitizer in Photodynamic Activity of N-Methylated and N-Oxidised Pyridylporphyrins**
Winner of the young medicinal chemist meeting in Croatia
Ms Martina MUSKOVIC
(UNIVERSITY OF RIJEKA, Rijeka, Croatia)
- 10:10** **Coffee Break**

YMCS competition presentation session IV

Session Chair

Mr Roman SINK
(UNIVERSITY OF LJUBLJANA FACULTY OF PHARMACY, Ljubljana, Slovenia)

- 10:30** **OC13 - Synthesis and Biological Evaluation of Bia 10-2474: an Irreversible and Aspecific Faah Inhibitor**
Winner of the young medicinal chemist meeting in The Netherlands
Dr Anthe JANSSEN
(LEIDEN UNIVERSITY, Leiden, The Netherlands)
- 10:50** **OC14 - Methylene - Cycloalkylacetate (mca) as Novel Neurotropic Agents**
Winner of the young medicinal chemist meeting in Israel
Mr David LANKRI
(HEBREW UNIVERSITY, Jerusalem, Israel)
- 11:10** **OC15 - Development of Release-and-Report Kinase Inhibitors as Molecular Tools for Investigating Neurodegenerative Disorders**
Winner of the young medicinal chemist meeting in Sweden

Programme

Dr Cassandra LEE FLEMING
(UNIVERSITY OF GOTHENBURG, Gothenburg, Sweden)

- 11:30** **OC16 - Piperazine Derivatives as a Novel, Active Histamine h3 Receptor Ligands**
Winner of the young medicinal chemist meeting in Poland

Dr Katarzyna SZCZEPANSKA
(JAGIELLONIAN UNIVERSITY MEDICAL COLLEGE, Krakow, Poland)

- 11:50** **Lunch & Poster presentation session 2 (Even numbers)**

YMCS competition presentation session V

Session Chair

Prof. Emmanouil FOUSTERIS
(UNIVERSITY OF PATRAS, Patras, Greece)

- 13:15** **OC17 - Development of Aminoxyrone as the First-in-Class hsp90 C-Terminal Domain Dimerization Inhibitor**
Winner of the young medicinal chemist meeting in Germany

Prof. Finn HANSEN
(UNIVERSITÄT LEIPZIG, Leipzig, Germany)

- 13:35** **OC18 - How Can We Inhibit a Protein that is Intrinsically Disordered? Androgen Receptor – epi-001 a Case Study**
Winner of the young medicinal chemist meeting in Spain

Dr Marta FRIGOLE-VIVAS
(INSTITUTE FOR RESEARCH IN BIOMEDICINE (IRB BARCELONA), Dresden, Germany)

- 13:55** **OC19 - Kinase Templated Abiotic Reaction: from Promiscuity to Selectivity**
Winner of the young medicinal chemist meeting in Switzerland

Mr Jacques SAARBACH
(UNIVERSITÉ DE GENÈVE, Geneva 4, Switzerland)

- 14:15** **OC20 - The Best of Three Worlds: Tackling Multidrug Resistance through Phytochemical, Biological and Computational Approaches**
Winner of the young medicinal chemist meeting in Portugal

Dr Ricardo FERREIRA
(UPPSALA UNIVERSITY, Uppsala, Sweden)

- 14:35** **OC21 - Targeting Zinc-Finger Proteins in Cancer and Viral Infections**
Winner of the young medicinal chemist meeting in Italy

Dr Mattia MORI
(UNIVERSITY OF SIENA, Siena, Italy)

- 14:55** **Voting break**

- 15:10** **KL02 - My Lessons in Drug Discovery**

Dr Marton CSEKEI
(SERVIER RESEARCH INSTITUTE OF MEDICINAL CHEMISTRY, Budapest, Hungary)

- 15:40** **Closing and award ceremony**