

Thursday September 6, 2018

13:45 Registration

14:30 Welcome and opening

Session Chair

Dr 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, Montpellier, 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 β 5i 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

Ms 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)

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.

Dr 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)

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 Erofili GIANNAKOPOULOU
(NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS, Athens, Greece)
- 09:10** **OC10 - Elucidation of the Antifungal Mechanism of Action of Bis-Guanylhydrazones**
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