

## 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 20S 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 $\beta$ /CK-1 $\gamma$ 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 Erofilii 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 Lipophylicity 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**