

### Thursday September 1, 2016

14:15 Registration

15:00 Welcome and opening

15:00 Session Chair

Prof. Koen AUGUSTYNS  
(UNIVERSITY OF ANTWERP, Antwerp, Belgium)

15:05 Case Histories of Fragment-Based Drug Discovery.

Dr David REES  
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

15:35 Heterocycles and Medicinal Chemistry: the Importance of Innovative Synthesis

Dr Anthony WOOD  
(PFIZER, Waltham, United States)

#### YMCS Competition Presentation Session I

16:05 **New Avenues in Protein Labeling - Exploiting Dna for Directing Chemical Reactions**  
**Winner of the young medicinal chemist meeting in Denmark (CP01)**

Dr Anne Louise Bank KODAL  
(NOVO NORDISK, Bagsværd, Denmark)

16:25 **Drug Design, Synthesis and Biological Evaluation of Antiretroviral and Anticancer Agents**  
**Winner of the young medicinal chemist meeting in Italy (CP02)**

Dr Valeria FAMILGLINI  
(UNIVERSITY OF ROME, Rome, Italy)

16:45 **Development of Potent, Cell-Active Inhibitors of the Mycobacterium Tuberculosis Cholesterol Oxidase Cyp125 (OC01)**

Ms Madeline KAVANAGH  
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

17:05 Flash Poster Presentations

#### FP01- Toward Libraries of Artificial Macrocycles

Mrs Eman ABD ELRAHEEM  
(GRONINGEN UNIVERSITY, Groningen, The Netherlands)

#### FP02 - Discovery, Structural Exploration and Biological Profiling of a Novel Class of Antimycobacterial Dpre1 Inhibitors

Ms Olga BALABON  
(UNIVERSITY OF ANTWERP, Wilrijk, Belgium)

#### FP03 - Orally Bioavailable Antimalarial 4(1h)-Quinolone Prodrugs with Single-Dose Cures

Dr Fabian BROCKMEYER  
(NORTHEASTERN UNIVERSITY, Germany)

#### FP04 - Development of Synthesis Methodology for Dna-Encoded Small Molecule Screening Libraries

Dr Mateja KLIKA SKOPIC  
(TECHNISCHE UNIVERSITÄT DORTMUND, Dortmund, Germany)

**FP05 - Fishing for an Off-Target": Deconvoluting the Molecular Mechanism of GPCR-Induced Macrophage Chemotaxis"**

Dr Maria CHATZOPOULOU  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

**FP06 - Design, Synthesis and Pharmacological Evaluation of Fluorescent Tools for Studying Cannabinoid Type 2 Receptor**

Ms Anna COOPER  
(UNIVERSITY OF OTAGO, Dunedin, New Zealand)

**FP07 - Development of Novel, Selective and Irreversible PI3K $\gamma$  Inhibitors**

Mr Sam DALTON  
(UNIVERSITY OF STRATHCLYDE, Glasgow, United Kingdom)

**FP08 - Identification of Novel Non-Natural Supramolecular Ligands as Stabilizers of 14-3-3 $\sigma$  Protein-Protein Interactions**

Dr Alba GIGANTE  
(DUISBURG ESSEN UNIVERSITY, Tres Cantos-Madrid, Spain)

**FP09 - Targets in Orphan Diseases and Their Repurposing Candidates - Analysis with a Knime Workflow Using Open Phacts**

Ms Jana GURINOVA  
(UNIVERSITY OF VIENNA, Vienna, Austria)

**FP10 - Selectivity Profiling of the Human Monoamine Transporters: A Case Study on Cathinone Analogs**

Ms Eva HELLSBERG  
(UNIVERSITY OF VIENNA, Vienna, Austria)

**FP11 - Photoswitchable 4-(Piperidin-4-yl)-1-Hydroxypyrazole Analogues for the GABA Type A Receptors**

Ms Henriette KIHL  
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

**FP12 - Extending Sar of Bile Acids as FXR/TGR5 Modulators: Synthesis and Biological Activity of Ring C Modified Cdca Derivatives**

Ms Serena MOSTARDA  
(UNIVERSITÀ DEGLI STUDI DI PERUGIA, Perugia, Italy)

**FP13 - Lead Optimisation of a Novel Class of Trypanosomacidal Agents**

Ms Harriet NEWSON  
(UNIVERSITY OF WESTERN AUSTRALIA, Australia)

**FP14 - Synthesis and Biological Evaluation of Diaromatic Guanidinium-Like Derivatives as Protein Kinase Inhibitors for the Treatment of Cancer**

Ms Viola PREVITALI  
(TRINITY COLLEGE DUBLIN, Dublin, Ireland)

**FP15 - Development of Novel 1,4-Benzodiazepines as Antitrypanosomal Agents**

Dr Santo PREVITI  
(UNIVERSITY OF MESSINA, Messina, Italy)

**FP16 - Determining the Binding Mode of 3-(1-Alkyl-1H-Imidazol-5-yl)-1H-Indoles**

Dr Adam HOGENDORF  
(MAJ INSTITUTE OF PHARMACOLOGY, POLISH ACADEMY OF SCIENCES, Krakow, Poland)

**FP17 - Targeting the Human Dihydroorotate Dehydrogenase (Hdhodh) by a Scaffold Hopping Bioisosteric Approach Using Hydroxylated Pentaatomic Heterocycles**

Dr Stefano SAINAS  
(UNIVERSITY OF TORINO, Torino, Italy)

**FP18 - Towards the Elucidation of the Mechanism of Action of Small Molecule Upregulators of Utrophin Using Chemical Proteomics**

Dr Aini VUORINEN  
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

**FP19 - Development of an Albumin-Binding Ligand for Prolonging the Plasma Half-Life of Peptide Therapeutics**

Mr Alessandro ZORZI  
(ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE , Lausanne, Switzerland)

**FP20 - Near-Infrared (Nir) Photothermal Therapy Using Biocompatible Palladium Nanoparticles**

Dr Belen RUBIO RUIZ  
(UNIVERSITY OF EDINBURGH, Edinburgh, United Kingdom)

**17:45**      **YMCS Poster presentation session & Networking drink**

**19:00**      **End of the day**

### Friday September 2, 2016

#### YMCS Competition Presentation Session II

- 08:30**     **Antimalarial Drug Discovery: Exploring the Mep Pathway**  
**Winner of the young medicinal chemist meeting in the United Kingdom (CP03)**  
Ms Kathryn PRICE  
(UNIVERSITY OF LIVERPOOL, Liverpool, United Kingdom)
- 08:50**     **Drugging the Undruggable: Targeting Challenging E3 Ligases**  
**Winner of the young medicinal chemist meeting in Spain (CP04)**  
Dr Carles GALDEANO  
(UNIVERSITAT DE BARCELONA, Barcelona, Spain)
- 09:10**     **Development of Highly Selective and Reversible Diacylglycerol Lipase Inhibitors**  
**Winner of the young medicinal chemist meeting in The Netherlands (CP05)**  
Dr Freek JANSSEN  
(LEIDEN UNIVERSITY, Nijmegen, The Netherlands)
- 09:30**     **Functional Lipidomics-Based Lead Discovery Reveals Novel Role of Phospholipids in Vitamin A Signaling**  
**Winner of the young medicinal chemist meeting in Germany (CP06)**  
Dr Andreas KOEBERLE  
(UNIVERSITY OF JENA, Jena, Germany)
- 09:50**     **Design, Synthesis and Biological Evaluation of Selective CDK Inhibitors based on Flavopiridol Structure**  
**Winner of the young medicinal chemist meeting in Greece (CP07)**  
Dr Nikitia MEXIA  
(UNIVERSITY OF ATHENS, Leeds, United Kingdom)
- 10:10**     **Coffee break**

#### YMCS Competition Presentation Session III

- 10:35**     **Design and Synthesis of 2,2'-Diindolylmethanes to Selectively Target Certain G-Quadruplex Dna Structures**  
**Winner of the young medicinal chemist meeting in Sweden (CP08)**  
Dr Madeleine LIVENDAHL  
(UMEA UNIVERSITY, Umeå, Sweden)
- 10:55**     **Stable, Effective, and Selective Anticancer Phenolato Titanium(IV) Complexes**  
**Winner of the young medicinal chemist meeting in Israel (CP09)**  
Dr Sigalit MEKER  
(THE HEBREW UNIVERSITY OF JERUSALEM, Kfar Yona, Israel)
- 11:15**     **Glyco-Conjugated Photosensitizers: From Synthesis to Validation in Cancer Photodynamic Therapy**  
**Winner of the young medicinal chemist meeting in Portugal (CP10)**  
Ms Patricia PEREIRA  
(UNIVERSIDADE DE AVEIRO, Aveiro, Portugal)
- 11:35**     **Discovery of Cct251921: A Potent, Selective and Orally Bioavailable Small Molecule Modulator of the Mediator Complex-Associated Kinases Cdk8 and Cdk19 (OC02)**  
Dr Aurelie MALLINGER  
(INSTITUTE OF CANCER RESEARCH, London, United Kingdom)
- 11:55**     **Lunch**

### YMCS Competition Presentation Session IV

- 13:15**    **How to Design Cell Permeable Non-Peptidic Macrocycles (OC03)**  
Dr Björn OVER  
(MACROCYCLE ADME, BEYOND RO5 AND NATURAL PRODUCT-FRAGMENTS, Landvetter, Sweden)
- 13:35**    **New 3d-Scaffolds for Fragment-Based Lead Discovery (Fbld): Exploration of Chemical Space Using Functionalized Spirohydantoin**  
**Winner of the young medicinal chemist meeting in France (CP11)**  
Mr Hugues PREVET  
(LABORATORY U1177 - UNIVERSITY OF LILLE, Lille, France)
- 13:55**    **Discovery Of Novel Atpase Inhibitors Of Dna Gyrase And Topoisomerase Iv Starting From Marine Sponge Alkaloid Oroidin**  
**Winner of the young medicinal chemist meeting in Slovenia (CP12)**  
Dr Tihomir TOMASIC  
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)
- 14:15**    **Purine Mimicking 3'-Ethynylribofuranose Nucleosides: New Opportunities for an Old Sugar Modification**  
**Winner of the young medicinal chemist meeting in Belgium (KVCV) (CP13)**  
Dr Fabian HULPIA  
(UGENT, Ghent, Belgium)
- 14:35**    **Experimental Platform for Characterization and High-Throughput Screening of Acetylcholinesterase Inhibitors**  
**Winner of the young medicinal chemist meeting in Poland (CP14)**  
Dr Piotr DRACZKOWSKI  
(UNIVERSITY OF LUBLIN, Lublin, Poland)
- 14:55**    **Novel Derivatives of the Tspo Ligand Dpa-714 For in Vivo Pet Imaging of Neuroinflammation (OC04)**  
Mrs Fanny CACHEUX  
(CEA, Orsay, France)
- 15:15**    **Voting Break**
- 15:30**    **Closing and award ceremony**