

Programme

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, Stevenage, Herts, SG1 2NY, United Kingdom)

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 - Developement of Synthesis Methodology for Dna-Encoded Small Molecule Screening Libraries

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

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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 γ Inhibitors

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

FP08 - Identification of Novel Non-Natural Supramolecular Ligands as Stabilizers of 14-3-3 σ 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 KIHLE
(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 Diaryl 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 (Hdh) by a Scaffold Hopping Bioisosteric Approach Using Hydroxylated Pentaatomic Heterocycles

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

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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**

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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**

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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)
Prof. 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, Beerse, 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**