

1st Alpine Winter Conference on Medicinal and Synthetic Chemistry

Programme

Sunday January 28, 2018

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| 17:00 | Opening Remarks |
| 17:15 | KL01 - Recent Developments in Strategies and Tactics Towards the Synthesis of Complex Secondary Metabolites as Enabling Tools for the Study of Biology and Medicine
Erick M. CARREIRA
(ETH ZÜRICH, Zürich, Switzerland) |
| 18:15 | Poster Session & Welcome Reception |
| 20:15 | End of Day 1 |

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Monday January 29, 2018

Session 1: Advances in Synthetic Methods

Session Chair

Nuno MAULIDE
(UNIVERSITY OF VIENNA, Vienna, Austria)

08:30 PL01 - Assembly Line Synthesis

Varinder K. AGGARWAL
(UNIVERSITY OF BRISTOL, Bristol, United Kingdom)

09:00 PL02 - Photochemical Reactions en route to Structurally Complex Molecules

Thorsten BACH
(TECHNISCHE UNIVERSITÄT MÜNCHEN, Garching, Germany)

09:30 Coffee Break

10:00 PL03 - Expanding the Potential of Organocatalysis with Light

Paolo MELCHIORRE
(INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA (ICIQ), Bologna, Italy)

10:30 OC01 - Exploring 3-D Pharmaceutical Space: New CH Functionalisation Reactions of Oxygen and Sulfur Heterocycles

Peter O'BRIEN
(UNIVERSITY OF YORK, York, United Kingdom)

11:00 End of the morning session

Session 2: Addressing Preclinical Toxicity – Approaches and Lessons Learned

Session Chair

Andy PEAT
(GLAXOSMITHKLINE, Durham, United States)

17:30 PL04 - Mechanism-Based Toxicities Associated With NAMPT Inhibition and Related Mitigation Strategies

Peter DRAGOVICH
(GENENTECH INC., San Francisco, United States)

18:00 PL05 - Utilizing in Depth Understanding of a Molecules Off-Target Profile to Tailor Clinical and Preclinical Safety Assessments

Douglas THOMSON
(CELLZOME GMBH, Heidelberg, Germany)

18:30 Coffee Break

19:00 PL06 - Reducing Bioactivation Potential of Drug Candidates: Implications for Preclinical Drug Optimization

Andreas BRINK
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

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- 19:30** **OC02 - Small Structural Changes Leading to Major Impact on Safety: Developing Safety Strategies in Medicinal Chemistry**
Martin PETTERSSON
(PFIZER, Cambridge, United States)
- 20:00** **Panel Discussion**
- 20:45** **End of Day 2**

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Tuesday January 30, 2018

Session 3: Advances in Lead Generation

Session Chair

Doris RIETHER
(BOEHRINGER INGELHEIM, Biberach an der Riss, Germany)

- 08:30 PL07 - ADAS (Affinity Directed Automated Synthesis): A New Technology to Accelerate Lead Generation**
Eva Maria MARTIN
(ELI LILLY, Madrid, Spain)
- 09:00 PL08 - A Chemist's Guide to Modern Phenotypic Drug Discovery**
Monika ERMANN
(EVOTEC LTD, Oxfordshire, United Kingdom)
- 09:30 Coffee Break**
- 10:00 OC03 - CDK8 Inhibitors with Pre-Engineered Long Residence Time, Exhibiting Efficacy in Tumor Xenograft Models**
Koen HEKKING
(MERCACHEM-SYNCOM, Nijmegen, The Netherlands)
- 10:30 PL09 - From Multiple Hit Series to (Pre)Clinical Candidates Using DNA-Encoded Library Technology**
Sanne SCHRODER GLAD
(NUEVOLUTION A/S, Copenhagen, Denmark)
- 11:00 End of the morning session**

Session 4: Chemical Biology in Drug and Target Discovery

Session Chair

Matthew HAYWARD
(PFIZER, Groton, United States)

- 17:30 PL10 - Fluorescent and Bioluminescent Sensor Proteins**
Kai JOHANSSON
(MAX-PLANCK INSTITUTE FOR MEDICAL RESEARCH, Heidelberg, Germany)
- 18:00 OC04 - Chemical Physiology of Antibody Conjugates and Natural Products**
Gonçalo BERNARDES
(INSTITUTO DE MEDICINA MOLECULAR, PORTUGAL & UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)
- 18:30 Coffee Break**
- 19:00 KL02 - Activity-based proteomics – Protein and Ligand Discovery on a Global Scale**
Benjamin CRAVATT
(THE SCRIPPS RESEARCH INSTITUTE, La Jolla, United States)
- 20:00 End of Day 3**

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Wednesday January 31, 2018

Session 5: Alternative Modalities

Session Chair

Philippe NANTERMET
(MERCK & CO. INC (MSD), West Point, United States)

08:30 PL11 - Intracellular Delivery of Macromolecules

David TELLERS
(MERCK & CO. INC (MSD), West Point, United States)

09:00 PL12 - New Modalities Probe and Hit Finding for Challenging Targets in Cardiovascular and Metabolic Diseases

Eric VALEUR
(ASTRAZENECA, IMED BIOTECH UNIT, Cambridge, United States)

09:30 Coffee Break

10:00 PL13 - Messenger RNA as a Novel Therapeutic Approach

Kerry BENENATO
(MODERNA THERAPEUTICS, Cambridge, United States)

10:30 OC05 - Proteolysis Targeting Chimera: A New Frontier in Medicinal Chemistry

Niall ANDERSON
(GLAXOSMITHKLINE, Hertfordshire, United Kingdom)

11:00 End of the morning session

Session 6: Late Stage Functionalization

Session Chair

Guido KOCH
(NOVARTIS PHARMA AG, Schlieren, Switzerland)

17:30 PL14 - New Chemical Tools for the Late Stage Functionalization of Biomolecules

Matthew GAUNT
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

18:00 PL15 - The Quest for Efficient Ligands in Asymmetric C-H Functionalizations

Nicolai CRAMER
(ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE, Lausanne, Switzerland)

18:30 Coffee Break

19:00 PL16 - Catalytic Approaches to Simplifying Synthesis

Darren J. DIXON
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

19:30 OC06 - Synthetic Routes to Oxindoles via Metal Catalysis

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Mark LAUTENS
(UNIVERSITY OF TORONTO, Toronto, ON, Canada)

20:00 **End of the Scientific Programme on Day 4**

21:00 **Conference Dinner**

23:00 **End of Day 4**

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Thursday February 1, 2018

Session 7: Challenges and Opportunities in Fragment Based Drug Discovery

Session Chair

Alison WOOLFORD
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

08:30 PL17 - Drug Discovery for Challenging Targets by X-ray Crystallographic Fragment Screening

Tom HEIGHTMAN
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

09:00 PL18 - The Impact of Fragments on Drug Discovery

Rod HUBBARD
(UNIVERSITY OF YORK & VERNALIS, Cambridge, United Kingdom)

09:30 Coffee Break

10:00 OC12 - Rational Design of Small-Molecules Inhibitors of Human Cyclophilins with a Pan Viral Activities by Fragment Based Drug Design Using a Linking Strategy

Jean-Francois GUICHOU
(CBS INSERM U1054, Montpellier, France)

10:30 OC07 - Fragment-Centric Methodologies for the Discovery of DOT1L Inhibitors

Christoph GAUL
(NOVARTIS, Basel, Switzerland)

11:00 End of the morning session

Session 8: Drug Discovery Tales

Session Chair

Sarah SKERRATT
(VERTEX PHARMACEUTICALS, London, United Kingdom)

17:10 OC08 - Discovery of Allosteric Malt1 Protease Inhibitors with High in Vivo Efficacy

Jean QUANCARD
(NOVARTIS, Basel, Switzerland)

17:30 OC09 - Discovery of Tak-041: A Potent and Selective Gpr139 Agonist for the Treatment of Negative Symptoms Associated with Schizophrenia

Holger MONENSCHIN
(TAKEDA CALIFORNIA, INC, San Diego, United States)

17:50 OC10 - Molecular Accessibility - Measuring and Understanding the Intracellular Free Concentration of Drugs During Lead Optimisation

(EYEDPHARMA)

18:10 OC11 - Discovery of a Ketohexokinase Inhibitor for the Treatment of Nafld/Nash: Fragment-to-Candidate via Structure-Based Drug Design and Parallel Chemistry

Brian RAYMER
(PFIZER, Cambridge, United States)

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- 18:30** **Coffee Break**
- 19:00** **KL03 - Novel Approaches in the Design of CNS Drug Candidates and PET Ligands**
Anabella VILLALOBOS
(BIOGEN, Cambridge, United States)
- 19:45** **Closing Remarks**
- 20:00** **End of Symposium**