

# 1st Alpine Winter Conference on Medicinal and Synthetic Chemistry

## Programme

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### Sunday January 28, 2018

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| 17:00 | Opening Remarks  |
| 17:15 | <b>KL01 - Recent Developments in Strategies and Tactics Towards the Synthesis of Complex Secondary Metabolites as Enabling Tools for the Study of Biology and Medicine</b><br>Erick M. CARREIRA<br>(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 Ketoheokinase 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**