

2nd Alpine Winter Conference on Medicinal and Synthetic Chemistry

Programme

Sunday January 19, 2020

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| 16:00 | Registration |
| 17:00 | Opening Remarks |
| 17:30 | Necessity is the Mother of Invention: Natural Products and the Chemistry They Inspire (KL01)
Prof. Sarah E. REISMAN
(CALIFORNIA INSTITUTE OF TECHNOLOGY, Pasadena, United States) |
| 18:30 | Poster Session & Welcome Reception |
| 20:30 | End of Day 1 |

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Monday January 20, 2020

08:30 **Session 1: Predictive ADME Sciences: Striking a Balance Between In Silico and Experimental Work?**

Session Chair

Dr Amit KALGUTKAR
(PFIZER, Groton, United States)

08:30 **Structural Attributes Influencing Unbound Tissue Distribution (PL01)**

Dr Li DI
(PFIZER, Groton, United States)

09:00 **Metabolism of Strained Rings: Tales of the Unexpected (PL02)**

Dr Martin HAYES
(ASTRAZENECA, Gothenburg, Sweden)

09:30 **Coffee Break**

10:00 **Leveraging In Silico ADMET Profiles and Ancillary Pharmacology to Influence Prioritization of Hit Series with Higher Probability of Success (PL03)**

Dr Falgun SHAH
(MERCK & CO., West Point, United States)

10:30 **Predicting ADME - Reality, Vision or Fantasy? (PL04)**

Dr Simone SCHADT
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

Dr Kenichi UMEHARA
(ROCHE PHARMACEUTICAL RESEARCH AND EARLY DEVELOPMENT, Basel, Switzerland)

11:00 **Outdoor Networking Activities**

15:45 **Networking Break**

16:00 **NovAliX Workshop: DNA-Encoded Libraries, an Integrated Platform for Hit Finding and Beyond**

Dr Julien MARIN
(NOVALIX, Illkirch, France)

17:00 **Session 2: Frontiers of Synthetic Chemistry**

Session Chair

Prof. Sarah E. REISMAN
(CALIFORNIA INSTITUTE OF TECHNOLOGY, Pasadena, United States)

17:00 **Break-it-to-Make-it Strategies for Complex Molecule Synthesis (PL05)**

Prof. Richmond SARPONG
(UNIVERSITY OF CALIFORNIA, BERKELEY, Berkeley, United States)

17:30 **New Avenues in Synthesis Enabled by Organic Photoredox Catalysis (PL06)**

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Prof. David NICEWICZ
(UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL, Chapel Hill, United States)

18:00 Coffee Break

18:30 Late-Stage Functionalizations (PL07)

Prof. Tobias RITTER
(MAX-PLANCK-INSTITUT FÜR KOHLENFORSCHUNG, Mulheim, Germany)

19:00 A Radical Way to Abeo-Steroids (PL08)

Prof. Philipp HERETSCH
(FREE UNIVERSITY OF BERLIN, Berlin, Germany)

19:30 Poster Session

20:30 End of Poster Session

21:00 Conference Dinner

23:00 End of Day 2

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Tuesday January 21, 2020

08:30 Session 3: Structure and Biophysics - Companions for Medicinal Chemistry

Session Chair

Dr Wolfgang JAHNKE
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

08:30 Membrane Proteins at the SGC – Challenges and Success Stories (PL09)

Dr Katharina DÜRR
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

09:00 The Mechanism of Outer Membrane Protein Insertion by BamA and its Role as a Target for Novel Antibiotic (PL10)

Prof. Sebastian HILLER
(UNIVERSITY OF BASEL, Basel, Switzerland)

09:30 Coffee Break

10:00 Discovery of ABL001, an Allosteric Inhibitor of BCR-ABL: Fragments, Biophysics, Structure and Chemistry (PL11)

Dr Wolfgang JAHNKE
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

10:30 Discovery of Small Molecule Fascin 1 Inhibitors Using Fragment-Based Drug Discovery (OC01)

Dr Stuart FRANCIS
(THE BEATSON INSTITUTE FOR CANCER RESEARCH, Glasgow, United Kingdom)

11:00 Outdoor Networking Activities

15:00 Networking Break & "Beyond-the-Science Leadership Development" Workshop

15:00 Beyond-the-Science Leadership Development

Session Chair

Dr Michelle CLAFFEY
(CLAFFEY LEADERSHIP, Norwich, United States)

Session Chair

17:00 Session 4: Protein Degradation: New Rules for Drug Discovery

Session Chair

Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

17:00 Targeted Protein Degradation (PL12)

Prof. Andy PHILLIPS
(C4 THERAPEUTICS, Watertown, United States)

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- 17:30** **Chemical Genomics Approaches to Targeted Protein Degradation (PL13)**
Dr Georg WINTER
(RESEARCH CENTER FOR MOLECULAR MEDICINE OF THE AUSTRIAN ACADEMY OF SCIENCES, Vienna, Austria)
- 18:00** **Four E3 Ligases, One Target: Towards Novel CDK6 Protacs (OC02)**
Dr Christian STEINEBACH
(UNIVERSITY OF BONN, Bonn, Germany)
- 18:30** **Coffee Break**
- 19:00** **Expanding the Druggable Genome through Cereblon-Mediated Protein Degradation (KL02)**
Dr Lawrence G. HAMANN
(BRISTOL-MYERS SQUIBB, San Francisco, United States)
- 20:00** **End of Day 3**

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Wednesday January 22, 2020

08:30 Session 5: Innovation and Inspiration from Natural Products

Session Chair

Prof. Thomas MAGAUER
(UNIVERSITY OF INNSBRUCK, Innsbruck, Austria)

08:30 Capturing Biological Activity in Natural Product Fragments: Success and Limitations (PL14)

Prof. Karl GADEMANN
(UNIVERSITY OF ZÜRICH, Zürich, Switzerland)

09:00 (De)Construction of Three-Dimensional Molecular Architectures (PL15)

Prof. Thomas MAGAUER
(UNIVERSITY OF INNSBRUCK, Innsbruck, Austria)

09:30 Coffee Break

10:00 Synthesis of Complex Antiplasmodial Isocyanoterpenes (PL16)

Prof. Christopher VANDERWAL
(UNIVERSITY OF CALIFORNIA, Irvine, United States)

10:30 Total Synthesis of Chivosazole F (OC03)

Dr Simon WILLIAMS
(SYNGENTA, Stein AG, Switzerland)

11:00 Outdoor Networking Activities

15:45 Networking Break & "Panel Discussion on Protein Degradation"

Panel Discussion on Protein Degradation

Session Chair

Dr Klemens HOEGENAUER
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

Prof. Andy PHILLIPS
(C4 THERAPEUTICS, Watertown, United States)

Dr Christian STEINEBACH
(UNIVERSITY OF BONN, Bonn, Germany)

Dr Georg WINTER
(RESEARCH CENTER FOR MOLECULAR MEDICINE OF THE AUSTRIAN ACADEMY OF SCIENCES, Vienna, Austria)

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17:00 **Session 6: Accelerating Drug Discovery by Intelligence Augmentation**

Session Chair

Dr Thomas TRIESELMAAN
(BOEHRINGER INGELHEIM PHARMA GMBH & CO. KG, Biberach an der Riss, Germany)

17:00 **Organic Synthesis on a Computer: Should Medicinal Chemists Care? (PL17)**

Prof. Bartosz A. GRZYBOWSKI
(ULSAN NATIONAL INSTITUTE OF SCIENCE & TECHNOLOGY, Ulsan, Korea, South)

17:30 **Exploring an Interface of Synthesis and Data Science (PL18)**

Prof. Timothy CERNAK
(UNIVERSITY OF MICHIGAN, Ann Arbor, United States)

18:00 **Accelerating R&D with Augmented Intelligence (PL19)**

Dr Matthias ZENTGRAF
(BOEHRINGER INGELHEIM, Biberach an der Riss, Germany)

18:30 **Coffee Break**

Session 7: Targeted Delivery - Strategies to Help your Drug Substances get to the Right Place

Session Chair

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

19:00 **Using Small Molecules to Engineer and Explore Human Immunity (PL20)**

(BIOIBÉRICA)
Prof. David SPIEGEL (YALE UNIVERSITY, New Haven, United States)

19:30 **Poster Session**

20:30 **End of Day 4**

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Thursday January 23, 2020

08:30 Session 7: Targeted Delivery - Strategies to Help your Drug Substances get to the Right Place

Session Chair

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

08:30 Discovery of Tumor-Targeted TLR7/8 Immune-Stimulating Antibody Conjugates (ISAC): A New Class of Immuno-Oncology Therapeutics (PL21)

Dr Brian SAFINA
(BOLT BIOTHERAPEUTICS, Redwood City, United States)

09:00 Intracellular and Tissue Specific Targeting of Therapeutic Modalities (PL22)

Dr Vadim DUDKIN
(JANSSEN DISCOVERY SCIENCES, Lansdale, United States)

09:30 Coffee Break

10:00 SBT6050, a HER2-Directed TLR8 Immunotac™ Therapeutic, is a Potent Human Myeloid Cell Agonist with Tumor-Localized Activity (PL23)

Dr Valerie ODEGARD
(SILVERBACK THERAPEUTICS, Seattle, United States)

10:30 Outdoor Networking Activities

15:45 Networking Break

Session 8: Drug Discovery Tales

Session Chair

Dr Lena RIPA
(ASTRAZENECA, Mölndal, Sweden)

16:00 Discovery of GDC-0334: a potent and orally bioavailable clinical candidate for the inhibition of TRPA1 (OC04)

Dr Vishal VERMA
(GENENTECH, South San Francisco, United States)

16:30 Investigating the Chameleonic Properties of RGD Integrin Antagonists for the Treatment of IPF (OC05)

Dr James THOMPSON
(GLAXOSMITHKLINE/UNIVERSITY OF STRATHCLYDE, Stevenage, United Kingdom)

17:00 Discovery of AZD3458 a Highly Selective PI3Ky Inhibitor: Combining Structure, HDX-MS and Binding Kinetics to Understand the Mode of Action (OC06)

Dr Nils PEMBERTON
(ASTRAZENECA, Mölndal, Sweden)

17:30 The Discovery of a Potent and Orally Bioavailable Macrocyclic Cyclophilin Inhibitor Based on The Structural Simplification of Sanglifehrin A (OC07)

Dr Vicky STEADMAN
(EUROFINS DISCOVERY, Macclesfield, United Kingdom)

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- 18:00** **Coffee Break**
- 18:30** **The Big Impact of Small Changes : Towards Best-in-Class EZH2 and LSD1 Inhibitors (OC08)**
Dr Julian LEVELL
(CONSTELLATION PHARMACEUTICALS, Cambridge, United States)
- 19:00** **Controlling the Fate and Function of Proteins with Photopharmacology (KL03)**
Prof. Dirk TRAUNER
(NEW YORK UNIVERSITY, New York, United States)
- 20:00** **Closing Remarks**
- 20:30** **End of Symposium**