

4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

Programme

Sunday 28/01/2024

13:00 **Registration**

14:45 **Opening Remarks**

Dr Klemens HOEGENAUER (NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)
Dr Karl Heinz KRAWINKLER (NOVARTIS PHARMA AG DEVELOPMENT, Basel, Switzerland)
Dr Antonia F. STEPAN (F. HOFFMANN-LA ROCHE LTD, Basel, Switzerland)

14:59 **Recent Developments in Synthetic Methodologies and their Impact**

Session Chair

Dr Fabrice GALLOU
(NOVARTIS PHARMA, Basel, Switzerland)

15:00 **Organic Reactions in Aqueous Medium enabled by Surfactants (PL01)**

Dr Niginia BORLINGHAUS
(UNIVERSITY OF KONSTANZ, Konstanz, Germany)

15:30 **Reagents and Catalysts with Translational Potential (PL02)**

Dr Josep CORNELLA COSTA
(MAX PLANCK INSTITUTE FOR COAL RESEARCH, Mülheim an der Ruhr, Germany)

16:00 **Coffee Break**

16:30 **From Batch to Flow: Advancing Synthetic Organic Chemistry through Technological Innovation (PL03)**

Prof. Timothy NOËL
(UNIVERSITY OF AMSTERDAM, Amsterdam, The Netherlands)

17:00 **Chemo-Biocatalytic Processes Enabled by a Continuous Flow Set Up (PL04)**

Prof. Francesca PARADISI
(UNIVERSITY OF BERN, Bern, Switzerland)

17:30 **Break**

17:45 **New Catalytic Approaches for Simplifying Complex Molecule Synthesis (KL01)**

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

18:45 **Welcome Reception, Sponsored by abcr**

20:15 **End of the day**

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From Underground to Mainstream: Neglected and Novel, Emerging Functional Groups for Drug Discovery

Session Chair

Dr Ulrich LÜCKING
(FORX THERAPEUTICS, Basel, Switzerland)

08:30 Boron Based Heterocycles and their Application in Drug Discovery (PL05)

Prof. Bhaskar DAS
(LONG ISLAND UNIVERSITY, Brooklyn, United States)

09:00 “Magic Chloro”: Profound Effects of the Chlorine Atom in Drug Discovery (PL06)

Dr Yoshihiro ISHIHARA
(VIVIDION THERAPEUTICS, San Diego, United States)

09:30 Coffee Break

10:00 Deuterium in Drug Design: From Deuterium Switch to De Novo Drug Discovery (PL07)

Prof. Tracey PIRALI
(UNIVERSITY OF PIEMONTE ORIENTALE, Novara, Italy)

10:30 New Functional Groups for Synthetic and Discovery Chemistry (PL08)

Prof. Michael WILLIS
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

11:00 Outdoor Networking Activities

16:00 Networking Break

16:15 In Silico Prediction of Phase I and II Metabolism: Guiding Optimisation of Drug Metabolism o_BRCompany Workshop by Optibriumc_BR

Dr Matthew SEGALL
(OPTIBRIUM LTD, Cambridge, United Kingdom)

Latest Advances and Approaches in Bioconjugation Drug Discovery

Session Chair

Dr Karl Heinz KRAWINKLER
(NOVARTIS PHARMA AG DEVELOPMENT, Basel, Switzerland)

17:00 Bicyclic Peptides as a Novel Therapeutic Modality (PL09)

Dr Philip MURRAY (BICYCLE THERAPEUTICS, Cambridge, United Kingdom)
(SOPLVIAS AG (WAS FUJIFILM))

17:30 Next-Generation Bioconjugates for Intra- and Extracellular Targeting (PL10)

Prof. Christian HACKENBERGER
(FMP BERLIN, Berlin, Germany)

18:00 Coffee Break

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- 18:30** **Creating Next-Generation Biotherapeutics Using Novel Chemistry Platform Technologies (PL11)**
Dr Vijaya R. PATTABIRAMAN
(BRIGHT PEAK THERAPEUTICS, Basel, Switzerland)
- 19:00** **Exploring the Versatility of Covalent and Supramolecular Bioconjugation in ADC and AOC (PL12)**
Dr Alain WAGNER
(CNRS/UNIVERSITY OF STRASBOURG, Illkirch, France)
- 19:30** **Poster Session 1 (odd numbers)**
- 20:30** **End of the Poster Session**

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Tuesday 30/01/2024

Human Dose Prediction in the Discovery Space

Session Chair

Dr Holger FISCHER
(F. HOFFMANN-LA ROCHE LTD., BASEL, Switzerland)

08:30 Early Human Dose Predictions in Lead Optimization (PL13)

Dr Johan BYLUND
(CTC CLINICAL TRIAL CONSULTANTS AB, Uppsala, Sweden)

09:00 Early Human Dose Prediction & Machine Learning Models - Can We Impact Lead Selection? (PL14)

Dr Gregori GEREBTZOFF
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

09:30 Coffee Break

10:00 SwiftPK: Development and Implementation of a High Throughput PBPK/PD Framework to Inform Drug Selection in Early Drug Discovery (PL15)

Dr Andres OLIVARES
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

10:30 Predicting Human Exposure and Dose of Compounds Targeting the Brain (PL16)

Dr Nicola COLCLOUGH
(ASTRAZENECA, Cambridge, United Kingdom)

11:00 Outdoor Networking Activities

15:30 Networking Break

Antiviral Drug Discovery

Session Chair

Dr Dafydd OWEN
(PFIZER, Cambridge, United States)

16:30 Discovery, Chemistry, and Preclinical Development of Pritelivir, a Novel Option for Acyclovir-Resistant Herpes Simplex Virus Infections (PL17)

Dr Alexander BIRKMANN
(AICURIS ANTI-INFECTIVE CURES AG, Wuppertal, Germany)

17:00 Targeting Viral RNA Degradation Via Small Molecules As a Novel Antiviral Strategy to Achieve HBV Cure (PL18)

Dr Dimitar GOTCHEV
(ARBUTUS BIOPHARMA, Doylestown, United States)

17:30 Coffee Break

18:00 Direct-Acting Antivirals with a Targeted Protein Degradation Mechanism (PL19)

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Prof. Priscilla YANG
(STANFORD UNIVERSITY, Stanford, United States)

18:30 Discovery of Obeldesivir; Oral Prodrug of Nucleoside GS-441524 That Exhibits Antiviral Efficacy in SARS-CoV-2-Infected African Green Monkeys (PL20)

Dr Rao KALLA
(GILEAD SCIENCES, Foster City, United States)

19:00 The Discovery of PAXLOVID (KL02)

Dr Dafydd OWEN
(PFIZER, Cambridge, United States)

20:00 End of the Scientific Programme

20:30 Conference Dinner

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Wednesday 31/01/2024

08:29 Radical Intermediates in Complex Molecule Synthesis

Session Chair

Prof. Nina HARTRAMPF
(UNIVERSITY OF ZURICH, Zürich, Switzerland)

08:30 Light-Mediated Nickel Catalysis Enabled by Donor-Acceptor Ligands (PL21)

Prof. Bart PIEBER (INSTITUTE OF SCIENCE AND TECHNOLOGY AUSTRIA (ISTA), Klosterneuburg, Austria)
(SOPLVIAS AG (WAS FUJIFILM))

09:00 Recent Adventures in Catalysis and Beyond (PL22)

Prof. Bill MORANDI
(ETH ZÜRICH, Zürich, Switzerland)

09:30 Coffee Break

10:00 Alkenes as Flexible Platforms for Asymmetric Transformations (PL23)

Prof. Cristina NEVADO
(UNIVERSITY OF ZURICH, Zurich, Switzerland)

10:30 Attempts to Deliver on the Promise of Natural Product Synthesis (PL24)

Prof. Ryan SHENVI
(SCRIPPS RESEARCH, La Jolla, United States)

11:00 Outdoor Networking Activities

16:00 Networking Break

16:15 AI for Medicinal Chemists: Novel Compounds Design and Retrosynthesis Prediction o_BRCompany Workshop by Iktosc_BR

Dr Quentin PERRON
(IKTOS, Paris, France)

16:59 Drug Discovery Tales I

Session Chair

Dr Scott WOLKENBERG
(JANSSEN PHARMACEUTICAL COMPANIES OF JOHNSON & JOHNSON, Spring House, United States)

17:00 NLRP3 Inhibitors for Neurodegenerative Disorders (OC01)

Dr Oscar MAMMOLITI
(JANSSEN RESEARCH & DEVELOPMENT, Beerse, Belgium)

17:30 Discovery of a Bivalent Protein Kinase CK2 Inhibitor with Activity in Renal Cell Carcinoma (OC02)

Dr Isabelle KRIMM
(CLB, Lyon, France)

17:50 Coffee Break

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- 18:20** **Discovery of BI 7446: A Potent Cyclic Dinucleotide Sting Agonist with Broad-Spectrum Variant Activity for the Treatment of Cancer (OC03)**
Dr Christian KUTTRUFF
(BOEHRINGER INGELHEIM PHARMA GMBH & CO. KG, Biberach, Germany)
- 18:40** **Discovery of [¹⁸F]RoSMA-18-D6 for PET Imaging of Cannabinoid Type 2 Receptors (OC04)**
Dr Luca GOBBI
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)
- 19:00** **Selective Inhibition of Tead Transcription and Impact on the Up-Stream Effector Kinases of the Hippo Pathway to Halt Metastatic Colorectal Cancer Cell Growth (OC05)**
Prof. Maria Paola COSTI
(UNIVERSITY OF MODENA AND REGGIO EMILIA, Modena, Italy)
- 19:20** **Poster Session 2 (even numbers)**
- 20:30** **End of the Poster Session**

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Thursday 01/02/2024

08:29 **Cryo-EM: Applications for Structure-Based Drug Discovery**

Session Chair

Dr Katharina DÜRR
(OMASS THERAPEUTICS, Oxford, United Kingdom)

08:30 **Deep Learning-Driven De Novo Drug Design Based on Gastric Proton Pump Structure (PL25)**

Prof. Kazuhiro ABE
(NAGOYA UNIVERSITY, Nagoya, Japan)

09:00 **Cryo-EM Enables Structure-Based Drug Design for Membrane Protein Targets at BI (PL26)**

Dr Rebecca EBENHOCH
(BOEHRINGER INGELHEIM, Biberach, Germany)

09:30 **Coffee Break**

10:00 **Single Particle CryoEM at 200 kV & Itchy GPRs (PL27)**

Prof. Jonathan F. FAY
(UNIVERSITY OF NORTH CAROLINA CHAPEL HILL, Chapel Hill, United States)

10:30 **Examples from Structure-Based Drug Discovery Using Cryo-EM at MSD (PL28)**

Dr Harini KRISHNAMURTHY
(MERCK, SHARP & DOHME, Blue Bell, United States)

11:00 **Outdoor Networking Activities**

16:00 **Networking Break**

16:59 **Drug Discovery Tales II**

Session Chair

Dr Scott WOLKENBERG
(JANSSEN PHARMACEUTICAL COMPANIES OF JOHNSON & JOHNSON, Spring House, United States)

17:00 **Discovery of a Novel Oral NO- and Heme-Independent sGC Activator Runcaciguat (BAY 1101042) (OC06)**

Dr Michael G. HAHN
(BAYER AG PHARMACEUTICALS, Wuppertal, Germany)

17:30 **Heterocyclic Compounds as Delta-5 Desaturase Inhibitors (OC07)**

Dr Ana MINATTI
(AMGEN INC, Copenhagen, Denmark)

18:00 **Coffee Break**

18:30 **Novel Approaches to Molecular Glue Discovery: Design of Clinical Candidate NVP-DKY709 an IKZF2 Degradar by Re-Programming of CRBN Selectivity and Screening for Cooperativity Using DNA Encoded Libraries (OC8)**

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Dr Frédéric ZECRI
(NOVARTIS, Cambridge, United States)

19:00 Discovery of LY3154885, a Dopamine D1 Receptor Positive Allosteric Modulator with an Improved Drug-Drug Interaction Risk Profile (OC09)

Dr Erik HEMBRE
(ELI LILLY AND COMPANY, Indianapolis, United States)

19:30 Site-Selective C—H Oxidations for Late-Stage Functionalizations (KL03)

Prof. M. Christina WHITE
(UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN, Urbana, United States)

20:30 Closing Remarks