

# 4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

## Programme

### Sunday January 28, 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**

# 4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

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### Monday January 29, 2024

#### 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**

# 4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

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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**

# 4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

## Programme

**Tuesday January 30, 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**

# 4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

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### Wednesday January 31, 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**

# 4th Alpine Winter Conference on Medicinal and Synthetic Chemistry

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### Thursday February 1, 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**