

Frontiers in Medicinal Chemistry
March 14 – 16, 2022, online

Scientific Program
Monday, March 14, 2022

8.15 a.m.

Welcome

F. von Nussbaum, M. Jung

Non-Mainstream Chemotypes

Chairs: W. Czechitzky, H. Dollinger

8.30 a.m.

Phosphine Oxides from a Medicinal Chemist's Perspective

C. Gnamm (Boehringer Ingelheim Pharma GmbH & Co. KG), Biberach/DE, P. Finkbeiner, Biberach/DE, J. P. Hehn, Biberach/DE, J. T. Kley, Biberach/DE

9.00 a.m.

N-Trifluoromethyl Amines and Azoles: An Underexplored Functional Group in the Medicinal Chemist's toolbox

S. Schiesser (AstraZeneca), Mölndal/SE

9.30 a.m.

The Lab Oddity prevails: Sulfoximines in Medicinal Chemistry revisited

U. Lücking (FoRx Therapeutics AG), Basel/SE

10.00 a.m.

Coffee Break & Meet the Speakers

Young Investigators

Chairs: C. Ducho, S. Laufer, B. Wunsch

10.15 a.m.

Covalent Proximity Scanning of a Distal Cysteine to Target PI3Kalpha

C. Borsari (University of Basel), Basel/CH, E. Keles, Basel/CH, J. McPhail, Victoria/CA, A. Schäfer, Zurich/CH, W. Goch, Warsaw/PL, W. Bal, Warsaw/PL, M. Gstaiger, Zurich/CH, J. Burke, Victoria/CA, M. P. Wymann, Basel/CH

10.30 a.m.

A small fluorescent ligand to investigate soluble epoxide hydrolase engagement in living cells

K. Hiesinger (University of Frankfurt), Frankfurt (Main)/DE, K. Hiesinger, Frankfurt (Main)/DE, J. Schoenfeld, Frankfurt (Main)/DE, S. Brunst, Frankfurt (Main)/DE, L. Burgers, Frankfurt (Main)/DE, P. Breunig, Frankfurt (Main)/DE, M. De Meglio, Frankfurt (Main)/DE, F. F. Lillich, Frankfurt (Main)/DE, L. Weizel, Frankfurt (Main)/DE, R. Fürst, Frankfurt (Main)/DE, J. Hefendehl, Frankfurt (Main)/DE, E. Proschak, Frankfurt (Main)/DE

10.45 a.m.

Addressing a Trapped High-Energy Water: Rational Design of Pyrimidoindole-Based Glycogen Synthase Kinase-3 β Inhibitors.

P. Koch (University of Regensburg), Regensburg/DE, S. Andreev, Regensburg/DE, T. Pantsar, Kuopio/FI

11.00 a.m.

Engineering Bioactive Dimeric Transcription Factor Analogs via Flow Synthesis and Palladium Rebound Mediated Protein Cross-Coupling

S. Pomplun (University of Leiden), Leiden/NL

11.15 a.m.

Targeting E3 Ligases and Deubiquitinases with PROTACs

C. Steinebach (University of Bonn), Bonn/DE, Y. L. D. Ng, Berlin/DE, A. Murgai, Berlin/DE, I. Sosič, Ljubljana/SI, J. Krönke, Berlin/DE, M. Gütschow, Bonn/DE

11.30 a.m.

Lunch Break, Meet the Speakers and Sponsor Presentation

Sponsor Presentation

11.30 - 11.45 Merck KGaA, Katrin Lautenschläger

Medicinal Chemistry and Target Highlights

Chairs: A. K. H. Hirsch, F. von Nussbaum

12.30 p.m.

Casein kinase II (CK2) as a novel drug target for SARS-CoV-2 infection

R. Grosse (University of Freiburg), Freiburg/DE

12.50 p.m.

Next-generation bioconjugates for intra- and extracellular targeting

C. P. R. Hackenberger (Leibniz Institut for Molekular Pharmacology (FMP), Berlin/DE

1.20 p.m.

N. N.

1.50 p.m.

Coffee Break & Meet the Speakers

Chemical Epigenetics

Chair: M. Jung

2.15 p.m.

Peptide-based chemical biology tools to study epigenetic proteins

A. Kawamura (University of Oxford), Oxford/UK

2.45 p.m.

Chemical Epigenetics: Bump and Hole and PROTACs

A. Ciulli (University of Dundee), Dundee/GB

3.15 p.m.

Potent and selective inhibitors for methyltransferases

R. Huang (Purdue University), West Lafayette/US

3.45 p.m.

The histone methyltransferase KMT9 is a new drug target for prostate cancer

R. Schüle (University of Freiburg), Freiburg/DE

4.15 p.m.

PhD prize award ceremony

Chair: G. Hessler

4.30 p.m.

Poster Session I

Scientific Program

Tuesday, March 15, 2022

First Disclosures & Fresh Case Studies

Chairs: H. Dollinger, F. von Nussbaum

8.30 a.m.

Design and Preclinical Characterization Program Towards Asundexian, an Oral Factor Xla Inhibitor for the Prevention and Treatment of Thromboembolic Disorders

A. Hillisch (Bayer AG), Wuppertal/DE, S. Röhrig (Bayer AG), Wuppertal/DE

9.00 a.m.

Design of SAR441255, a Potent Unimolecular Peptidic Triple GLP-1/GIP/GCG Receptor Agonist and its Effects on Weight Loss and Glycemic Control

M. Bossart (Sanofi Deutschland GmbH), Frankfurt (Main)/DE, M. Wagner, Frankfurt (Main)/DE, R. Elvert, Frankfurt (Main)/DE, A. Evers, Frankfurt (Main)/DE, T. Hübschle, Frankfurt (Main)/DE, T. Kloeckener, Frankfurt (Main)/DE, K. Lorenz, Frankfurt (Main)/DE, C. Moessinger, Frankfurt (Main)/DE, O. Eriksson, Uppsala/SE, I. Velikyan, Uppsala/SE, S. Pierrou, Uppsala/SE, L. Johansson, Uppsala/SE, I. Nowotny, Frankfurt (Main)/DE, A. Nitsche, Frankfurt (Main)/DE, A. Konkar, Frankfurt (Main)/DE

9.30 a.m.

Overcoming optimization challenges of Tankyrase inhibitors with different chemotypes and binding modes

H.-P. Buchstaller (Merck KGaA), Darmstadt/DE, C. Esdar, Darmstadt/DE, P. Czodrowski, Darmstadt/DE, D. Dorsch, Darmstadt/DE, D. Kuhn, Darmstadt/DE, B. Leuthner, Darmstadt/DE, D. Musil, Darmstadt/DE, F. Rohdich, Darmstadt/DE, R. Schneider, Darmstadt/DE, A. Wegener, Darmstadt/DE, S. Weigt, Darmstadt/DE, D. Wienke, Darmstadt/DE

10.00 a.m.

Coffee Break & Meet the Speakers

Trends in Medicinal Chemistry

Chairs: B. Wünsch, M. Jung

10.30 a.m.

Structural Modifications Yield Novel Insights Into the Intriguing Pharmacodynamic Potential of Anti-inflammatory Nitro-Fatty Acids

G. Manolikakes, Kaiserslautern/DE, K. J. Hock, Kaiserslautern/DE, K. Zacharowski, Frankfurt/DE, J. Roos, Langen/DE, T. J. Maier, Langen/DE, N. Hellmuth, Frankfurt/DE, C. Brat, Frankfurt/DE, O. Awad, Langen/DE, S. George, Frankfurt/DE, A. Kahnt, Frankfurt/DE, T. Bauer, Langen/DE, H. P. Huynh Phuoc, Langen/DE, D. Steinhilber, Frankfurt/DE, C. Angioni, Frankfurt/DE, M. Hassan, Kaiserslautern/DE

11.00 a.m.

Fit for purpose: On the suitability of reactions for DNA-encoded library design

A. Brunschweiler, Dortmund/DE

11.30 a.m.

Expanding the Druggable Target Landscape in Cardiovascular, Renal and Metabolic Diseases

M. Lemurell (AstraZeneca), Mölndal/SE

12.00 p.m.

Natural product-inspired macrocycles for FK506-binding proteins

F. Hausch (TU Darmstadt), Darmstadt/DE

12.30 p.m.

Lunch Break, Meet the Speakers and Sponsor Presentation

Sponsor Presentation

12.30-12.45 Nuvisan GmbH, Markus Kroll

1.30 p.m.

Poster Session II

Innovation Awards

Chair: H. Dollinger

2.30 p.m.

Laudatio Innovation Award Medicinal/Pharmaceutical Chemistry 2022

2.35 p.m.

Development of New Therapeutics for the Treatment of Neurodegenerative Diseases

S. Pockes (University of Regensburg), Regensburg/DE

2.45 p.m.

Laudatio Innovation Award Medicinal/Pharmaceutical Chemistry 2022

2.50 p.m.

High-resolution probes for microtubules and for oxidoreductases

O. Thorn-Seshold (University of Munich), München/DE

Next Generation Drugs

Chairs: M. Gehringer, C. Méndez Pérez

3.00 p.m.

Targeted protein degradation: genetic determinants and drug discovery opportunities

C. Mayor-Ruiz (IRB Barcelona), Barcelona/ES

3.30 p.m.

Discovery of Inupadenant, a novel A2A receptor antagonist that retains activity in adenosine-rich microenvironments

S. Van der Plas, Gosselies/BE

4.00 p.m.

Development of Reversible Covalent Inhibitors as Chemical Probes and Clinical Candidates

T. D. Owens (Principia Biopharma a Sanofi Company.), South San Francisco/US

4.30 p.m.

Coffee Break & Meet the Speakers

Plenary Lecture

Chairs: M. Jung, F. von Nussbaum

5.00 p.m.

Target Protein Degradation Drugs

C. De Savi (Kymera Therapeutics, Inc.), Watertown/US

Scientific Program

Wednesday, March 16, 2022

Macrocycles

Chair: U. Lücking

8.30 a.m.

Synthetic Opportunities and Challenges for Macrocyclic Kinase Inhibitors

T. Hanke (University of Frankfurt), Frankfurt (Main)/DE, J. A. Amrhein, Frankfurt (Main)/DE, S. Knapp, Frankfurt (Main)/DE

9.00 a.m.

SAR by 1D NMR for Structure Based Drug Design of Macrocycles

E. Chiarparin (AstraZeneca), Cambridge/GB

9.30 a.m.

Design, synthesis and screening of large libraries of macrocyclic compounds for addressing intracellular targets

C. Heinis (EPFL), Lausanne/CH

10.00 a.m.

Coffee Break & Meet the Speakers

Friedrich Stolz-Prize

Chairs: A. K. H. Hirsch, F. von Nussbaum

10.30 a.m.

Discovery of Novel sGC Stimulators Riociguat, Vericiguat & sGC Activator RuncaciguatAI - Retrosynthesis and Automation

J. Mittendorf, Wuppertal/DE, M. Follmann, Wuppertal/DE, M. G. Hahn, Wuppertal/DE

Chair: G. Hessler

11.00 a.m.

Universal Chemical Discovery and Synthesis Machines and Chemputation

L. Cronin (University of Glasgow), Glasgow/UK

11.30 a.m.

Leveraging the increase of Fsp³ into drug molecules using flow technologies and automation

I. Abdiaj (Janssen Pharmaceutical Companies of J&J), Toledo/ES, J. M. Alcazar, Toledo/ES

12.00 p.m.

A Perspective on AI and Automation for the Medicinal Chemistry Lab

C. W. Coley (MIT), Cambridge/US

Closing remarks and Poster Prizes

Chairs: M. Jung, F. von Nussbaum

NextGenMedChem Workshop

1.20 p.m. NextGenMedChem Workshop: Starting a Career in Medicinal Chemistry

Workshop BioSolve IT

Chair: A. Neumann

2.30 p.m. Interactive Design of Small Molecule Inhibitors