



GESELLSCHAFT DEUTSCHER CHEMIKER



Fachgruppe Medizinische Chemie

Frontiers in Medicinal Chemistry

March 8 – 10, 2021 · Online



TECHNISCHE
UNIVERSITÄT
DARMSTADT



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Society

Division of
Medicinal Chemistry &
Chemical Biology

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Monday, March 8, 2021

*Chair: Franz von Nussbaum*8.30 a.m. **WELCOME**8.40 a.m. **OPENING LECTURE****Chemical proteomic strategies to fight multiresistant bacteria**S. Sieber (Technical University of Munich), Garching/DE**Degraders and Molecular Glues***Chair: Franz von Nussbaum*9.30 a.m. **Dissecting molecular glue action**N. Thomä (Friedrich Miescher Institute for Biomedical Research), Basel/CH10.00 a.m. **Cryo EM of Cullin-RING E3 Ligation Mechanisms**B. Schulman (Max Planck Institute for Biochemistry), Heidelberg/DE10.30 a.m. **bacPROTACs: Hijacking a Bacterial Proteasome**K. Rumpel (Boehringer Ingelheim), Vienna/AT11.00 a.m. **COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS****Antiviral Agents***Chair: Christian Ducho*11.30 a.m. **Design of Nucleotide Prodrugs for Antiviral Chemotherapy – the TriPPPProApproach**C. Meier (University of Hamburg), Hamburg/DE12.00 p.m. **Allosteric Inhibition of Flaviviral Proteases**T. Schirmeister (University of Mainz), Mainz/DE**Exhibitor presentations***Chair: Matthias Gehringer*12.30 p.m. **Pharmacelsus GmbH****Hepatocytes sandwich cultures as a versatile in vitro tool for drug metabolism and clearance prediction**L. Horbal, Saarbrücken/DE12.45 p.m. **Nuvisan ICB GmbH****Discovery of ATR inhibitor BAY-1895344, SOS1-Probe BAY-293 and insights into a novel scientific CRO**M. Menke, Berlin/DE, C. Sachse, Berlin/DE1.00 p.m. **LUNCH BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS**

Monday, March 8, 2021

Young Investigators*Chair: Bernhard Wunsch*2.00 p.m. **Development of barcoding strategies for DNA-encoded library synthesis and identification of TEAD-YAP inhibitors**A. Brunschweiler, (Technical University Dortmund), Dortmund/DE2.15 p.m. **Towards macrocyclic complement C3 inhibitors with prolonged target residence time – insights in structure-activity relationships and mode-of-action of compstatin**C. Lamers, (University of Basel), Basel/CH, B. Wagner, Basel/CH, P. Gros, Utrecht/NL, J. D. Lambris, Philadelphia/US, D. Ricklin, Basel/CH2.30 p.m. **Discovery of Dual Covalent Inhibitors of the Protein Kinases BMX and BTK**M. Gehringer, (University of Tübingen), Tübingen/DE, M. Forster, Tübingen/DE, X. J. Liang, Tübingen/DE, M. Schröder, Frankfurt/DE, S. Gerstenecker, Tübingen/DE, A. Chaikvad, Frankfurt/DE, S. Knapp, Frankfurt/DE, S. Laufer, Tübingen/DE2.45 p.m. **Development of Novel CD73 Inhibitors and PET Tracers for the Imaging of Cd73 Expression in Cancer**A. Junker, (University of Münster), Münster/DE, C. Dobelmann, Münster/DE, K. A. Jacobson, Bethesda/US, C. E. Müller, Bonn/DE**PhD Prizes***Chair: Gerhard Hessler*3.00 p.m. **PhD Prizes 2020 & 2021 (2 x 5 min)**3.20 p.m. **COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS****Highlights in Medicinal Chemistry***Chair: Tatjana Ross*3.30 p.m. **Pharmacologic insights from cryo-EM structures of autoinhibited and active-state structures of BRAF/MEK/14-3-3 complexes**Michael Eck (Dana-Farber Cancer Institute), Boston/US4.00 p.m. **Receptor deorphanization by ultra large scale docking**J. Irwin (University of California), San Francisco/US4.30 p.m. **Computational Chemistry AI applications change the way we work in early Drug Discovery: Scientific and operational learnings**D. Kuhn (Merck Healthcare KGaA), Darmstadt/DE5.00 p.m. **COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS**5.30 p.m. **POSTER SESSION I (5.30 – 7.00 p.m.)**

Tuesday, March 9, 2021

First Disclosures & Case Studies

Chair: Stefan Laufer

- 8.30 a.m. **Target-Based Identification and Optimization of Toll-like Receptor 7/8 Antagonists**
D. Behnke (Novartis Pharma AG), Basel/CH
- 9.00 a.m. **Discovery and Optimization of Next Generation Reversible Methionine Aminopeptidase-2 Inhibitors – Identification of clinical compound M8891**
T. Heinrich (Merck Healthcare KGaA), Darmstadt/DE
- 9.30 a.m. **Potent, Selective & Bioavailable Covalent Inhibitors of CDK7**
I. Stansfield (Janssen Pharmaceuticals), Beerse/BE
- 10.00 a.m. **Stepwise Design of advanced γ -Secretase Modulators with an Unconventional Phenyl Ring Bioisostere**
R. M. Rodriguez Sarmiento (F. Hoffmann-La Roche Ltd), Basel/CH
- 10.30 a.m. COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS

Covalent Binders and Fragments

Chair: Boris Schmidt

- 11.00 a.m. **Covalent ligand directed release chemistry**
N. London (Weizmann Institute of Science), Rehovot/IL
- 11.30 a.m. **Expanding the Scope for Targeted Covalent Inhibitors: Peptido Sulfonyl Fluorides and Thiosulfonates**
R. M. J. Liskamp (Glasgow University), Glasgow/GB
- 12.00 p.m. **Covalent fragment approaches in drug discovery**
G. M. Keserü (Research Centre for Natural Sciences), Budapest/HU

Exhibitor presentations

Chair: Eleonora Diamanti

- 12.30 p.m. **Crelux GmbH, a WuXi AppTec Company**
Unlock the true potential of DNA-encoded library technology in your own lab: Hit finding by using DELopen and DELight
N. Tschammer, Martinsried/DE
- 12.45 p.m. **Chemspeed Technologies AG**
Standardized, Digitalized and Accelerated Solutions for Medicinal Chemistry
S. Eller, Füllinsdorf/CH
- 1.00 p.m. LUNCH BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS

Tuesday, March 9, 2021

Medicinal Chemistry Highlights

Chair: Anna K. H. Hirsch

- 2.00 p.m. **Selection and optimization of 1,3-diaryl-pyrazin-6-one-5-carboxylic amides towards BAY 2416964, an AhR Antagonist in clinical trials**
N. Schmees, (Nuvisan ICB GmbH), Berlin/DE, I. Gutcher, Berlin/DE, U. Roehn, Berlin/DE, H. Irlbacher, Berlin/DE, D. Stoeckigt, Berlin/DE, B. Bader, Berlin/DE, L. Roesse, Berlin/DE, B. Kreft, Berlin/DE, M. Platten, Heidelberg/DE, R. Carretero, Heidelberg/DE, I. V. Hartung, Darmstadt/DE
- 2.30 p.m. **Flow-Based Synthesis of Chemically Modified Peptides and Proteins**
N. Hartrampf, (University of Zurich), Zurich/CH
- 2.45 p.m. **Discovery of nucleic acid binding molecules from combinatorial biohybrid nucleobase peptide libraries**
S. Pomplun, (MIT), Cambridge/US, Z. P. Gates, Cambridge/US, G. Zhang, Cambridge/US, A. J. Quartararo, Cambridge/US, B. L. Pentelute, Cambridge/US
- 3.00 p.m. **Discovery of antibacterial agents inhibiting the energy-coupling factor (ECF) transporters by structure-based virtual screening**
E. Diamanti, (HIPS), Saarbrücken/DE, I. Setyawati, Groningen/NL, S. Bousis, Saarbrücken/DE, L. Monjas Gómez, Groningen/NL, L. Swier, Groningen/NL, J. Hauptenthal, Saarbrücken/DE, P. Gibson, Lausanne/CH, C. Volz, Saarbrücken/DE, W. Stanek, Groningen/NL, M. Jäger, Groningen/NL, J. Herrmann, Saarbrücken/DE, J.-W. Veening, Lausanne/CH, R. Müller, Saarbrücken/DE, D. Slotboom, Groningen/NL, A. K. H. Hirsch, Saarbrücken/DE
- 3.15 p.m. **Rational Design of Selective HDAC10 Chemical Probes**
A. K. Miller, (DKFZ), Heidelberg/DE
- 3.30 p.m. **Glutathione peroxidases - novel targets of anti-inflammatory drugs?**
S. C. Koeberle, (University of Innsbruck), Innsbruck/AT, O. Werz, Jena/DE, A. Koeberle, Innsbruck/AT, A. P. Kipp, Jena/DE
- 3.45 p.m. **Synthesis and characterisation of irreversible transglutaminase 2-inhibitors with albumin binding moiety**
R. Wodtke, (Helmholtz-Zentrum Dresden-Rossendorf), Dresden/DE, P. Schlitterlau, Dresden/DE, F. Brandt, Dresden/DE, M. Laube, Dresden/DE, K. Kopka, Dresden/DE, H.-J. Pietzsch, Dresden/DE, J. Pietzsch, Dresden/DE, R. Löser, Dresden/DE
- 4.00 p.m. COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS

Tuesday, March 9, 2021

Innovation Prize

Chair: Horst Dollinger, Christa Müller

- 4.30 p.m. **Synthesis of Natural Products for Drug Development**
N. Schützenmeister, (University of Vienna), Wien/AT
- 4.50 p.m. **Rational design of inhibitors of CNS kinases**
P Koch, (University of Tübingen), Tübingen/DE
- 5.10 p.m. COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS
- 5.30 p.m. **POSTER SESSION II (5.30 – 7.00 p.m.)**

Wednesday, March 10, 2021

Cryptic Binding Pockets

Chair: Felix Hausch

- 8.30 a.m. **Inhibitors of the NAD⁺-dependent lysine deacylases hSirt2 and smSirt2 as potential drugs and chemical tools**
M. Jung (University of Freiburg), Freiburg/DE
- 9.00 a.m. **Allosteric regulation and targeting of intramolecular cryptic binding pockets in tyrosine kinases**
O. Hantschel (University of Marburg), Marburg/DE
- 9.30 a.m. **Computational Mapping of the Druggability of Cryptic Pockets in Proteins**
R. Wade (HITS), Heidelberg/DE
- 10.00 a.m. COFFEE BREAK, EXHIBITION LOUNGE & MEET THE SPEAKERS
- Chair: Tatjana Ross*

10.30 a.m. POSTER PRIZES

Novel Methods in Medicinal Chemistry

Chair: Jean-Louis Reymond

- 10.45 a.m. **Structural studies of substrate and inhibitor binding to multidrug transporters by cryo-electron microscopy**
K. Locher (ETH Zurich), Zurich/CH
- 11.15 a.m. **RoboRXN: An AI-driven cloud-accessible autonomous chemical laboratory**
T. Laino (IBM Research Europe), Zurich/CH
- 11.45 a.m. **Closing Remarks**
Felix Hausch, Franz von Nussbaum, Jean-Louis Reymond



DARMSTADT

The General Meetings of the GDCh and DPhG
take place at another point of time.
Members will be informed.

Wednesday, March 10, 2021

Workshops

12.00 p.m. – 1.00 p.m.	David Peralta, Editor-in-Chief ChemMedChem, Wiley-VCH 5 Rules for Effective Writing in the Sciences
1.00 p.m. – 2.30 p.m.	Meet the Industr(ies): Life as a Medicinal Chemist in the new PharmaEco System Great opportunity for students, PhDs and postdocs to meet representatives from the pharmaceutical industries 1.00 – 1.20 p.m. Introduction (F. von Nussbaum, F. Hausch, T. Ross) Short self-introduction by industry representatives Tatjana Ross/Merck KGaA María Méndez Pérez /Sanofi Christian Kuttruf & Silke Buschbom-Helmke/Boehringer-Ingelheim Julien Lefranc/Nuvisan Franca Klingler/MSD Andreas Christoforow/Abbvie 1.20 – 2.20 p.m. 6 x 10min Speed-Dating with industry representatives 2.20 – 2.30 p.m. Wrap-up and Outlook
2.30 p.m. – 4.00 p.m.	Modelling-in-Medchem Workshop: Alexander Neumann, BioSolveIT From Fragment to Lead: Interactive Design of SARS-CoV-2 Mpro inhibitors

▶ POSTER

The deadline for abstract submission for selected talks (Highlights in Medicinal Chemistry) and short talks: **January 15, 2021**

The deadline for poster submissions: **until February 15, 2021**

www.gdch.de/medchem2021

There will be an online poster wall and a virtual exhibiton area.

Prizes will be awarded to the best posters on **Wednesday, March 10, 2021 at 10.30 a.m.**

▶ DATES

Deadlines

January 25, 2021 Cancellation of participation
February 25, 2021 Registration

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▶ REGISTRATION

Please register online not later than **February 25, 2021**

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The participation link will be sent to you by e-mail approx. one week before the event.

Upon online registration, payment by credit card, direct debit or bank transfer (only with German bank account) is possible. The invoice will be sent to you automatically.

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REGISTRATION FEES¹⁾

GDCh-, DPhG-, SCG- and member of EuChemS-member societies	€ 150,-
Member, job seeker or retired	€ 90,-
Non-member	€ 180,-
Student** (GDCh-, DPhG, SCG- and member of EuChemS-member societies)	€ 40,-
Student** (Non-member)	€ 60,-
Gold-member (with over 50 years of GDCh membership)	free of charge

* Not taxable under German law – exempt from tax under Swiss law.)

** valid Student-ID required

CANCELLATION

Requests for cancellation made prior to **January 25, 2021** will be subject to a € 25,- administration fee. After that date the full amount of the invoice has to be paid. Requests for refund will not be accepted; however, registration may be transferred to another member of your organisation. In this case please send a note to the GDCh event team.

If the meeting is cancelled for whatever reason, fees paid will be refunded. Further recourse is excluded.

INFORMATION BEFORE AND AFTER THE MEETING

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