



GESELLSCHAFT DEUTSCHER CHEMIKER



Fachgruppe Medizinische Chemie

Frontiers in Medicinal Chemistry

March 22 – 25, 2020 · Freiburg



www.gdch.de/medchem2020



▶ SCIENTIFIC COMMITTEE

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Sunday, March 22, 2020

Seminarraum 03 002

4.00 p.m. PRE-CONFERENCE WORKSHOP

6.00 p.m.

Modeling for Anyone

(further information can be found on the conference webpage)

Register to this free workshop at:
workshop-registration@biosolveit.comContact:
Dr. Franca Klingler, BioSolveIT

Hörsaal Rundbau

6.00 p.m. **Welcome**

6.30 p.m.

OPENING LECTURE**Targeting protein modification: from chemical biology to drug discovery**E. Tate, London/GB

Foyer

7.30 p.m. **POSTER SESSION I and GET TOGETHER**

Monday, March 23, 2020

Hörsaal Rundbau

- 8.30 a.m. **Functionalizing Ligands and Inhibitors with Electrophilic Traps to Identify Protein Binding Sites**
M. D. Witte, Groningen/NL, A. K. H. Hirsch, Saarland/DE, G. Medard, Munich/DE, B. Kuster, Munich/DE, M. R. Groves, Groningen/NL, A. J. van der Zouwen, Groningen/NL, J. Lohse, Groningen/NL, H. E. Wieske, Groningen/NL, K. F. Hohmann, Groningen/NL, R. van der Vlag, Groningen/NL, E. van der Pol, Groningen/NL, R. Stenecker, Groningen/NL, W. Wang, Groningen/NL, N. van Oosterwijk, Groningen/NL, S. Bousis, Saarland/DE
- 9.00 a.m. **Cysteine Protease Selective Activity-Based Probes for Molecular Imaging Applications and Protease Research**
G. Blum, Jerusalem/IL
- 9.30 a.m. **Hit-to-Lead with DNA-Encoded Libraries: Autotaxin and DDR1**
A. L. Satz, Basel/CH
- 10.00 a.m. COFFEE BREAK
- 10.30 a.m. **Macrocyclic Peptides as Chemical Tools for Studying Enzymes**
A. Kawamura, Oxford/GB
- 11.00 a.m. **Transition Metal-Catalyzed Addition of Pronucleophiles to Alkynes and Allenes: Key Step for the Synthesis of Bioactive Macrocycles**
B. Breit, Freiburg/DE
- 11.30 a.m. **Targeting Cancer**
D. Rauh, Dortmund/DE
- 12.00 a.m. LUNCH BREAK
- 1.00 p.m. **YOUNG INVESTIGATORS SESSION**
N^ω-carbamoylated Arginines: an Avenue to Radio- or Fluorescence Labeled and Cyclic Ligands of Peptidergic GPCRs
M. Keller, Regensburg/DE

Monday, March 23, 2020

Hörsaal Rundbau

- 1.15 p.m. **Encapsulins as prodrug activating nanoreactors**
C. Jessen-Trefzer, Freiburg/DE
- 1.30 p.m. **Short Lecture 1**
- 1.45 p.m. **Short Lecture 2**
- 2.00 p.m. **PhD Prizes**
- 2.15 p.m. COFFEE BREAK
- 2.45 p.m. **Pharmacologic Insights from Cryo-EM Structures of Autoinhibited and Active-state Structures of BRAF/MEK/14-3-3 Complexes**
M. Eck, Boston/US
- 3.15 p.m. **Target Based Identification and Optimization of Toll-Like Receptor 7 and 8 Antagonists**
T. Knoepfel, Basel/CH, C. Betschart, Basel/CH, R. Glatthar, Basel/CH, D. Behnke, Basel/CH, E. Vangrevelighe, Basel/CH, T. Junt, Basel/CH, S. Hawtin, Basel/CH, P. Loetscher, Basel/CH, J. Blank, Basel/CH, M. Faller, Basel/CH, R. Feifel, Basel/CH, P. Alper, San Diego/US, P.-Y. Michellys, San Diego/US, J. Deane, San Diego/US
- 3.45 p.m. **DXS as a Target to Block Terpenoid Biosynthesis in Plasmodium and Other Human Pathogens**
D. Merkler, Tampa/US, R. H. Y. Jiang, Tampa/US
- 4.15 p.m. COFFEE BREAK
- 4.45 p.m. **The discovery of BI-3406: an orally active SOS1: KRAS inhibitor for the treatment of KRAS driven tumors**
P. Ettmayer, Vienna/AT
- 5.15 p.m. **Short Lecture 3**
- 5.45 p.m. BREAK

Monday, March 23, 2020

Hörsaal Rundbau

6.00 p.m. **GENERAL MEETING** (guests are welcome)
of the GDCh Division on Medicinal Chemistry

**Mitgliederversammlung der GDCh-Fachgruppe
Medizinische Chemie**
(Gäste sind herzlich willkommen)

Agenda/Tagesordnung:

1. Bericht des Vorsitzenden der Fachgruppe
2. Veranstaltungen der Fachgruppe
3. Zusammenarbeit mit anderen nationalen und internationalen Organisationen
4. Preise
5. Mitgliederstand
6. Verschiedenes

6.45 p.m. **GENERAL MEETING** (guests are welcome)
of the DPhG Division of Pharmaceutical/
Medicinal Chemistry

**Mitgliederversammlung der DPhG-Fachgruppe
Medizinische Chemie**
(Gäste sind herzlich willkommen)

Agenda/Tagesordnung:

1. Bericht des Vorsitzenden
2. Zukünftige Tagungen
3. Innovationspreis und weitere wissenschaftliche Preise, Wahl der Jurymitglieder
4. Verschiedenes

Tuesday, March 24, 2020

Hörsaal Rundbau

9.00 a.m. **Design of Nucleotide Prodrugs for Antiviral
Chemotherapy – the TriPPPPro-Approach**
C. Meier, Hamburg/DE

9.30 a.m. **The ER Quality Control of Glycoprotein Folding as
Therapeutic Target – from Target Validation and
Structures to Drug Development**
N. Zitzmann, Oxford/GB

10.00 a.m. **COFFEE BREAK**

10.30 a.m. **Allosteric Covalent Inhibitors of the Mutant
GTPase KRAS^{G12C}**
D. Cassar, Cambridge/GB

11.00 a.m. **Discovery of LNP023, a First-in-Class, Oral Factor
B Inhibitor for Treatment of Rare Alternative
Complement Pathway Driven Diseases**
S. Flohr, Basel/CH

11.30 a.m. **Discovery, Synthesis and Structure-Activity
Relationship of Tetraniliprole (VAYEGO™),
a Novel Diamide Insecticide**
M. Willot, Monheim/DE, R. Fischer, Monheim/DE,
C. Funke, Monheim/DE, E. R. Gesing, Monheim/DE,
N. Godley, Monheim/DE, C. Grondal, Monheim/DE,
M. Heil, Monheim/DE, A. Hense, Monheim/DE,
S. Kuebbeler, Monheim/DE, P. Loesel, Monheim/DE,
O. Malsam, Monheim/DE, S. Pazenok, Monheim/DE,
H.-J. Wroblowsky, Monheim/DE

11.55 a.m. **Innovation Prize**

12.15 p.m. **LUNCH BREAK**

1.00 p.m. **POSTER SESSION II**

2.00 p.m. **Bringing it All Together – Towards a Versatile
Platform for Automated Ligand Design**
H. Briem, Berlin/DE

2.30 p.m. **Exploring Virtual Chemical Spaces and Generative
Neural Networks: How to Get the Most for Your
Drug Design Project**
C. Grebner, Frankfurt (Main)/DE

3.00 p.m. **COFFEE BREAK**

Tuesday, March 24, 2020

Hörsaal Rundbau

- 3.30 p.m. **Navigate your Chemistry-Case Studies of CETSA® in Drug Discovery**
S. Lundgren, Solna/SE
- 4.00 p.m. **tba**
- 4.30 p.m. **Integration of Biophysical Data with Structure-guided Design to Drive Modern Drug Discovery**
G. Siegal, Leiden/NL
- 5.00 p.m. **Poster Prizes**
- 5.30 p.m. Departure for Dinner
- 6.00 p.m. **Conference Dinner**

Wednesday, March 25, 2020

Hörsaal Rundbau

- 9.00 a.m. **PLENARY LECTURE**
Chemically Induced Protein Degradation Using PROTACs
A. Ciulli, Dundee/UK
- 10.00 a.m. **Bringing Light to Epigenetics**
O. Vazquez, Marburg/DE, L. Albert, Marburg/DE, B. Heinrich, Marburg/DE, L. Zhang, Marburg/DE
- 10.30 a.m. **Modulation of KMT9 During Tumorigenesis**
R. Schüle, Freiburg/DE
- 11.00 a.m. Coffee Break
- 11.30 a.m. **Discovery of Small Molecules Targeting Protein Methyltransferases**
J. Jin, New York/US
- 12.00 p.m. **Identification of LSD1 Inhibitors and KDM5C Inhibitors as Candidate Therapeutic Agents**
T. Suzuki, Osaka/JP
- 12.30 p.m. **Targeting Chromatin Binding Domains in Cancer**
E. C. Dykhuizen, West Lafayette/US
- 1.00 p.m. **Closing Remarks**

► POSTER

The deadline for poster submissions extended until **January 31, 2020**

www.gdch.de/medchem2020

Poster format: Portrait A0 (height: 118.9 cm, width: 84.1 cm)

Prizes will be awarded to the best posters on **Tuesday, March 24, 2020 at 5.00 p.m.**

▶ SOCIAL PROGRAM

Sunday, March 22, 2020

7.30 p.m.

Get-together and Poster Session I

Albert-Ludwigs-Universität Freiburg
 „Foyer Rundbau“
 Faculty of Chemistry and Pharmacy
 Alberstr. 21
 79104 Freiburg
 (free of charge, booking required)

Monday, March 23, 2020

8.00 p.m.

Guided City Tour, approx. 1,5 hrs

Price per person € 7.50
 (booking required)

Meeting point:
 Rathausplatz, near by Bertold Schwarz-fountain



Tuesday, March 24, 2020

6.00 p.m.

Congress Dinner

Market Hall “Freiburger Markthalle”
 Grünwälderstrasse 4
 79098 Freiburg, Germany

Price per Person: € 50,- (Buffet and three drinks included)
 (booking required)

▶ VENUE

Albert-Ludwigs-Universität Freiburg

“Hörsaal Rundbau”
 Faculty of Chemistry and Pharmacy
 Alberstr. 21
 79104 Freiburg

www.uni-freiburg.de/universitaet/kontakt-und-wegweiser/anfahrt

▶ TRAVEL INFORMATION

Arrival by car

Use highway exit “Freiburg Mitte” and follow the signs to „Hauptbahnhof (main train station)” along Schnewlinstraße and Bismarckallee, pass the main station and keep straight on along Stefan-Meier-Straße, then turn right into Albertstraße, the venue is at Albertstraße 21 (on the left side)

Arrival by Train

From Freiburg main station, exit city center: turn to the left and follow Stefan-Meier-Straße for about 5 minutes, then turn right into Albertstraße, the venue is at Albertstraße 21 (on the left side)

The “Deutsche Bahn” offers attractive conditions for travelling to GDCh-events. Further information can be found on following link en.gdch.de/railway

▶ ACCOMMODATION

HRS – Hotel Reservation Service will gladly assist in booking accommodation in all categories. Please apply no later than date **February 1, 2020**.

HRS – Hotel Reservation Service
 Blaubach 32
 50676 Köln

Please book online www.hrs.de or through the conference webpage.

Phone: +49 221 2077-7320
 Email: event-online@hrs.de

The customers will be held accountable for non-occupancy of reserved rooms.

REGISTRATION

Please register online not later than **February 10, 2020**

www.gdch.de/medchem2020

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Event Team / MedChem 2020

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All tickets and congress papers (incl. book of abstracts) will be handed to the participants upon check-in at the registration desk. Participants are requested to wear their congress badges at all times for identification and admittance to the conference rooms.

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 FEES^{*)}

GDCh-, DPhG- and member of EuChemS-member societies	€ 310,-
Member, job seeker or retired	€ 190,-
Non-member	€ 360,-
Student** (GDCh-, DPhG- and member of EuChemS-member societies)	€ 80,-
Student** (Non-member)	€ 120,-
Gold-member (with over 50 years of GDCh membership)	free of charge

* The registration fees are not liable to value added tax (tax exemption additional § 4 Nr. 22a UStG.)

** valid Student-ID required

If fees are paid in advance, but **after March 9, 2019**, we kindly ask participants to show proof of payment when claiming their tickets and congress papers at the registration desk. Credit cards (Amex, Mastercard, Visa) will be accepted.

CANCELLATION

Requests for cancellation made prior to **February 9, 2020** 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.

BEVERAGES

Coffee, tea, and soft drinks will be provided for free during the breaks.

LUNCH

Lunch will be served in the "Mensa" and can be bought upon registration:

Price per meal incl. one drink € 6,70.

DATES

Deadlines

January 31, 2020	Submission of posters
February 10, 2020	Registration
February 10, 2020	Cancellation of participation

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INFORMATION BEFORE AND AFTER THE MEETING

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Executive director: Professor Dr. Wolfram Koch

Registered Charity No.: VR 4453 Registergericht Frankfurt/Main

INFORMATION AND REGISTRATION DURING THE CONFERENCE

Opening hours of the conference office:

Foyer of the Lecture Hall University of Freiburg:

Sunday, March 22, 2020	4.00 p.m. – 6.30 p.m.
Monday, March 23, 2020	8.00 a.m. – 5.00 p.m.
Tuesday, March 24, 2020	8.30 a.m. – 4.30 p.m.
Wednesday, March 25, 2020	8.15 a.m. – 12.00 p.m.

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FURTHER CHEMICAL SOCIETY

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(German Pharmaceutical Society (DPHG))

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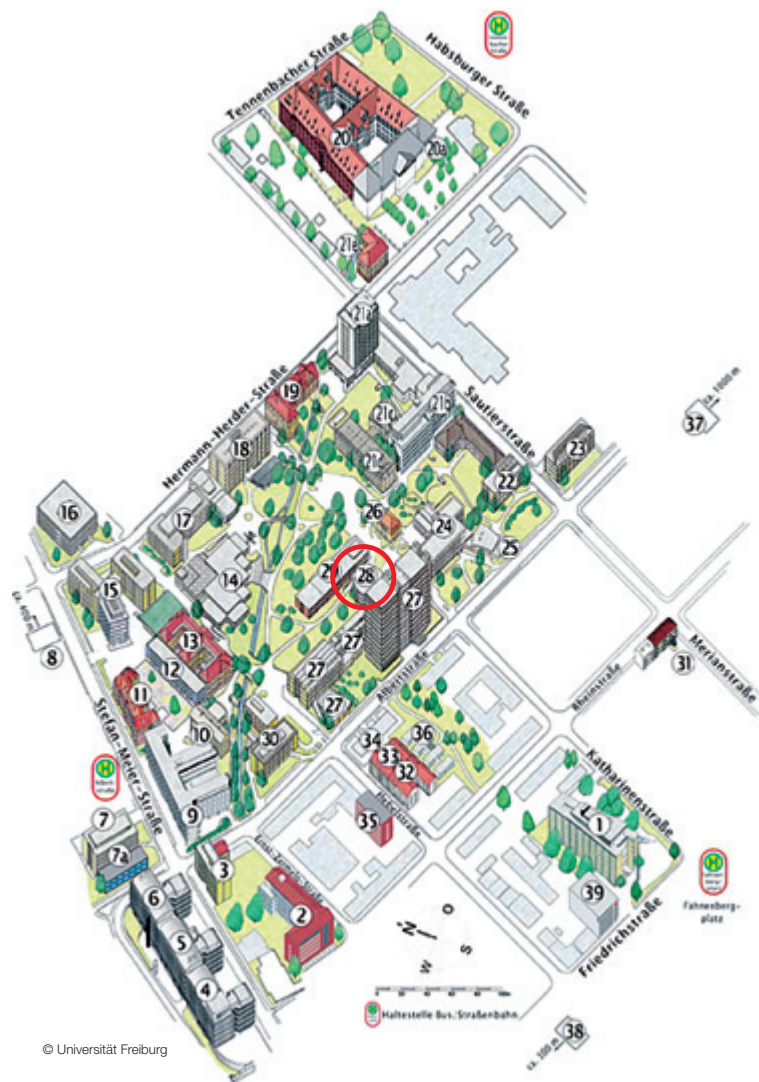
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ACKNOWLEDGEMENTS

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