



GESELLSCHAFT DEUTSCHER CHEMIKER



Medizinische
Chemie

Fachgruppe Medizinische Chemie

Frontiers in Medicinal Chemistry

March 11 – 14, 2018 · Jena

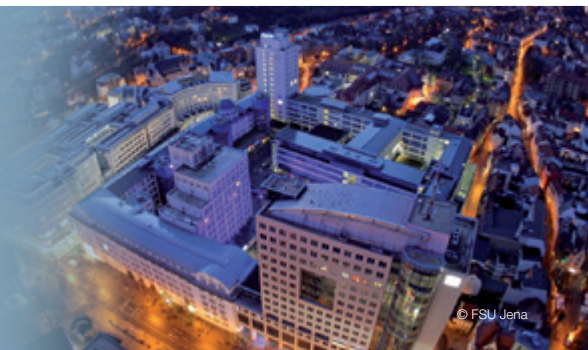


FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

DPhG

Deutsche
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www.gdch.de/medchem2018



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Sunday, March 11, 2018

Lecture Hall

6.00 p.m. **Welcome**

6.30 p.m. **OPENING LECTURE**
**Peptide Drugs to Target GPCR– State of the Art
and Innovative Applications**
A. Beck-Sickinger, Leipzig/DE

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



Monday, March 12, 2018

Lecture Hall

Natural Product-inspired Drugs Including Macrocycles

- 8.30 a.m. **Macrocyclic Peptide Natural Product Synthesis: Sharp Tool for Complex Targets**
H.-D. Arndt, Jena/DE
- 9.15 a.m. **Total Synthesis of Complex Polyketide Macrolides: Chemical Tools in Cancer Research**
D. Menche, Bonn/DE
- 10.00 a.m. COFFEE BREAK
- 10.30 a.m. **New Perspectives for Natural Products and Total Synthesis in Modern Drug Discovery**
C. Pöverlein, Frankfurt (Main)/DE
- 11.15 a.m. **On Nature's Strategies to Optimize the Biological Profile of Polyketides**
M. Kalesse, Hannover/DE, A. Naini, Hannover/DE, H.-H. Lu, Nanjing/RC
- 12.00 p.m. The *Klaus-Grohe-Preis für Medizinische Chemie* awards outstanding contributions of young doctors who work in the field of medicinal chemistry and/or active pharmaceutical ingredients.
In 2018 the Klaus-Grohe-Stiftung (foundation) awards the prize to Dr. Mateja Kljka Škopič, Dortmund and Dr. Matthias Schiedel, Oxford/UK
- 12.45 p.m. LUNCH BREAK
- 1.30 p.m. POSTER SESSION II

Innovative Anti-cancer Therapies

- 2.45 p.m. **Purinergic Targets in Cancer Immunotherapy**
C. Müller, Bonn/DE
- 3.30 p.m. **Novel mRNA Cancer Immunotherapies**
R. Jabulowsky, Mainz/DE
- 4.15 p.m. COFFEE BREAK
- 4.45 p.m. **A Reversible Covalent Approach to Selective FGFR4 Inhibition**
N. Buschmann, Basel/CH, J. Trappe, T. Gabriel, F. Hofmann, B. Sellers, R. A. Fairhurst, T. Knoepfel, P. Furet, C. Leblanc, R. Mah, M. Kiffe, D. Graus-Porta, A. Weiss, J. Kinyamu-Akunda, M. Wartmann, Basel/CH

Monday, March 12, 2018

Lecture Hall

- 5.30 p.m. **tba**
U. Köhl
- 6.15 p.m. **General Meeting GDCh** (guests are welcome)
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 DPhG** (guests are welcome)
Agenda/Tagesordnung:
1. Bericht des Vorsitzenden
2. Zukünftige Tagungen
3. Innovationspreis und weitere wissenschaftliche Preise, Wahl der Jurymitglieder
4. Verschiedenes



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Tuesday, March 13, 2018

Lecture Hall

Highlights in Medicinal Chemistry and Technology

- 8.30 a.m. **Discovery of Potent and Highly Selective Inhibitors of Calpain for the Treatment of Alzheimer's Disease**
A. Kling, Ludwigshafen/DE, A. Moeller, Ludwigshafen/DE
- 9.15 a.m. **Monitoring the Antagonist-Protein and Protein-Protein Interactions with NMR Spectroscopy: Inhibitors of p53-Mdm2 and Immune Checkpoints PD-1/PD-L1**
T. Holak, Krakow/PL
- 10.00 a.m. COFFEE BREAK
- 10.30 a.m. **Allosteric Inhibitors of Flaviviral NS3/NS2B Proteases**
T. Schirmeister, Mainz/DE
- 11.15 a.m. **Discovery of BAY 1142524, a Potent Selective and Orally Active Chymase Inhibitor for the Treatment of Cardiac Diseases**
C. Fuerstner, Wuppertal/DE, A. Tersteegen, V. Geiß, E. Hartmann, B. Albrecht-Küpper, H. Tinel, J. Ackerstaff, H. Meier, A. Straub, J. Mittendorf, J. Schamberger, Wuppertal/DE, M. Schäfer, Berlin/DE, K. Boerngen, H. Jörißen, D. Zubov, K. Zimmermann, Wuppertal/DE
- 12.00 p.m. **Synthesizing and Tuning Artificial Macrocycles for Difficult Targets and Membrane Permeation-Tuning Artificial Macrocycles for Difficult Targets and Membrane Permeation**
A. Dömling, Groningen/NL, E. Abdelraheem, S. Shaabani, M. C. Rudrakshula, Groningen/NL
- 12.15 p.m. **Antibody Paratope Mimetic Peptides**
J. Eichler, Erlangen/DE, C. Haußner, Erlangen/DE, B. Schmidt, Regensburg/DE
- 12.30 p.m. LUNCH BREAK
- 1:15 p.m. POSTER SESSION III

Tuesday, March 13, 2018

Lecture Hall

Young Investigators

- 2.30 p.m. **Innovation Prize I**
- 3.00 p.m. **H₂neupna-trastuzumab: Evaluation of a Novel Bifunctional Chelator for ¹¹¹In Radiopharmaceuticals and Immuno-SPECT Imaging**
S. Spreckelmeyer, Berlin/DE, C. F. Ramogida, J. Rousseau, K. Arane, I. Bratanovic, N. Colpo, U. Jermilova, G. M. Dias, I. Dude, M. Jaraquemada-Pelaez, F. Benard, P. Schaffer, C. Orvig, Vancouver/CA
- 3.15 p.m. **Natural Products and Their de novo Mimetics as Retinoid X Receptor Modulators**
D. Merk, Zurich/CH, G. Schneider, Zurich/CH
- 3.30 p.m. **M. tuberculosis Thioredoxin Reductase Inhibitors with Activity on Mycobacterial Growth in Infected Macrophages**
O. Koch, Dortmund/DE, L. Bering, J. Pretzel, Dortmund/DE, M. Schneefeld, N. Reiling, Borstel/DE, F.-C. Bange, Hannover/DE
- 3.45 p.m. **Rational Design and Diversity-oriented Synthesis of Peptoid-Based Histone Deacetylase (HDAC) Inhibitors for the Epigenetic Therapy of Cancer**
F. K. Hansen, Leipzig/DE, V. Krieger, D. Diedrich, A. Hamacher, C. G. W. Gertzen, Düsseldorf/DE, J. Senger, Freiburg/DE, T. Kurz, Düsseldorf/DE, M. Jung, Freiburg/DE, H. Gohlke, M. U. Kassack, Düsseldorf/DE
- 4.00 p.m. COFFEE BREAK
- In Silico Toxicology**
- 4.30 p.m. **In silico Toxicology – from Prediction of Transporter Interaction Profiles to Toxicological Read Across and Beyond**
G. Ecker, Wien/AT
- 5.15 p.m. **In Silico Prediction of ADMET Properties of Small Molecules**
J. Kirchmair, Hamburg/DE
- 6.00 p.m. **In-silico Drug Hazard Prediction: Computational Models for Toxicity Assessment and Case Studies in Pharmaceutical R&D**
F. Schmidt, Frankfurt (Main)/DE, J. Wenzel, A. Czich, Frankfurt (Main)/DE

Wednesday, March 14, 2018

Lecture Hall

Inflammation and Resolution

- 8.30 a.m. **Tailored Design of Sugar-modified α -GalCer Analogues for Th1-polarized Immune Responses**
S. Van Calenberg, Gent/BE
- 9.15 a.m. **Ultrashort Lectures/Poster Awards**
- 9.35 a.m. **Ph. D. Awards**
- 10.05 a.m. **Inhibitors of the Mitotic Kinase MPS1: From Screening Hits to a Preclinical Drug Candidate**
S. Hoelder, London/GB, F. Broaccatelli, R. Burke, S. A. Eccles, F. Raynaud, S. Linardopoulos, R. L. M. Van Montfort, J. Blagg, J. Schmitt, L. O'Fee, H. Saville, A. De Haven Brandon, R. Baker, J. Roberts, G. Box, M. Valenti, A. T. Henley, K. Walsh, H. Woodward, P. Innocenti, K.-M. J. Cheung, S. Naud, S. Solanki, I. M. Westwood, A. Faisal, G. W-Y. Mak, A. Hayes, P. Sheldrake, B. Mattijssen, London/GB
- 10.20 a.m. **Discovery and Investigation of Transient Covalent KLK6 Inhibitors**
A. Miller, Heidelberg/DE, E. De Vita, N. Gunkel, Heidelberg/DE
- 10.35 a.m. COFFEE BREAK
- 11.00 a.m. **The Signaling Pathways of Regulated Necrosis as Therapeutic Targets**
A. Linkermann, Dresden/DE
- 11.45 a.m. **5-Lipoxygenase as Target for Inhibition of Inflammation and Promotion of Resolution**
D. Steinhilber, Frankfurt (Main)/DE
- 12.30 p.m. **Closing Remarks**

POSTER

Deadline for poster submissions: January 31, 2018 (extended)

www.gdch.de/medchem2018

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

Prizes will be awarded to the best three posters. The winning poster presenters will be allotted 5 minutes to present their work on March 14, 2018. Therefore, all poster presenters should be prepared to give such an ultra-short lecture (5 min, 2-3 slides).

SOCIAL PROGRAM

Sunday, March 11, 2018

7.30 p.m.

Get-together and 1st Poster Session

Foyer
Campus Ernst-Abbe-Platz
Carl-Zeiss-Straße 3
07743 Jena, Germany
(free of charge, booking required)

Monday, March 12, 2018

7.30 p.m.

Guided discovery tour through Jena

Binoculars, star projector and the black-red-gold flag – all discovered in Jena. The guided tour will end in a local brewery with the possibility to attend a beer degustation.

Language: German

Price per person € 10,-
(booking required, limited tickets)

Meeting point: Campus Carl-Zeiss-Straße 3, Jena



Tuesday, March 13, 2018

8.00 p.m.

Social Evening (dinner and party)

Volksbad Jena
Knebelstraße 10
07743 Jena, Germany

Price per person € 30,- incl. buffet and € 10,- beverages voucher
(booking required)

The Volksbad Jena is within walking distance to the conference venue (800 m). When exiting the main building walk across the square (Ernst-Abbe-Platz) and turn right on Leutragraben. Turn left on Engelplatz (at the post office) and follow the street Grietgasse. Turn right on "Am Volksbad". At the end of the street, the Volksbad is on your right hand side.

▶ VENUE

University of Jena

Campus Ernst-Abbe-Platz
Carl-Zeiss-Straße 3
07743 Jena, Germany

▶ TRAVEL INFORMATION

Arrival by car

A 4 either direction Dresden or Frankfurt take exit 54 "Jena Zentrum" and follow the signs toward the city center (Stadtrodaer Straße, B88).

Arrival by Train/Public Transportation

Arrival at Jena West

Exit the station and turn left. At the end of the street (100 m) turn right on Westbahnhofstraße. The street makes a left turn and turns into Schillerstraße. Follow the street until you cross the tracks of the tram. After about 50 m, the building on the left side of the street opens and you will see Ernst-Abbe-Platz. Enter the square through the opening.

Arrival at Jena Paradies

Exit the station and cross the street (Knebelstraße). Keeping the bus terminal to your right, follow the street Grietgasse (making a left turn) until you face the post office. Turn right (Schillerstraße) and follow until you cross the tracks of the tram. After about 50 m, the building on the left side of the street opens and you will see Ernst-Abbe-Platz. Enter the square through the opening.

The "Deutsche Bahn" offers attractive conditions for travelling to GDCh-events. Further information can be found on following link www.gdch.de/bahn

▶ DATES

Deadlines

January 31, 2018	Submission of posters
February 1, 2018	Personal registration
February 1, 2018	Room reservation
February 11, 2018	Cancellation of participation

▶ COPYRIGHT PERMISSION

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▶ ACCOMMODATION

HRS – Hotel Reservation Service will gladly assist in booking accommodation in all categories. Please apply no later than date **February 1, 2018**.

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 1, 2018**

www.gdch.de/medchem2018

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.

Claudia Birkner – Event Team

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Germany

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Internet: www.gdch.de

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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GENERAL INFORMATION

REGISTRATION FEES¹⁾

GDCh-member, DPhG-member and member of EuCheMS-member societies	€ 290,-
Member, unemployed or retired	€ 170,-
Non-member	€ 340,-
Student** (GDCh-member, DPhG-member and member of EuCheMS-member societies)	€ 75,-
Student** (Non-member)	€ 100,-
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 1, 2018**, 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 11, 2018** 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 GDCh, event team.

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

SCHOLARSHIPS

The GDCh Division of Medicinal Chemistry offers a limited number of scholarships to student division members in education presenting a scientific contribution. Please send your application (form on the internet at www.gdch.de/medchem) until **January 31, 2018**, latest.

BEVERAGES

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

GENERAL INFORMATION

LUNCH

Lunch can be taken in the nearby cafeteria (Mensa). Individual payment.

An overview about restaurants within walking distance will be provided at the conference office.

INFORMATION BEFORE AND AFTER THE MEETING

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.

Claudia Birkner – Event Team

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Internet: www.gdch.de

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 Campus Ernst-Abbe-Platz, University of Jena:

Sunday, March 11, 2018	4.00 p.m. – 6.30 p.m.
Monday, March 12, 2018	8.00 a.m. – 5.00 p.m.
Tuesday, March 13, 2018	8.00 a.m. – 4.30 p.m.
Wednesday, March 14, 2018	8.00 a.m. – 12.00 a.m.

Phone: +49 171 679 2995

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FURTHER CHEMICAL SOCIETIES

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(Date: January 19, 2018/tg)

GENERAL INFORMATION



ACKNOWLEDGEMENTS

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