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GESELLSCHAFT DEUTSCHER CHEMIKER



Medizinische
Chemie

Fachgruppe Medizinische Chemie

Frontiers in Medicinal Chemistry

March 13 – 16, 2016 · Bonn



DPhG

Deutsche
Pharmazeutische
Gesellschaft e.V.

www.gdch.de/medchem2016



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Sunday, March 13, 2016

Lecture Hall X

- 18:00 **Welcome to “Frontiers in Medicinal Chemistry”**
- 18:30 **OPENING LECTURE**
Molecular Diversity and Re-emergence of Natural Products in Drug Discovery
R. J.Quinn, Brisbane/AU
- 19:30 **GET TOGETHER and POSTER SESSION**



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Monday, March 14, 2016

Lecture Hall X

Target Identification & Lead Discovery

- 8:30 **Design of Long-acting GLP-1 Analogs Applicable for Once Weekly Dosing**
J. Lau, Måløv/DK
- 9:05 **Discovery of a Negative Allosteric Modulator of the mGlu5 receptor by Fragment Based Drug Discovery**
M. Congreve, Welwyn Garden City/GB, S. Aves, K. Bennett, A. Dore, J. Patel, B. Tehan, F. Marshall, Welwyn Garden City/GB
- 9:40 **Aptamers for screening and therapy**
G. Mayer, Bonn/DE
- 10:15 COFFEE BREAK
- 10:45 **Fatty acid receptors as drug targets**
S. Offermanns, Bad Nauheim/DE
- 11:20 **G protein coupled receptor conformational dynamics and ligand selectivity: a new opportunity for drug design?**
J.-L. Banères, Montpellier/FR, S. Mary, M. Damian, J.-A. Fehrentz, J. Martinez, J. Marie, Montpellier/FR
- 11:55 **Impact of Target-based Approaches on the Discovery of First-in-class Drugs**
J. Eder, Basel/CH
- 12:30 LUNCH
- 12:30 **SPONSORTALK** (12:30 – 13:00)
***In vivo* Pharmacokinetics during Early Drug Development: When Do *in vivo* Data Facilitate Decision Making?**
What is the best time to include early *in vivo* studies and how to choose the most efficient study design tailored to early drug & lead development?
S. Urschel, Saarbrücken/DE
- 13:40 **POSTER SESSION**

Allosteric Modulators & Modulation of Protein-Protein Interactions

- 14:45 **Structural disorder and allostery: new challenges in drug development**
P. Tompa, Brussels/BE
- 15:20 **Allosteric modulation of the hERG channel – impact on cardiotoxicity**
A. P. IJzerman, Leiden/NL, Z. Yu, L. H. Heitman, Leiden/NL
- 15:55 COFFEE BREAK

Monday, March 14, 2016

Lecture Hall X

Allosteric Modulators & Modulation of Protein-Protein Interactions

- 16:30 **Combining AB technology, structural biology and molecular dynamics to define new PPI opportunities**
A. Henry, Brussels/BE
- 17:05 **Fragment-based protein ligands through protein-assisted fragment ligation: application for antiviral and anticancer targets**
J. Rademann, Berlin/DE
- 17:40 **Short talk**
- 17:50 **Short talk**
- 18:00 **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 (Innovationspreis in Medizinisch/ Pharmazeutischer Chemie; Promotionspreise)
 5. Entwicklung der Fachgruppe
 6. Verschiedenes
- 18:45 **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
 4. Verschiedenes
- 20:00 **Social Program**

Tuesday, March 15, 2016

Lecture Hall X

Antibacterial Drugs

- 8:30 **Antibiotic crisis: Status, problems and solutions (from the past)?**
P. Hammann, Frankfurt (Main)/DE
- 9:05 **Interference with bacterial quorum sensing – a novel anti-virulence strategy**
R. W. Hartmann, Saarbrücken/DE
- 9:40 **Bacterial and fungal pathogens as sources for new peptide drugs**
R. Süßmuth, Berlin/DE
- 10:15 COFFEE BREAK
- 10:50 **Development of drugs for Mycobacterium tuberculosis**
P. Brodin, Lille/FR
- 11:25 **Dissecting the role of purinergic receptor and ATP through malaria parasites life cycle**
C. R. S. Garcia, Sao Paulo/BR
- 11:35 **Short talk**
- 11:45 **Short talk**
- 11:55 **Klaus-Grohe-Prize**
- 12:30 LUNCH
- 13:40 **POSTER SESSION**

Structural Biology

- 14:45 **Envolving GPCRs to Favorable Biophysical Properties: Enabling Drug Screening Studies**
A. Plückthun, Zürich/CH
- 15:20 **Innovation Prize**
- 15:35 **Short talk**
- 15:45 **Short talk**
- 15:55 **SPONSORTALK**
A New Visual Alert System for Structural Biology and MedChem
M. Gastreich, Sankt Augustin/DE
- 16:05 COFFEE BREAK

Tuesday, March 15, 2016

Lecture Hall X

Structural Biology

- 16:30 **Crystal Structures of Purinergic Receptors**
Q. Zhao, Shanghai/CN, D. Zhang, K. Zhang, Shanghai/CN, J. Zhang, Shanghai/CN, Z. Gao, Bethesda/US, H. Jiang, Shanghai/CN, V. Cherezov, V. Katritch, La Jolla/US, C. Müller, Bonn/DE, R. Stevens, La Jolla/US, B. Wu, Shanghai/CN
- 17:05 **Structure, function and inhibition of the ectonucleotidases CD39 and CD73 in purinergic signalling**
N. Sträter, Leipzig/DE, J. Pippel, E R. Scaletti, K. Knapp, M. Krauss, M. Zebisch, Leipzig/DE
- 17:40 **Short talk**
- 17:50 **Short talk**

Highlights in Medicinal Chemistry & Technology I

- 18:00 **A Chemical Approach to Controlling Cell Fate**
S. Ding, San Francisco/US



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Wednesday, March 16, 2016

Lecture Hall X

Highlights in Medicinal Chemistry & Technology II

- 8:30 **CRISPR Screening in the Study of Human Disease**
W. Wei, Beijing/CN, S. Zhu, Y. Zhou, Beijing/CN
- 9:05 **Ultrashort Lectures, Poster Prizes**
- 9:25 **PhD Prizes**
- 10:00 **Innovation Prize**
- 10:15 **COFFEE BREAK**
- 10:50 **Soluble guanylate cyclase (sGC) stimulator vericiguat as a potential treatment for heart failure**
M. Follmann, Wuppertal/DE, J. Ackerstaff, J. P. Stasch, P. Sandner, F. Wunder, G. Redlich, D. Lang, A. Kern, P. Fey, N. Griebenow, E. M. Becker-Pelster, A. Kretschmer, V. Geiss, V. M. Li, A. Straub, J. Mittendorf, R. Jautelat, H. Schirok, K. H. Schlemmer, A. Knorr, W. Kroh, Wuppertal/DE
- 11:15 **Bioisosteric Hinge-Binding Motifs for Tofacitinib-Derived JAK3-selective Probes**
S. A. Laufer, Tübingen/DE, M. Gehringer, E. Pfaffenrot, M. Forster, S. M. Bauer, Tübingen/DE
- 11:40 **AGC Kinase Inhibitors**
O. Plettenburg, Frankfurt (Main)/DE
- 12:05 **Synthesis Design Through the Lens of Flow Chemistry**
T. F. Jamison, Cambridge/US
- 12:40 **Closing Remarks**

POSTER

Deadline for poster submissions: January 31, 2016 (extended)

www.gdch.de/medchem2016

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 16, 2016. Therefore, all poster presenters should be prepared to give such an ultra-short lecture (5 min, 2-3 slides).

SOCIAL PROGRAM

Sunday, March 13, 2016

19:30

Get-together and 1st Poster Session

Aula of the University main building
Am Hof 1 / Regina-Pacis-Weg 1
53113 Bonn, Germany
(free of charge, booking required)

Monday, March 14, 2016

20:00

Guided tour with a night watchman (“Nachtwächterführung”) through Bonn’s city center

Price per person € 10,-* booking required
Meeting point: In front of the entrance “Am Hof” of the University Main building (also see map on page 14/15)

Guided gastronomical tour “Drink doch ene met” (with stories about Bonn’s traditional restaurants and bars in the historic city center + visit of three bars)

Price per person € 7,-* (drinks not included), booking required
Meeting point: In front of the entrance “Am Hof” of the University Main building (also see map on page 14/15)

Tuesday, March 15, 2016

20:00

Social Evening (dinner and party)

Maritim Hotel Bonn
Godesberger Allee
53175 Bonn, Germany
Price per person € 20,-* incl. buffet and drinks
booking required

The Maritim Hotel can be reached via metro. Starting e.g. from “Bonn Hbf” (central station) or “Universität/Markt” take metro line 16 (destination “Bad Godesberg”), line 63 (destination “Bad Godesberg”) or line 66 (destination “Bad Honnef”). Get off at station “Olof-Palme-Allee”. If you look into the direction the metro takes you can see the Maritim Hotel on the left (Travel duration: ca. 9 min, one-way ticket Preisstufe 1b: € 2.80). The last metro back from “Olof-Palme-Allee” to Bonn city center leaves at 2.21 h.

* including 19% VAT

▶ VENUE

University of Bonn

Main building (Castle)
Am Hof 1 / Regina-Pacis-Weg 1
53113 Bonn
Germany

▶ TRAVEL INFORMATION

Further travel information including parking information can be found on the conference webpage and also:

www.uni-bonn.de/die-universitaet/anfahrt_uni-bonn_webversion.pdf (German)

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

▶ REGISTRATION

Please register online not later than **February 1, 2016**

www.gdch.de/medchem2016

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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 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, SCT-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 card required

If fees are paid in advance, but **after March 1, 2016**, 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 1, 2016** 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, congress 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, 2016**, latest.

Scholarships are also offered by the DPhG. For details please refer to www.dphg.de.

▶ BEVERAGES

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

▶ LUNCH

A small lunch snack will be served and is included.
An overview about restaurants nearby offering lunch will be provided at the conference desk.

▶ ACCOMMODATION

HRS – Hotel Reservation Service will gladly assist in booking accommodation in all categories. Please apply no later than date **February 1, 2016**.

HRS – Hotel Reservation Service
Blaubach 32
50676 Köln

Please book online

www.hrs.de/web3?clientId=ZGVfX2Zyb250aWVycw,2
or through the conference webpage.

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

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

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▶ INFORMATION BEFORE AND AFTER THE MEETING

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Executive director: Professor Dr. Wolfram Koch
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▶ INFORMATION AND REGISTRATION DURING THE CONFERENCE

Opening hours of the conference office:
Foyer of the Aula, University of Bonn:

Sunday, March 13, 2016	16:00 – 18:30 hrs
Monday, March 14, 2016	8:00 – 17:00 hrs
Tuesday, March 15, 2016	8:00 – 16:30 hrs
Wednesday, March 16, 2016	8:00 – 12:00 hrs

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▶ FURTHER CHEMICAL SOCIETIES

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▶ DATES

Deadlines

January 31, 2016	Submission of posters
February 1, 2016	Personal registration
February 1, 2016	Cancellation of participation
February 1, 2016	Room reservation

(Date: January 18, 2016/tg)

BONN Inner City Map



ACKNOWLEDGEMENTS

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(Preliminary list January 11, 2016)



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