**SCIENTIFIC COMMITTEE**

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P. George  Longvilliers/FR
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S. Laufer  Tübingen/DE
V. Lisowski  Montpellier/FR
C. E. Müller  Bonn/DE
E. Ottow  Berlin/DE
J.-P. Rocher  Lyon/FR
J. Sapi  Reims/FR (SCT president)
L. van Hijfte  Illkirch/FR
F. von Nussbaum  Berlin/DE

**October 1, 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
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>Design of Long-acting GLP-1 Analogs Applicable for Once Weekly Dosing</td>
<td>J. Lau, Måløv/DK</td>
</tr>
<tr>
<td>9:05</td>
<td>Discovery of a Negative Allosteric Modulator of the mGlu5 receptor by Fragment Based Drug Discovery</td>
<td>M. Congreve, Welwyn Garden City/GB, S. Aves, K. Bennett, A. Dore, J. Patel, B. Tehan, F. Marshall, Welwyn Garden City/GB</td>
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<tr>
<td>9:40</td>
<td>Aptamers for screening and therapy</td>
<td>G. Mayer, Bonn/DE</td>
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<td>10:15</td>
<td>COFFEE BREAK</td>
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<tr>
<td>10:45</td>
<td>Fatty acid receptors as drug targets</td>
<td>S. Offermanns, Bad Nauheim/DE</td>
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<tr>
<td>11:55</td>
<td>Impact of Target-based Approaches on the Discovery of First-in-class Drugs</td>
<td>J. Eder, Basel/CH</td>
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<td>12:30</td>
<td>LUNCH</td>
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<tr>
<td>12:30</td>
<td>SPONSORTALK (12:30 – 13:00)</td>
<td>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 &amp; lead development?</td>
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<td>13:40</td>
<td>POSTER SESSION</td>
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<td>14:45</td>
<td>Structural disorder and allostery: new challenges in drug development</td>
<td>P. Tompa, Brussels/BE</td>
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<td>15:20</td>
<td>Allosteric modulation of the hERG channel – impact on cardiotoxicity</td>
<td>A. P. IJzerman, Leiden/NL, Z. Yu, L. H. Heitman, Leiden/NL</td>
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<td>15:55</td>
<td>COFFEE BREAK</td>
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<tbody>
<tr>
<td>16:30</td>
<td>Combining AB technology, structural biology and molecular dynamics to define new PPI opportunities</td>
<td>A. Henry, Brussels/BE</td>
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<td>17:05</td>
<td>Fragment-based protein ligands through protein-assisted fragment ligation: application for antiviral and anticancer targets</td>
<td>J. Rademann, Berlin/DE</td>
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<td>17:40</td>
<td>Short talk</td>
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<tr>
<td>18:00</td>
<td>GENERAL MEETING (guests are welcome) of the GDCh Division on Medicinal Chemistry</td>
<td>Mitgliederversammlung der GDCh-Fachgruppe Medizinische Chemie (Gäste sind herzlich willkommen)</td>
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<td></td>
<td>Agenda/Tagesordnung:</td>
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<tr>
<td></td>
<td>1. Bericht des Vorsitzenden der Fachgruppe</td>
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<td>2. Veranstaltungen der Fachgruppe</td>
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<td>3. Zusammenarbeit mit anderen nationalen und internationalen Organisationen</td>
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<td>4. Preise (Innovationspreis in Medizinisch/Pharmazeutischer Chemie; Promotionspreise)</td>
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<td>5. Entwicklung der Fachgruppe</td>
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<td>6. Verschiedenes</td>
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<tr>
<td>18:45</td>
<td>GENERAL MEETING (guests are welcome) of the DPhG Division of Pharmaceutical/Medicinal Chemistry</td>
<td>Mitgliederversammlung der DPhG-Fachgruppe Medizinische Chemie (Gäste sind herzlich willkommen)</td>
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<td>Agenda/Tagesordnung:</td>
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<td>1. Bericht des Vorsitzenden</td>
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<td>2. zukünftige Tagungen</td>
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<td>3. Innovationspreis und weitere wissenschaftliche Preise</td>
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<td></td>
<td>4. Verschiedenes</td>
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<tr>
<td>20:00</td>
<td>Social Program</td>
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### Antibacterial Drugs

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<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Speaker/Institution</th>
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<tbody>
<tr>
<td>8:30</td>
<td>Antibiotic crisis: Status, problems and solutions (from the past)?</td>
<td>P. Hammann, Frankfurt (Main)/DE</td>
</tr>
<tr>
<td>9:05</td>
<td>Interference with bacterial quorum sensing – a novel anti-virulence</td>
<td>R. W. Hartmann, Saarbrücken/DE</td>
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<tr>
<td></td>
<td>strategy</td>
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<tr>
<td>9:40</td>
<td>Bacterial and fungal pathogens as sources for new peptide drugs</td>
<td>R. Süßmuth, Berlin/DE</td>
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#### Tuesday, March 15, 2016

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<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Speaker/Institution</th>
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<tbody>
<tr>
<td>10:15</td>
<td><strong>COFFEE BREAK</strong></td>
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<tr>
<td>10:50</td>
<td>Development of drugs for Mycobacterium tuberculosis</td>
<td>P. Brodin, Lille/FR</td>
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<tr>
<td>11:25</td>
<td>Dissecting the role of purinergic receptor and ATP through malaria</td>
<td>C. R. S. Garcia, Sao Paulo/BR</td>
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<td>parasites life cycle</td>
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<tr>
<td>11:35</td>
<td><strong>Short talk</strong></td>
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<td>11:45</td>
<td><strong>Short talk</strong></td>
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<td>11:55</td>
<td><strong>Klaus-Grohe-Prize</strong></td>
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<td>12:30</td>
<td><strong>LUNCH</strong></td>
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<td><strong>POSTER SESSION</strong></td>
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### Structural Biology

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<tr>
<th>Time</th>
<th>Title</th>
<th>Speaker/Institution</th>
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</thead>
<tbody>
<tr>
<td>16:30</td>
<td>Crystal Structures of Purinergic Receptors</td>
<td>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</td>
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<td>CD73 in purinergic signalling</td>
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<td>17:40</td>
<td><strong>Short talk</strong></td>
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#### Tuesday, March 15, 2016

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

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](http://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

REGISTRATION FEES

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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60486 Frankfurt/Main
Germany
Phone: +49 69 7917-366
E-mail: tg@gdch.de
Internet: www.gdch.de

Executive director: Professor Dr. Wolfram Koch
Registered Charity No.: VR 4453 Registergericht Frankfurt/Main

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

University of Bonn, main building entrance „Am Hof“

Meeting point (social program):

© OpenStreetMap contributor

ca. 4 km Maritim-Hotel
SPONSORS

(Preliminary list January 11, 2016)

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