Frontiers in Medicinal Chemistry
March 13 – 16, 2016 · Bonn

www.gdch.de/medchem2016
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
### Monday, March 14, 2016

#### Lecture Hall X

**Target Identification & Lead Discovery**

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</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>
</tr>
<tr>
<td>9:40</td>
<td>Aptamers for screening and therapy</td>
<td>G. Mayer, Bonn/DE</td>
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<tr>
<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>
</tr>
<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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<tr>
<td>12:30</td>
<td>LUNCH</td>
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<tr>
<td>12:30</td>
<td><strong>SPONSORTALK</strong> (12:30 – 13:00)</td>
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<tr>
<td></td>
<td><em>In vivo</em> Pharmacokinetics during Early Drug Development: When Do <em>in vivo</em> Data Facilitate Decision Making?</td>
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<tr>
<td></td>
<td>What is the best time to include early <em>in vivo</em> studies and how to choose the most efficient study design tailored to early drug &amp; lead development?</td>
<td>S. Urschel, Saarbrücken/DE</td>
</tr>
<tr>
<td>13:40</td>
<td><strong>POSTER SESSION</strong></td>
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**Allosteric Modulators & Modulation of Protein-Protein Interactions**

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>14:45</td>
<td>Structural disorder and allostery: new challenges in drug development</td>
<td>P. Tompa, Brussels/BE</td>
</tr>
<tr>
<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>
</tr>
<tr>
<td>15:55</td>
<td>COFFEE BREAK</td>
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<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>
</tr>
<tr>
<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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<tr>
<td>17:40</td>
<td>Short talk</td>
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<tr>
<td>17:50</td>
<td>Short talk</td>
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<tr>
<td>18:00</td>
<td><strong>GENERAL MEETING</strong> (guests are welcome) of the GDCh Division on Medicinal Chemistry</td>
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<tr>
<td></td>
<td>Mitgliederversammlung der GDCh-Fachgruppe Medizinische Chemie (Gäste sind herzlich willkommen)</td>
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<tr>
<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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<tr>
<td></td>
<td>2. Veranstaltungen der Fachgruppe</td>
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<td></td>
<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></td>
<td>5. Entwicklung der Fachgruppe</td>
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<td></td>
<td>6. Verschiedenes</td>
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<tr>
<td>18:45</td>
<td><strong>GENERAL MEETING</strong> (guests are welcome) of the DPhG Division of Pharmaceutical/Medicinal Chemistry</td>
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<tr>
<td></td>
<td>Mitgliederversammlung der DPhG-Fachgruppe Medizinische Chemie (Gäste sind herzlich willkommen)</td>
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<tr>
<td></td>
<td>Agenda/Tagesordnung:</td>
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<tr>
<td></td>
<td>1. Bericht des Vorsitzenden</td>
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<td></td>
<td>2. zukünftige Tagungen</td>
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<tr>
<td></td>
<td>3. Innovationspreis und weitere wissenschaftliche Preise</td>
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<tr>
<td></td>
<td>4. Verschiedenes</td>
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<tr>
<td>20:00</td>
<td><strong>Social Program</strong></td>
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### Antibacterial Drugs

**Tuesday, March 15, 2016**  
**Lecture Hall X**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
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</thead>
<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 strategy</td>
<td>R. W. Hartmann, Saarbrücken/DE</td>
</tr>
<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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<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>
</tr>
<tr>
<td>11:25</td>
<td>Dissecting the role of purinergic receptor and ATP through malaria parasites life cycle</td>
<td>C. R. S. Garcia, Sao Paulo/BR</td>
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<tr>
<td>11:35</td>
<td><strong>Short talk</strong></td>
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<tr>
<td>11:45</td>
<td><strong>Short talk</strong></td>
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<tr>
<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>13:40</td>
<td><strong>POSTER SESSION</strong></td>
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### Structural Biology

**Tuesday, March 15, 2016**  
**Lecture Hall X**

<table>
<thead>
<tr>
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</tr>
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<tbody>
<tr>
<td>16:30</td>
<td><strong>Crystal Structures of Purinergic Receptors</strong></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>
</tr>
<tr>
<td>17:40</td>
<td><strong>Short talk</strong></td>
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<tr>
<td>17:50</td>
<td><strong>Short talk</strong></td>
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<tr>
<td>18:00</td>
<td><strong>Highlights in Medicinal Chemistry &amp; Technology I</strong></td>
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<tr>
<td>14:45</td>
<td><strong>Envolving GPCRs to Favorable Biophysical Properties: Enabling Drug Screening Studies</strong></td>
<td>A. Plückthun, Zürich/CH</td>
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<tr>
<td>15:20</td>
<td><strong>Innovation Prize</strong></td>
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<tr>
<td>15:35</td>
<td><strong>Short talk</strong></td>
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<tr>
<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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<tr>
<td>16:05</td>
<td><strong>COFFEE BREAK</strong></td>
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</tbody>
</table>
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).
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

<table>
<thead>
<tr>
<th>Category</th>
<th>Fee</th>
</tr>
</thead>
<tbody>
<tr>
<td>GDCh-member, DPhG-member and member of EuCheMS-member societies</td>
<td>€ 290,-</td>
</tr>
<tr>
<td>Member, unemployed or retired</td>
<td>€ 170,-</td>
</tr>
<tr>
<td>Non-member</td>
<td>€ 340,-</td>
</tr>
<tr>
<td>Student** (GDCh-member, DPhG-member, SCT-member and member of EuCheMS-member societies)</td>
<td>€ 75,-</td>
</tr>
<tr>
<td>Student** (Non-member)</td>
<td>€ 100,-</td>
</tr>
<tr>
<td>Gold-member (with over 50 years of GDCh membership)</td>
<td>free of charge</td>
</tr>
</tbody>
</table>

* 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**

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.
Claudia Birkner - Congress Team
P. O. Box 90 04 40
60444 Frankfurt/Main
Varrentrappstr. 40-42
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

(Date: January 18, 2016/tg)

**INFORMATION AND REGISTRATION DURING THE CONFERENCE**

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

<table>
<thead>
<tr>
<th>Date</th>
<th>Hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sunday, March 13, 2016</td>
<td>16:00 – 18:30 hrs</td>
</tr>
<tr>
<td>Monday, March 14, 2016</td>
<td>8:00 – 17:00 hrs</td>
</tr>
<tr>
<td>Tuesday, March 15, 2016</td>
<td>8:00 – 16:30 hrs</td>
</tr>
<tr>
<td>Wednesday, March 16, 2016</td>
<td>8:00 – 12:00 hrs</td>
</tr>
</tbody>
</table>

Phone: +49 171 679-2995
Fax: +49 69 7917 1366

**FURTHER CHEMICAL SOCIETIES**

**Deutsche Pharmazeutische Gesellschaft e.V.**
(German Pharmaceutical Society (DPhG))
Varrentrappstr. 40-42
60486 Frankfurt/Main
Germany
Phone: +49 69 7191596-0
Fax: +49 69 7191596-29
E-mail: info@dphg.de
Internet: www.dphg.de

**Société de Chimie Thérapeutique**
(Centre d’Etudes Pharmaceutiques
5, rue Jean-Baptiste Clément
92296 Chatenay Malabry Cedex
France
Phone: +33 1 46 83 56 84
Fax: +33 1 46 83 53 23
E-mail: sct@sct-asso.fr
Internet: www.sct-asso.fr

**DATES**

<table>
<thead>
<tr>
<th>Deadlines</th>
<th>Submission of posters</th>
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</thead>
<tbody>
<tr>
<td>January 31, 2016</td>
<td>Personal registration</td>
</tr>
<tr>
<td>February 1, 2016</td>
<td>Cancellation of participation</td>
</tr>
<tr>
<td>February 1, 2016</td>
<td>Room reservation</td>
</tr>
</tbody>
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(Date: January 18, 2016/tg)
SPONSORS

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BioSolveIT GmbH
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Charnwood Molecular Ltd.
ChemPur Feinchemikalien und Forschungsbedarf GmbH
IBA GmbH
Interchim
LABC-Labortechnik Zilger GmbH
NanoTemper Technologies GmbH
Pharmacelsus GmbH
Reach Separations

MEDIA PARTNERS

Wiley-VCH Verlag GmbH & Co. KGaA

EXHIBITORS

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Enzo Life Sciences GmbH
Xantec bioanalytics GmbH