



GESELLSCHAFT DEUTSCHER CHEMIKER



Medizinische  
Chemie

Fachgruppe Medizinische Chemie

# Frontiers in Medicinal Chemistry

March 15 – 18, 2015 · Marburg

Philipps



Universität  
Marburg



**SCS**  
Swiss Chemical  
Society

**DPhG**

Deutsche  
Pharmazeutische  
Gesellschaft e.V.

[www.gdch.de/medchem2015](http://www.gdch.de/medchem2015)



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T. Steinmetzer	Marburg
C. Wegscheid-Gerlach	Marburg

Sunday, March 15, 2015

Lecture Hall

- 18.00 Welcome to „Frontiers in Medicinal Chemistry“
- 18.30 **OPENING LECTURE**  
**Molecular Obesity, Potency and Other Addictions in Medicinal Chemistry**  
M. Hann, Stevenage/GB
- 19.30 **GET TOGETHER and POSTER SESSION**



Monday, March 16, 2015

Lecture Hall

## RNA Therapeutics

- 8.30 **Locked and Unlocked Nucleic Acid (LNA and UNA) in Drug Discovery**  
J. Wengel, Odense/DK
- 9.15 **LNA Drug Platform – from Bench to Bedside**  
H. Ørum, Hørsholm/DK
- 10:00 COFFEE BREAK
- 10.30 **Making Drugs out of siRNAs**  
M. Manoharan, Cambridge/US
- 11.15 **Structure-based Design of Riboswitch Ligands**  
R. Brenk, Mainz/DE
- 11.40 **Targeting RNA with Drug-like Ligands**  
J. Hall, Zürich/CH

12.05 LUNCH

13.20 POSTER SESSION

## CNS-Neurodegeneration

- 14.30 **Glutamyl Cyclases (QCs) – Emerging Anti-inflammatory and Dementia Targets: Discovery, Target Validation and Drug Discovery**  
H.-U. Demuth, Halle (Saale)/DE
- 15.15 **Regulation of Apoptosis by Small Molecule Activators and Inhibitors of Bcl-2 Family Proteins**  
D. Andrews, Toronto/CA
- 16.00 COFFEE BREAK
- 16.30 **Inhibition of Bid-dependent Death Pathways – Novel Targets for Mitochondrial Protection**  
C. Culmsee, Marburg/DE
- 17.15 **Selective Inhibitors for the Psychiatric Risk Factor FKBP51 Enabled by an Induced-fit Mechanism**  
F. Hausch, München/DE

Monday, March 16, 2015

Lecture Hall

- 17.40 **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. Vorstellung des Vorsitzenden der Fachgruppe
  2. Bericht des Vorsitzenden der Fachgruppe
  3. Veranstaltungen der Fachgruppe
    - GDCh-Wissenschaftsforum Chemie vom 30.08.-02.09.2015 in Dresden
    - Frontiers in Medicinal Chemistry 2015
    - Frontiers in Medicinal Chemistry 2016
    - Future in Medicinal Chemistry Workshop
    - Summer School Medicinal Chemistry
  4. Zusammenarbeit mit anderen nationalen und internationalen Organisationen
  5. Preise (Innovationspreis in Medizinisch/Pharmazeutischer Chemie; Promotionspreis)
  6. Entwicklung der Fachgruppe
  7. Verschiedenes

Lecture Hall

- 18.25 **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. Tagungsstipendien für Doktoranden
  4. Innovationspreis Medizinische/Pharmazeutische Chemie
  5. Zukunftspapier „Pharmazie 2020“
  6. Verschiedenes

19.30 **Social Program**

Tuesday, March 17, 2015

Lecture Hall

## Antiinfectives and Antivirals

- 8.30 **Griselimycins – Magic Bullets Against Mycobacterium Tuberculosis?**  
R. Müller, Saarbrücken/DE
- 9.15 **Approaches to Overcome Resistance to Antibiotics**  
C. Zumbrunn, Allschwil/CH
- 10.00 **COFFEE BREAK**
- 10.30 **Establishment and Application of Cell Culture Systems to Develop Antiviral Drugs**  
R. Bartenschlager, Heidelberg/DE
- 11.15 **Discovery and Structure-guided Optimization of Adenain Inhibitors**  
E. Altmann, Basel/CH
- 11.40 **Virus-activating Host Cell Proteases Provide Potential Drug Targets for the Treatment of Influenza Virus Infections**  
E. Böttcher-Friebertshäuser, Marburg/DE
- 12.05 **LUNCH**
- 13.20 **POSTER SESSION**

## Highlights in Technology and Medicinal Chemistry

- 14.30 **Analysis of Binding Kinetics and Thermodynamics of DPPiV Inhibitors and Their Relationship to Structure**  
H. Nar, Biberach (Riss)/DE
- 15.45 **Drug-Target Residence Time and Applications to Lead Optimization**  
R. Copeland, Cambridge/US
- 16.00 **COFFEE BREAK**
- 16.30 **Target Family-centric Privileged Structures: Unexploited Opportunities for Medicinal Chemistry**  
G. Müller, Nijmegen/NL
- 17.15 **Design of Kinase Inhibitors from INPHARMA-NMR Data**  
T. Carlomango, Heidelberg/DE

Tuesday, March 17, 2015

Lecture Hall

## Highlights in Technology and Medicinal Chemistry

- 18.00 **Allostery at the Chemokine Receptor CXCR3: Discovery of First Highly Potent Baised Negative and Positive Allosteric Modulators**  
N. Tschammer, Erlangen/DE
- 18.25 **Development of Potent Ligands by the Three-dimensional Structural Diversity-oriented Strategy Based on the Characteristic Stereo- and Stereoelectronic Feature of Cyclopropane**  
S. Shuto, Hokkaido/JP
- 20.00 **Conference Dinner**



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Wednesday, March 18, 2015

Lecture Hall

## Innovative Novel Drug Releases

- 8.30 **Development of Covalent Inhibitors for Bruton's Tyrosine Kinase – Round Two**  
Z. Pan, Shenzen/CN
- 9.15 **Ultrashort lectures, poster prizes**
- 9.35 **Innovation prize**
- 10.00 **COFFEE BREAK**
- 10.30 **Creating Novel FXIa Inhibitors Through Fragment Based Lead Generation and Structure Aided Drug Design**  
O. Fjellström, Mölndal/SE
- 11.15 **The Discovery of Modulators of HCV NS5A – Daclatasvir and Synergists**  
N. Meanwell, Wallingford/US
- 12.00 **Discovery of CETP Inhibitors with Reduced Lipophilicity**  
T. Trieselmann, Biberach (Riss)/DE
- 12.25 **Closing remarks**



## POSTER

Deadline for poster submissions: **January 15, 2015**[www.gdch.de/medchem2015](http://www.gdch.de/medchem2015)

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 followed by a 5 minute discussion on March 19, 2015. Therefore, all poster presenters should be prepared to give such an ultrashort lecture (5 min, 2-3 slides).

## SOCIAL PROGRAM

Sunday, March 15, 2015

19.30

**Get-together and 1<sup>st</sup> Poster Session**

Foyer of the lecture hall building (Hörsaalgebäude)  
Biegenstr. 14  
35037 Marburg, Germany  
(free of charge, booking required)

Monday, March 16, 2015

19.30

**Guided Tour through the interactive laboratory****“Chemikum Marburg”** including hands-on experiments

Price per person € 10,-\* booking required (max 40 persons)  
Meeting point: conference office

**Guided Tour through Marburgs historic city center**

Price per person € 5,-\* booking required  
Meeting point: conference office

\* including 19% VAT

Tuesday, March 17, 2015

20.00

**Conference Dinner**

Restaurant im Kaufhaus Ahrens  
Universitätsstr. 14 - 22  
35037 Marburg, Germany  
(approx. 700 m near the lecture hall)

**Note: all participants of the meeting are invited to attend the dinner.**

(free of charge, booking required, drinks included).



## ▶ VENUE

### Philipps-Universität Marburg

Hörsaalgebäude (lecture hall building)  
Biegenstr. 14  
35037 Marburg  
Germany

## ▶ TRAVEL INFORMATION

### Arrival by car

#### From North (Kassel)

Leave the urban motorway at the Marburg-Bahnhofstrasse exit. Take a right at the first traffic light onto Bahnhofstrasse in the direction of the city center. Stay in the left lane until you reach the next traffic light at Elisabeth Church (Elisabethkirche) and then turn left onto Deutschhausstrasse. Now go straight on at the next traffic light and follow the right bend onto Biegenstrasse. After about 300m you will see a church to your right and right next to it an entry to the parking lot.

#### From South (Frankfurt)

Leave the urban motorway at the Marburg-Mitte exit (near the Esso petrol station) and take a right turn. Stay in the right lane until you reach the next traffic light, then take a right turn in the direction of the city center. Now continue on in the right lane. At the third traffic light, and after crossing the bridge over the Lahn river, take a right at the next traffic light and stay in the left lane. Go past the Cineplex cinema on your right, and then change to the left lane before you reach the second pedestrian crossing, then take a left turn. You have reached the lecture hall building.

### Arrival by Train/Public Transportation

After arrival at Marburg main station take a municipal bus number 2, 3, 6, 7 or C. Get off at "Rudolphsplatz", or take a taxi in front of the Marburg main station and ask the driver to take you to Biegenstrasse 14. You have reached lecture hall building.

See also: [www.uni-marburg.de/profile-en/anfahrt](http://www.uni-marburg.de/profile-en/anfahrt)

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

## ▶ REGISTRATION

Please register online not later than **February 1, 2015**

[www.gdch.de/medchem2015](http://www.gdch.de/medchem2015)

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.

### Congress Team / MedChem 2015

Postfach 90 04 40  
60444 Frankfurt/Main  
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Phone: +49 69 7917-366 (Claudia Birkner)

e-mail: [tg@gdch.de](mailto:tg@gdch.de)

Internet: [www.gdch.de](http://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 FEES<sup>1)</sup>

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 card required

If fees are paid in advance, but **after March 1, 2015**, 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, 2015** 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](http://www.gdch.de/medchem)) until **January 31, 2015**, latest.

For DPhG scholarships please contact the DPhG directly.

## GENERAL INFORMATION

### BEVERAGES

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

### LUNCH

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, 2015**.

HRS – Hotel Reservation Service  
Blaubach 32  
50676 Köln

#### Please book online

[www.hrs.de/web3?clientId=ZGVfX2Zyb250aWVycw,2](http://www.hrs.de/web3?clientId=ZGVfX2Zyb250aWVycw,2)  
or through the conference webpage.

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

#### Congress Team / MedChem 2015

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Internet: [www.gdch.de](http://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 the Lecture Hall Philipps-Universität Marburg

<b>Sunday, March 15, 2015</b>	<b>16.00 – 18.30 hrs</b>
<b>Monday, March 16, 2015</b>	<b>8.00 – 17.00 hrs</b>
<b>Tuesday, March 17, 2015</b>	<b>8.00 – 16.30 hrs</b>
<b>Wednesday, March 18, 2015</b>	<b>8.00 – 12.00 hrs</b>

Phone: +49 175 335 4803

Fax: +49 69 7917 1366

## DATES

### Deadlines

January 15, 2015	Submission of posters
February 1, 2015	Personal registration
February 1, 2015	Cancellation of participation
February 1, 2015	Room reservation

## FURTHER CHEMICAL SOCIETIES

### German Pharmaceutical Society

(Deutsche Pharmazeutische Gesellschaft e.V.)  
Hamburger Allee 26-28  
60486 Frankfurt/Main  
Germany

Phone: +49 69 7191596-0

Fax: +49 69 7191596-29

E-mail: [info@dphg.de](mailto:info@dphg.de)

Internet: [www.dphg.de](http://www.dphg.de)

### Swiss Chemical Society (SCS)

(Schweizerische Chemische Gesellschaft, SCG)  
Schwarztorstr. 9  
CH-3007 Bern  
Switzerland

Phone: +41 31 310-4090

Fax: +41 31 310-4029

E-mail: [info@scg.ch](mailto:info@scg.ch)

Internet: [www.scg.ch](http://www.scg.ch)

Preliminary list of sponsors December 17, 2014



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# MAP

