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GESELLSCHAFT DEUTSCHER CHEMIKER



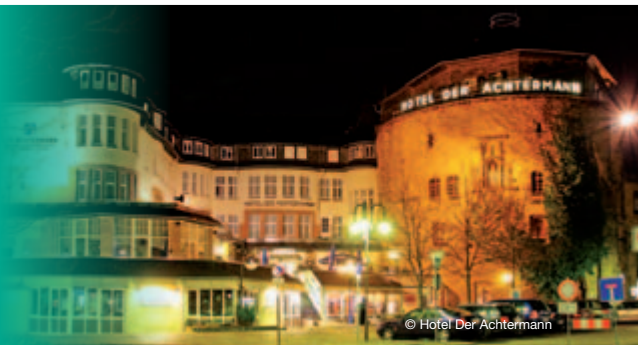
Fachgruppe
Chemie – Information – Computer

GCC 2012

8th German
Conference on Chemoinformatics

November 11 – 13, 2012
Goslar · Germany

www.gdch.de/gcc2012



© Hotel Der Achtermann



The division "Chemie-Information-Computer" (CIC: Chemistry-Information-Computer) of the Gesellschaft Deutscher Chemiker e.V. (German Chemical Society) cordially invites you to participate in the

**8. German Conference on Chemoinformatics
November 11-13, 2012, Goslar**

In the spirit of previous meetings organized by the "Chemie-Information-Computer" division of the Gesellschaft Deutscher Chemiker e.V., the topics of our international symposium will span a wide range of contributions related to computer aided processes in chemistry, and to chemical information. The conference is aimed at providing a scientific event of excellence, attractive to both industrial and academic scientists in this field. The scientific programme will include plenary lectures as well as presentation of posters, projects and software. The conference language is English.

On Sunday, November 11, a free-software session with tutorials on a number of open source projects in chemoinformatics will be offered.

Pre-conference workshops will be given by Chemical Computing Group and ChemAxon.

**INFORMATION BEFORE AND
AFTER THE CONFERENCE**

Gesellschaft Deutscher Chemiker e.V.
(German Chemical Society)
Congress Team / GCC 2012
P.O. Box 90 04 40
60444 Frankfurt am Main, Germany

Varrentrappstr. 40-42
60486 Frankfurt am Main, Germany

Phone: +49 69 7917-358 (Silvia Kirrwald)
E-mail: tg@gdch.de
Website: www.gdch.de

Executive Director: Professor Dr. Wolfram Koch
Registered Charity No.: VR 4453
Registergericht Frankfurt am Main

INFORMATION DURING THE CONFERENCE

The conference office will be located in front of "Großer Saal".

Opening hours:

Sunday, November 11, 2012	13:00 – 18:00 hrs
Monday, November 12, 2012	08:00 – 16:00 hrs
Tuesday, November 13, 2012	08:00 – 12:00 hrs

Phone: +49 5231 7000-909

**INFORMATION ABOUT
THE SCIENTIFIC PROGRAMME**

Dr. Frank Oellien
MSD Animal Health Innovation GmbH
Drug Discovery/Molecular Discovery Sciences
Zur Propstei
55270 Schwabenheim
Germany
E-mail: Frank.Oellien@msd.de

DEADLINES

October 10, 2012	Room reservation
October 14, 2012	Personal registration
October 15, 2012	Cancellation of participation
November 1, 2012	Submission of last minute poster

► SCIENTIFIC ADVISORY BOARD

J. Bajorath	Bonn/DE
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► SPONSORING

We appreciate as main conference sponsor:



CHEMICAL
COMPUTING
GROUP

Sunday, November 11, 2012

Großer Saal

14:00 **FREE SOFTWARE SESSION**

Get your Chemistry right with KNIME
T. Meinl, Konstanz/D

Barbarasaal

15:00 **SOFTWARE EXHIBITION BY COMPANIES**

Großer Saal

16:00 **PRE-CONFERENCE WORKSHOPS**

The Latest Developments in MOE – the Molecular Operating Environment
S. Maginn, Cambridge/GB

17:00 **Using ChemAxon's Discovery Toolkit within Workflow Tools; KNIME and Pipeline Pilot**

A. Allardyce, Budapest/H

18:30 **Dinner**

Großer Saal

19:45 **Conference opening**20:00 **EVENING LECTURE**

The Digital Native
R. Marcinko, Stanford/USA

Monday, November 12, 2012

Großer Saal

Molecular Modelling I09:00 **KEYNOTE**

Targeting Protein Dynamics in Drug Design
R. Wade, Heidelberg/DE

09:40 **Protein Modeling and Molecular Dynamic Studies of Two New Surfactant Proteins**

F. W. Rausch, Halle/DE, Brandt, Halle/DE, M. Schicht,
L. Bräuer, F. Paulsen, Erlangen/DE

10:05 **The MoSGrid – E-Science Gateway: Molecular Simulations in a Distributed Computing Environment**

L. Packschies, Köln/DE, G. Birkenheuer, Paderborn/D,
D. Blunk, S. Breuers, Köln/DE, A. Brinkmann, Paderborn/DE, L. de la Garza, Tübingen/DE, I. dos Santos Vieira, Dortmund/DE, G. Fels, Paderborn/DE, S. Gesing, Tübingen/DE, R. Grunzke, Dresden/DE, S. Herres-Pawlis, München/DE, O. Kohlbacher, J. Krüger, Tübingen/DE, M. Kruse, U. Lang, Köln/DE, R. Müller-Pfefferkorn, Dresden/DE, P. Schäfer, Berlin/DE, T. Schlemmer, Dresden/DE, C. Schärfe, Tübingen/DE, T. Steinke, Berlin/DE, K.-D. Warzecha, Köln/DE, A. Zink, Tübingen/DE

10:30 **Coffee Break & Exhibition****Chemoinformatics and Drug Discovery I**11:00 **KEYNOTE**

Reproducibility in Cheminformatics and Computational Chemistry Research: Certainly We Can Do Better than this
G. Landrum, Basel/CH

11:40 **Statistical Modeling of Value Distributions of Similarity Coefficients in Virtual Screening and its Application to Predicting Fingerprint Search Performance**

M. Vogt, Bonn/DE, J. Bajorath, Bonn/DE

12:05 **FMCS: A Novel Algorithm for the Multiple MCS Problem**

A. Dalke, Göteborg/SE, J. Hastings, Hinxton/GB

12:30 **How to Pick a Winning Team: Approaches towards the Selection of Computationally Derived Protein Structures for Ensemble-Based Virtual Screening**

B. Sander, Southampton/GB, O. Korb, Cambridge/GB,
J. Cole, Cambridge/GB, J. Essex, Southampton/GB

12:50 **Lunch**

Monday, November 12, 2012

Großer Saal

Chemoinformatics and Drug Discovery I

- 14:00 **Let's Talk About Rings**
M. Rarey, Hamburg/DE, A. Kolodzik, Hamburg/DE,
S. Urbaczek, Hamburg/DE
- 14:25 **Toxicological Knowledge Discovery by Mining Emerging Patterns from Toxicity Data**
R. Sherhod, Sheffield/GB, V. Gillet, Sheffield/GB,
T. Hanser, Leeds/GB, P. Judson, Leeds/GB, J. Vessey, Leeds/GB
- 14:50 **Conference Photo**

Awards

- 15:10 **GMELIN-BEILSTEIN-DENKMÜNZE**
Awardee:
Engelbert Zaß, Zürich/CH
Laudatory Speech:
René Deplanque, Berlin/DE
- FIZ CHEMIE BERLIN-AWARD**
Awardees:
Florian Pfeiffer, Stuttgart/DE
A Polynomial Based Vibrational Multiconfiguration Self-Consistent Field Program
Anselm Horn, Erlangen/DE
Computational Investigations of the Amyloid-beta Peptide from Alzheimer's Disease
Lectures of the Award Winners
- 16:30 **Postersession & Exhibition**

Tuesday, November 13, 2012

Großer Saal

Computational Materials Science and Nanotechnology

- 09:00 **KEYNOTE**
Computational Prediction of Heterogeneous Interface Properties at the Atomic Level
C. Ciacchi, Bremen/DE
- 09:40 **Theoretical and Experimental Study of the pH-Dependent Interaction of Amino Acids and MFI-Type Zeolite**
K. Stueckenschneider, Dortmund/DE, J. Merz, Dortmund/DE,
V. Milman, Cambridge/GB, G. Schembecker, Dortmund/DE
- 10:05 **Coffee Break & Exhibition**

Chemoinformatics and Drug Discovery II

- 10:30 **KEYNOTE**
Cheminformatics Approaches for Bridging Chemical, Protein Target and Phenotypic Space
A. Bender, Cambridge/GB
- 11:10 **Quantifying the Shifts in Physicochemical Property Space Introduced by the Metabolism of Small Organic Molecules**
J. Kirchmaier, Cambridge/GB, A. Howlett, Cambridge/GB,
J. Peironcelly, Leiden/NL, D. Murrell, Cambridge/GB,
M. Williamson, Cambridge/GB, S. Adams, Cambridge/GB,
T. Hankemeier, Leiden/NL, L. van Buren, Vlaardingen/NL,
G. Duchateau, Vlaardingen/NL, W. Klaffke, Vlaardingen/NL,
R. Glen, Cambridge/GB
- 11:35 **3D-QSAR Reloaded: Open3DALIGN Meets COSMOsar3D**
P. Tosco, Turin/I, A. Klamt, Leverkusen/DE
- 12:00 **Dataset Overlap Density Analysis**
A. H. Göller, Wuppertal/DE
- 12:30 **GENERAL MEETING OF THE GDCh DIVISION CIC**
- 13:00 **Lunch**
- 13:45 **POSTER AWARDS**

Tuesday, November 13, 2012

Großer Saal

Chemical Information, Patents and Databases

- 14:00 **KEYNOTE**
The Long and Winding Road to Chemical Information
E. Zaß, Zürich/CH
- 14:40 **Efficient Maximum Common Subgraph (MCS) Searching of Large Chemical Databases**
R. A. Sayle, Cambridge/GB, J. Batista, Alderley Park/GB, J. Grant, Alderley Park/GB
- 15:05 **IUPAC International Identifier for Chemical Reactions**
G. Grethe, Alameda /USA
- 15:30 **Coffee Break & Exhibition**

Molecular Modelling II

- 16:00 **KEYNOTE**
Challenges in Agrochemicals Design
K.-J. Schleifer, Ludwigshafen/DE
- 16:40 **Development of a Pharmacophore Model for Pharmacological Chaperones Targeting Mutant Trafficking-Deficient CNG Channels**
C. Schärfe, Tübingen/DE, J. Taeger, Tübingen/DE, P. Reuter, Tübingen/DE, N. Fischer, Tübingen/DE, J. Krüger, Tübingen/DE, B. Wissinger, Tübingen/DE, O. Kohlbacher, Tübingen/DE
- 17:05 **Modifications to Glucose-6-Phosphate Dehydrogenase for Industrial Applications: Predictions and Tests**
M. Mosisch, Hamburg/DE, J. Simons, Hamburg-Harburg/DE, L. Hilterhaus, Hamburg-Harburg/DE, A. Torda, Hamburg/DE
- 18:00 **CONFERENCE DINNER**

POSTER

Please note that it is possible to submit last minute posters online until **November 1, 2012** at

www.gdch.de/gcc2012

(No guarantee for last-minute-posters to be published in the book of abstracts)

There is a total limit of 60 posters for the conference.

EXHIBITION

The scientific programme will be accompanied by an exhibition of software applications, hardware solutions and scientific literature.

The exhibition is organised by

Dr. Frank Oellien
 MSD Animal Health Innovation GmbH
 Drug Discovery/Molecular Discovery Sciences
 Zur Propstei
 55270 Schwabenheim
 Germany
 E-mail: Frank.Oellien@msd.de



► SOCIAL PROGRAMME

Sunday, November 11, 2012

18:30

Dinner

The buffet and softdrinks (water and apple juice) are included in the registration fee. All other beverages have to be paid separately.

Monday, November 12, 2012

16:30

Postersession

Beer and pretzel are included in the registration fee.

Tuesday, November 13, 2012

18:00

Conference Dinner

The buffet and softdrinks (water and apple juice) are included in the registration fee. All other beverages have to be paid separately.

Booking is required for the dinner on Tuesday!

► LUNCH AND COFFEE BREAKS

The participant fee includes lunch and coffee breaks (softdrinks excluded).

► INTERNET ACCESS

The conference hotel provides a wireless LAN (WLAN) hotspot of the Deutsche Telekom. If internet access is required details about pricing and configuration can be obtained from www.t-com.de/hotspots.

► REGISTRATION

Please register online via internet not later than **October 14, 2012**.

www.gdch.de/gcc2012

Because of the strong increase of the number of attendees during the last conferences, we have to impose a limit for the number of conference participants (200 max).

All tickets and conference papers (incl. book of abstracts) will be given to participants upon check-in at the conference office.

Participants are requested to wear their conference badges at all times for identification and admittance to the conference rooms.

Upon online-registration payment by credit card or direct debit (only with German bank account) is preferred. If you want to pay by bank transfer (free of bank commission) please do not forget to print out the invoice at the end of your online registration.

Please pay the fees to the following account (free of bank commission):

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.

Commerzbank AG Frankfurt am Main

Bank no.: 500 800 00

Account no.: 4 900 200 00

Code: 5370 / GCC 2012

Attention

Participants from EU countries except Germany please use IBAN (International Bank Account Number) and SWIFT-BIC (Bank Identifier Code) instead of bank account and bank name:

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.

Commerzbank AG Frankfurt am Main

Frankenallee 71-81

60327 Frankfurt am Main, Germany

IBAN: DE85 5008 0000 0490 0200 00

SWIFT BIC: COBADEFFXXX

Code 5370 / GCC 2012

REGISTRATION FEES

GDCh-member and member of EuCheMS-member societies	€ 350,-
Member, unemployed or retired	€ 200,-
Non-member	€ 420,-
Student – GDCh-/EuCheMS-member (valid student card required)	€ 150,-
Student – Non-member (valid student card required)	€ 190,-
GDCh Gold member (with over 50 years of GDCh membership)	free of charge

If fees are paid in advance, but after **November 1, 2012**, we kindly ask participants to show proof of payment when claiming their tickets and congress papers at the conference office. **Onsite payment only by electronic cash or credit card (Mastercard, Visa).**

CANCELLATION

Written cancellations received on or before **October 15, 2012**, will be refunded less 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 conference is cancelled for whatever reason, fees paid will be refunded. Further recourse is excluded.

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HOTEL ACCOMMODATION

The hotel provides accommodation for all participants in single (from € 70,- to € 90,- per room/night) or double bed rooms (from € 105,- to € 125,- per room/night).

Arrangements should be made directly with the hotel under the keyword “CIC 2012” not later than October 10, 2012.

Hotel Der Achtermann

Rosentorstraße 20
38640 Goslar, Germany

Phone: +49 5321 7000-200

Fax: +49 5321 7000-999

E-mail: reservierung@der-achtermann.de

Website: www.hotel-der-achtermann.de

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

LOCATION

The meeting will take place at the Hotel Der Achtermann
Rosentorstraße 20,
38640 Goslar, Germany



Goslar is located at the heart of Germany and famous for its ore mine (UNESCO World Heritage Site) and its old town. The conference hotel “Der Achtermann” is within 3 minutes walking distance from Goslar main station.



▶ TRAVEL INFORMATION

By train:

IC/ICE to Hanover main station, “Regional Express” train directly to Goslar main station.

By plane:

Flight to Hanover airport (www.hannover-airport.de), train to Hanover main station, “Regional Express” train directly to Goslar main station.

By car:

After entering Goslar follow the traffic signs “Tagungszentrum” and park your car at the “Parkhaus Zentrum”. You can reach the hotel entrance on the 1st storey of the carpark.

