3. GERMAN CONFERENCE ON CHEMoinformatics

November 11 – 13, 2007
Goslar, Germany

21. CIC-Workshop 2007
The division Chemistry-Information-Computer of the Gesellschaft Deutscher Chemiker e.V. (German Chemical Society) cordially invites you to participate in the

3. German Conference on Chemoinformatics
   (21. CIC-Workshop)
   November 11–13, 2007, Goslar

In the spirit of previous meetings organized by the “Chemistry-Information-Computer” division (CIC) 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. We wish to attract 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 in combination with a business marketplace of chemoinformatics vendors.
We appreciate as main conference sponsor:

**Bayer Business Services**

Bayer Business Services, Leverkusen

We are grateful for the support of our publishing partner:

**Chemistry Central Journal**

Chemistry Central Journal, London

A supplement containing the abstracts of the conference will be published in Chemistry Central Journal.

We also gratefully acknowledge the generous financial support by the Deutsche Forschungsgemeinschaft (German Research Foundation).
Sunday, November 11, 2007

14.00 **Free Software Session**
A number of open source projects in chemoinformatics will be offered.

14.00 **Software Exhibition by companies**

14.00 **Market Place**
The chemoinformatics marketplace gives exhibitors the opportunity to present themselves in a way that goes beyond the possibilities of a regular exhibition booth. During this time (Sunday, November 11, 14:00 – 17:00) exhibitors may offer different kinds of events like talks, product reviews, hands-on tutorials. This year Accelrys and Chemical Computing Group will organize the market place. The specific events will also be announced on our conference homepage and are bookable by participants as part of the registration process.

- **A data pipelining approach for data retrieval, organisation and reporting**
  Accelrys
  Room Rosentor

- **Hands-on introduction to new applications in MOE 2007**
  Chemical Computing Group

17.00 **Opening – with short introduction of the exhibitors**
(approx. 12 minutes each)

18.30 **Dinner**

20.00 **EVENING LECTURE**
The Chemoinformatics Manifesto
Tropsha, A., Chapel Hill/USA

Großer Saal

Monday, November 12, 2007

**Chemoinformatics and Drug Development**

09.00 **KEYNOTE**
Foundations of Molecular Similarity Analysis
Bajorath, J., Bonn/D

09.40 **Natural Product-likeness Score and Its Application for Prioritization of Compound Libraries**

10.05 **Beyond Descriptor Vectors: QSAR Modelling using Structural Similarity**
Hinselmann, G., Tuebingen/D, Fechner, N. H., Tuebingen/D, Jahn, A., Tuebingen/D

10.30 **Coffee Break**

11.00 **Side effect profile prediction – Early addressing of big pharma’s worst nightmare**

11.25 **Is Learning Drugs the Same as Learning Non-Drugs?**
Brown, R. D., San Diego/USA, Rogers, D., San Diego/USA

11.50 **A computational protocol to Fragment-Based Drug Design at PDB scale**

12.15 **Conference photo with all participants**

12.30 **Lunch**

14.00 **FIZ CHEMIE Berlin Award with lectures of the winners**

15.00 **Award of the Gmelin-Beilstein-Denkmünze with lecture of the winner**

16.00 **CIC GENERAL MEETING**

17.00 **POSTER SESSION**
Tuesday, November 13, 2007

Computational Material Science and Nanotechnology

09.00 KEYNOTE
An approximate DFT-method to computational nanotechnology
Frauenheim, T., Bremen/D

09.40 Modeling of nanomaterials: recent applications and new tools development
Goldbeck-Wood, G., Cambridge/GB

10.05 MFD-simulation of surface coatings – an extension to solid/fluid molecular modelling models
Richter, D.S., Essen/D, Engels, C., Essen/D, Kuhn, H., Essen/D

10.30 Coffee Break

Chemical Information

11.00 KEYNOTE
An Overview of Large Chemical Structure Databases
Heller, S. R., Gaithersburg/USA

11.40 Using Chemical Structure In Open-Source Chemical Text Mining
Corbett, P. T., Cambridge/GB, Murray-Rust, P., Cambridge/GB

12.05 Breaking the Language Barrier: Chemical Nomenclature around the Globe
Sayle, R. A., Santa Fe/USA

12.30 Lunch

13.45 Poster Awards

Molecular Modeling

14.00 KEYNOTE
Black Swans and White Tablets
Oprea, T., Albuquerque/USA

14.40 Assignment of Protonation States and Geometries to Macromolecular Structures Using Unary Quadratic Optimization
Labute, P., Montreal/CDN

15.05 Coarse-Grained Molecular Models for High-Throughput and Multi-Scale Functional Investigations
Hamacher, K., Darmstadt/D

15.30 Coffee Break

16.00 KEYNOTE
Protein Structure-based Drug Design: Applications, Limitations and Future Developments
Hillisch, A., Wuppertal/D

16.40 DrugScore<sup>Fr</sup>: Profiling Protein-Ligand Interactions using Fingerprint Simplicity paired with Knowledge-Based Potential Fields
Pfeffer, P., Marburg/D, Neudert, G., Marburg/D, Klebe, G., Marburg/D

17.05 Development of new in silico methods to identify ligands for orphan GPCR
Weill, N., Strasbourg/F, Rognan, D., Strasbourg/F

18.00 Conference Dinner
LAST-MINUTE-POSTER

Please note that it is possible to submit last-minute-poster online until **November 5, 2007** at

www.gdch.de/gcc2007

EXHIBITION

The scientific programme will be accompanied by an exhibition of instruments, accessories and scientific literature. The exhibition is organized by

Frank Oellien  
Intervet Innovation GmbH  
Zur Propstei  
D-55270 Schwabenheim  
E-Mail: Frank.Oellien@intervet.com

SOCIAL PROGRAM

- **Sunday, November 11, 2007** 18.30 hrs
  - Dinner
  - The buffet is included in the participation fee. Beverages have to be paid separately.

- **Monday, November 12, 2007** 18.00 hrs
  - Postersession
  - Beer and pretzel are included in the participation fee.

- **Tuesday, November 13, 2007** 18.00 hrs
  - Dinner
  - The buffet is included in the participation fee. Beverages have to be paid separately.

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.

LOCATION

The meeting will take place at the  
Hotel Der Achtermann  
Rosentorstraße 20  
D-38640 Goslar

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 Hannover main station, „Regional Express“ train directly to Goslar main station.

By plane:  
Flight to Hannover airport (www.hannover-airport.de), train to Hannover 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.
REGISTRATION

Please register online via internet not later than **October 19, 2007**

[www.gdch.de/gcc2007](http://www.gdch.de/gcc2007)

All tickets and congress papers (incl. book of abstracts) will be given to 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 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.**
Dresdner Bank AG Frankfurt am Main
Routing Number (BLZ) 500 800 00
Account No. (Kto.Nr.) 4 900 200 00
Code: 5316 / CIC-Workshop 2007

**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.**
Dresdner Bank AG Frankfurt am Main
IBAN DE85 5008 0000 0490 0200 00
SWIFT-BIC DRES DE FF
Code: 5316 / CIC-Workshop 2007

REGISTRATION FEES

<table>
<thead>
<tr>
<th>Category</th>
<th>Fee</th>
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<tbody>
<tr>
<td>GDCh-member and member of FECS-member societies</td>
<td>€ 240,-</td>
</tr>
<tr>
<td>Member, unemployed and retired</td>
<td>€ 140,-</td>
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<tr>
<td>Non-member</td>
<td>€ 320,-</td>
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<tr>
<td>Student – GDCh-member (valid student card required)</td>
<td>€ 90,-</td>
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<tr>
<td>Student – Non-member (valid student card required)</td>
<td>€ 100,-</td>
</tr>
<tr>
<td>Gold member (as of 50 years of age GDCh membership)</td>
<td>free of charge</td>
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If fees are paid in advance, but **after October 26, 2007**, we kindly ask participants to show proof of payment when claiming their tickets and congress papers at the congress Office. Credit cards (Mastercard, VISA) will be accepted.

CANCELLATION

Written cancellations received on or **before October 22, 2007** 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 organization. In this case please send a note to GDCh, congress department.

If the conference is cancelled for whatever reason, fees paid will be refunded. Further recourse is excluded.
HOTEL ACCOMMODATION

The hotel provides accommodation for all participants in single (€ 62,- per room/night) or double bed rooms (€ 106,- per room/night).

Arrangements should be made directly with the hotel under the keyword “CIC 2007” not later than October 19, 2007.

Hotel Der Achtermann
Rosentorstraße 20
D-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.

INFORMATION CONCERNING THE SCIENTIFIC PROGRAMME

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Fachbereich Angewandte Naturwissenschaften
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INFORMATION BEFORE AND AFTER THE MEETING

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Website: www.gdch.de

Executive Director: Professor Dr. Wolfram Koch
Registernummer beim Vereinsregister: VR 4453
Registergericht Frankfurt am Main

INFORMATION DURING THE MEETING

The conference office will be located in front of the Großer Saal.
Opening hours:

Sunday, September 11, 2007 13.00 – 18.30 hrs
Monday, September 12, 2007 08.00 – 16.00 hrs
Tuesday, September 13, 2007 08.00 – 13.00 hrs
Phone: +49 5231 7000-909

DEADLINES

October 19, 2007 Room reservation
October 19, 2007 Personal registration
October 22, 2007 Cancellation of participation
November 5, 2007 Submission of last-minute-poster
No guarantee to be published in the book of abstracts