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GESELLSCHAFT DEUTSCHER CHEMIKER

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GDCh-Fachgruppe
Chemie – Information – Computer

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3. GERMAN CONFERENCE ON CHEMOINFORMATICS

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November 11 – 13, 2007
Goslar, Germany

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21. CIC-Workshop 2007

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GDCh
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DEUTSCHER CHEMIKER

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Veranstaltungen
GDCh-Veranstaltungen – Ihr P
Herzlich Willkommen

Hier finden Sie aktuellen Informationen zu allen Tagungen und weiteren Veranstaltungen.
Wir, der Bereich Veranstaltungen der GDCh realisieren für unsere 70 Fortbildungskurse und über 20 Tagungen jährlich.
Nutzen auch Sie unser Know-How für Ihre Veranstaltung! Weitere Infos freuen uns, Sie bei unseren Veranstaltungen begrüßen zu dürfen.
Ihr GDCh-Veranstaltungs-Team



GDCh-Fachgruppe
Chemie – Information –
Computer

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.

FORTBILDUNG 2007

996/07 **Wirtschaftsinformation für die Chemieindustrie**
Fachinformation aus Internet und professionellen Datenquellen
28. – 29. November 2007 · Köln
Kursleiter: Ulrich Kämper

FORTBILDUNG 2008

- 932/08 **REACH – Grundlagen und Bedeutung für Hersteller und Anwender von Chemikalien und Produkten**
28. Februar 2008 · Frankfurt am Main
Kursleiter: MinR a.D. Prof. Dr. Ulrich Schlottmann
- 885/08 **Kundengewinnung und Kundenbindung für leistungsstarke Anbieter im Bereich der Chemischen Industrie**
Fortbildungskurs in Anbindung an die analytica 2008
3. April 2008 · München
Kursleiter: Dr. Andreas Lotz
- 997/08 **Kritischer Umgang mit Informationsquellen in der Chemie**
SciFinder, CrossFire, Web of Science et al. – ihre Stärken und Schwächen
(in Zusammenarbeit mit dem FIZ-CHEMIE Berlin unter Nutzung der Lehrinhalte CHEMGAROO)
13. – 14. November 2008 · Frankfurt am Main
Kursleiter: Dr. Engelbert Zaß

Informationen zu diesen und weiteren Fortbildungskursen für 2007 und 2008 finden Sie im Internet unter **www.gdch.de/fortbildung**.

Anmeldung/Information:

E-Mail: fb@gdch.de
Tel.: +49 69 7917-291/-364
Fax: +49 69 7917-485
Internet: www.gdch.de/fortbildung

Gesellschaft Deutscher Chemiker e.V.
Fortbildung
Postfach 90 04 40
D-60444 Frankfurt am Main

PROGRAMME

▶ SCIENTIFIC COMMITTEE

A. Zielesny	Recklinghausen, Committee-Chairman
R. Herges	Kiel, Committee Co-Chairman
F. Oellien	Schwabenheim, Committee Co-Chairman
J. Bajorath	Bonn
G. Fels	Paderborn
J. Gasteiger	Erlangen
S. Heller	Gaithersburg/USA
F.-P. Hoever	Leverkusen
P. Murray-Rust	Cambridge/UK
M. Rarey	Hamburg
G. Schneider	Frankfurt am Main
C. Steinbeck	Achern, CIC-Chairman
H. Thiele	Bremen
A. Varnek	Strasbourg/F

▶ SPONSORING

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).

PROGRAMME

Sunday, November 11, 2007

Großer Saal

14.00 **Free Software Session**

A number of open source projects in chemoinformatics will be offered.

Barbarasaal

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.

to be announced

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

Großer Saal

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

18.30 **Dinner**

Großer Saal

20.00 **EVENING LECTURE**

The Chemoinformatics Manifesto

Tropsha, A., Chapel Hill/USA

PROGRAMME

Monday, November 12, 2007

Großer Saal

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**

Ertl, P., Basel/CH, Roggo, S., Basel/CH, Schuffenhauer, A., Basel/CH

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**

Scheiber, J., Cambridge/USA, Jenkins, J. L., Cambridge/USA, Bender, A., Cambridge/USA, Whitebread, S., Cambridge/USA, Hamon, J., Basel/CH, Urban, L., Cambridge/USA, Azzaoui, K., Basel/CH, Glick, M., Cambridge/USA, Davies, J. W., Cambridge/USA

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**

Moriaud, F., Palaiseau/F, Henry, T., Palaiseau/F, Adcock, S. A., Palaiseau/F, Vorotynev, A. M., Palaiseau/F, Martin, L., Palaiseau/F, Doppelt, O., Palaiseau/F, De Brevern, A. G., Paris/F, Delfaud, F., Palaiseau/F

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-Denk Münze with lecture of the winner**

16.00 **CIC GENERAL MEETING**

Großer Saal

17.00 **POSTER SESSION**

Foyer

PROGRAMME

Tuesday, November 13, 2007

Großer Saal

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**

Großer Saal

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**

Großer Saal

PROGRAMME

Tuesday, November 13, 2007

Großer Saal

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^{FP}: 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/E, Rognan, D., Strasbourg/F
- 18.00 **Conference Dinner**

GENERAL INFORMATION

▶ 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.

GENERAL INFORMATION

▶ 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.

GENERAL INFORMATION

REGISTRATION

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

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

GENERAL INFORMATION

REGISTRATION FEES

GDCh-member and member of FECS-member societies	€ 240,-
Member, unemployed and retired	€ 140,-
Non-member	€ 320,-
Student – GDCh-member (valid student card required)	€ 90,-
Student – Non-member (valid student card required)	€ 100,-
Gold member (as of 50 years of age GDCh membership)	free of charge

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
August-Schmidt-Ring 10
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INFORMATION BEFORE AND AFTER THE MEETING

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(German Chemical Society)
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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

MAP OF GOSLAR

