PROGRAMME

GDCh

Gesellschaft Deutscher Chemiker

CIC

Fachgruppe
Chemie – Information – Computer

GCC 2015

11th German Conference on Chemoinformatics

November 08 – 10, 2015
FULDA · Germany

www.gdch.de/gcc2015

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

11th German Conference on Chemoinformatics
November 08 – 10, 2015 · FULDA

The conference will reflect and highlight the new role of chem-informatics in the modern information world. It will span a wide range of subjects related to the use of computers in chemistry, pharmacy, materials science and biology; from chem- and bioinformatics to explicit modelling and from industrial applications to fundamental academic research.

The scientific programme will include plenary and contributed lectures, posters and software presentations. The language of the conference is English.

On Sunday, November 08, Pre-conference workshops will be given by KNIME and OpenEye. Afterwards, the conference starts with three keynote talks in the Sunday Highlights session.

On Monday, November 09, „Research Telegrams“ gives PhD students the opportunity to present their current work in form of short talks. Furthermore, every young researcher is invited for open discussions and/or exchange with others in the Moonlight-Session.

SCIENTIFIC ADVISORY BOARD

Frank Böckler	Tübingen/DE
Tim Clark	Erlangen/DE
Thomas Engel	München/DE (CIC Division Chair)
John Essex	Southampton/UK
Uli Fechner	Frankfurt/DE
Guido Kirsten	Köln/DE
Oliver Koch	Dortmund/DE (Conference Co-Chair)
Jan Kriegl	Biberach/DE
Frank Oellien	Schwabenheim/DE
Matthias Rarey	Hamburg/DE
Gisbert Schneider	Zürich/CH
Wolfgang Sippl	Halle/DE
Alexander Tropsha	Chapel Hill/USA
Wendy Warr	Holmes Chapel/UK
Gerhard Wolber	Berlin/DE (Conference Chair)

Sunday, November 08, 2015

11:00 **Registration**

12:00–13:30 **SOFTWARE SESSION** (Pre-Conf. Workshops)

Salon Bonifatius

Knime: "Getting your chemistry right with KNIME"

Salon Köln

OpenEye: "OpenEye toolkits and iPython notebooks"
A do-it-yourself workshop around chemo-informatic problems

13:45–14:00 **OPENING REMARKS** Festsaal
G. Wolber, Berlin/DE

SUNDAY HIGHLIGHTS — Festsaal

Session Chair: G. Kirsten, Köln/DE

14:00–14:40 KEYNOTE
3D-e-Chem: Structure-Based Navigation of Medicinal Chemistry Space
C. de Graaf, Amsterdam/NL

14:40–15:20 KEYNOTE
Why I do not like Monte Carlo
A. Torda, Hamburg/DE

15:20–16:00 KEYNOTE
Predictive Modelling for Biologics – Chemoinformatics meets Bioinformatics
S. Güssregen, Frankfurt (Main)/DE

16:00–16:30 COFFEE BREAK AND EXHIBITION

Sunday, November 08, 2015

Festsaal

CHEMOINFORMATICS AND DRUG DISCOVERY – SESSION I

16:30–17:10 KEYNOTE
Target deconvolution of phenotypic screens using formal concept analysis
N. Richmond, Middlesex/GB

17:10–17:35 **Toxicity Prediction using Deep Learning**
G. Klambauer, Linz/AT, T. Unterthiner, Linz/AT, A. Mayr, Linz/AT, S. Hochreiter, Linz/AT

17:35–18:00 **Discovering Unprecedented Catalytic Reactions by Chemical Machine Reasoning**
M. Segler, Münster/DE, M. Waller, Münster/DE

18:30 **DINNER** Apollo Saal/Roter Saal

EVENING LECTURE — Festsaal

Session Chair: G. Wolber, Berlin/DE

20:00 **Fight against growing crime: Forensic Science Research**
S. Pleik, Wiesbaden/DE

Monday, November 09, 2015

Festsaal

PROTEIN MODELLING AND SIMULATION

09:00–09:40 KEYNOTE
Effect of surfaces in modulating protein folding and aggregation mechanisms
J.-E. Shea, Santa Barbara/US, Z. Levine, Santa Barbara/US, R. Mullen, Santa Barbara/US

09:40–10:05 **Mesoscopic Simulation of Biomolecular Systems**
A. Zielesny, Recklinghausen/DE, K. van den Broek, Munich/DE, M. Epple, Essen/DE, H. Kuhn, Essen/DE, A. Truszkowski, Recklinghausen/DE

10:05–10:30 **Automated mesoscale approach to biomolecular affinity calculations**
J. Fraaije, Leiden/NL, R. Serral Gracia, Leiden/NL

10:30–11:00 COFFEE BREAK AND EXHIBITION

HOT TOPICS AND NEW DEVELOPMENTS

11:00–11:40 KEYNOTE
Computational solvation modeling: from simple liquids to biomolecules
S. Kast, Dortmund/DE

11:40–12:05 **An integrated chemical, biological and pathological in silico approach towards identifying potent drug combinations**
K. C. Bulusu, Cambridge/GB, A. Bender, Cambridge/GB

12:05–12:30 **Statistical Modeling in Material Sciences**
H. Senderowitz, Ramat-Gan/IL, A. Yosipof, Ramat Gan/IL, O. Nahum, Ramat Gan/IL

12:45–13:00 **Photo session**

13:00 LUNCH — Apollo Saal/Roter Saal

Monday, November 09, 2015

Festsaal

RESEARCH TELEGRAMS

14:15–14:30 **Development of Methods for the Efficient Comparison of Protein Binding Sites**
T. Krotzky, Marburg/DE

14:30–14:45 **Fragment-Based Design of Viral Protease Inhibitors by Virtual Screening and Chemical Space Sampling**
R. Schulz, Berlin/DE, G. Wolber, Berlin/DE

14:45–15:00 **Identification and Prepocessing of Alternative Protein Binding Site Conformations for Modeling Protein Flexibility**
S. Bietz, Hamburg/DE, M. Rarey, Hamburg/DE

15:15–15:30 **ChemPLP^{XB}: Implementation of QM-based terms for the recognition of halogen bonding in drug design**
M. Zimmermann, Tübingen/DE, A. Lange, Tübingen/DE, M. Ruff, Tübingen/DE, J. Heidrich, Tübingen/DE, I. Onila, Tübingen/DE, T. Exner, Tübingen/DE, F. Boeckler, Tübingen/DE

15:30–15:45 **Dynamic and mechanistic models for ligand-dependent modulation of G protein coupled receptors**
M. Bermudez, Berlin/DE, G. Wolber, Berlin/DE

15:45–16:00 **Computer Design of Ionic Liquids for CO_2 Absorption**
D. Firaha, Bonn/DE, O. Hollóczki, Bonn/DE, B. Kirchner, Bonn/DE

from 16:00 COFFEE BREAK AND EXHIBITION

16:00–17:30 **POSTERSESSION I** (even No.) — Foyer

17:30–19:00 **POSTERSESSION II** (odd No.) — Foyer

19:00–20:00 **General Meeting of the GDCh division CIC** — Festsaal

20:00 **CONFERENCE DINNER** — Wappensaal/Dianasaal

22:00 **Moonlight-Session** — Salon Köln
open for young researchers

Tuesday, November 10, 2015

Festsaal

CHEMOINFORMATICS AND DRUG DISCOVERY – SESSION II

09:00–09:40 KEYNOTE
Molecular Basis for the Long Duration of Action of Tiotropium for the Muscarinic M3 Receptor – Insights from Molecular Dynamics Simulations
C.S. Tautermann, Biberach/DE

09:40–10:05 **Prioritization of less-explored protein kinases as drug targets**
A. Volkamer, Heidelberg/DE, S. Eid, Heidelberg/DE, S. Turk, Heidelberg/DE, F. Rippmann, Darmstadt/DE, S. Fulle, Heidelberg/DE

10:05–10:30 **A Three-Site Mechanism for Agonist/Antagonist Action on the Vasopressin Receptors**
N. Saleh, Erlangen/DE, G. Saladino, London/GB, F. L. Gervasio, London/GB, E. Haensele, Portsmouth/GB, L. Banting, Portsmouth/GB, D. C. Whitley, Portsmouth/GB, J. Sopkova-de Oliveira Santos, Caen Cedex/FR, R. Bureau, Caen Cedex/FR, T. Clark, Erlangen/DE

10:30 COFFEE BREAK AND EXHIBITION

AWARD SESSION

Session Chairs: T. Engel, München/DE, G. Wolber, Berlin/DE

11:00–11:20 **CIC-Award for Computational Chemistry**

11:20–11:40 MASTER THESIS AWARD 2014
Analysis of µs MD simulations of the p53 core domain
A. Sandmann, Erlangen/DE, H. Lanig, Erlangen/DE

11:40–12:00 MASTER THESIS AWARDS 2015
Theoretical approach to conformational preconfiguration of drug-like molecules in solution
P. J. Kibies, Dortmund/DE, S. M. Kast, Dortmund/DE

Tuesday, November 10, 2015

Festsaal

12:00–12:20 **Using Support Vector Regression to Develop a Quantum Chemical-based Scoring Function for the Recognition of Halogen Bonds Targeting Methionine**
M. Ruff, Tübingen/DE, F. M. Boeckler, Tübingen/DE

12:30 LUNCH

MOLECULAR MODELLING

14:00–14:40 KEYNOTE
Recent progress in exploring the role of water in protein-ligand binding
J. Essex, Southampton/UK

14:40–15:05 **Ab initio derived descriptors as a promising perspective for regioselectivity prediction of metabolic reactions**
A. R. Finkelmann, Zürich/CH, A. H. Göller, Wuppertal/DE, G. Schneider, Zürich/CH

15:05–15:30 **Integrating Chemoinformatics and Quantum Chemistry for computational electrochemistry: The search for new electrolyte materials**
M. Korth, Ulm/DE, T. Husch, Ulm/DE, C. Schütter, Ulm/DE, A. Balducci, Ulm/DE

15:30 **CLOSING REMARKS and NETWORKING APÉRO**

POSTER

Please note that it is possible to submit last minute posters online until **October 29, 2015** at

www.gdch.de/gcc2015

(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 organized by

Dr. Oliver Koch
Technische Universität Dortmund
Fakultät Chemie – Chemische Biologie
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Dr. Guido Kirsten
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SOCIAL PROGRAMME

Sunday, November 08, 2015 **18:30**

Dinner

The buffet and water are included in the registration fee. All other beverages have to be paid separately.

Monday, November 09, 2015 **16:00 – 19:00**

Postersession I and II

Beer and pretzel are included in the registration fee.

Monday, November 09, 2015 **20:00**

Conference Dinner

The buffet and water are included in the registration fee. All other beverages have to be paid separately.

LUNCH AND COFFEE BREAKS

The registration fee includes lunch and coffee breaks.

DINNER

Dinners are included in the registration fee on November 08 and November 09. Drinks except water are not included.

Booking is required for both dinners (Sunday and Monday)!

INTERNET ACCESS

WLAN-Voucher for one day is included. Additional WLAN-Vouchers can be booked on site via hotspot.

LOCATION

The meeting will take place at the

MARITIM Hotel am Schlossgarten Fulda
Pauluspromenade 2
36037 Fulda
Germany

Fulda is located at the heart of Germany and famous for its baroque old town. The conference hotel "MARITIM Hotel am Schlossgarten" is within 10 minutes walking distance from Fulda main station.

TRAVEL INFORMATION

The Maritim Hotel am Schlossgarten Fulda is located in a park area right in the city's historic downtown area.

The central railway station with excellent ICE (high-speed train) connection can be reached in just a few minutes walking distance.

Distance to central railway station: 1 km
Distance to motorway: 4 km
Distance to Frankfurt airport: 100 km
Distance to downtown: 0.5 km

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GENERAL INFORMATION

HOTEL ACCOMMODATION

The MARITIM Hotel provides accommodation for participants in single (from € 126 to € 157 per room/night).

Alternatively accommodations are available in the IBIS Hotel in single bed room € 72 per room/night or in the Holiday Inn Fulda in single bed room € 88 per room/night.

All rates are including breakfast.

For more information see our conference webpage

www.gdch.de/gcc2015

Arrangements should be made directly with the hotel of choice under the **keyword "GCC 2015"**.

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

REGISTRATION

Please register online via internet:

www.gdch.de/gcc2015

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, direct debit or bank transfer (only with German bank account) is possible. The invoice will be sent to you automatically.

Please pay the fees to the following account:

GESELLSCHAFT DEUTSCHER CHEMIKER e.V.
Commerzbank AG Frankfurt am Main
IBAN: DE85 5008 0000 0490 0200 00
SWIFT BIC: DRESDEFFXXX
Code 520031 / GCC 2015

REGISTRATION FEES*

	until July 15, 2015	from July 16, 2015
Student – GDCh-Member and Member of EuCheMS-member societies (valid student card required)	€ 200,-	€ 220,-
Student – Non-Member (valid student card required)	€ 250,-	€ 275,-
GDCh-Member and Member of EuCheMS-member societies	€ 450,-	€ 495,-
Member, unemployed or retired	€ 200,-	€ 220,-
Non-Member	€ 500,-	€ 550,-
GDCh Gold member (with over 50 years of GDCh Membership)	free of charge	free of charge

*) The registration fees are not liable to value added tax (tax exemption additional § 4 Nr. 22a UStG.)

If fees are paid in advance, but after **October 24, 2015**, 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, AMEX).**

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

CANCELLATION

Please note: Registration is binding upon receipt by the GDCh. Every participant must register separately. In case of cancellation 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.

INFORMATION BEFORE AND AFTER THE CONFERENCE

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(German Chemical Society)
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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 the Conference Room.

Opening hours:

Sunday, November 08, 2015	11.00 – 18.00 hrs
Monday, November 09, 2015	08.00 – 16.00 hrs
Tuesday, November 10, 2015	08.00 – 12.00 hrs

INFORMATION ABOUT THE SCIENTIFIC PROGRAMME

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As of September 22, 2015