



GESELLSCHAFT DEUTSCHER CHEMIKER



Fachgruppe  
Chemie – Information – Computer

# **GCC 2016**

**12<sup>th</sup> German  
Conference on Chemoinformatics**

**November 6 – 8, 2016  
Fulda · Germany**

[www.gdch.de/gcc2016](http://www.gdch.de/gcc2016)



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

**12<sup>th</sup> German Conference on Chemoinformatics  
November 6 – 8, 2016 · Fulda**

The conference will reflect and highlight the new role of cheminformatics 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.

On Sunday, November 06, software workshops will be given by KNIME and Schrödinger. Afterwards, the conference starts with three keynote talks in the Sunday Highlights session.

On Monday, November 07, „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.

The language of the conference is English.

### ▶ SCIENTIFIC ADVISORY BOARD

<b>Frank Böckler</b>	Tübingen/DE
<b>Tim Clark</b>	Erlangen/DE
<b>Thomas Engel</b>	Munich/DE (CIC Division and Conference Chair)
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<b>Wendy Warr</b>	Holmes Chapel/GB
<b>Gerhard Wolber</b>	Berlin/DE

## Sunday, November 6, 2016

11:00 Registration

## 12:00 Software Workshops

**KNIME:**  
The KNIME Analytics Platform –  
Bringing Science to your Data

Salon Ulm

**Schrödinger:**  
More than a New Sight – An Introduction to  
Maestro 11

Salon Köln

## 13:45 OPENING REMARKS

T. Engel, Munich/DE

Festsaal

## Sunday Highlights

*Session Chair: T. Clark, Erlangen/DE*

## 14:00 KEYNOTE

**Investigating Allosteric Regulation Through  
Simulations and Modelling**

F. L. Gervasio, London/GB

## 14:40 KEYNOTE

**De novo design: from drug discovery to the design of  
novel chemicals from biomasses**

V. Gillet, Sheffield/GB

## 15:20 KEYNOTE

**Using small molecule biological profiling data in lead  
discovery**

A. M. Wassermann, Boston/US

## 16:00 COFFEE BREAK AND EXHIBITION

## Sunday, November 6, 2016

Festsaal

## Chemoinformatics and Drug Discovery I

*Session Chair: G. Wolber, Berlin/DE*

## 16:30 KEYNOTE

**The Cool in Drug Discovery**

J. Boström, Göteborg/SE

## 17:10 The analysis of protein and ligand building blocks with impact on rational molecular design

O. Koch, Dortmund/DE

## 17:35 Kinome wide off-target prediction by mining structural and profiling data

S. Fulle, Heidelberg/DE, B. Merget, A. Volkamer, S. Turk,  
S. Eid, Heidelberg/DE, F. Rippmann, Darmstadt/DE

## 19:00 SOCIAL EVENT &amp; DINNER

Hohmanns Brauhaus Fulda

(booking required, limited to 100 places)

Monday, November 7, 2016

Festsaal

## Software Updates I

Session Chair: N.N.

08:20 **Growing ligands to where only water has gone before – Can solvent mapping drive optimization of a fragment based campaign?**

G. Stahl, Cologne/DE, G. L. Warren, Santa Fe/US

08:40 **3D-RISM – effects of improved electrostatic models**  
M. D. Mackey, Litlington/GB, S. Tomasio, Litlington/GB

## Protein Modelling and Molecular Modelling

Session Chair: M. Rarey, Hamburg/DE

## 09:00 KEYNOTE

**New Developments in Delivering Public Access to Data From the National Center for Computational Toxicology at the EPA**

T. Williams, Durham/US

09:40 **3D-e-Chem: An integrated cheminformatics platform. Case studies on GPCR bioactivity data.**

M. Vass, Amsterdam/NL, R. McGuire, Oss/NL,  
S. Verhoeven, A. J. Kooistra, I. J. P. de Esch, R. Leurs, C. de Graaf, Amsterdam/NL

10:05 **EMPIRE: New Dimensions for Quantum-Chemical Molecular Modelling**

M. Hennemann, Erlangen/DE, J. T. Margraf, T. Clark, Erlangen/DE

## 10:30 COFFEE BREAK &amp; EXHIBITION

## Hot Topics and New Developments

Session Chair: S. Güssregen, Frankfurt (Main)/DE

## 11:00 KEYNOTE

**Structural Biology in vitro and in situ with cryo-electron microscopy**

F. Förster, Utrecht/NL, S. Pfeffer, Martinsried/DE

11:40 **Practices in Structure Based Drug Design: A Huge Waste of Money?**

P. Schmidtke, Paris/FR, D. Alvarez-Garcia, M. Oberlin, Paris/FR

12:05 **Will the correct drugs please stand up?**

C. Southan, Edinburgh/GB, E. Faccenda, S. J. Harding, J. L. Sharman, A. J. Pawson, J. A. Davies, Edinburgh/GB

12:45 **Conference photo call**

13:00 **LUNCH**

Apollo Saal &amp; Roter Saal

Monday, November 7, 2016

Festsaal

## Research Telegrams

14:15 **An intra-domain allosteric network modulates the calcium affinity of the C-type lectin receptor Langerin**  
S. Aleksic, Berlin/DE, J. Hanske, C. Rademacher, Potsdam/DE, B. G. Keller, Berlin/DE

14:30 **Binding Site Shape Clustering and Shape Complementarity to Increase Selectivity of PTP1B Inhibitors**  
A. Nass, Berlin/DE, G. Wolber, Berlin/DE

14:45 **Hydrogen Bond Interaction Geometries in Proteins: A Large-Scale Statistical Study**  
E. Nittinger, Hamburg/DE, T. Inhester, Hamburg/DE,  
G. Lange, R. Klein, Frankfurt/DE, M. Rarey, Hamburg/DE

15:00 **ProcAuxInfo – Extending the RInChI to store reaction data**  
P.-M. Jacob, Cambridge/GB, T. Lan, A. Lapkin, Cambridge/GB

15:15 **Scalable Local Coupled Cluster Methods**  
M. Schwilk, Stuttgart/DE, Q. Ma, C. Köppl, H.-J. Werner, Stuttgart/DE

15:30 **Analysis of antiviral chemical space based on ChEMBL data**  
A. A. Orlov, Moscow/RU, A. A. Nikitina, D. I. Osolodkin, V. A. Palyulin, N. S. Zefirov, Moscow/RU

15:45 **Discovery of a novel relationship between two proteins by an advanced privileged scaffold approach**  
L. Humbeck, Dortmund/DE, J. Pretzel, O. Koch, Dortmund/DE

16:00 **Ligand-Sensing Cores in Protein Space**  
T. Brinkjost, Dortmund/DE, C. Ehrh, P. Mutzel, O. Koch, Dortmund/DE

## 16:15 COFFEE BREAK &amp; EXHIBITION

16:15 **POSTER SESSION** (uneven No.) Foyer

17:30 **POSTER SESSION** (odd No.) (17:30 – 18:45) Foyer

19:00 **CONFERENCE DINNER**  
 Diana Keller & Wappensaal

Salon Ulm

21:00 **MOONLIGHT SESSION**  
 Open room for young scientists

Tuesday, November 8, 2016

Festsaal

**Software Updates II***Session Chair: G. Kirsten, Cologne/DE*08:20 **Free Energy Calculations Applied to Protein Homology Models**D. Cappel, Mannheim/DE08:40 **Blind challenge on the prediction of alkane-water distribution: Calculations beating experimental accuracy**A. Klamt, Leverkusen/DE, J. Reinisch, F. Eckert, K. Wichmann, Leverkusen/DE**Cheminformatics and Big Data***Session Chair: W. Warr, Holmes Chapel/GB*09:00 **KEYNOTE****Enabling decisions in Drug Discovery by leveraging "Big" Biomedical Data**J. Scheiber, Munich/DE09:40 **Recommender Systems for Chemistry Papers**P. T. Corbett, Cambridge/GB, C. R. Batchelor, J. R. White, N. J. Bailey, J. Boyle, Cambridge/GB10:05 **The Synthetically Accessible Virtual Inventory (SAVI) System**W. D. Ihlenfeldt, Königstein/DE, Y. Pevzner, M. C. Nicklaus, Frederick/US10:30 **COFFEE BREAK & EXHIBITION****Molecular Modelling***Session Chair: S. Kast, Dortmund/DE*11:00 **KEYNOTE****Thermodynamics and kinetics of ligand-protein binding through molecular simulations**A. Cavalli, Bologna/IT11:40 **Method for the automated compilation of datasets of accurate protein-bound ligand structures**J. Kirchmair, Hamburg/DE, N. O. Friedrich, A. Meyder, K. Sommer, M. Rarey, Hamburg/DE12:05 **A stochastic approach to explain how proteins protect against oxidative damage**H. Thomas, Erlangen/DE, T. Clark, M. Hennemann, I. Maqboul, Erlangen/DE12:30 **LUNCH**

Apollo Saal &amp; Roter Saal

Tuesday, November 8, 2016

Festsaal

**Award Session***Session Chair: T. Engel, Munich/DE, G. Kirsten, Cologne/DE*13:45 **CIC-Award for Computational Chemistry**14:00 **Master Thesis Award 2016****Tailor-Made Scoring Functions: Protein Ligand Interaction Fingerprints based on Proteinatom Scoring Function Contributions**J. Jasper, Dortmund/DE14:20 **PhD Thesis Award 2016****From Raw PDB Files to Protonated Binding Site Ensembles: Adaptive Solutions for the Case-Specific Preprocessing of Protein Structures**S. Bietz, Hamburg/DE14:45 **COFFEE BREAK & EXHIBITION****Chemoinformatics and Drug Discovery Session II***Session Chairs: A. Tropsha, Chapel Hill/US*15:00 **From Low Affinity, High Micromolar Fragments to the First Selective Nanomolar Inhibitors of Human Paics Enzyme Without any X-Ray Structures**C. Mpamhanga, Stevenage/GB, P. Coombs, S. Osborne, J. Large, E. Smiljanic-Hurley, D. Harding, N.-I. Zaynab, M. Newman, C. Southern, J. Brownlees, K. Ansell, D. Whalley, H. Saunders, T. Debra, Stevenage/GB, N. Visser, D. Peeper, Amsterdam/NL15:25 **Reaction prediction tools for both idea generation in new synthesis route planning and for de novo molecule design**V. Eigner-Pitto, Munich/DE, F. F. Huerta, Södertälje/SE, M.G. Hutchings, H. Saller, P. Loew, Munich/DE15:50 **KEYNOTE****The "NOMAD (Novel Materials Discovery) Center of Excellence": Challenges and Solutions to Build a Code-independent Data Base for Computational Materials Science and its implication in Computational Chemistry**F. Illas, Barcelona/ES16:30 **CLOSING REMARKS and NETWORKING APERO**T. Engel, Munich/DE

**POSTER**

Please note that it is possible to submit last minute posters online until **October 6, 2016** at

[www.gdch.de/gcc2016](http://www.gdch.de/gcc2016)

(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. Guido Kirsten  
 E-Mail: [gcc-exhibition@dr-kirsten.de](mailto:gcc-exhibition@dr-kirsten.de)



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**SOCIAL PROGRAMME**

**Sunday, November 6, 2016** **19:00**

**Beer tasting and dinner at Hohmanns Brauhaus Fulda**

Hohmanns Brauhaus Fulda  
 Florengasse 3-5, 36037 Fulda  
 Germany  
[www.hohmanns-brauhaus.de](http://www.hohmanns-brauhaus.de)  
 (free of charge, water included, booking required)

**Monday, November 7, 2016** **16:15 – 18:45**

**Poster Session, Coffee Break & Exhibition**

**Monday, November 7, 2016** **19:00**

**Conference Dinner**

MARITIM Hotel am Schlossgarten Fulda  
 Diana Keller & Wappensaal  
 Pauluspromenade 2  
 36037 Fulda  
 Germany  
 (free of charge, water included, booking required)



**LUNCH AND COFFEE BREAKS**

The registration fee includes lunch and coffee breaks.

**DINNER**

Dinners are included in the registration fee on November 6 and November 7. Drinks except water are not included.

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

**INTERNET ACCESS**

WLAN is included for Maritim hotel guests. WLAN-Voucher for non-hotel guests can be booked on site at the reception desk.

### 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.



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### 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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### HOTEL ACCOMMODATION

The MARITIM Hotel provides accommodation in single (from € 130 to € 162 per room/night).

Alternatively accommodations are available in the IBIS Hotel in Single bed room from € 78 per room/night or in the Holiday Inn Fulda in Single bed room from € 95 per room/night.

All rates are including breakfast.

For more information see our conference webpage:

[www.gdch.de/gcc2016](http://www.gdch.de/gcc2016)

Arrangements should be made directly with the hotel of choice under the **keyword "GCC 2016"**.

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

### REGISTRATION

Please register online via internet:

[www.gdch.de/gcc2016](http://www.gdch.de/gcc2016)

**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 520050 / GCC 2016**



## REGISTRATION FEES\*

Student – GDCh-Member and Member of EuCheMS-member societies (valid student card required)	€ 220,-
Student – Non-Member (valid student card required)	€ 275,-
GDCh-Member and Member of EuCheMS-member societies	€ 495,-
Member, unemployed or retired	€ 220,-
Non-Member	€ 550,-
GDCh 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.)

If fees are paid in advance, but after **October 23, 2016**, 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

Gesellschaft Deutscher Chemiker e.V.  
(German Chemical Society)  
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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 the Conference Room.

Opening hours:

Sunday, November 6, 2016	11.00 – 18.00 hrs
Monday, November 7, 2016	08.00 – 16.00 hrs
Tuesday, November 8, 2016	08.00 – 12.00 hrs

## INFORMATION ABOUT

## THE SCIENTIFIC PROGRAMME

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