

► CIC IN SHORT

Computers in Chemistry (CIC) is a division of the German Chemical Society (Gesellschaft Deutscher Chemiker e.V.) that covers all aspects of computer-based generation, processing and documentation of information and knowledge in chemistry.

Founded in 1982, CIC brings together scientists from various disciplines to foster and propel development and applications in this field, with particular emphasis on

- ✿ the annual „German Conference on Cheminformatics“ (formerly CIC workshop)
- ✿ promotion of cheminformatics, computational chemistry and chemical information as part of the curriculum at universities and higher teaching institutions
- ✿ support of working groups on particular aspects of interest to CIC
- ✿ promoting cooperation and knowledge exchange between universities and industry
- ✿ supporting the open-source idea for the development of chemistry software in the academic environment
- ✿ fostering the relationship between international institutions working in this field, in particular to EuChemS and ACS
- ✿ usage of modern communication platforms like social networks

<https://www.gdch.de/cic>
https://twitter.com/GDCh_CIC
 #GCC2022 (Twitter hashtag)

► SPONSORS

All sponsors may be found on the conference website:

<https://www.gdch.de/gcc2022>

► ACCOMMODATION

Garmisch-Partenkirchen with the conference hotel “Dorint Sporthotel” and the Zugspitze is located south of Munich in the German Alps and can be easily reached by train from Munich. Arrangements should be made directly with the conference hotel under the keyword “GCC2022” no later than February 02, 2022. The attendees will be held accountable for non-occupancy of reserved rooms.

Lower-priced accommodations (e.g. guesthouses and apartments) are available within few minutes walking distance of the conference venue.

► INFORMATION ABOUT THE SCIENTIFIC PROGRAMME

Prof. Dr. Stefan Kast
 Fakultät für Chemie und Chemische Biologie
 Technische Universität Dortmund
 Otto-Hahn-Str. 4a
 44227 Dortmund
 Germany
 Phone: +49 231 755-3906
 E-mail: stefan.kast@tu-dortmund.de

► SOFTWARE WORKSHOPS AND EXHIBITION

The conference programme contains a slot for pre-conference software workshops. Our sponsors will introduce the latest software developments to the participants. If you are interested in offering workshops, sponsoring or exhibiting please contact Dr. Stefan Güssregen at gcc-exhibition@chemoinformatics.info.

► INFORMATION ABOUT THE ORGANISATION

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

Varrentrappstr. 40-42
 60486 Frankfurt am Main, Germany

Phone: +49 69 7917-358
 E-mail: tg@gdch.de
 Homepage: <https://www.gdch.de/tagungen>

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

The photo of the conference hotel is copyrighted by Dorint Sporthotel.
 Date: 01.09.2021



GESELLSCHAFT DEUTSCHER CHEMIKER



Division
 Computers in Chemistry

GCC 2022 / EuroSAMPL

17th German Conference on
 Cheminformatics and
 EuroSAMPL Satellite Workshop

May 08 – 12, 2022
 Garmisch-Partenkirchen
 Germany

<https://www.gdch.de/gcc2022>

Highlights 2022

40th anniversary of the foundation
 of the CIC Division
 2nd EuroSAMPL Workshop



INVITATION

The division Computers in Chemistry (CIC) of the German Chemical Society (Gesellschaft Deutscher Chemiker e.V.) cordially invites you to participate in the

**17th German Conference on Cheminformatics
and EuroSAMPL Satellite Workshop
May 08 – 12, 2022 in Garmisch-Partenkirchen, Germany**

► VENUE

"Dorint Sporthotel" Mittenwalder Straße 59,
82467 Garmisch-Partenkirchen, Germany
<https://hotel-garmisch-partenkirchen.dorint.com>

► AIM OF THE CONFERENCE

The **GCC (May 08-10)** reflects and highlights the important role of cheminformatics, which connects the modern information and data-driven world with computational modelling of molecular systems. It spans a wide range of subjects related to the use of computers in chemistry, pharmacy, materials science and biology; from informatics and data science to atomistic modelling, and from fundamental academic research to industrial applications. The scientific programme will include plenary and contributed lectures, posters and software presentations.

The **EuroSAMPL satellite workshop (May 11-12, 2022)** will encompass invited lectures and contributions from participants during the recent SAMPL challenge on predicting host-guest binding and small molecule physicochemical properties, covering also aspects of industry-academia data exchange.

The language of the conferences is English.

► SOCIAL EVENTS

- 🌸 **Monday 09: 40th anniversary talk by Wendy Warr**
- 🌸 **Tuesday 10: Conference day at ZUGSPITZE, Germany's highest mountaintop**
- 🌸 **Wednesday 11: Morning is reserved for individual excursions.**

► CONFIRMED INVITED SPEAKERS

Bernd Beck	Boehringer-Ingelheim/DE
Natasja Brooijmans	Scorpion Therapeutics/US
Lee Cronin	University of Glasgow/UK
Andreas Göller	Bayer/DE
Anna Kohlmann	Black Diamond Therapeutics/US
Jens Meiler	Universität Leipzig/DE
David Mobley	UC Irvine/US
Sereina Riniker	ETH Zürich/CH
Adrian Roitberg	University of Florida/US
Tamar Schlick	New York University/US
Jana Selent	University Pompeu Fabra/ES
Wendy Warr	Holmes Chapel/UK

The current list of speakers is available at:

<https://www.gdch.de/gcc2022>

INVITATION

► SCIENTIFIC COMMITTEE

Karl-Heinz Baringhaus	Frankfurt/DE
Frank Böckler	Tübingen/DE
Evan Bolton	Washington/US
Mirko Buchholz	Halle/DE
Tim Clark	Erlangen/DE
Stefan Güssregen	Frankfurt/DE (Conference Co-Chair)
Wolf-D. Ihlenfeldt	Königstein/DE
Stefan M. Kast	Dortmund/DE (Conference Chair)
Oliver Koch	Münster/DE
Christian Kramer	Basel/CH
Greg Landrum	Basel/CH
David Mobley	Irvine/US
Frank Oellien	Ludwigshafen/DE
Matthias Rarey	Hamburg/DE
Sereina Riniker	Zürich/CH
Josef Scheiber	Munich/DE
Nadine Schneider	Basel/CH
Alexander Tropsha	Chapel Hill/US
Andrea Volkamer	Berlin/DE
Wendy Warr	Holmes Chapel/UK
Gerhard Wolber	Berlin/DE

► GCC TOPICS

- 🌸 **Cheminformatics and Drug Discovery**
- 🌸 **Big Data and Deep Learning**
- 🌸 **Chemical Information and Databases**
- 🌸 **Protein Structure and Modelling**
- 🌸 **Molecular Modelling, Simulation and Design**
- 🌸 **Property Prediction**

► CONTRIBUTION TYPES (GCC)

We offer three different formats for scientific contributions: talks (20 min.), research telegrams (12 min.) and posters. Young academics (Ph.D. students only) are encouraged to select the format of research telegrams as an opportunity to present the highlights of their research to a wider audience. Ph.D. student submissions as full talks will compete against all contributions in this category, cannot be moved to the format of research telegrams if declined, and are not eligible for the Lecture Award.

Please submit an abstract of your contribution using our online submission system available at:

<https://www.gdch.de/gcc2022>

Sample abstracts can be found on this website. No editing is done by the scientific committee. You will receive a reference code for each submission. The scientific committee reserves the right to accept, reject or assign submissions to a different format. Oral contributions from SAMPL participants are selected by the organizers upon invitation. SAMPL participants intending to show posters can submit their titles and abstracts via the registration system.

INVITATION

► SCHOLARSHIPS

Scholarships will be offered to a limited number of bachelor, master, diploma and Ph.D. students who are the main author of a full talk, research telegram or poster. Please send your application to the German Chemical Society until February 27, 2022.

More information about scholarships is available on the conference website:

<https://www.gdch.de/gcc2022>

► POSTER AND LECTURE AWARD

Prizes will be awarded for the two best posters and the best research telegram presentation by a young academic.

► CIC AWARD FOR COMPUTATIONAL CHEMISTRY

We invite research group leaders to propose candidates for the CIC Award for Computational Chemistry for outstanding master, diploma and doctoral theses until December 15, 2021.

More details can be found on the CIC website.

► REGISTRATION

Registration will open January 1st 2022 and close as soon as 170 seats are reached. Please register online at:

<https://www.gdch.de/gcc2022>

Registration fees for GCC and EuroSAMPL are listed on the conference website.

► DEADLINES

Submission of oral contributions (GCC)	January 09, 2022
Submission of research telegrams (GCC)	January 09, 2022
Submission of posters (GCC)	March 15, 2022
Submission of posters (EuroSAMPL)	March 15, 2022
Scholarships	February 27, 2022
Room reservation	February 02, 2022

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

► HEALTH AND SAFETY

We hope that vaccination campaigns proceed further, allowing us to look forward to an exciting in-person meeting. Details of the hygiene and safety concept will be communicated in due time.

Please note that proof of a full vaccination status (COVID-19 vaccines approved in Germany only, certificate required) is mandatory for attendance.

Please keep in mind that legal requirements and restrictions can change at any time. We advise to select flexible travel options and to consider taking out travel cancellation insurance.