

# The International Conference on Chemical Structures scientific program is online!

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## Keywords

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## chem-bla-ics

Now that most speakers confirmed their talk by registering for the conference, it was time to upload the preliminary [scientific program](#) of the [International Conference on Chemical Structures \(#2022ICCS\)](#).

The conference will have 5 sessions:

- Analysis of Large Chemical Data Sets,
- Structure-Activity and Structure-Property Prediction,
- Dealing with Biological Complexity,
- Structure-Based Approaches, and
- Cheminformatics Approaches.

I am also a bit disappointed that the nanoinformatics community did not submit much work. I guess that like the gaps with the nanomedicine community, the link with the cheminformatics community is also a bit weak.

I am also delighted that two [BiGCaT](#) researchers (Denise Slenter and Ammar Ammar) will present their research in Noordwijkerhout. I am looking forward to seeing you all in June. You can [register here](#). Keep in mind the number of places is limited and the registration is filling up quickly.

| Sunday, June 12, 2022 |  |
|-----------------------|--|
| 12:00 - 18:00         | REGISTRATION   |
| 15:00 - 17:00         | PRE-CONFERENCE WORKSHOPS (abstracts)   |
| 15:00 - 17:00         | De novo design of novel compounds to meet multiple property constraints<br>Chemical Computing Group                              |
| 17:00 - 18:00         | FREE TIME  |
| 18:00 - 18:15         | WELCOME  |
| 18:15 - 19:00         | KEYNOTE ADDRESS - CSA Trust Mike Lynch Award   |
| 19:00 - 22:00         | RECEPTION DINNER   |
| Monday, June 13, 2022 |  |
| 8:30 - 11:30          | Analysis of Large Chemical Data Sets   |
| 8:30 - 9:00           | 25 years of small molecule optimization at Novartis: A retrospective analysis of chemical series evolution<br>Maximilian Beckert |
| 9:00 - 9:30           | GeoMine: On-The-Fly Geometric Pattern Mining in Binding Sites<br>Joel Greif  |
| 9:30 - 10:00          | Papyrus - A large scale curated dataset aimed at bioactivity predictions<br>Oliver Jacques Maurice Beaugignon                    |

Part of the scientific program of the ICCS 2022.