chem-bla-ics

The International Conference on Chemical Structures scientific program is online!

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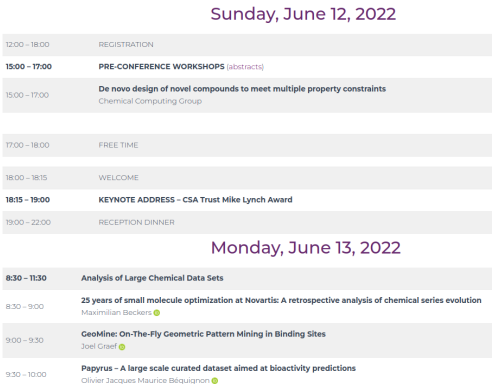
Keywords

Iccs

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.



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** 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** Maximilian Beckers
9:00 – 9:30	**GeoMine: On-The-Fly Geometric Pattern Mining in Binding Sites** Joel Graef
9:30 – 10:00	**Papyrus – A large scale curated dataset aimed at bioactivity predictions** Olivier Jacques Maurice Béquignon

Part of the scientific program of the ICCS 2022.

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.