

12th International Conference on Chemical Structures

June 12 – 16, 2022 ♦ Noordwijkerhout ♦ The Netherlands

Scientific Topics:

- ❑ Cheminformatics Approaches
- ❑ Structure-Activity and Structure-Property Prediction
- ❑ Structure-Based Approaches
- ❑ Artificial Intelligence Approaches
- ❑ Analysis of Large Chemistry Spaces
- ❑ Dealing with Biological Complexity
- ❑ and all other aspects of Computational Molecular Design

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Cheminformatics

- Molecular similarity and diversity
- Mining of chemical literature and patents
- Spectroscopy and structure elucidation
- Reaction handling

Structure-Activity and Structure-Property Prediction

- Consensus and federated methods
- Assessment of uncertainties in predictive modeling
- Graphical methods for SAR analysis
- Multi- and Many-objective optimization

Structure-Based Drug Design

- Advances in molecular dynamics and free energy calculation
- Structure-based and rational drug design
- Modeling of protein-ligand and protein-protein recognition
- Computer-assisted protein design/engineering

Artificial Intelligence Approaches

- Deep learning and sparse-data modelling
- de novo generation
- Representation learning
- Synthetic accessibility and retrosynthesis approaches

Analysis of Large Chemistry Spaces

- Design, profiling, and comparison of compound collections
- DNA Encoded Libraries (DEL)
- Advances in (low-, mid- and high-level) data fusion techniques
- Findable, Accessible, Interoperable, and Reusable (FAIR) data

Dealing with Biological Complexity

- Analysis and prediction of poly-pharmacology and selectivity
- Advances in metabolomics
- Nanoinformatics modelling
- Natural product drug discovery

We also welcome contributions in other aspects of the computer handling of chemical structure information, such as: automatic structure elucidation, combinatorial chemistry and diversity analysis, electronic publishing, MM or QM/MM simulations, modeling of ADME properties, material sciences, analysis and prediction of crystal structures, grid and cloud computing in cheminformatics.

Visit the conference website at

www.iccs-nl.org

for more information, including details on
online abstract submission and conference registration.
The deadline for submission of abstracts is February 28th, 2022.