

June 1-5 2014 ♦ Noordwijkerhout ♦ The Netherlands

The 10<sup>th</sup> International Conference on Chemical Structures (ICCS) and the 10<sup>th</sup> German Conference on Chemoinformatics (GCC) are seeking presentations for the following plenary sessions:

### Cheminformatics

- advances in structure representation
- molecular similarity and diversity
- chemical information visualization
- reaction handling and electronic lab notebooks (ELNs)

### Structure-Activity and Structure-Property Prediction

- industrialized and large-scale model building
- multi-objective optimization and multi-property prediction
- assessment of uncertainties in predictive modeling
- graphical methods for SAR analysis

### Structure-Based Drug Design and Virtual Screening

- improved understanding of protein-ligand interactions
- modeling of protein-protein interactions (PPIs)
- modeling of challenging targets
- advances in antibody modeling

### Analysis of Large Chemistry Spaces

- design, profiling, comparison of compound collections and screening sets
- machine learning and knowledge extraction from databases
- improved visualization of disparate data types
- mining of chemical literature and patents

### Integration of Chemical Information with other Resources

- advances in chemogenomics
- integration of medical and biological information
- semantic technologies as a driving force of integration
- chemical information using mobile technologies and social media

### Dealing with Biological Complexity

- analysis and prediction of poly-pharmacology
- analysis of high-content screening data
- pathways and biological networks
- druggability of targets

The conference is focusing on novel research and emerging technologies. We encourage submission of papers on both applications and case studies as well as on method development and algorithmic work. The final program will be a balance of these two aspects.

### Joint Organizers

- Division of Chemical Information of the American Chemical Society (ACS)
- Chemical Structure Association Trust (CSA Trust)
- Division of Chemical Information and Computer Science of the Chemical Society of Japan (CSJ)
- Chemistry-Information-Computer Division of the German Chemical Society (GDCh)
- Royal Netherlands Chemical Society (KNCV)
- Chemical Information and Computer Applications Group of the Royal Society of Chemistry (RSC)
- Swiss Chemical Society (SCS)

Contributions can be submitted for any of the above and related areas, but we also welcome contributions in any aspect of the computer handling of chemical structure information, such as:

- automatic structure elucidation
- combinatorial chemistry, diversity analysis
- web technology and its effect on chemical information
- electronic publishing
- MM or QM/MM simulations
- practical free energy calculations
- modeling of ADME properties
- material sciences
- analysis and prediction of crystal structures
- grid and cloud computing in cheminformatics

Before and after the official conference program free workshops will be offered by the Chemical Computing Group, the Cambridge Crystallographic Data Centre, Certara, and OpenEye.

Visit the conference website at

[www.int-conf-chem-structures.org](http://www.int-conf-chem-structures.org)

for more information, including details on  
online abstract submission and conference registration.  
The deadline for submission of abstracts is January 31<sup>st</sup>, 2014.