

Ninth International Conference on Chemical Structures, June 5–9, 2011, Noordwijkerhout, The Netherlands

This issue of the *Journal of Chemical Information and Modeling* (JCIM) contains papers presented at the Ninth International Conference on Chemical Structures (ICCS, www.int-conf-chem-structures.org). These conferences are held triennially at the Congress Center in Noordwijkerhout, The Netherlands. The *Journal of Chemical Information and Modeling* and its predecessor, the *Journal of Chemical Information and Computer Sciences*, have published papers from the last seven conferences in special issues. (I had the pleasure of editing the first two in book form as “Chemical Structures” and “Chemical Structures 2”.)

ICCS brings together an international audience interested in handling chemical structures and related topics. Participants discuss research and development in the processing, storage, retrieval, and use of chemical structures. The main scientific program was divided into six plenary sessions: structure–activity and structure–property prediction, structure-based drug design and virtual screening, integrated chemical information, analysis of large chemistry spaces, cheminformatics, and dealing with biological complexity. In addition, an extended poster session was held. There were 35 oral and 77 poster presentations. Dr. Engelbert Zass, of ETH Zürich, Switzerland, was awarded the CSA Trust Mike Lynch Award and delivered the keynote address. A commercial exhibition with 18 leading scientific software suppliers accompanied the scientific program. The conference again featured a sailing cruise on the IJsselmeer with splendid weather and ample opportunity for scientific discussion and networking.

There were 191 participants from 20 different countries. The potential number of participants exceeded the Congress Center’s capacity, as it did the previous time in 2008, and a waiting list again had to be operated. Seventy-five percent of the participants were from Germany, the United Kingdom, the United States, and The Netherlands, and 20% of the participants were PhD students who were able to use the opportunity to discuss their work with experts in the field. About half of the students were supported by ICCS bursaries.

The conference fosters cooperation among organizations and researchers involved in the merging fields of cheminformatics and bioinformatics. The ninth conference was jointly organized by the Division of Chemical Information of the American Chemical Society (CINF), the Chemical Structure Association Trust (CSA Trust), the Division of Chemical Information and Computer Science of the Chemical Society of Japan (CSJ), the Chemistry-Information-Computer Division of the German Chemical Society (GDCh CIC), the Royal Netherlands Chemical Society (KNCV), the Chemical Information and Computer Applications Group of the Royal Society of Chemistry (RSC CICAG), and the Swiss Chemical Society (SCS).

A great deal of credit for the success of the meeting goes to the Scientific Advisory Board: Peter Ertl of Novartis, Kimito Funatsu of the University of Tokyo, Val Gillet of the University of Sheffield, Rajarshi Guha of the NIH Chemical Genomics

Center, Michael Lajiness of Eli Lilly and Company, Jordi Mestres of Hospital del Mar Research Institute, Matthias Rarey of the University of Hamburg, Keith Taylor of Accelrys, Lothar Terfloth of Molecular Networks, Markus Wagener then of Merck Sharp and Dohme (now at Grünenthal), and Patrick Walters of Vertex Pharmaceuticals. These 11 people reviewed all the abstracts submitted for oral or poster presentation. All the related papers submitted to the *Journal of Chemical Information and Modeling* after the conference have been subject to the journal’s usual peer review process.

Finally, as a previous organizer of this meeting and a nine-time editor, I want to thank especially Keith Taylor and Markus Wagener, the 2011 co-chairs, for their immense enthusiasm and highly efficient organization. The 10th International Conference on Chemical Structures will take place at the same venue on June 1–5, 2014.

Wendy A. Warr, Associate Editor, *Journal of Chemical Information and Modeling*

Special Issue: 2011 Noordwijkerhout Cheminformatics

Published: February 6, 2012