

10th ICCS/GCC Conference: 40 Years of Cheminformatics

In 2014, two international conferences dedicated to all aspects of cheminformatics, molecular modeling and related applications of computers in chemistry were having their tenth anniversary. To celebrate the ongoing success of both conference series, which go back to the roots of cheminformatics some 40 years ago, the 10th International Conference on Chemical Structures (ICCS) and the 10th German Conference on Chemoinformatics (GCC) were jointly held June 1–5, 2014 in Noordwijkerhout, The Netherlands. This is to continue a long and successful history, which started for the triennial ICCS with a NATO Advanced Study Workshop in 1973 and for the GCC with a CIC workshop in Hochfilzen, Austria, in 1986. Today, both conferences are among the most important events in this area of science. The special virtual issue of the Journal of Chemical Information and Modeling available at <http://pubs.acs.org/page/vi/cheminformaticsat40.html> contains selected papers from the 10th ICCS/GCC giving an accurate picture of the state-of-the-art in the computer handling and manipulation of chemical structures.

The conference did attract more than 200 attendees from over 20 countries with the majority originating from Germany, the UK, Switzerland, USA, and The Netherlands. As in previous years, the capacity of the conference was quickly reached, proving the tremendous popularity of the event. Among the attendees were also 40 Ph.D. students who took the opportunity to discuss their work with leading scientists in the field. Because of generous donations by sponsors, about one-third of the students could be supported with conference bursaries.

The main scientific program of the conference was divided into six sessions dedicated to Cheminformatics, Structure-Activity and Structure-Property Prediction, Structure-Based Drug Design and Virtual Screening, Analysis of Large Chemistry Spaces, Integration of Chemical Information with other Resources and Dealing with Biological Complexity. The plenary sessions with a total of 34 oral presentations were complemented by two poster sessions with together 83 posters. A commercial exhibition with 17 leading scientific software suppliers accompanied the scientific program. Full details of the program can be found on the ICCS/GCC 2014 website at <http://www.int-conf-chem-structures.org>.

The conference opened with the presentation of the CSA Trust Mike Lynch Award to the “InChI Team” (Steve Heller, Alan McNaught, Igor Pletnev, Steve Stein, Dmitrii Tchekhovskoiin) in recognition of their outstanding accomplishments in the conception and development of the IUPAC International Chemical Identifier (InChI). On behalf of the team, Steve Heller presented the history and highlights of the standardization project.

Besides a strong scientific program with a wide spectrum of contributions ranging from methods development to applications of cheminformatics and modeling in various areas, it has always been our focus to provide a framework for scientific exchange and stimulating discussions. Thus, the program of the conference and its location in a former monastery were selected

to encourage interaction between participants with different backgrounds and to bring together scientists from academia and industry. The excursion to nearby Amsterdam with its canals and museums provided ample opportunity to continue and intensify discussions and networking.

We acknowledge all those who have contributed to the success of ICCS/GCC 2014. In particular, we thank the Scientific Advisory Board who reviewed all the abstracts: P. Ertl, K. Funatsu, V. Gillet, C. de Graaf, R. Guha, O. Koch, J. Kriegl, M. Lajiness, J. Mestres, M. Rarey, K.T. Taylor, L. Terfloth, A. Tropsha, M. Wagener, W.P. Walters, W. Warr, and E. Willighagen. All related papers submitted to the special virtual issue of the Journal of Chemical Information and Modeling were subject to the journal’s usual peer-review process. We also thank all organizing societies (American Chemical Society, Chemical Structure Association Trust, Chemical Society of Japan, German Chemical Society, Royal Netherlands Chemical Society, Royal Society of Chemistry, Swiss Chemical Society, European Association of Chemical and Molecular Sciences) for their support. We are especially grateful to the sponsors of the conference. We also thank all of the session chairs, presenters, and attendees who made this conference such an enriching and enjoyable event!

Both conferences will continue their regular schedule, with the 11th International Conference on Chemical Structures taking place at the same venue in Noordwijkerhout, The Netherlands, on June 11–15, 2017, and the 11th German Conference on Chemoinformatics in Fulda, Germany, on November 8–10, 2015.

We wish you a very good and interesting reading.

Markus Wagener, Chair ICCS

Frank Oellien, Co-Chair ICCS

Uli Fechner, Chair GCC

Matthias Rarey, Editor of the Virtual Special Issue
 ICCS/GCC

■ AUTHOR INFORMATION

Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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