The 17th European Symposium on Quantitative Structure-Activity Relationships & Omics Technologies and Systems Biology

21 - 26 September 2008, Uppsala, Sweden

The 17th Euro-QSAR symposium (www.qsar2008.org) was the latest meeting in a series of events that have become one of the most prominent international symposia held in Europe in the field of computer-assisted molecular design. The program of the symposium spanned six days of lectures and a continuous poster exhibition.

The scientific talks featured a variety of method descriptions and application studies. Some highlights were (in no specific order): Jeremy K. Nicholson gave an illuminating lecture on a pharmaco-metabonomic approach to the study of drug toxicity and metabolism using statistical methods on metabolic biomarker data obtained using nuclear magnetic resonance and mass spectrometry. His observations on the effect of gut microbial activity on the health of an individual made us think more carefully what we are eating. He stated that “you are only 2% human, the rest is bugs.”
Gabriele Cruciani introduced a new method for the prediction of pK_a of drug-sized organic molecules with multiple protonation sites using molecular interaction fields as input for statistical modeling. The accurate prediction of pK_a is of utmost importance because the pK_a of a compound affects its solubility and lipophilicity and, therefore, its bioavailability as well as the capability to penetrate the blood-brain barrier.
Jianxin Duan gave a talk on a novel algorithm for the superimposition and similarity comparison of flexible models of drug-sized molecules. Their method is based on finding atomic triads that are used align the structures before a computing a similarity score. Dr. Duan's presentation was of personal interest to me as it considers a method that achieves the same endpoint as the computer program ShaEP developed by our group and presented in a poster titled “ShaEP: Molecular alignment based on shape and electrostatics”. We also presented another poster titled “High-Quality Molecular Electrostatic Potential Reproduction Using Conformation-Dependent Partial Charges Obtained by Electronegativity Equalization”.

The mutual research interests were discussed during the poster sessions and other informal activities during the six days. Based on this experience and the previous ones at the same series of symposia, I will definitely attend the next Euro-QSAR meeting at Rhodes, Greece in 2010. In 2012, the symposium will be held in Vienna, Austria. I warmly recommend these meetings to those interested in computer-assisted molecular design and drug development.

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