The 16th European Symposium on Quantitative Structure-Activity Relationships & Molecular Modelling

10 - 17 September 2006, Civitavecchia, Italy

The 16th Euro-QSAR symposium (http://www.euro-qsar2006.org/) was the latest meeting in a series of events that have become one of the most prominent European get-together for scientist in the field of computational drug design and molecular modelling. Despite the attribute "Euro", the symposium attracted participants from all over the world.

The scientific talks featured a variety of method descriptions and application studies. Some highlights were (in no specific order): Lennart Eriksson gave an illuminating outline of the divide-and-conquer type approach one should take to building quantitative statistical models. Manuel Pastor introduced a new method for finding the "hot spots" in molecular interaction fields. Tudor Oprea and Alexander Tropsha presented the Molecular Libraries Initiative of the National Institute of Health and the PubChem public database of chemical structures and their biological activity. A few talks concentrated on modelling drug metabolism; Eric Johnson and Lovisa Afzelius provided insight on the flexibility of the cytochrome P450 family of enzymes on the atomic level of detail.

Of most personal interest were presentations related to modelling the protein-ligand interactions using molecular docking. Many of the studies in the oral and poster presentations involved docking at some stage of the workflow. Ingo Reulecke presented a poster about a new method for assessing the goodness of *in silico* generated protein-ligand complex structures. The methods takes into account the solvation effects of the change in polar and apolar molecular surface area upon binding and formation of hydrogen bonds. Several studies presented different technical aspects of the generation of molecular geometries. Our research involves the generation of ligand conformations and it was presented in a poster titled "Generating conformer ensembles using a genetic algorithm".

The symposium sprouted new international and national contacts. The mutual interests were discussed lively during the poster sessions and other less formal activities during the six days. Email correspondence about a prospective international collaboration is on-going. The experience fortified my conception of the Euro-QSAR series of meetings as *the* event in computer-assisted drug design and molecular modelling in Europe.

I gratefully acknowledge National Graduate School in Informational and Structural Biology, BioCity Systems Biology Programme, and Stiftelsens för Åbo Akademi forskningsinstitut for their financial support.

Turku 21. November 2006,
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