

Euro-QSAR 2008, Uppsala, Sweden

by Pekka Tiikkainen

One of the most important meetings on the field of computer-aided drug design (CADD), Euro-QSAR 2008, took place in Uppsala from 21st to 26th September. Conference venue was the newly built Uppsala Conference and Concert building right in the city center.

The emphasis of this year's meeting was on system biology and the meeting's first session was dedicated for it. Mainly the posters and talks still handled more traditional aspects of CADD such as virtual screening and QSAR models. Of the talks given, three were particularly interesting to me personally. The first one was a very lively presentation of limits and pitfalls of QSAR models given by Arthur Doweiko from Bristol-Myers Squibb. Second memorable talk was given by Professor Yvonne Martin of Abbott Laboratories on belief theory for combining results from different ligand-based virtual screening tools. The third talk well worth listening was given by Professor Knut Baumann from Braunschweig University. The talk presented unbiased benchmark sets for ligand-based virtual screening.

I was given the honour of giving a 15-minute presentation on one of my projects. The talk was titled "Linking chemical and biological similarity of small molecules". This was based on my (hopefully) soon-to-be-published manuscript. As in all meetings, Euro-QSAR gave also an important opportunity for networking with fellow scientists in the field.