# QSAR affinity fingerprints: Further exploration of chemogenomic space

Dehaen W.1, Škuta C.1,2 Svozil D.1,2

1 CZ-OPENSCREEN: National Infrastructure for Chemical Biology, Department of Informatics and Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology Prague, Prague, Czech Republic.

2 CZ-OPEN-SCREEN: National Infrastructure for Chemical Biology, Institute of Molecular Genetics, AS CR v.v.i., Prague, Czech Republic.

Chemogenomic space describes the relationship between chemical and genomic space and one logical entrance point to it is the ligand-target space, i.e. the activity of all possible ligands to all possible targets. Most of these activities are empirically not known, leading to a very sparse experimental ligand-target matrix. Using the ChEMBL database of measured target-ligand activities and QSAR we attempt to construct models for each target to fill in this chemogenomic space, and with this modelled ligand-target matrix as a starting point, we construct a series of ligand fingerprints based on QSAR-predicted activity at various targets.   
  
Various aspects of these QSAR affinity fingerprints (QAFFP) will be discussed in this poster, including the predictive value at targets outside of the fingerprint, the effect of target selection to build the fingerprint, the biological relevance of these fingerprints, the effect of different machine learning techniques on the predictive strength of the fingerprints, comparison with structure based fingerprints and combination of QAFFP with structural fingerprints to build a hybrid fingerprint.