

QSAR methods

OCHEM was designed as a user-friendly web tool for model development.

It provides an access to about 10 different machine learning methods and more than 20 different descriptors.

OCHEM can easily develop models with >300k molecules and has handled data matrices with up to 2×10^{11} entries (~300k molecules X 700,000 descriptors). For analysis of ToxCast data more than 20k models [were developed](#) as analysed [elsewhere](#).

The [following tutorial](#) explains the development of models using OCHEM.