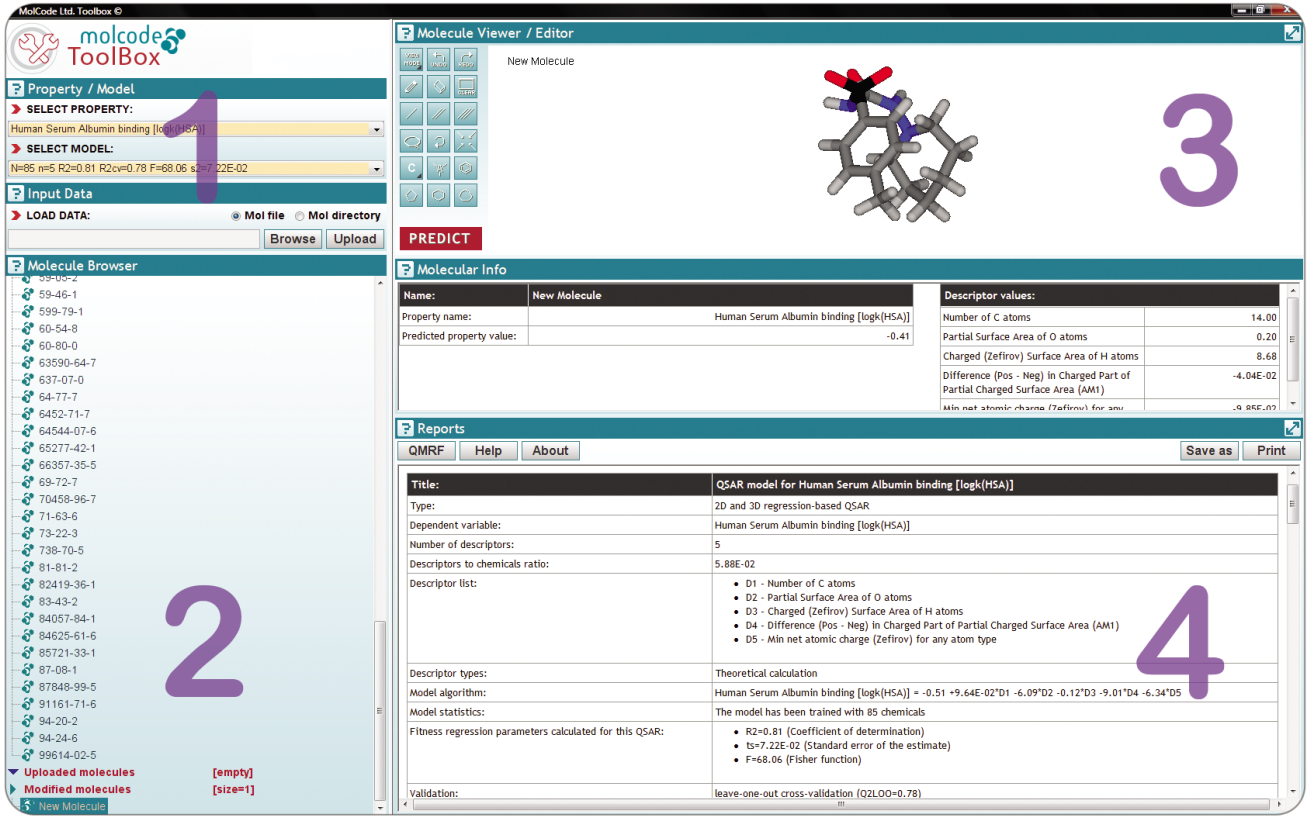
4 Four easy steps to explore the Molcode Toolbox



1 Browse through your files, simultaneously upload and optimize your mol files. Select a property and appropriate model to predict theoretical values.

2 Navigate through the library of compounds. Investigate structures of interest. Check their structure and property-descriptor values in the molecule viewer and molecular information tables.

3 Draw, correct or modify your structures or modify the existing ones from our models set. Predict the values of the new molecules and save them in the Toolbox.

4 Create a QMRF report for overall statistics and predictions of all sets currently loaded in the Molcode Toolbox. Investigate the molecular descriptor values and analyze the results.

Useful information

Molcode Toolbox uses semiempirical quantum mechanics to calculate molecular features (descriptors) for all compounds. Prior to these calculations, molecular mechanics is also applied.
We also develop custom Toolboxes for our clients needs, if there is a need unmet by standard Toolboxes.