ADMEWORKS Predictor Release Notes

ADMEWORKS Predictor 6.0

- Display of Prediction Reliability: Based on statistical similarity of the predicted compound with the training set of the model.
- Reporting Functionality: Predictor results and their corresponding details can be exported to a PDF file.
- Display of Actual Experimental Value: Predictor has the option to display the actual experimental values, instead of predicted values, if they are available in the training set of the models.

ADMEWORKS Predictor 5.0

- New Look-and-Feel: Faster and more convenient GUI based on AJAX technologies.
- Support for MO-G descriptors: MO-G is a general-purpose semi-empirical molecular orbital library developed by Fujitsu for the study of chemical structures and reactions. The semi-empirical Hamiltonians MNDO, AM1, PM3 and PM5 are used in the electronic part of the calculation to obtain molecular orbitals, the heat of formation and its derivative with respect to molecular geometry.
- Copy&Paste from ChemDraw (Pro and Ultra only) to Molecular Editor.

ADMEWORKS Predictor 4.5

- New SVM regression model.

ADMEWORKS Predictor 4.0

- New combined substructure descriptors.
- Permanent CORINA library.

ADMEWORKS Predictor 3.1

- User private folder (upload, download, delete files).
- Generation of molecules to a SDF file in user's private folder.
- External parameters can be used as descriptors.
- Stepwise Qualitative model.
- New math functions.