

## ADMEWORKS ModelBuilder Release Notes

### ADMEWORKS ModelBuilder 7.10

- Display discriminant score (or Critical Value) in hidden columns of all qualitative models.
- Missing Values policy change. Default value = "Don't Replace".
- iMLR "automatic" recalculation (feature selection).
- Unify all dialogs to display substructures not just the name of the substructure descriptors SCOUNT and SC.
- User should be able to identify samples that have been modified by "wash molecules".
- Add "Select ALL/Deselect ALL" button in SDF and CSV export dialog.
- Conversion tool to migrate User descriptor groups.
- Wash Molecules: Remove duplicates should be separated from "remove conflicting samples".
- iMLR history plot is overlapping the labels.

### ADMEWORKS ModelBuilder 7.6

- New filter options available in 'Extract Substructures' feature.
- SubstructureSearch support for halogens, non-metals, etc.
- New implementation of existed descriptors: DMFRAG, CTYPE, DEDGE, DFLEX, DKAPPA, DMALP, DMCHI, DMCON, DMGEO, DMOMI, DPEND, ECCEN, SAVOL.
- New Descriptors: HBOND (Hydrogen bonds), ESTAT (Electrotopological State Indices), AUTOCOR (AutoCorrelation).

### ADMEWORKS ModelBuilder 6.0

- Multi-core CPU support: Takes advantage of the multi-cores to speed up calculations of descriptors and analyses.
- Improvement of the Model Wizard: New criteria to ease ranking of models automatically created by Model Wizard.
- Support Vector Regression Feature Selection: New Feature Selection method to support quantitative data analysis.
- Improvement of Wash molecules: Repairs molecules to be readable by ModelBuilder descriptor generators.
- Improvement of Graph functions: Improvements in dendrograms and class division graphs for better analysis of the samples.

### ADMEWORKS ModelBuilder 5.0

- Particle Swarm Optimization.
- MO-G descriptors.
- All quantitative models (including PLS and RSVM) display not only R2 but also RMSE values.

#### **ADMEWORKS ModelBuilder 4.5**

- New SVM regression model.
- Automatic generation of substructures from training set for use in Substructure Descriptors set.

#### **ADMEWORKS ModelBuilder 4.0**

- ModelWizard - a tool for the quick, automated creation of classification and regression models.
- “Wash molecules” - option used for repairing/removing bad or incompatible structures.
- New combined substructure descriptors.
- Permanent CORINA library.

#### **ADMEWORKS ModelBuilder 3.1**

- Added Cross-Validation R2 (CVR2) to Genetic Algorithm's objective functions.
- Added Cross-Validation R2 (CVR2) to:
  - Stepwise MLR
  - RFSBoost-LDA
  - Interactive DF
  - Interactive MLR
  - Iterative SVMFS
  - Iterative SVMFS MIXED
  - Boost-LDA FS
- External parameters can be used as descriptors.
- Automatic selection of descriptors based on a CSV file.
- Parameter selection using a given list (CSV).
- New math functions.