

ADMEWORKS ModelBuilder

ADMEWORKS ModelBuilder is a tool dedicated for building QSAR/QSPR models that can later be used for predicting various chemical and biological properties of compounds. A set of data on molecular structures and their respective experimental values of the property of interest is a prerequisite for every model building. Two classes of models (Qualitative and Quantitative) can be built using various algorithms.



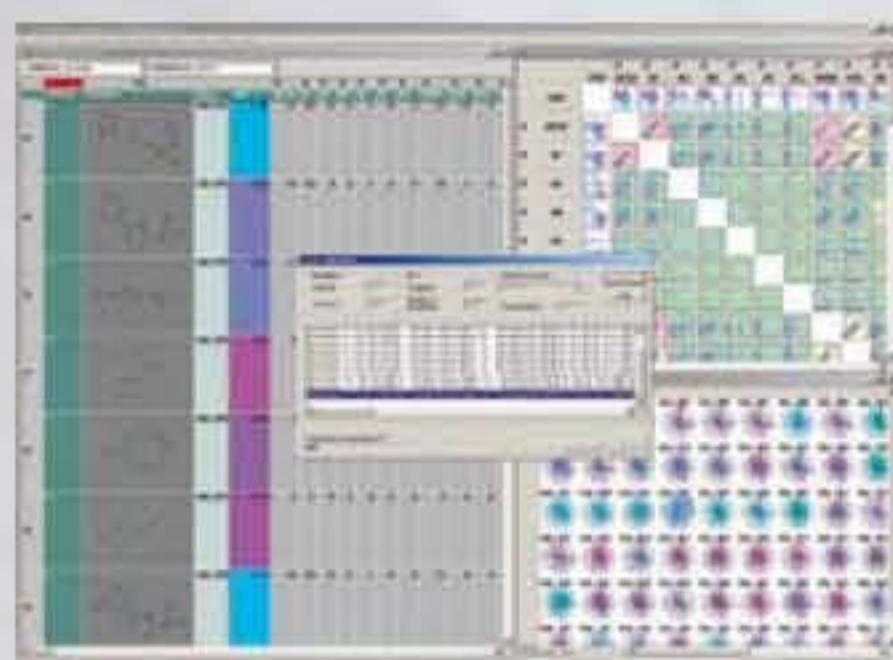
The models are based on values of physicochemical, topological, geometrical, and electronic properties derived from the molecular structure - called descriptors. Descriptor generator programs in ADMEWORKS ModelBuilder come mostly from ADAPT (the software system created by Professor Peter Jurs and coworkers at the Pennsylvania State University to study molecular structure - biological activity relationships SAR and molecular structure - physicochemical property relationships SPR) and MOPAC (general-purpose semiempirical molecular orbital package developed by Professor James Stewart).

Models created in Model Builder are easily imported into ADMEWORKS Predictor (optional product) which is a high-speed virtual (In Silico) screening

system intended for simultaneous evaluation of the ADMET properties of compounds. Simultaneous evaluation of the pharmacological as well as the ADMET properties of compounds is useful in the discovery phase to produce balanced quality hits, and also in the lead optimization phase to lessen the occurrence of faulty leads.

System Specifications

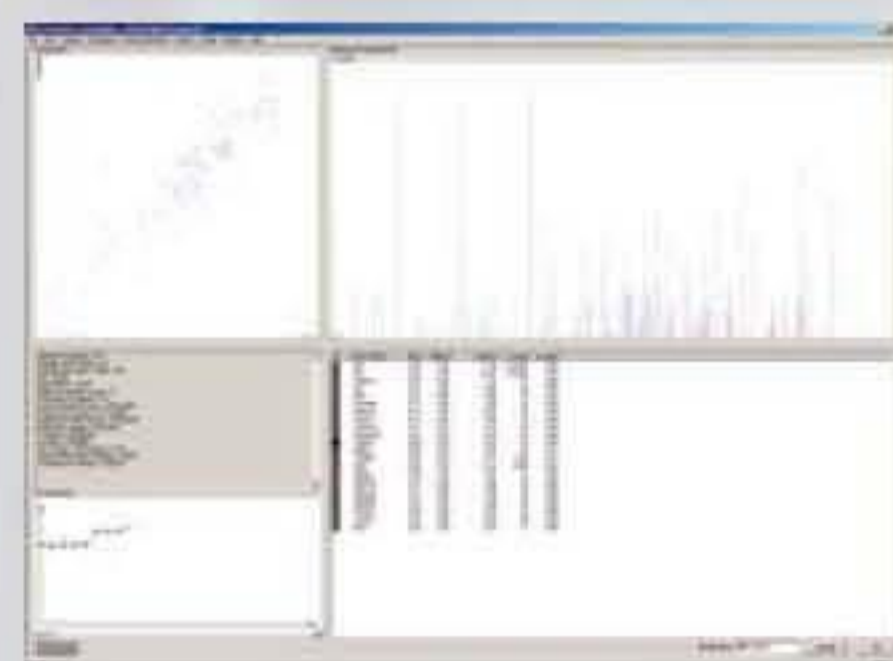
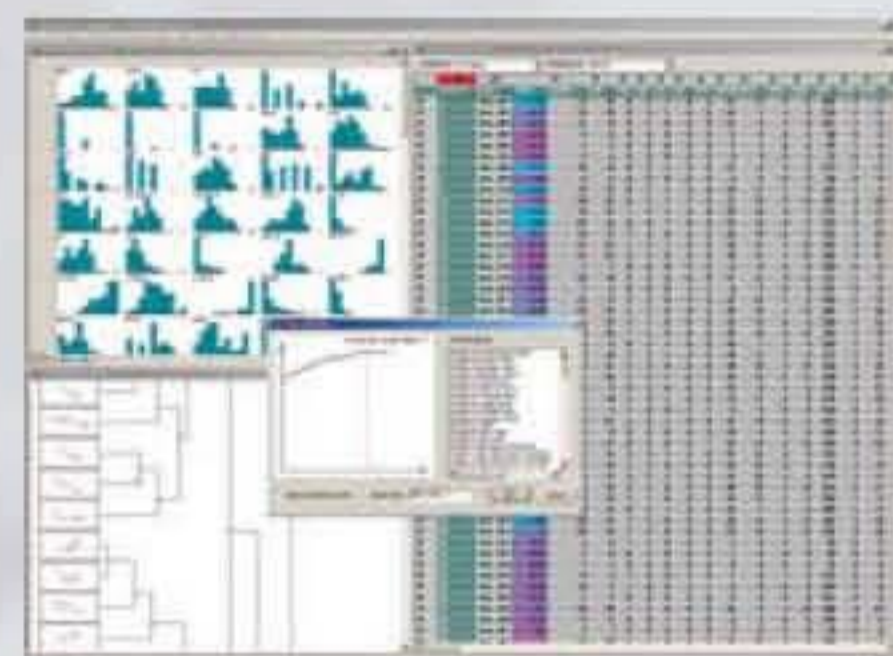
- Quantitative/qualitative structure-activity relation's analysis.
- Multiple statistical methods for generating predictive models: Perceptron, Iterative Least Squares Method, Multiple Linear Regression, Stepwise Regression, Leap-and-Bounds Regression, Genetic Algorithm, Fuzzy Adaptive Least Squares, k Nearest Neighbors, ADA Boost and Support Vector Machine.



- Customizable cross-validation of models.
- Multivariate/pattern recognition data analysis.
- ADMET data analysis.
- Near 400 predefined descriptors and an unlimited number of substructure-related descriptors.
- Interactive graphs that display property distribution, predicted vs. actual activity, property correlations, clustering of samples and properties and others.
- Interactive graphical feature and outlier

selection tools.

- Automated statistical tools for feature and sample selection.
- SDF and CSV file import/export.



Hardware and software requirements

- Suggested hardware configuration: Intel Pentium 4 2.0 GHz or higher, 512 MB RAM or more, 500MB HDD space or more.
- Operating Systems: Windows 2000/XP.