ModelBuilder

ADMEWORKS/ModelBuilder is a tool for building mathematical models that can later be used for predicting various chemical and biological properties of compounds.

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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 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 from MOPAC.

ModelBuilder seamlessly integrates with ADMEWORKS Predictor. Models created in ModelBuilder are easily imported into ADMEWORKS Predictor, allowing a quick comparison of the models, and the selection of only the best ones. Features includes:

- Quantitative/qualitative Structure-Activity Relation's analysis
- Advanced results visualization capabilities
- Multiple statistical methods for generating predictive models: Perceptron, Iterative Least Squares Method, Multiple Linear Regression, Stepwise Regression, Leap-and-Bounds Regression, and Genetic Algorithm
- Customizable cross-validation of models
- Multivariate/pattern recognition data analysis
- ADMET data analysis
- More than 300 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

Models

Two types of models can be built using system:

- Qualitative (Discriminant Function)
- Quantitative (Multiple Linear Regression)

A qualitative model categorizes molecules into classes. An example of such is a model that predicts if a molecule fits in a carcinogenic or non-carcinogenic class. Conversely, a

quantitative model produces a numerical value for its prediction. A water solubility model serves as a good example of a quantitative model.

Applications

Use ADMEWORKS ModelBuilder to:

- Predict properties of compounds
- Perform ADMET analysis
- Virtually screen large libraries for molecules with desirable property profiles
- Support hit finding and lead optimisation decisions
- Data mine databases and compound libraries
- Speed up innovation

Predictor

ADMEWORKS/Predictor is a high-speed virtual screening system intended for simultaneous evaluation of ADMET properties of compounds.

The system employs a number of models to predict ADMET properties. The models are based on values of topological, geometric, physicochemical and substructure descriptors derived from the molecular structures.

ADMEWORKS Predictor is a virtual screening system intended for evaluation of the ADMET properties of compounds. With ADMEWORKS Predictor it is possible to prioritize while simultaneously evaluating the ADME and the pharmaceutical properties.

By freely ranking the properties according to their relative importance, ADMEWORKS Predictor allows for a more focused screening of compounds, stressing only the properties that are of highest interest.

ADMEWORKS Predictor seamlessly integrates with ADMEWORKS ModelBuilder, which allows the creation of customized models to be used in predicting compound properties. Models created in ADMEWORKS ModelBuilder are easily imported into ADMEWORKS Predictor, allowing a quick comparison of the models, and the selection of only the best ones.

ADMEWORKS Predictor also provides support for legacy systems and models through a comprehensible interface, and is highly scalable by allowing integration with other third party computational tools. Features include:

- Store molecular structures and properties in a central database
- Manage and control via a web browser
- Divide work into convenient worksheets
- Handle many users in a corporate environment
- Run all-at-once predictions via a web browser
- View structures using a highly functional 3D structure viewer

- Import/export MOL, SDF files
- Filter and sort results

Prediction Models

Models related to Adsorption and Distribution

- LogP
- Solubility
- Lipinski's Rule of Five
- Lead-likeness
- Human intestinal absorption (HIA)
- Blood-brain barrier (BBB)
- P-glycoprotein transporter (Pgp)

Models related to Metabolism

- CYP2D6 Substrate
- CYP3A4 Inhibitor
- CYP3A4 Substrate

Models related to Toxicity

- Carcinogenicity
- Mutagenicity (Ames TA100/TA98)
- Chromosomal aberration
- hERG inhibition
- Skin sensitization
- Biodegradability
- Bioconcentration factor (BCF)

For more information:

https://www.fujitsu.com/jp/group/kyushu/en/solutions/industry/lifescience/admeworks/#anc-01