SimulationsPlus

ADMET Predictor®

ADMET MODELER™

ADMET Modeler is a QSAR/QSPR model building module in ADMET Predictor®. It automates the difficult and tedious process of building high quality predictive QSAR/QSPR models from experimental data sets.

The following modeling methods are offered in ADMET Modeler™:

- Kohonen Self-Organizing Maps
- Artificial Neural Network Ensembles for regression and binary classification models
- Support Vector Machine Ensembles for regression and classification models
- Kernel Partial Least Squares and Ordinary PLS for regression
- Multiple Linear Regression

Better models tunable to your chemistry space

The product of this new methodology is not only greater speed, but also better models. Now a wider set of architectures can be fitted rapidly, so more options can be investigated to see which is best. The DELTA model approach is the methodology of choice for extension of pre-built models using additional data from internal or public sources.

>300 Atomic and Molecular Descriptors

A large palette of atomic and molecular descriptors is available. The modeling algorithm automatically removes low variance and correlated descriptors. Several test set selection methods are available such as Kohonen maps and K-means.

Faster Modeling

When the original predictive models for physicochemical and biopharmaceutical properties for ADMET Predictor® were developed using a generic modeling software, the time required to develop each model using all of the above steps was as much as 2-3 months. Now, similar models can be built in a matter of hours.

Descriptor Sensitivity Analysis provides greater interpretability

After automatic identification of the most influential descriptors, a series of new chemical derivatives of the compound in question can be easily designed – derivatives that push the property of interest in the desired direction.

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Interested in collaborating?

Email us! info@simulations-plus.com

Rev. 12/06/2023