SimulationsPlus

AP ADMET Predictor

MS

MEDCHEM STUDIO™

The MedChem Studio Module, contains tools for data visualization, compound clustering, high throughput screening analysis, lead identification and prioritization, *de novo* design, scaffold hopping, lead optimization, and much more!

MedChem Studio is now free of charge for all our users for extended data analysis capabilities.

What is the MedChem Studio™ Module?

Visualize SARs: MedChem Studio can generate fingerprints (keys) using different methods including Extended-Connectivity Fingerprints (ECFPs) in order to elucidate SAR and visualize structure alerts. One can easily identify keys that most correlate with a compound property.

Intuitive Class Generation

MedChem Studio's class generation technology reproduces a chemist's reasoning by automatically organizing molecules into chemical families based on shared scaffolds. Molecular properties can then be analyzed at the class level, providing clearer insight into chemo type assets and liabilities.

- ✓ Uses maximum common substructures (MCSs) rather than fingerprints, so results are chemically intuitive
- ✓ Generates scaffolds from the data rather than reading them from a pre-defined list, so novel structural motifs can be discovered
- ✓ Provides an ideal starting point for local QSAR generation, molecule design, and other analysis tasks
- ✓ User-defined scaffolds can also be used to generate classes
- ✓ "Frameworks" class generation option similar to the Murcko assemblies method

Formatted Databases

One can also create a database (library) of compounds that can be searched very quickly. The library can be screened by structure, text, or similarity. The similarity searches can be performed on a single molecule or a file of structures.

Matched molecular pair analysis (MMPA)

Matched molecular pair analysis can be used to identify activity cliffs in a data set or to perform an analysis to identify and possibly exploit structural trends in property values:

R Group Analysis

- ✓ Once the core has been defined the software can automatically generate a substituent table.
- ✓ The R Group Analyzer provides advanced capabilities for the analysis of substituent effects.

simulations-plus.com/admetpredictor

Interested in collaborating?

Email us! info@simulations-plus.com