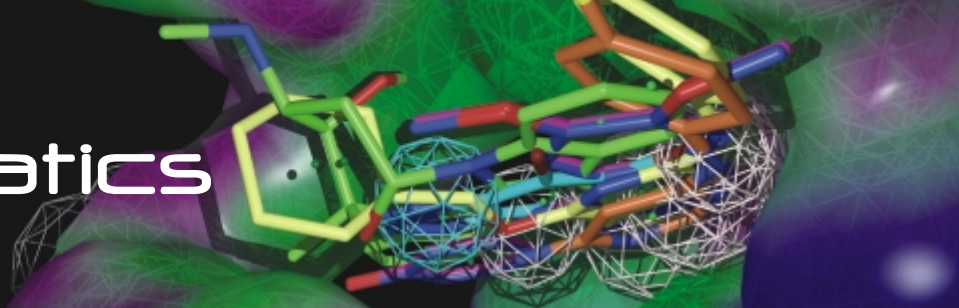


Cheminformatics and QSAR



- 300+ Molecular Descriptors
- Similarity
- Diversity
- Fingerprints
- Clustering
- Diverse Subset
- PCA
- QSAR/QSPR Predictive Modeling
- Consensus Modeling

MOE™ provides a suite of applications for manipulating and analyzing large collections of compounds, building property models, consensus models and SD command line tools.

Molecular Descriptors. Calculate over 300 molecular descriptors including topological indices, structural keys, E-state indices, physical properties (such as LogP, molecular weight and molar refractivity), topological polar surface area and CCG's VSA descriptors with wide applicability to both biological activity and ADME property prediction. Use descriptors for classification, clustering, filtering and predictive model construction. Add custom descriptors using MOE's built-in ScientificVector Language.

Similarity, Diversity and Fingerprints. Perform similarity searching and diverse subset selection using Descriptor, Conformation and Molecular Fingerprint methodologies. Choose between a number of fingerprint systems including 2, 3 and 4-point pharmacophore fingerprints in 2D or 3D and MACCS key fingerprints.

HighThroughput Conformational Search. Construct conformation databases using a parallelized fragment-based approach. Molecules are subdivided into overlapping fragments each of which is subjected to a rigorous stochastic search. The fragment conformations are rapidly assembled by superposing the overlap atoms. A database of fragments is maintained (and augmented as the search proceeds) making conformation generation of combinatorial libraries very fast.

Automatic 2D Depiction. Quickly generate publication quality depictions of small molecules in 2D using a unique algorithm. The algorithm has been validated using a dataset of ~70,000 structures. Calculate 2D depictions for each molecule in a database and create depictions during ASCII import of SMILES strings.

QSAR/QSPR Predictive Modeling. Build QSAR/QSPR models using linear, probabilistic and decision-tree methodologies. CCG's unique Binary QSAR methodology is ideal for building pass/fail models from high error content data. Linear models include PCR and PLS methodologies and can support biological activity or ADME assessments.

Consensus Modeling. Combine linear, binary, fingerprint, and pharmacophore models into a single composite model. Save and apply the constructed models to collections of compounds for clustering, selection, filtering applications or designing focused combinatorial libraries.

SD Pipeline Command Line Tools. Operate directly on SD files for structure depiction, acid/base protonation state, database filtering, sorting and descriptor calculations. Remove records that do not satisfy a series of filters (e.g. lead-like, reactive groups, drug-like, etc..), sort records and remove duplicate entries from SD files. Calculate descriptors and write the output to SD or ASCII formats.

MOE

Molecular Operating Environment

Protein Modeling and Bioinformatics
Pharmacophore Modeling
Structure-Based Design

Method Development and Deployment
Molecular Modeling and Simulations
High Throughput Discovery

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