

Selector™

CHARACTERIZE AND SAMPLE COMPOUND LIBRARIES



Selector characterizes, compares, and samples sets of compounds. Clustering tools identify relationships between compounds based on their similarity. Selector can create diverse or representative subsets, filter compound lists based on properties, find compounds similar to a lead compound, and compare the diversity of sets of compounds.

Features

- Applicable to dozens or hundreds of thousands of compounds
- Uses data from the SYBYL® Molecular Spreadsheet™ or UNITY® databases
- Expands the property descriptors of the Molecular Spreadsheet
- A variety of diversity property descriptors
- Analysis tools include Jarvis-Patrick, Reciprocal Nearest Neighbor, Hierarchical Clustering and Staged Clustering
- Explicit scaling of unrelated properties
- UNITY database comparison utility

Many properties can be calculated from individual molecular structures. Together, these properties define a structural "space" for a compound library. Using these properties to characterize the library, Selector helps define diversity scales and select compounds based on this information. Selector is important since many compounds in the corporate library are literally irreplaceable. By optimizing the diversity of the library of compounds selected for testing - while minimizing the use of rare and unique samples - Selector fulfills the promise of generating value from compound libraries.

From Something or From Nothing

Selector can be used throughout the drug discovery process. In early stages of exploration, the need may be to sample very different structures in order to search for multiple starting points for further development. When the chemical neighborhood of active compounds becomes better characterized, optimal sampling may call for more thorough mining of all possible compounds in that vicinity. Selector can be used to choose which compounds from a library will be tested in a particular biochemical or biological screen, or to determine which reagents should be chosen from among those available to create a new combinatorial library.

Diverse Ways to Measure Structure Diversity

Molecular diversity can be measured in a variety of ways. Selector allows the use of a large number of methods to measure diversity, including:

- Molecular Fingerprints and Tanimoto Indices
- Pharmacophore Distance Triplets
- Substituent Parameters
- Latest Connectivity Indices from HDI

- Integrated ClogP and CMR from Principal Components Analysis
- QSAR with CoMFA® Field Contributions
- Support of Advanced CoMFA Cluster Columns

Multiple Selection Methods

Selector can be used to optimize diversity (useful when selecting a library of compounds to be run in a new, unknown biological screen), or to optimize similarity (useful when expanding on an existing lead compound).

Additionally, Selector can use a list-based or a cluster-based method to group structures. In the list method, the single compound which has not yet been selected, and is most (or least) similar to those which have already been selected, is determined, and that compound is added to the list. In the clustering method, the library structures are pre-grouped into clusters that contain molecules that are close together in a structure space involving all the property values. Similar lists are created by selecting compounds from the same cluster; dissimilar lists are created by selecting compounds from different clusters.

Powerful Data Organization and Analysis Tools

Selector organizes data in SYBYL's powerful Molecular Spreadsheet format. The Molecular Spreadsheet offers traditional spreadsheet functionality, including saving, searching, sorting, filtering, and graphing. Graphs created from spreadsheet data are hyperlinked back to the table to provide convenient communication between graphical and tabular displays. Results can be output to a file, printer, or an HTML table.

Hardware and Software Requirements

Selector requires a separate license, and runs on workstations operating under IRIX® (SGI®) or Linux® (x86).

Complementary Software

Integration of Selector in the SYBYL expert molecular modeling environment allows users to access SYBYL's powerful molecular design and analysis tools.

- **Advanced CoMFA** for refining and enhancing 3D QSAR models.
- **ClogP/CMR** for including molar refractivity and logP in QSAR and ADME models.
- **Concord®** for generating accurate 3D coordinates.
- **DiverseSolutions®** for designing, comparing, or selecting compound libraries.
- **Molconn-Z™** for computing a wide range of topological indices based on molecular structure.
- **QSAR with CoMFA** for building predictive structure-activity and structure-property models.
- **StereoPlex®** for expanding the stereochemical diversity of a database.
- **UNITY** for locating compounds in databases that match a pharmacophore or fit a receptor site.



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