

Data Management

- Database development and updating
- Undesirable molecule elimination
- Library comparisons
- Duplicate structure identification and elimination
- Data format conversion (SDF, ISIS/Base, MOL, LST, Excel, JCAMP-LINK, NIST MS)

Data Entry

- Structure drawing
- Spectral information entry
- Other data entry

Diversity Analysis

- Molecular diversity analysis
- Database comparison and sorting by diversity
- Similarity index calculation for any chemical compound with all other compounds in any database
- Complete similarity matrix calculation for any database of chemical compounds
- Whole diversity estimation of any compound database
- Diverse subset selection of compounds from any database
- Selective import of a subset of dissimilar compounds from an external database
- Heterocycles diversity analysis and database sorting

Physico-chemical Property Calculations

- Lipophilicity (cLogP and cLogD)
- Solubility (LogSw)
- Intestinal absorption in humans (FA)

Drug-like Characteristic Selection Parameters

Lipinski Rule of Five requirements can be incorporated into any compound selection process

- H-bond donors < 5
- H-bond acceptors < 10
- Log P < 5
- Mol. Weight < 500
- Free-rotation bonds < 10

Consulting and Programming

- Medicinal chemistry and organic synthesis
- Internet chemical database setup and development
- Custom programming