

Molecular Diversity and Similarity

- Molecular Diversity Analysis
- Comparing and sorting databases by diversity
- Calculation of similarity indexes for any chemical compound with all compounds in any database
- Calculation of the complete similarity matrix for any database of chemical compounds
- Estimation of the whole diversity of any database of chemical compounds
- Selection of a diverse subset of compounds from any database of chemical compounds
- Selective import of a subset of dissimilar compounds from external database
- Heterocycles diversity analysis
- Heterocycles database generation
- Sorting databases by heterocycles diversity

Algorithms Used in Calculations

- Centroid algorithm
- Cluster Sampling
- Sum(Min.Dissimilarities) maximization
- Min.Dissimilarities maximization
- Sum(Dissimilarities) maximization
- Stepwise Elimination