

3D Searching

This module teaches experienced ISIS/Base users how to retrieve molecules based on the three-dimensional, spatial relationships of functional and chemical groups. Three search methods are highlighted: 3D substructure searching, submodel searching, and conformationally flexible substructure searching.

Course Objectives

The participant will be able to:

- ◆ Construct search queries that define 3D objects such as geometric centers, lines, and planes
- ◆ Specify geometric constraints, such as the distance between two points, angles, and exclusion spheres
- ◆ Construct a submodel query based on the 3D model of a compound with known activity
- ◆ Retrieve potentially active compounds by manipulating stored conformations to find those that fit the query
- ◆ Set search parameters to reduce search time

Prerequisites

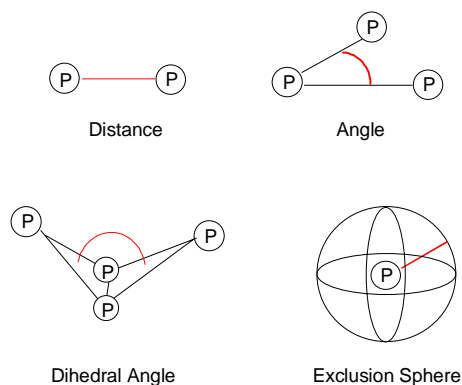
Molecule Searching
Drawing Molecules

Course Length

1/2 day

Examples from the Class

3D geometric constraints



Interpretation of a published pharmacophore for central nervous system drugs

