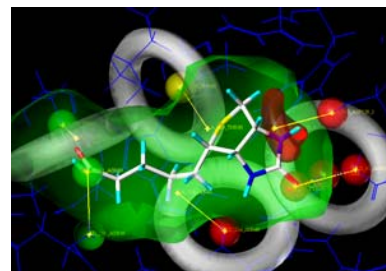


3D-DATABASE SEARCHING

This course focuses on achieving optimal database search results by improving search performance and query definition. Learners will conduct searches on 3D databases, and explore options to maximize search performance. They will define both ligand-based and receptor-based queries, and enhance queries to restrict or expand the desired search results.



Who Should Attend

Researchers who use structure-based design or ligand-based design techniques. Molecular modelers and chemists who want to find new compounds that match their current models.

Requirements

Before attending this course, participants should be able to perform the following tasks in SYBYL: Manipulate molecules with a mouse, create molecular spreadsheets and add columns of associated properties, prepare a ligand-receptor complex with correct SYBYL atom types and appropriate hydrogens, and create a pharmacophoric alignment of molecules. These topics are covered in the courses [Receptor-Ligand Modeling for New Modelers](#) and [Ligand-Based Modeling for New Modelers](#), and [Pharmacophore Model Analysis](#).

What You Will Learn

- ▶ Choose appropriate settings to translate datasets and create databases.
- ▶ Evaluate database search performance.
- ▶ Adjust settings to enhance search performance.
- ▶ Find molecules in a database that can be aligned to features in an active molecule.
- ▶ Find molecules in a database that can be aligned to interact with a given receptor.

Course Topics

Search for Hits

- ▶ Prepare Datasets
- ▶ Conduct Flexible Searches
- ▶ Use Expanded Search Options

Create Queries

- ▶ Develop Ligand-Based Queries
- ▶ Construct Queries from Receptor-Ligand Complexes
- ▶ Generate Cavity-Based Queries

Enhance Queries

- ▶ Employ Markush Atoms
- ▶ Refine Feature Definitions
- ▶ Introduce Variability

Course Objectives

1. Convert SD files to SLN files and UNITY databases.
2. Conduct flexible searches and determine the search performance, using coverage, selectivity, and enrichment, and load the hits into a molecular spreadsheet for viewing.
3. Use expanded search options in flexible searches, including both "per search" options and "per database" options.
4. Develop ligand-based 3D queries using ligand atoms, donors, acceptors, and hydrophobic features.
5. Develop 3D queries from ligand-receptor complexes. The query features will be placed using atom positions in the ligand and the receptors.
6. Develop 3D queries from receptor cavities. The query features will be placed using donors, acceptors and hydrophobic groups in the receptor.
7. Create Markush atom types to find specific types of atoms.
8. Refine feature definitions by modifying and reordering 3DSLN rules.
9. Introduce variability to a query by using partial-match constraints.

Modules Used

SYBYL/Base, UNITY, and Biopolymer.

Course Length

1 day

Schedule and Registration

For a schedule of Training Workshops and online registration, please visit

www.tripos.com/training

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