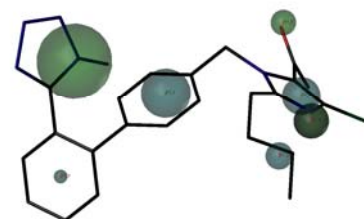


PHARMACOPHORE MODEL ANALYSIS

This course covers methods for pharmacophore model development on structures of known ligands. Users will gain hands-on experience creating pharmacophore models, and then using these models to find other molecules capable of fitting the pharmacophore model.



Who Should Attend

Molecular modelers and chemists who employ ligand-based design techniques. Researchers who are investigating the 3D-requirements for biological activity in the absence of a receptor structure.

Requirements

Before attending this course, participants should be able to perform the following tasks in SYBYL: Manipulate molecules using a mouse, display structures from a molecular spreadsheet. These topics are covered in the course [Ligand-Based Modeling for New Modelers](#).

What You Will Learn

- ▶ Determine the geometric requirements for ligand activity.
- ▶ Find compounds that match a pharmacophore model.
- ▶ Improve database search results by enhancing queries.
- ▶ Evaluate how well compounds align to a pharmacophore model.

Course Topics

Develop Pharmacophore Models

- ▶ Create GASP Models
- ▶ Create GALAHAD Models
- ▶ Align Compounds to GALAHAD Models

Search Databases

- ▶ Modify 3D Queries
- ▶ Conduct Database Searches

Course Objectives

1. Generate and examine pharmacophore models for a given dataset.
2. Identify models that have favorable scores.
3. Align compounds to a pharmacophore model and view the alignment.
4. Modify the features and constraints of a 3D query generated from a pharmacophore model.
5. Conduct database searches and assess the enrichment factor for queries.

Modules Used

SYBYL/Base, GALAHAD, GASP and UNITY.

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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