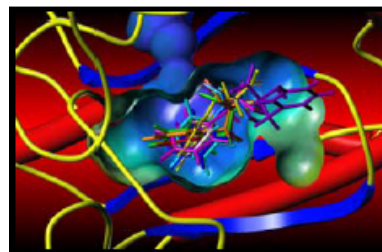


## VIRTUAL SCREENING

This course concentrates on both ligand-based and structures-based virtual screening of molecules. When the receptor structure is not known, a set of active ligands is aligned, and the aligned set of compounds is used as a similarity template to find other molecules with similar shapes and placement of features. When the receptor structure is known, ligands are screened by docking them into the receptor.



### Who Should Attend

Chemists and biologists who screen large sets of compounds for lead identification.

### Requirements

Before attending this course, participants should be able to perform the following tasks in SYBYL: Manipulate molecules with a mouse, create molecular spreadsheets, add columns to molecular spreadsheets, display structures from molecular spreadsheets, and prepare protein-ligand complexes. These topics are covered in the course [Receptor-Ligand Modeling for New Modelers](#).

### What You Will Learn

- ▶ Use similarity to find promising ligands when no receptor structure is available.
- ▶ Use docking to find promising ligands when a receptor structure is available.
- ▶ Increase the percentage of actives in your datasets by eliminating poorly binding compounds.

### Course Topics

#### Screen Ligands without a Receptor Structure

- ▶ Create Template for Alignment
- ▶ Align Ligands to Template

#### Screen Ligands Using a Receptor Structure

- ▶ Display Binding Site
- ▶ Dock Multiple Ligands
- ▶ View Docking Results

## Course Objectives

1. Create a template of aligned active compounds to be used for screening purposes.
2. Identify compounds with the most favorable scores when aligning to a template.
3. Display the binding site of a ligand-receptor complex with hydrogen bonds indicated between the ligand and the receptor.
4. Dock a set of molecules into a defined receptor site.
5. View poses of docked ligands in a receptor site, and identify the compounds with the most favorable scores.

## Modules Used

SYBYL/Base, Biopolymer, CSCORE, Surflex-Dock, and Surflex-Sim.

## Course Length

1 day

## Schedule and Registration

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

[www.tripos.com/training](http://www.tripos.com/training)

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