Reaction Searching

This module introduces strategies and techniques for reaction searching based on structural features, desired chemical transformations, or associated data. Participants practice a variety of search strategies culminating in a workshop to optimize a published reaction scheme. This module uses the Reaction Browser application. A half-day version is offered to transition users from previous reaction searching applications to the Reaction Browser 2.0.

Course Objectives

The participant will be able to:

- Search for reactions using substructures of reaction components
- Specify stereochemical requirements in reaction queries
- Retrieve reactions that involve structurally similar molecules and/or chemically similar transformations
- Apply logical operators to search criteria
- View all reactions within the same scheme or individual path
- Cluster hit lists
- Search for reactions based on text or numeric data

Prerequisites

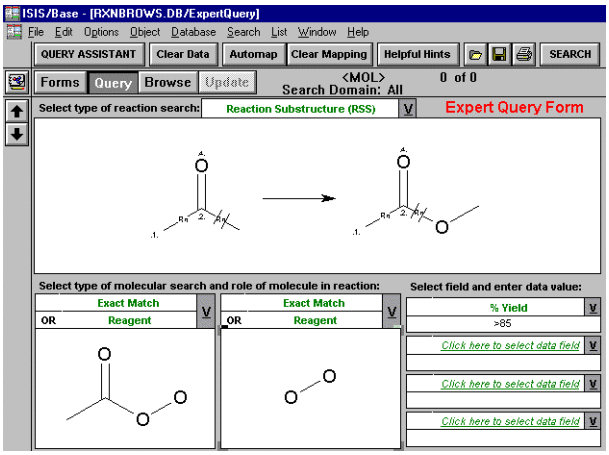
Drawing Molecules

Course Length

1 day

Examples from the Class

Searching with the Expert Query form



Clustering a hit list