

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

The screenshot shows the ISIS/Base Expert Query form. At the top, it displays the title "ISIS/Base - [RXNBROWS.DB/ExpertQuery]" and a menu bar. Below the menu bar are buttons for "QUERY ASSISTANT", "Clear Data", "Automap", "Clear Mapping", "Helpful Hints", and "SEARCH". The main area shows a search domain of "<MOL>" with "0 of 0" results. The search type is set to "Reaction Structure (RSS)". A chemical reaction scheme is displayed in the center, showing a ketone reacting to form an enol ether. Below the reaction, there are two sections for molecular search criteria. The first section is labeled "Select type of molecular search and role of molecule in reaction:" and contains two "Exact Match" criteria for "Reagent". The second section is labeled "Select field and enter data value:" and contains three criteria for "% Yield" with a value of ">85".

Clustering a hit list

The screenshot shows the ISIS/Base Summary window. At the top, it displays the title "ISIS/Base - [RXNBROWS.DB/Summary]" and a menu bar. Below the menu bar are buttons for "Main List", "Scheme", "Derivs/Paths", "Examples", "CLUSTER", "Cluster #", and "View Scheme". The main area shows a hit list with columns for "Ref. lib", "Cluster #", "Item #", and "Variation". The first entry is "Ref. lib 95.1.1" with "Cluster # 1" and "Item # 1". The variation is "Wang, K. K.; Chu, K.-H.; J Org Chem [JOCEAH] 1992, 57, 5175". Below the hit list, there is a "Literature Reference" section with the following text: "Brown, C. A.; Yamashita, A.; J Chem Soc, Chem Commun 1976, 994". A "Select Clustering Options" dialog box is open, showing a list of fields to cluster on: "Article", "Rxn Class (Broad)", "Rxn Class (Medium)", "Rxn Class (Narrow)", "Reagent (Fmla)", "Solvent (Fmla)", "Author", "Journal", and "Journal Year". The "Cluster entire list" option is selected. There are "Uncluster" and "Cluster" buttons at the bottom of the dialog box.