

Searching Local Databases

This module presents techniques for searching local ISIS/Base databases. Participants search molecule and reaction databases using both structure and data queries. Participants learn how to sort search results, print records, and incorporate structures and data into word-processed reports.

Course Objectives

The participant will be able to:

- ◆ Retrieve molecules based on molecular formula, full structure match, and substructure search
- ◆ Retrieve reactions based on the substructures of component molecules
- ◆ Retrieve molecules and reactions based on associated text and numeric data, such as ID number, chemical properties, and reaction conditions
- ◆ Sort and save search results, and combine the results from different searches
- ◆ Print structures and data
- ◆ Copy and paste structures and data into a word-processing document

Prerequisites

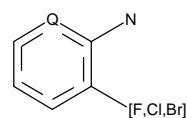
Drawing Molecules

Course Length

1/2 day

Examples from the Class

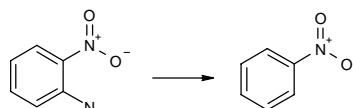
Molecule substructure query features



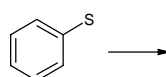
Query Atoms		Query Bonds	
A	any atom except H	Any	any type of bond
Q	any atom except H or C	Aromatic	aromatic bond
List	any atom on the list	S/D	single or double bond
Not List	any atom except those on the list		

Reaction substructure search queries

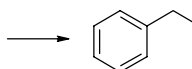
Both reactant and product constraint



No product constraint



No reactant constraint



Data search queries

Molecular Weight
between 150 180

Sample hits	Rules
175.9 151.2	BETWEEN specifies a range