

# Molecule Searching

This module teaches the new ISIS/Base user how to search for compounds based on structural features and desired chemical or biological properties. Participants practice a variety of search strategies by searching the Available Chemicals Directory. This module is available in the standard ISIS/Base version or the ACD Finder version.

## Course Objectives

The participant will be able to:

- ◆ Represent chemical questions as structure queries and conduct substructure, flexmatch, and similarity searches
- ◆ Retrieve molecules based on associated data, such as ID number, molecular formula, name, or other data values
- ◆ Sort and save search results, and combine results from different searches
- ◆ Print structures and data, or copy and paste structures and data to a word-processing program

## Prerequisites

Drawing Molecules

## Course Length

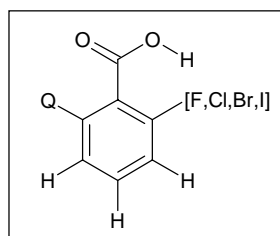
1 day

## Editions Available

- ◆ Standard ISIS/Base
- ◆ ACD Finder

## Examples from the Class

### Substructure searching



- Hydrogens prevent esters and substitution at 3-, 4-, and 5-positions
- Q atom allows any heteroatom at 2-position
- Atom list allows any halogen at 6-position

### Formula searching

- Syntax: <symbol><number> <symbol><number>...
- Separate the <symbol><number> units with a space

### Data searching

	Sample hits
<b>Molecular Weight</b> between 150 180	175.9 151.2
<b>Name</b> like "%benz%"	benzoic acid azobenzene
<b>ID Number</b> Like "B-88_5"	B-8805 B-8815