

# Rgroup Searching

This module teaches experienced ISIS/Base users how to create more complex and powerful substructure search queries. By using Rgroup queries, users can retrieve molecules that contain a common core structure but have different functional groups at specific sites.

## Course Objectives

The participant will be able to:

- ◆ Construct Rgroup queries that define a core structure, specific substitution sites, and the functional groups allowed at each site
- ◆ Control the number of times that a particular Rgroup can appear on the core structure
- ◆ Specify Rgroup members that contain Rgroups themselves (nested Rgroups)
- ◆ Control the presence of one Rgroup depending on the presence of another Rgroup (if/then logic)

## Prerequisites

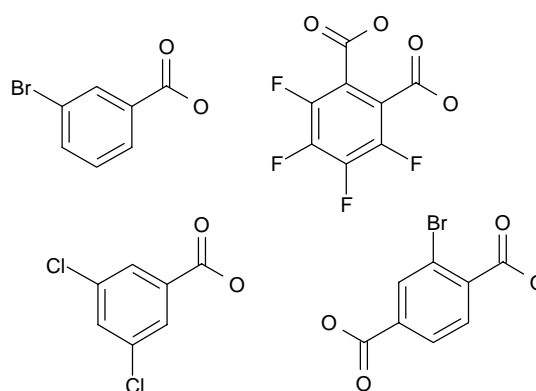
Molecule Searching  
Drawing Molecules

## Course Length

1/2 day

## Examples from the Class

*How to retrieve phthalic acid or halogenated benzoic acid derivatives?*



*Using standard SSS queries, you would need three queries to specify the halogen derivatives and three more queries for the 1,2-, 1,3-, and 1,4-phthalic acids.*

*A single Rgroup query can represent all six combinations.*

