

## Retrieving Chemical Data

This module teaches the new user of ISIS for Microsoft Excel how to search for compounds based on structural features and desired chemical or biological properties. Participants practice a variety of search strategies on both local and remote databases and retrieve structures, text and numeric data, and substituents into an Excel worksheet.

### Course Objectives

The participant will be able to:

- ◆ Retrieve selected fields of data into an Excel worksheet
- ◆ Find database records based on specific criteria
- ◆ Represent chemical questions as structure queries and conduct substructure, similarity, and Rgroup searches
- ◆ Exchange data with ISIS/Base users and with other software applications

### Prerequisites

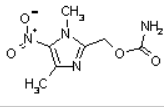
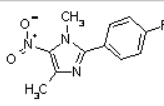
Drawing Molecules

### Course Length

1 day

### Examples from the Class

#### Structure and data table

1	A	B	C	D	E
ID	Structure	Mol.wt	Bio Act	Mutagenicity	
2	000101		214.18	5.33	2
3	000102		235.22	4.37	15

#### Query to search two data fields

**Search Chem**

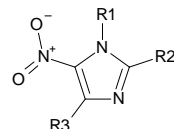
Search domain: All (160 records)

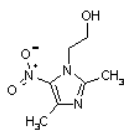

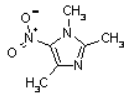

List name: Chem-1  Temporary

Search criteria:

Act_Class	Bio_Act
Unsorted	Unsorted
like "%Hill%"	> 4.5

#### Rgroup table



	A	B	C	D	E
5	000103			X <sub>2</sub> -CH <sub>3</sub>	H <sub>3</sub> C X <sub>3</sub>
6	000104			X <sub>2</sub> -CH <sub>3</sub>	H <sub>3</sub> C X <sub>3</sub>