Creating Structure-Activity Relationship Tables

This module teaches ISIS/Base users how to transfer structures and data from ISIS/Base into a Microsoft Excel spreadsheet, where the data can be sorted and graphed. Participants learn how to create different table formats and how to display compounds as whole structures, or as a core structure and a table of substituents.

Course Objectives

The participant will be able to:

- Create Excel spreadsheets that contain structures and related data
- Sort the structures and data in the spreadsheet
- Create spreadsheets of core structures and their Rgroup substituents
- Use text abbreviations to represent substituents

Prerequisites

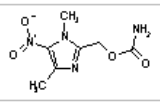
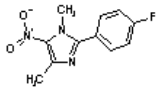
Molecule Searching
Drawing Molecules

Course Length

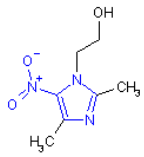
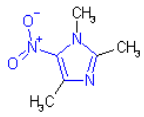
1/2 day

Examples from the Class

Structure and data table

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

Rgroup table

	A	B	C	D	E
1	**ID**	**Structure map**	**R1**	**R2**	**R3**
2	000103				
3	000104				

Substituent table

	A	B	C	D
1	**ID**	**R1**	**R2**	**R3**
2	000101	-CH3	-CH2OC(O)NH2	-CH3
3	000102	-CH3	-Ph(4-F)	-CH3
4	000103	-CH2CH2OH	-CH3	-CH3
5	000104	-CH3	-CH3	-CH3
6	000105	-CH3	-CH3	-CH2CH2OH
7	000106	-CH3	-CH2OH	-CH2CH2OH