



ICM-Chemist How-To Guide

Version 3.6-1g

Last Updated 12/01/2009

ICM-Chemist

HOW TO IMPORT, SKETCH AND EDIT CHEMICALS

How to access the ICM Molecular Editor.

1. Click here

ICM Molecule Editor [new file *] Acebutolol

File Edit View Templates Help

The screenshot shows the ICM Molecule Editor window with the chemical structure of Acebutolol. The structure is a benzene ring with a propyl chain attached to one carbon, a propyl chain attached to another carbon, and a propyl chain attached to a third carbon. The propyl chain on the right is highlighted with a blue arrow pointing to the nitrogen atom. The properties table on the right lists various molecular descriptors.

Name	Value
1 Formula	C18H27NO3
2 Smiles	CC(C)NCCOC1=CC=C(C(=O)C)N1C(=O)CC
3 IUPAC	1-(4-((2S)-2-(2S)-2-methylpropylamino)ethoxy)phenyl)propan-1-one
4 MolWeight	336.42
5 HBA	5
6 HBD	3
7 RotB	11
8 DrugLikeness	0.9
9 MolHfi	-17
10 MolLogP	1.6
11 MolLogS	-3.7
12 MolPSA	72
13 Volume	358
14 Bad Groups	
15 Groups	Ph Am Ket Eth Hyc

2. Start sketching

```
Startup> Loading aliases...
Startup> Loading modules.._macro_rebel
...ICM startup file executed...
icm/def>
```



no selection

How to sketch chemicals in the ICM Molecular Editor.

1c. Click Templates menu for even more templates

1a. Select atoms and bonds here

ICM Molecule Editor [new file *] Acebutolol

File Edit View Templates Help

Acebutolol

Name	Value
1 Formula	C18H27NO5
2 Smiles	CC(C)NCCOC(O)c1ccc(cc1)C(=O)NCC(=O)CC
3 IUPAC	1-(4-((2S)-2-(2-(2S)-2-methylaminoethoxy)acetyl)phenyl)ethanone
4 MolWeight	338
5 HBA	5
6 HBD	3
7 RotB	11
8 DrugLikeness	0.9
9 MoldHi	-17
10 MolLogP	1.6
11 MolLogS	-3.7
12 MolPSA	72
13 Volume	358
14 Bad Groups	
15 Groups	Phenyl Amino Ketone Ether Hydroxyl

1b. Select rings here

2. Click on the canvas to start sketching

```
Startup> Loading aliases...
Startup> Loading modules..._macro_rebel
...ICM startup file executed...
icm/def>
```

no selection

tables (1 item)

example 1 rows 2 cols 0 he

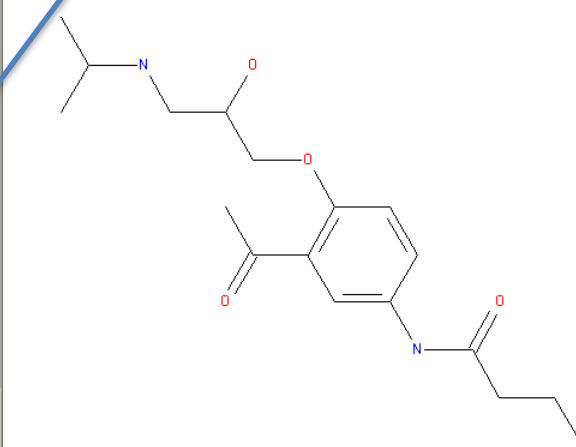
mol	NAME
racemic	Acebutolol

2. New chemical spreadsheet

ICM Molecule Editor [new file *] Acebutolol

File Edit View Templates Help

Acebutolol



Name	Value
1 Formula	C18H27NO3
2 Smiles	CC(=O)Nc1ccc(OCC(C)N)cc1C
3 IUPAC	1-(4-((S)-1-((S)-1-hydroxypropan-2-ylamino)ethyl)phenoxy)propan-2-one
4 MolWeight	336.42
5 HBA	5
6 HBD	3
7 RotB	11
8 DrugLikeness	0.9
9 MoldHf	-17
10 MolLogP	1.6
11 MolLogS	-3.7
12 MolPSA	72
13 Volume	356
14 Bad Groups	
15 Groups	Phe Am Am Ket Eth Hyc

1. Click here and enter when prompted the name of spreadsheet and chemical name.

How to save a 2D sketch into a chemical spreadsheet.

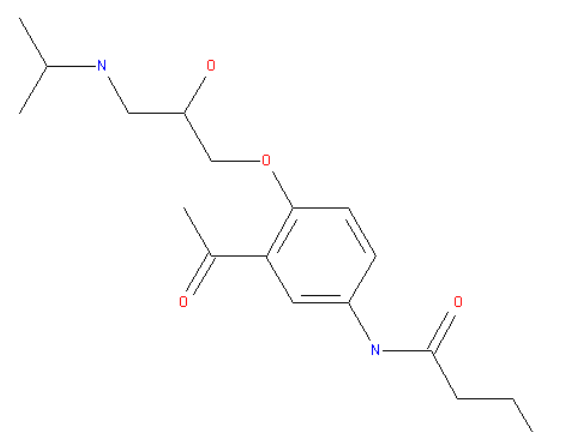
```
icm/def> delete myTable
icm/def> read table mol name=Name("example",unique) input =s_out
Info> table 'example' ( 0 headers, 1 arrays[1] ) created
icm/def>
```

1. Click here

ICM Molecule Editor [new file *] Acebutolol

File Edit View Templates Help

Acebutolol



The image shows the chemical structure of Acebutolol, a beta-blocker. It consists of a central benzene ring with a propylamino group (-NHCH2CH2CH3) at the para position, an isopropylamino group (-NHCH(CH3)2) at the other para position, and a 2-(4-isobutylphenoxy)ethyl group (-OCH2CH2OC6H4CH2CH2CH3) at the meta position.

Name	Value
1 Formula	C18H27NO3
2 Smiles	CC(C)NCCOC1=CC=C(C(=O)NCCC)C=C1
3 IUPAC	1-(4-((2-(4-isobutylphenoxy)ethyl)oxy)phenyl)propan-1-amine
4 MolWeight	336
5 HBA	5
6 HBD	3
7 RotB	11
8 DrugLikeness	0.9
9 MoldHi	-17
10 MolLogP	1.6
11 MolPSA	-3.7
12 MolPSA	72
13 Volume	358
14 Bad Groups	
15 Groups	Ph Am Am Ket Eth Hyc

Note: More save options can be accessed by going to File/Save as...

```
Startup> Loading aliases...
Startup> Loading modules.._macro_rebel
...ICM startup file executed...
icm/def>
```

no selection

Edit Add Smile

ICM Molecule Editor [new file *] Acebutolol

File Edit View Templates Help

- Undo Ctrl+Z
- Redo Ctrl+Y
- Copy Ctrl+C
- Copy as SMILES
- Cut Ctrl+X
- Paste Ctrl+V
- Select All Ctrl+A
- Flip X Ctrl+Shift+X
- Flip Y Ctrl+Shift+Y
- Zoom In Ctrl++
- Zoom Out Ctrl+-
- Center Ctrl+T
- Assign 2D Coordinates
- Delete Del
- Add Smiles Ctrl+M
- Edit Name
- Edit Comment

Name	Value
1 Formula	C18 H28 N2 O4
2 Smiles	CCCC(NC1=CC=C(C=C1)O)
3 IUPAC	1-(3-acetyl-4-(2-hydroxy-3-
4 MolWeight	336.2049
5 HBA	5
6 HBD	3
7 RotB	11
8 DrugLikeness	0.91
9 MoldHf	-170.17
10 MolLogP	1.68
11 MolLogS	-3.77
12 MolPSA	72.22
13 Volume	358.44
14 Bad Groups	
15 Groups	Phenyl Amide Amine Ketone (Carbonyl) Ether Hydroxyl

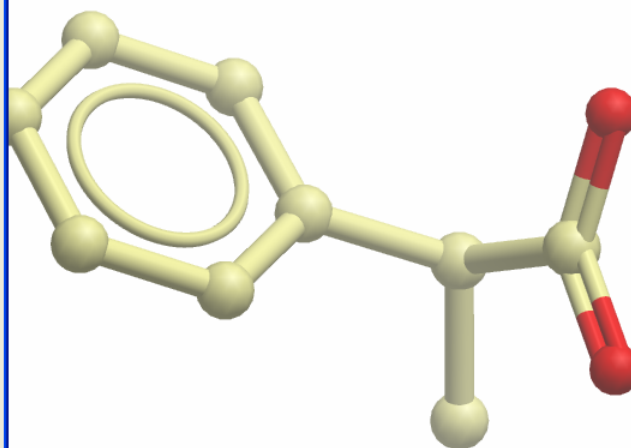
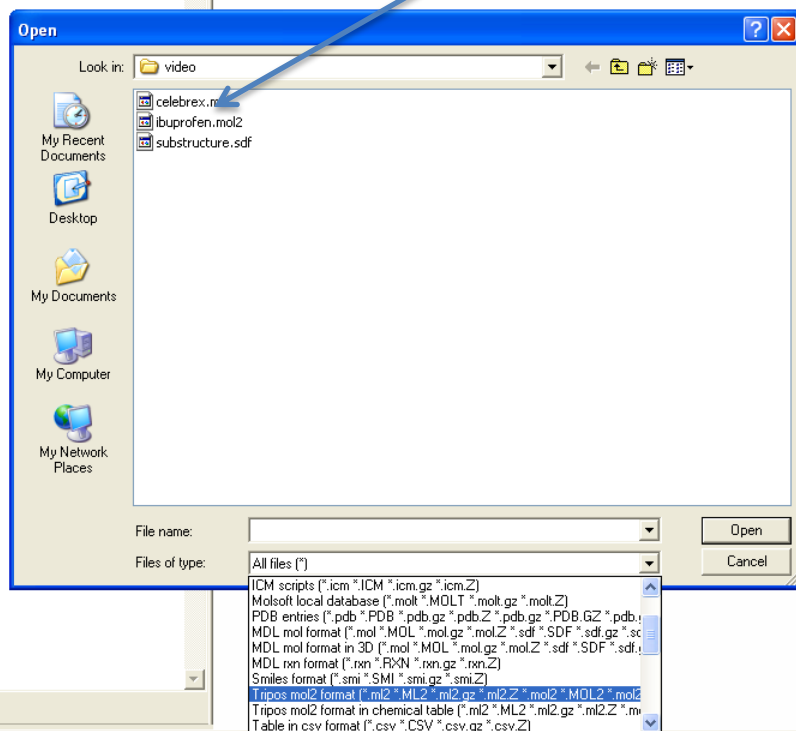
How to use SMILES strings to sketch a chemical.

Example of a SMILES string C1C=CC=CC=1

```
icm/def> read table mol name=Name("example",unique) input =s_out
Info> table 'example' ( 0 headers, 1 arrays[1]) created
icm/def> delete example
icm/def>
```

1. File/Open

2. Locate file



mol	NAME	molid	molWeight	molLogP	molLogS	molPSA	smiles
	C10H8N2O		392196	172.1	1.511	-2.531	28.11 NIC=C1C
	C12H12N2O		1604910	200.1	1.625	-3.214	28.13 C1C=NN(C=C1)C(C=C(C=C1))C(=O)C

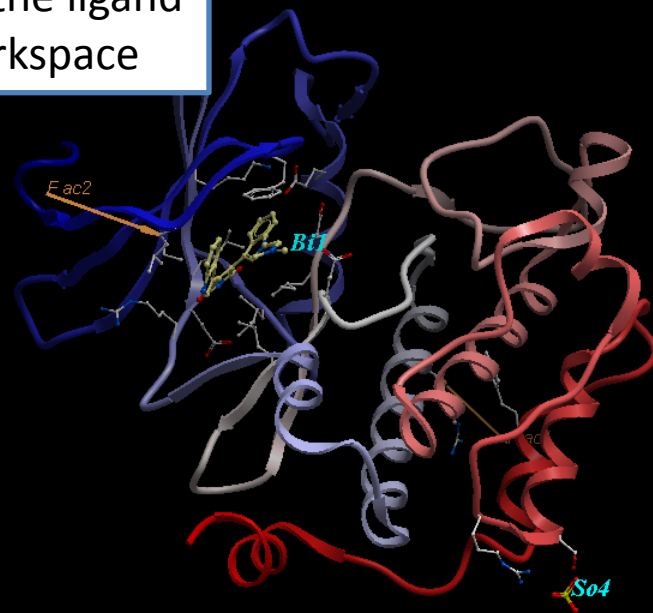
- SDF and mol files will open in chemical spreadsheet format.
- Mol2 will open up in the graphical display.

How to extract a 2D sketch of a ligand in complex with a PDB structure.

1. Click here to search the PDB

2. Right click on the ligand in the ICM workspace

3. Click Edit/ Edit Compound and the ICM Molecular Editor will be displayed.



```
Info> PDB index loaded from C:/Program Files/Molsoft LLC/Molsoft ICM-Chemist_4/data/inx/PDB.tab
Warning> [375] 32 missing SEQRES residues (met ..) before pro [a 33 ]
icm/1xws> editSelection a_1xws.abi1 yes no no
Info> tmp_p_s_totz_terms_s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/1xws> editSelection a_1xws.abi1 yes no no
Info> tmp_p_s_totz_terms_s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/1xws>
```

ICM-Chemist

WORKING WITH CHEMICAL SPREADHSHEETS

How to add columns into a chemical spreadsheet.

1. Right click on a column header and select "insert column".

4. Select the argument (s)

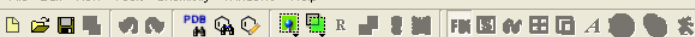
2. Click the main type of argument you want to add.
E.g. mol for chemical functions.

3. Press the "Add To List" button

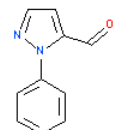
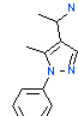
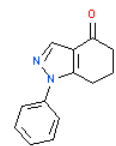
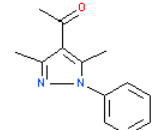
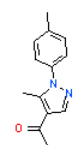
Insert Column dialog box showing the "Function" dropdown set to "Multiple Functions", the "Main argument" dropdown set to "mol", and the "Add To List" button highlighted.

Function	Name	Category	Description
<input checked="" type="checkbox"/> MolWeight(mol)	molWeight	Chemical	Molecular weight
<input type="checkbox"/> MolFormula(mol)	molFormula	Chemical	Chemical formula, e.g. C2H6O
<input type="checkbox"/> IupacName(mol)	iupacName	Chemical	IUPAC nomenclature name
<input type="checkbox"/> MolLogP(mol)	molLogP	Chemical	Octanol water partition, -Log(C _{ow} /C _w)
<input type="checkbox"/> MolLogS(mol)	molLogS	Chemical	Water solubility -Log(C _{aggr})
<input type="checkbox"/> MolPSA(mol)	molPSA	Chemical	Polar surface area
<input type="checkbox"/> MolVolume(mol)	molVolume	Chemical	Molecular volume
<input type="checkbox"/> MolDf(mol)	molDf	Chemical	Heats of formation from elements
<input type="checkbox"/> DrugLikeness(mol)	drugLikeness	Chemical	Empirical drug-likeness
<input type="checkbox"/> Smiles(mol, mode='asis')	smiles	Chemical	SMILES/SMARTS: string notation o...
<input type="checkbox"/> BadGroups(mol)	badGroups	Chemical	Unwanted or reactive chemical func...
<input type="checkbox"/> Nof_Atoms(mol, atom='')	nof_Atoms	Chemical	Number of atoms
<input type="checkbox"/> Nof_Molecules(mol)	nof_Molecules	Chemical	Number of individual molecules
<input type="checkbox"/> Nof_Fragments(mol, smarts='', type=)	nof_Fragments	Chemical	Number of SMARTS pattern occur...
<input type="checkbox"/> Nof_Chirals(mol, type='any')	nof_Chirals	Chemical	Number of chiral centers, R,S, or (R)
<input type="checkbox"/> Nof_Rings(mol)	nof_Rings	Chemical	Number of rings in the SSSR

```
Info> tmpm,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
```



no selection
 tables (1 item)
 substructure 10000 rows 9 cols 0 header

	mol	NAME	molid	molwei					
1		C10H8N2O	39210	17	N(C=C1)C=O)(N=C1)C(=CC1)C=CC=1				2
2			1604910	20	C1(C=NN(C=1)C1C=CC=CC=1)C(=O)C				2
3		racemic C7H8N2	1604911	20	N(C1C)N=CC=1(C(N)C)C1=CC=CC=C1				2
4		C13H12N2O	510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1)C)C2C=CC=CC=2)C(=O)CC1	1
5		C13H14N2O	1526405	214.1	1.886	-3.387	28.48	N(N=C(C1C(=O)C)C)(C=1)C1=CC=CC=C1	2
6		C13H14N2O	1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1)C)C2C=CC(=CC=1)C)C(=O)C	2

1. Right click on a column header and select "Sort"

How to sort a column(s) in a chemical spreadsheet.

- molWeight (real)
- Hide Column(s)
- Freeze Column
- Paste Column(s) Ctrl+V
- Edit Mode
- Rename Column...
- Delete Column(s)
- Insert Column...
- Add External Columns...
- Column Statistics...
- Sort**
- Filter
- Learn...
- Group by Column...
- Format...

```
Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
```

How to change the view of a chemical spreadsheet – form, table and grid.

1. For grid view select the columns you wish to display in the grid. Click on the column header to select (click and hold CTRL key for non-contiguous selections or SHIFT key for range)

2a. Right click anywhere on the spreadsheet and select "Table View"

2b. Or you can use the buttons here.

	NAME	molid	molw	molv	molc	molr	molh	molm
1	C10H8N2O	392196	172.1	1.511	-2.531	28.11	N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1	2
2	C12H12N2O	1604910	200.1					2
3	racemic C12H15N3	1604911	201.1	0				2
4								
5								
6	C13H14N2O	1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1)C1C=CC(=CC=1)C)(=O)C	2
7								
8								
886							N(N=C(C1C(=O)C)C)(C=1)C1=CC=CC=C1	2

```

Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
    
```

How to copy, cut, and paste columns and rows in a chemical spreadsheet.

mol	NAME	molWt	molWt	molWt	molWt	molWt	molWt	molWt	molWt	molWt
1	C10H8N2O	392.198	172.1	1.511	-2.531	28.11	N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1			2
	C12H12N2O	198.198	172.1	1.511	-2.531	28.11	C1=C(N)C(=O)C1C(=CC=CC=C1)C(=O)C			2
	C12H15N3						CC=1C(N)C1=CC=CC=C1			2
	C3H12N2O	510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1C1)C2C=CC=CC=2)C(=O)CC1			1
	C13H14N2O	1526405	214.1	1.886	-3.387	28.48	N(N=C(C1C(=O)C)C)(C=1C)C1=CC=CC=C1			2
			214.1	2.026	-3.669	28.13	C1(C=NN(C=1C)C1C=CC(=CC=1)C)C(=O)C			2

1. Select a column or row by clicking on the header. (click and hold CTRL key for non-contiguous selections or SHIFT key for range)

2b. To copy, cut and paste rows – right click here on a selected column(s)

2a. To copy, cut and paste rows – right click here on a selected row(s)

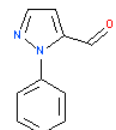



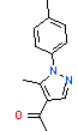
```

Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
    
```

How to hide rows in a chemical spreadsheet.

1. Select row(s) (click and hold CTRL key for non-contiguous selections or SHIFT key for range)

2. Right click here and select "Hide Rows"

mol	NAME	molid	molWt	molWt	molWt	molWt	molWt	molWt	molWt	molWt
	C10H8N2O		392196	172.1	1.511	-2.531	28.11	N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1		2
	racemic C12H15N3		1604911	201.1	0.5295	-3.096	34.66	N(C1C)N=CC=1C(N)C1=CC=CC=C1		2
	C13H12N2O		510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1C1)C2C=CC=CC=2)C(=O)CC1		1
	C13H14N2O		1526405	214.1	1.886	-3.387	28.48	N(N=C(C1C(=O)C)C)(C=1C)C1=CC=CC=C1		2
	C13H14N2O		1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1C)C1C=CC(=CC=1)C)C(=O)C		2

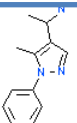
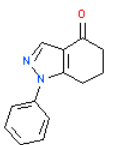
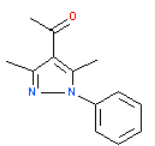
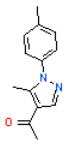
```
Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
```

How to hide columns in a chemical spreadsheet.

1. Select column(s) (click and hold CTRL key for non-contiguous selections or SHIFT key for range)

2. Right click here and select "Hide Column(s)"

no selection
tables
subst

	NAME	molid							
	C13H16N2O		2.531	28.11		N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1		2	
	C12H12N2O		3.214	28.13		C1(C=NN(C=1)C1C=CC=CC=1)C(=O)C		2	
3			3.096	34.66		N(C1C)N=CC=1C(N)C1=CC=CC=C1		2	
4		C13H12N2O	510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1)C)C2C=CC=CC=2)C(=O)CC1	1
5		C13H14N2O	1526405	214.1	1.886	-3.387	28.48	N(N=C(C1C(=O)C)C)(C=1)C1=CC=CC=C1	2
6		C13H14N2O	1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1)C)C=CC(=CC=1)C)C(=O)C	2

- molid (int)
- Hide Column(s)**
- Freeze Column
- Column Histogram
- Copy Column(s) Ctrl+C
- Cut Column(s)
- Paste Column(s) Ctrl+V
- Edit Mode
- Rename Column...
- Delete Column(s)
- Insert Column...
- Add External Columns...
- Column Statistics...
- Sort
- Filter
- Learn...
- Group by Column...
- Format...

```
Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
```


How to save a chemical spreadsheet in sdf format.

1. Right click on the spreadsheet header tab

2. Select "Save As.."

	NAME	molid	molWeight						
1	C10H8N2O	392196	172.1	1.511	-2.531	28.11	<chem>N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1</chem>	2	
2	C12H12N2O	1604910	200.1	1.625	-3.214	28.13	<chem>C1(C=NN(C=1)C1C=CC=CC=1)C(=O)C</chem>	2	
3						-3.096	34.66	<chem>N(C1C)N=CC=1C(N)C1C=CC=CC=C1</chem>	2
4	C13H12N2O	510572	212.1	1.912	-3.61	27.46	<chem>C1(C=NN(C=1)C2C=CC=CC=2)C(=O)CC1</chem>	1	
5	C13H14N2O	1526405	214.1	1.886	-3.387	28.48	<chem>N(N=C(C1C(=O)C)C)C(=1)C1=CC=CC=C1</chem>	2	
6	C13H14N2O	1604831	214.1	2.026	-3.669	28.13	<chem>C1(C=NN(C=1)C1C=CC(=CC=1)C)C(=O)C</chem>	2	

```
Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
```

How to export a chemical spreadsheet into Excel.

1. Right click on the spreadsheet header tab

2. Select "Export To Excel"

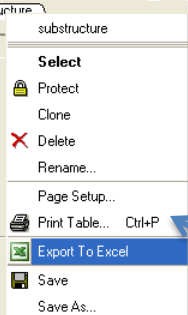
	NAME	molid	molWeight						
1	C10H8N2O		392196	172.1	1.511	-2.531	28.11	N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1	2
2	C12H12N2O		1604910	200.1	1.625	-3.214	28.13	C1(C=NN(C=1)C1C=CC=CC=1)C(=O)C	2
3								N(C1C)N=CC=1C(N)C1C=CC=CC=1	2
4	C13H12N2O		510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1)C)C2C=CC=CC=2)C(=O)CC1	1
5	C13H14N2O		1526405	214.1	1.886	-3.387	28.48	N(N=C(C1C(=O)C)C)(C=1)C1=CC=CC=C1	2
6	C13H14N2O		1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1)C1C=CC(=CC=1)C)C(=O)C	2

```
Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>
```



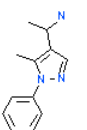
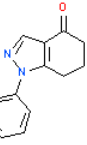
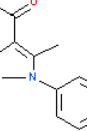
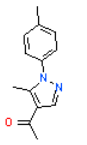
table: 10000 rows, 9 columns



1. Right click on the spreadsheet header tab



2. Select "Print Table"

	substructure	NAME	molid	molWeight	molLogP	molLogS	molPSA	smiles	nof RotB
1		C10H8N2O		392196	172.1	1.511	-2.531	28.11 N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1	2
2		C12H12N2O		1604910	200.1	1.625	-3.214	28.13 C1(C=NN(C=1)C1C=CC=CC=1)C(=O)C	2
3								N(C1C)N=CC=1(C(N)C)C1=CC=CC=C1	2
4		C13H12N2O		510572	212.1	1.912	-3.61	27.46 C1(C=NN(C=1)C)C2C=CC=CC=2)C(=O)CC1	1
5		C13H14N2O		1526405	214.1	1.886	-3.387	28.48 N(N=C(C1C(=O)C)C)(C=1)C1=CC=CC=C1	2
6		C13H14N2O		1604831	214.1	2.026	-3.669	28.13 C1(C=NN(C=1)C1C=CC(=CC=1)C)C(=O)C	2

All

```

Info> tmp_p,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/ixws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"
Info> table 'substructure' ( 0 headers, 8 arrays[10000]) created
icm/def>

```

binding_data Molsoft Chemist 3.6-1g [NewProject *] (1 table)

File Edit View Tools Chemistry Windows Help

no selection
tables (1 item)
binding_data 64 rows 11 columns

1. Right click on the column header you wish to filter

2. Select Filter Custom or From List...

mol	ki uM	molWeight (real)	molVolume	molLogP	molWeight	molVolume	molLogP	molWeight	molVolume	molLogP
<chem>C1=CC=C(C=C1)C2=NC=NC=C2</chem>	6.375	303	1.925	-4.668	52.56	222.2	98.47	0.007176	3	2
<chem>C1=CC=C(C=C1)C2=NC=NC=C2</chem>	6.525	373.1	4.255	-5.809	42.92	310.4	79.3	0.6977	3	1
<chem>C1=CC=C(C=C1)C2=NC=NC=C2</chem>	6.6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3	1
<chem>C1=CC=C(C=C1)C2=NC=NC=C2</chem>	6.675	331	2.759	-5.176	42.63	260.4	95.06	0.2819	3	1

How to filter columns in a chemical spreadsheet (1).

```
Info> 1 column 'molLogS' added to table 'binding_data'  
icm/def> add column binding_data function="MolLogP(mol)" index=3 name="molLogP" append format="%.2f"  
Info> 1 column 'molLogP' added to table 'binding_data'  
icm/def> add column binding_data function="MolWeight(mol)" index=3 name="molWeight" append format="%.3f"  
Info> 1 column 'molWeight' added to table 'binding_data'  
icm/def>
```

How to filter columns in a chemical spreadsheet (2).

The screenshot shows the Molsoft Chemist 3.6-1g interface. The main window displays a table with columns: mol, ki uM, molWeight, molLogP, molLogS, molPS, and several unlabeled columns. The 'molWeight' column is highlighted with a blue box and a callout: "2. This symbol indicates the column is filtered". A dialog box titled "Custom filter on 'molWeight'" is open, showing two conditions: "is greater than 300" and "is less than 600". A callout "1. Enter filters" points to the "600" value. The bottom console shows the following commands:

```
Info> 1 column 'molLogS' added to table 'binding_data'  
icm/def> add column binding_data function="MolLogP(mol)" index=3 name="molLogP" append format="%.2f"  
Info> 1 column 'molLogP' added to table 'binding_data'  
icm/def> add column binding_data function="MolWeight(mol)" index=3 name="molWeight" append format="%.3f"  
Info> 1 column 'molWeight' added to table 'binding_data'  
icm/def>
```

mol	ki uM	molWeight	molLogP	molLogS	molPS						
<chem>C1=NC2=C(N1)N=CN=C2</chem>	471	471	4.775	-7.196	42.74	336	134.4	0.05017	3	1	
<chem>C1=NC2=C(N1)N=CN=C2</chem>	6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3	1	
<chem>C1=NC2=C(N1)N=CN=C2</chem>	6.375	303	1.925	-4.668	52.56	222.2	98.47	0.007176	3	2	
<chem>C1=NC2=C(N1)N=CN=C2</chem>	6.525	600	3	3	3	3	3	3	3	1	
<chem>C1=NC2=C(N1)N=CN=C2</chem>	6.6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3	1	
<chem>C1=NC2=C(N1)N=CN=C2</chem>	6.675	331	2.759	-5.176	42.63	260.4	95.06	0.2819	3	1	
<chem>C1=NC2=C(N1)N=CN=C2</chem>	7.275	345.1	3.102	-5.125	41						

2. This symbol indicates the column is filtered

Custom filter on 'molWeight'

is greater than 300

And Or

is less than 600

Case Sensitive

OK Cancel

1. Enter filters

To remove a filter right click on the column that is filtered and select Filter/Clear

1. Right click on the mol column

2. Select Chemical Find and Replace

How to use find and replace in a chemical spreadsheet.

3. Use the editor to sketch the group you want to find

4. Use the editor to sketch the group you want to replace with

You can also do text find and replace by right clicking anywhere on the table and select Find and Replace.

mol

- mol
- Hide Column(s)
- Freeze Column
- Copy Column(s) Ctrl+C
- Cut Column(s)
- Paste Column(s) Ctrl+V
- Edit Mode
- Rename Column...
- Set Compound Names From ...
- Delete Column(s)
- Color Structure By
- Clear Selection Color
- Insert Column...
- Add External Columns...
- Column Statistics...
- Sort
- Filter
- Group by Column...
- Assign 2D Coordinates...
- Rotate for Best Fit
- Split Into Fragments
- Chemical Find and Replace...
- Set 3D Browse Mode
- Chemical View Options...
- Format...

Chemical Find and Replace

Search For: Br [Br]

Replace With: Cl [Cl]

Find Find All Replace Replace All Help Close

```

Info> 1 column 'molLogS' added to table 'binding_data'
icm/def> add column binding_data function="MolLogP(mol)" index=3 name="molLogP" append format="%.2f"
Info> 1 column 'molLogP' added to table 'binding_data'
icm/def> add column binding_data function="MolWeight(mol)" index=3 name="molWeight" append format="%.3f"
Info> 1 column 'molWeight' added to table 'binding_data'
icm/def>

```

How to mark and label rows in a chemical spreadsheet.

1. Select the row(s) you wish to label by clicking on the row number. Click and hold CTRL key for non-contiguous selections or SHIFT key for range.

2. Right click on the selected row and choose "Mark Selected Rows" Select a color label.

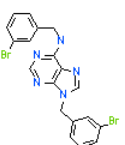
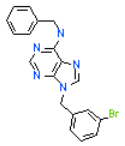
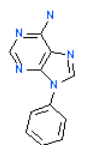
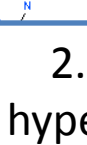
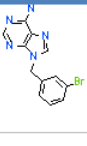
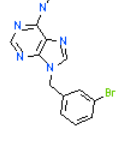
3. You can select marked (labeled) rows here.

The screenshot shows the Molsoft Chemist 3.6-1g interface with a spreadsheet titled 'binding_data'. The spreadsheet has columns: mol, ki_uM, molWeight, molLogP, molLogS, molPSI, and several unlabeled columns. Rows 5 and 6 are highlighted in blue. A context menu is open over row 5, showing options like 'Mark Selected Rows' (selected), 'Select Marked Rows', 'Copy Row(s)', 'Paste', 'Print Table...', and 'Export To Excel'. A sub-menu for 'Mark Selected Rows' is also open, showing color options: 1 (red), 2 (orange), 3 (green), 4 (blue), and 5 (magenta). The '0 No Label' option is also visible. Chemical structures are shown for the 'mol' column.

mol	ki_uM	molWeight	molLogP	molLogS	molPSI						
<chem>BrC1=CC=C(C=C1)N2C=NC(=C2)N</chem>	6	471	4.775	-7.196	42.74	336	134.4	0.05017	3	1	
					-6.126	42.74	314	128.1	0.07959	3	1
					-3.533	53.02	183.3	88.27	-0.3593	3	2
					-4.688	52.56					
<chem>BrC1=CC=C(C=C1)N2C=NC(=C2)N</chem>	6.6	311	2.206	-4.619	43.16	240.4	99.96	0.129	3	1	
<chem>BrC1=CC=C(C=C1)N2C=NC(=C2)N</chem>	6.675	331									

```
Info> 1 column 'molLogS' added to table 'binding_data'
icm/def> add column binding_data function="MolLogP(mol)" index=3 name="molLogP" append format="%.2f"
Info> 1 column 'molLogP' added to table 'binding_data'
icm/def> add column binding_data function="MolWeight(mol)" index=3 name="molWeight" append format="%.3f"
Info> 1 column 'molWeight' added to table 'binding_data'
icm/def>
```

no selection
 tables (1 item)
 binding_data 64 rows 12 col


	mol	ki uM	molWeight	molLogP	molLogS	molPSA	molVolume	molHf	drugLikeness	nof HBA	nof HBD	pdb
1		6		471	4.775					3		1abc
2		6		393.1	3.924					3		2abc
3		6		211.1				-0.3593		3		23abc
4		6.375		303				0.007176		3		24abc
5				373.1				0.6977		3		15abc
6		6.6		317	2.206	-4.615						16abc
		6.675		331	2.759	-5.176	42.63	260.4	95.06	0.2819	3	17abc

1. Right click on the column header and select "Format"

Column Format: pdb


Font

Bold Italic

Font Color 

Font Size

Background

Single Color 

Alignment

Default Left Right Center Justify

Hyper Link

Format

Display Name

OK Apply Cancel

2. Choose hyperlink type here

3. Click OK and the hyperlink will be generated

```
icm/def> binding_data.pdb[4] = "4abc"
icm/def> binding_data.pdb[5] = "5abc"
icm/def> binding_data.pdb[6] = "6abc"
icm/def> binding_data.pdb[7] = "7abc"
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1%1%1" name="" color="" "
```


no selection
 tables (1 item)
 binding_data 64 rows 12 cols

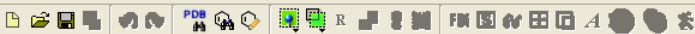
	mol	ki uM	molWeight	molLogP	molLogS	molPSA	molVolume	molHf	drugLikeness	nof HBA	nof HBD	pdb
1		6		4.71	4.775	-7.196	42.74	336	134.4	0.05017	3	11abc
		6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3		12abc
				1.1	1.376	-3.533	53.02	183.3	88.27	-0.3593	3	23abc
4				303	1.925	-4.668	52.56	222.2	98.47	0.007176	3	24abc
5				31.1	4.255	-5.809	42.92	310.4	79.3	0.6977	3	15abc
6				317						0.129	3	16abc
		6.675		331	2.759	-5.176	42.63	260.4	95.06	0.2819	3	17abc

1. Right click on the 2D chemical.

- binding_data
- Edit Cells by Double-click
- Table View
- Stored Views
- Find and Replace in Table Ctrl+F
- Color By
- Clustering...
- Learn...
- Analysis
- Columns Plot...
- Column Histogram...
- Row Selection
- Save/Export Image
- Edit Molecule...
- Query Molecule
- Chemistry
- Cell mol[2]
- Mark Row
- Select Marked Rows
- Copy 2D Molecule Ctrl+C**
- Paste Ctrl+V
- Print Table... Ctrl+P
- Export To Excel

2. Select "Copy 2D Molecule"

```
icm/def> binding_data.pdb[4] = "4abc"
icm/def> binding_data.pdb[5] = "5abc"
icm/def> binding_data.pdb[6] = "6abc"
icm/def> binding_data.pdb[7] = "7abc"
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1%1</a>" name="" color=""'
icm/def>
```



no selection
 tables (1 item)
 binding_data 64 rows 12 columns

	mol	ki uM	molWeight	molLogP	molLogS	molPS						
1			6	471	4.775	-7.196	42.74	336	134.4	0.05017	3	11abc
2			393.1	3.924	-6.126	42.74	314	128.1	0.07959	3	12abc	
3			6					88.27	-0.3593	3	23abc	
4		6.375					98.47	0.007176	3	24abc		
5		6.525	373.1	4.255	-5.809	42.92	310.4	79.3	0.6977	3	15abc	
6		6.6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3	16abc	
		6.675	331	2.759	-5.176	42.63	260.4	95.06	0.2819	3	17abc	

How to edit data inside a chemical spreadsheet.

1. Click here

2. Edit data by double clicking on the data.

```
icm/def> binding_data.pdb[4] = "4abc"
icm/def> binding_data.pdb[5] = "5abc"
icm/def> binding_data.pdb[6] = "6abc"
icm/def> binding_data.pdb[7] = "7abc"
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1%1</a>" name="" color=""
icm/def>
```

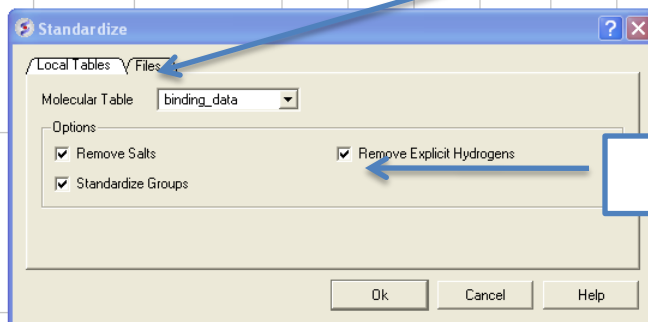
- Standardize...
- Annotate by Substructure...
- Predict
- Convert Smiles to 2D...
- Convert Structure to Smiles...
- 2D Depiction...
- Generate Tautomers...
- Convert To Racemic...
- Generate Stereoisomers...
- Align/Color By 2D Scaffold...
- Cluster Set
- Compare Two Sets...
- Merge Two Sets...
- Sort Table...
- Select Duplicates...
- Create/Modify Markush...
- Enumerate by Scaffold...
- R-Group Decomposition...
- Enumerate by Reaction...

1. Chemistry/Standardize

How to remove salts, explicit hydrogens and standardize chemical groups.

3. Select Files tab for batch mode

2. Select here



```

icm/def> binding_data.pdb[4] = "4abc"
icm/def> binding_data.pdb[5] = "5abc"
icm/def> binding_data.pdb[6] = "6abc"
icm/def> binding_data.pdb[7] = "7abc"
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1%1</a>" name="" color=""
icm/def>

```

How to calculate chemical properties in a spreadsheet.

1. Chemistry/Calculate Properties

Calculate Chemical Properties

Function: Function Multiple Functions

Arguments: Main argument: mol

New column location: Insert after before in-place at end column: mol

New column name: name

Add To List

Function	Name	Category	Description
<input checked="" type="checkbox"/> MolWeight(mol)	molWeight	Chemical	Molecular weight
<input checked="" type="checkbox"/> MolFormula(mol)	molFormula	Chemical	Chemical formula, e.g. C2H6O
<input type="checkbox"/> IupacName(mol)	iupacName	Chemical	IUPAC nomenclature name
<input type="checkbox"/> MolLogP(mol)	molLogP	Chemical	Octanol water partition, -Log(C _w /C _o)
<input checked="" type="checkbox"/> MolLogS(mol)	molLogS	Chemical	Water solubility -Log(C _{agg})
<input checked="" type="checkbox"/> MolPSA(mol)	molPSA	Chemical	Polar surface area
<input checked="" type="checkbox"/> MolVolume(mol)	molVolume	Chemical	Molecular volume
<input type="checkbox"/> MolDH(mol)	molDH	Chemical	Heats of formation from elements
<input type="checkbox"/> DrugLikeness(mol)	drugLikeness	Chemical	Empirical drug-likeness
<input type="checkbox"/> Smiles(mol, mode='asis')	smiles	Chemical	SMILES/SMARTS: string notation o...
<input type="checkbox"/> BadGroups(mol)	badGroups	Chemical	Unwanted or reactive chemical func...
<input type="checkbox"/> Nof_Atoms(mol, atom='')	nof_Atoms	Chemical	Number of atoms
<input type="checkbox"/> Nof_Molecules(mol)	nof_Molecules	Chemical	Number of individual molecules
<input type="checkbox"/> Nof_Fragments(mol, smarts='', type=)	nof_Fragments	Chemical	Number of SMARTS pattern occur...
<input type="checkbox"/> Nof_Chirals(mol, type='any')	nof_Chirals	Chemical	Number of chiral centers, R,S, or (R)
<input type="checkbox"/> Nof_Rings(mol)	nof_Rings	Chemical	Number of rings in the SSSR

OK Cancel

2. Select properties

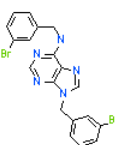

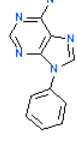
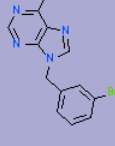
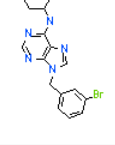
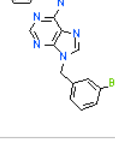
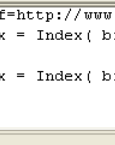
3. Properties will be displayed in new columns

```
icm/def> binding_data.pdb[4] = "4abc"  
icm/def> binding_data.pdb[5] = "5abc"  
icm/def> binding_data.pdb[6] = "6abc"  
icm/def> binding_data.pdb[7] = "7abc"  
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1%1</a>" name="" color=""  
icm/def>
```

- Standardize...
- Annotate by Substructure...
- Predict
- Convert Smiles to 2D...
- Convert Structure to Smiles...
- 2D Depiction...
- Generate Tautomers...
- Convert To Racemic...
- Generate Stereoisomers...
- Align/Color By 2D Scaffold...
- Cluster Set
- Compare Two Sets...
- Merge Two Sets...
- Sort Table...
- Select Duplicates...
- Create/Modify Markush...
- Enumerate by Scaffold...
- R-Group Decomposition...
- Enumerate by Reaction...

no selection

tables (1 it
binding_data

	mol	ki uM	molWeight	molLogP	molLogS	molPS							
			6	471	4.775	-7.196	42.74	336	134.4	0.05017	3		11abc
			6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3		12abc
			6	211.1	1.376	-3.533	53.02	183.3	88.27	-0.3593	3		23abc
			6.375				222.2	98.47	0.007176	3			24abc
4			6.525	373.1	4.255	-5.809	42.92	310.4	79.3	0.6977	3		15abc
5			6	393.1									
6			6.6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3		16abc

1. Chemistry/Select Duplicates...

2. Enter table/spreadsheet name

Find duplicated entries in set

Table: binding_data

Use Chirality Use Salt

Ok Cancel

3. Duplicate compounds will be selected and highlighted in blue

```
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1%1</a>" name="" color=""
icm/def> find table binding_data select index = Index( binding_data.mol exact stereo )
Info> 1 hits selected in binding_data
icm/def> find table binding_data select index = Index( binding_data.mol exact stereo )
Info> 1 hits selected in binding_data
icm/def>
```

How to identify duplicate chemicals in a spreadsheet.

How to compare two chemical spreadsheets.

1. Chemistry/Compare Two Sets...

2. Choose the tables you want to compare

3. Select the comparison method and output

mol	ki uM	molWeight	molLogP	molLogS	molPS					
	6	471	4.775	-7.196	42.74	336	134.4	0.05017	3	11abc
	24		-6.126	42.74	314	128.1	0.07959	3	12abc	
	6	211								23abc
							0.007176	3		24abc
	6.929	373.1	4.255	-5.809	42.92	310.4	79.3	0.6977	3	15abc
	6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3	12abc
	6.6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3	16abc

```
icm/def> find table binding_data select index = Index( binding_data.mol exact stereo )
Info> 1 hits selected in binding_data
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no no ""
Info> table 'binding_data_assay2' ( 0 headers, 2 arrays[23] ) created
icm/def> delete binding_data_assay2.NAME
icm/def>
```

How to merge two chemical spreadsheets.

File Edit View Tools Chemistry Windows Help

Calculate Properties

- Standardize...
- Annotate by Substructure...
- Predict
- Convert Smiles to 2D...
- Convert Structure to Smiles...
- 2D Depiction...
- Generate Tautomers...
- Convert To Racemic...
- Generate Stereoisomers...
- Align/Color By 2D Scaffold...
- Cluster Set
- Compare Two Sets...
- Merge Two Sets...**
- Sort Table...
- Select Duplicates...
- Create/Modify Markush...
- Enumerate by Scaffold...
- R-Group Decomposition...
- Enumerate by Reaction...

1. Chemistry/Merge Two Sets...

2. Choose the tables you want to compare

Merge Two Sets

Table A: binding_data by Column: mol

inner left right

Table B: binding_data_assay2 by Column: mol

Result Name: T_join

Hint:
 inner - only molecules present in BOTH A and B tables are kept
 left - ALL rows of A are kept
 right - ALL rows of B are kept

Ok Cancel Help

3. Select the way you want to merge them

```
icm/def> find table binding_data select index = Index( binding_data.mol exact stereo )
Info> 1 hits selected in binding_data
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no no ""
Info> table 'binding_data_assay2' ( 0 headers, 2 arrays[23] ) created
icm/def> delete binding_data_assay2.NAME_
icm/def>
```

ICM-Chemist

HOW TO PERFORM CHEMICAL SEARCHING

How to setup a chemical search.

1. Click here

2. Chemical search window will be displayed

binding_data_assay2 Molsoft Chemist 3.6-1g [NewProject] (2 tables)

mol	ki uM	molWeight	molLogP	molLogS	molPSA	molVolume	moldHf	drugLikeness	nof HBA	nof HBD	pdb
1		6	4.775	-7.196	42.74	336	134.4	0.05017	3		11abc
2		6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3	12abc
5		6.6	2.206	-4.619	43.16	240.4	99.96	0.129	3		6abc

ICM Chemical Search: [new file *] Molcart not connected

Data Source: Table | File | Molcart | binding_data

Query Options: Search type: Substructure, Max distance: 0.4, Number of matches: any, Match stereo, Ignore salt, Selected only, Maximum # of hits: 10000

Results: Count hits only, Select in source, Hide unmatched, Save results to: result, Overwrite, Highlight match, Rotate by match, Display as grid, Store query, Append, Hide after Search, Search

```
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no no ""
Info> 1 hits selected in binding_data
icm/def> delete binding_data_assay2.NAME_
icm/def> web "http://www.rcsb.org/pdb/explore/explore.do?structuresId=2abc"
icm/def>
```

How to draw a chemical search query.

1. Use bonds, atoms, and templates to sketch

2. Right click on an atom to select filters such as ring membership, connectivity,

mol	ki uM	molWeight	molLogP	molLogS	molPSA	molVolume	moldHf	drugLikeness	nof HBA	nof HBD	pdb
1		6	4.775	-7.196	42.74	336	134.4	0.05017	3		11abc
2		6	393.1								12abc
3		6.6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3	16abc

```
Info> 1 hits selected in binding_data
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no no ""
Info> table 'binding_data_assay2' ( 0 headers, 2 arrays[23]) created
icm/def> delete binding_data_assay2.NAME_
icm/def> web "http://www.rcsb.org/pdb/explore/explore.do?structuresId=2abc"
icm/def>
```

How to add conditions to your chemical search.

The screenshot shows the Molsoft Chemist 3.6-1g interface. The main window displays a table of chemical data with columns for mol, ki uM, molWeight, molLogP, molLogS, molPS, and various numerical values. A chemical structure of a brominated benzimidazole derivative is shown in the top left. A search window titled "ICM Chemical Search: [new file *] Molcart not connected" is open, showing a chemical structure of C14H22 and a table of search conditions. The search window has a menu bar (File, Edit, View, Templates, Help) and a toolbar. The "Data Source" is set to "binding_data". The "Query Options" include "Search type" (Substructure), "Max distance" (0.4), and "Number of matches" (any). There are checkboxes for "Match stereo", "Ignore salt", "Selected only", "Highlight match", "Rotate by match", "Display as grid", "Store query", and "Append". A "Search" button is at the bottom right. A table at the bottom of the search window lists conditions:

	FieldName	Relation	Value
1	molWeight	>	200
2		AND	
3	molWeight	<	600

Annotations include a blue box with the text "1. Right click here and select 'Add condition'" pointing to the "Add condition" button, and another blue box with the text "2. Double click and use drop down arrows to enter condition" pointing to the "molWeight" field in the table. A command window at the bottom left shows the following commands:

```
Info> 1 hits selected in bind
icm/def> openFile "V:\\training
Info> table 'binding_data_asse
icm/def> delete binding_data_ase
icm/def> web "http://www.rcsb.o
icm/def>
```

1. Right click here and select "Add condition"

2. Double click and use drop down arrows to enter condition

How to search chemical spreadsheets, local databases and MolCart.

1. Select what you want to search here

2. Select your query options

ICM Chemical Search: [new file *] Molcart not connected

Data Source: binding_data, binding_data, binding_data_assay2

Query Options: Search type: Substructure, Max distance: 0.4, Number of matches: any, Match stereo: , Selected only: , Ignore salt: , Maximum # of hits: 10000

	FieldName	Relation	Value
1	molWeight	>	200
2		AND	
3	molWeight	<	600

```
Info> 1 hits selected in binding_data
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no no ""
Info> table 'binding_data_assay2' ( 0 headers, 2 arrays[23]) created
icm/def> delete binding_data_assay2.NAME_
icm/def> web "http://www.rcsb.org/pdb/explore/explore.do?structureId=2abc"
icm/def>
```

How to send a chemical search query.

The screenshot shows the Molsoft Chemist 3.6-1g interface. The main window displays a table with columns: mol, ki uM, molWeight, molLogP, molLogS, molPSA, molVolume, moldHf, drugLikeness, nof HBA, nof HBD, and pdb. The first row shows a molecule with a brominated benzimidazole core. A dialog box titled "ICM Chemical Search: [new file *] Molcart not connected" is open, showing search options for "binding_data". The search type is set to "Substructure", and the maximum number of hits is 10000. A callout box points to the "Search" button with the text "1. Select how you want to display the results". Another callout box points to the "Search" button with the text "2. Press Search".

mol	ki uM	molWeight	molLogP	molLogS	molPSA	molVolume	moldHf	drugLikeness	nof HBA	nof HBD	pdb
1		6	471	4.775	-7.196	42.74	336	134.4	0.05017	3	11abc
2		6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3	12abc
3		6	317	2.206	-4.619	43.16	240.4	99.96	0.129	3	

ICM Chemical Search: [new file *] Molcart not connected

Data Source: binding_data

Query Options:

- Search type: Substructure
- Max distance: 0.4
- Number of matches: any
- Match stereo:
- Ignore salt:
- Selected only:
- Maximum # of hits: 10000

Results:

- Count hits only:
- Select in source:
- Hide unmatched:
- Save results to:
- Table: result
- Overwrite:
- Highlight match:
- Rotate by match:
- Display as grid:
- Store query:
- Append:
- Hide after Search:

Search

1. Select how you want to display the results

2. Press Search

```
Info> 1 hits selected in binding_data
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no no ""
Info> table 'binding_data_assay2' ( 0 headers, 2 arrays[23]) created
icm/def> delete binding_data_assay2.NAME_
icm/def> web "http://www.rcsb.org/pdb/explore/explore.do?structuresId=2abc"
icm/def>
```

ICM-Chemist

HOW TO WORK WITH PHARMACOPHORES

How to search a 2D pharmacophore.

1. Click on chemical search button and sketch

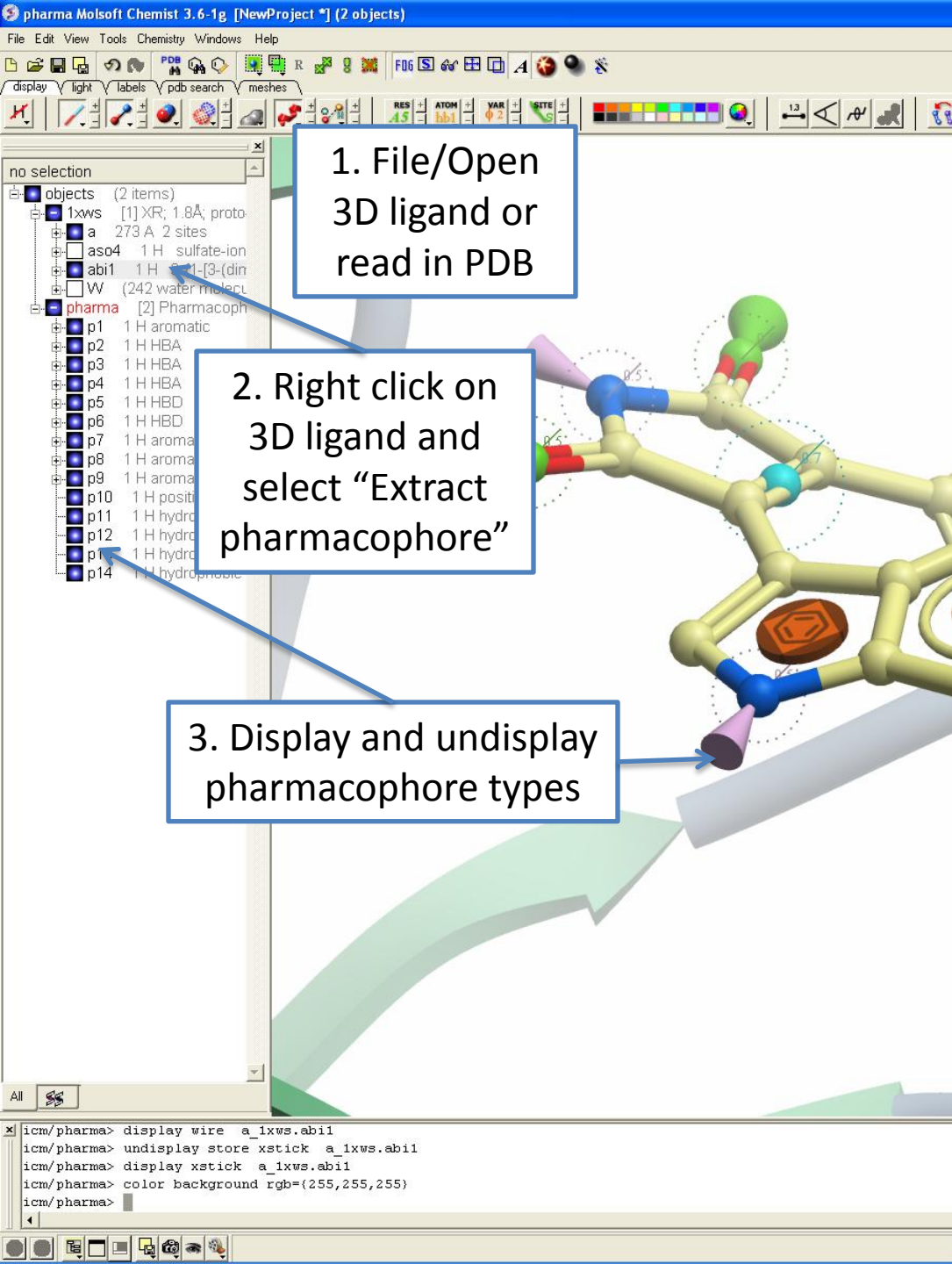
Distance bond

Pharmacophore types

2. Select query options and search

The screenshot shows the Molsoft Chemist 3.6-1g interface. The main window displays a table with columns: molWeight, molLogP, molLogS, molPSA, molVolume, molHf, drugLikeness, nof HBA, nof HBD, and pdb. The table contains two rows of data. A dialog box titled "ICM Chemical Search: [new file *] Molcart not connected" is open, showing a chemical sketch of C2H7X2 with a distance bond between two atoms. The dialog box has several sections: "Data Source" (Table, File, Molcart), "Query Options" (Search type: Substructure, Max distance: 0.4, Number of matches: any, Match stereo, Ignore salt), "Pharmacophore types" (Hydrogen bond acceptor, Hydrogen bond donor), and "Results" (Count hits only, Select in source, Matched, Save results to: File, Molcart, Overwrite, Right match, Rotate by match, Store query, Append, Hide after Search, Search). The bottom of the dialog box shows a "Text search" field and a "Search" button. The background window shows a chemical structure of a benzimidazole derivative with a bromine atom. The bottom status bar shows the command prompt with the following text:

```
Info> 1 hits selected in binding_data  
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\binding_data_assay2.sdf" 0 yes no no ""  
Info> table 'binding_data_assay2' ( 0 headers, 2 arrays[23]) created  
icm/def> delete binding_data_assay2.NAME_  
icm/def> web "http://www.rcsb.org/pdb/explore/explore.do?structuresId=2abc"  
icm/def>
```



How to extract a 3D pharmacophore from a 3D ligand.

1. File/Open
3D ligand or
read in PDB

2. Right click on
3D ligand and
select "Extract
pharmacophore"

3. Display and undisplay
pharmacophore types

no selection

objects (2 items)

- 1xws [1] XR; 1.8Å; proto
- a 273 A 2 sites
- aso4 1 H sulfate-ion
- abi1 1 H 3-(-[3-(dir
- W (242 water molecu
- pharma [2] Pharmacoph
- p1 1 H aromatic
- p2 1 H HBA
- p3 1 H HBA
- p4 1 H HBA
- p5 1 H HBD
- p6 1 H HBD
- p7 1 H aromatic
- p8 1 H aromatic
- p9 1 H aromatic
- p10 1 H aromatic
- p11 1 H hydrophobic
- p12 1 H hydrophobic
- p13 1 H hydrophobic
- p14 1 H hydrophobic

1. Right click on a pharmacophore point and select the "Pharmacophore" menu

- a_pharma.p6/6/Qv11
- Skin Mesh
- Edit
- Advanced
- Label
- Center...
- Connect to Molecule
- Disconnect
- Annotate Selection...
- Neighbors...
- Select
- Pharmacophore

- Edit Point...
- Clone Point
- Remove Direction

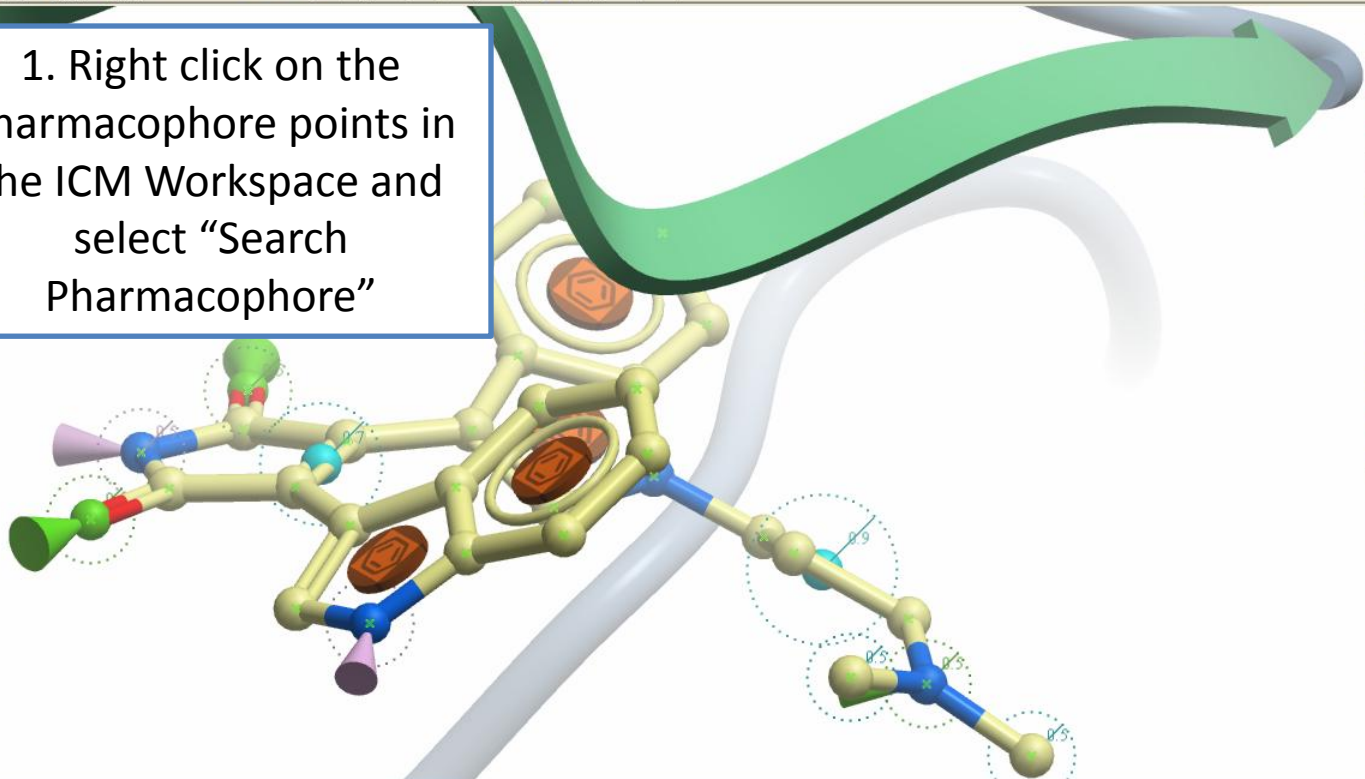
Use connect to move a point

Edit move and clone

```
icm/pharma> display wire
icm/pharma> undisplay store xstick a_1xws.ab11
icm/pharma> display xstick a_1xws.ab11
icm/pharma> color background rgb=(255,255,255)
icm/pharma>
```

How to send a 3D pharmacophore search query.

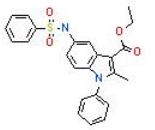
1. Right click on the pharmacophore points in the ICM Workspace and select "Search Pharmacophore"



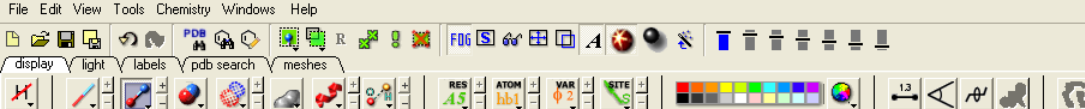
- a_pharma
- Clone...
- Set to Current
- Convert PDB...
- Convert PDB Chemical...
- Make Ca-Trace Object...
- Skin Mesh
- Read full PDB entry...
- Convert to non-ICM...
- Generate Biomolecules...
- Clear Default Display...
- Properties
- Edit
- Search Pharmacophore...**
- Advanced
- Center...
- Connect to Object
- Disconnect (Esc)
- Extract Sequence(s)
- Sort Molecules by Size
- Neighbors...
- Select
- Protect
- Pharmacophore
- Undisplay
- Delete
- Rename...
- Save As...
- Open Records
- Close Records

	mol	NAME	molid	confid	L	D
1		3D	5	438	0	7
2		3D	5	439	0	8
		3D	5	440	0	9

2. Search a table with chemicals that have 3D coordinates



How color a 2D chemical sketch by pharmacophore feature.



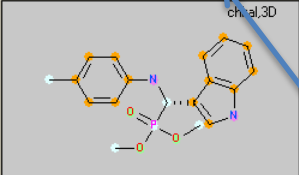
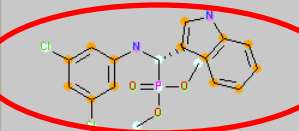

no selection

- objects (1 item)
 - pharma [1] Pharmacophore
 - p3 1 H HBA
 - p5 1 H HBD
 - p7 1 H aromatic
 - p8 1 H aromatic
- tables (2 items)
 - t_3D 9994 rows 6 cols 0 he
 - ph4_res 7 rows 8 cols 3 he
- script (1 item)
- run

- mol
 - Hide Column(s)
 - Show Column(s)
 - Freeze Column
 - Copy Column(s) Ctrl+C
 - Cut Column(s)
 - Paste Column(s) Ctrl+V
 - Edit Mode
 - Rename Column...
 - Set Compound Names From...
 - Delete Column(s)
 - Color Structure By
 - MolLogP
 - By Fragment Frequency
 - By Pharmacophore Features
 - Off
 - Edit Color Gradient...
 - Clear Selection Color
 - Insert Column...
 - Add External Columns...
 - Column Statistics...
 - Sort
 - Filter
 - Group by Column...
 - Assign 2D Coordinates...
 - Rotate for Best Fit
 - Split Into Fragments
 - Chemical Find and Replace...
 - Unset 3D Browse Mode
 - Unlock All
 - Chemical View Options...
 - Format...

2. Select Color Structure By/ By Pharmacophore Features

1. Right click on column header

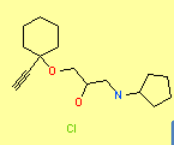
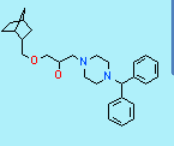
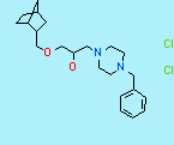
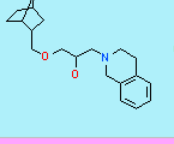
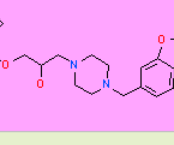
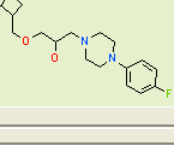
	mol	NAME	molid	confid	L	rmsd	score	
1	chiral,3D		824	190184		0.007595	100	
	chiral,3D		880					
3	chiral,3D		880	226603		0.018	100	

ICM-Chemist

HOW TO PERFORM CHEMICAL CLUSTERING

How to perform chemical clustering.

no selection
tables (1 item)
my_database 10001 rows 8 cols 1 head

	mol	NAME	molid	vendors	molWeight
1		racemic C16H28ClNO2		129 chembridge:9140902 lifechemicals:F3314-0008	30
2					50
3		racemic C22H36Cl2N2O2		561323 lifechemicals:F3354-0180	43
4		racemic C20H30ClNO2		561330 lifechemicals:F3354-0198	35
5		racemic C23H36Cl2N2O4		561322 lifechemicals:F3354-0185	47
6		racemic C21H33Cl2FN2O2		561324 lifechemicals:F3354-0183	43

1. Click on the "Run Clustering" button

Header Tree
0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0.

- C16H28ClNO2
- C28H40Cl2N2O2
- C22H36Cl2N2O2
- C20H30ClNO2
- C23H36Cl2N2O4
- C21H33Cl2FN2O2
- C21H33Cl2FN2O2
- C21H34Cl2N2O2
- C22H32ClF3N2O2
- C17H34Cl2N2O3
- C15H28ClNO3
- C21H3ON2
- C26H36N2O4
- C23H34N2
- C22H30N2O4
- C14H16N2
- C22H30N2O4
- C14H2ON2
- C21H3ON2
- C19H28N2
- C14H17N
- C23H35N3
- C18H26N2
- C15H21N
- C22H28N2
- C18H25FN2
- C18H25FN2
- C18H25FN2
- C18H25ClN2
- C18H25BrN2
- C18H25BrN2
- C17H23NO
- C19H25FN2
- C19H25FN2
- C19H25FN2
- C19H25ClN2
- C19H26N2
- C19H25BrN2
- C19H25BrN2
- C19H25BrN2
- C20H25F3N2
- C21H27ClN2O4
- C21H27ClN2O4
- C25H30N2O4
- C18H25N3
- C18H25N3
- C18H25N3
- C17H25N3
- C17H25N3
- C21H27N3
- C25H30N2O
- C19H25BrN2O

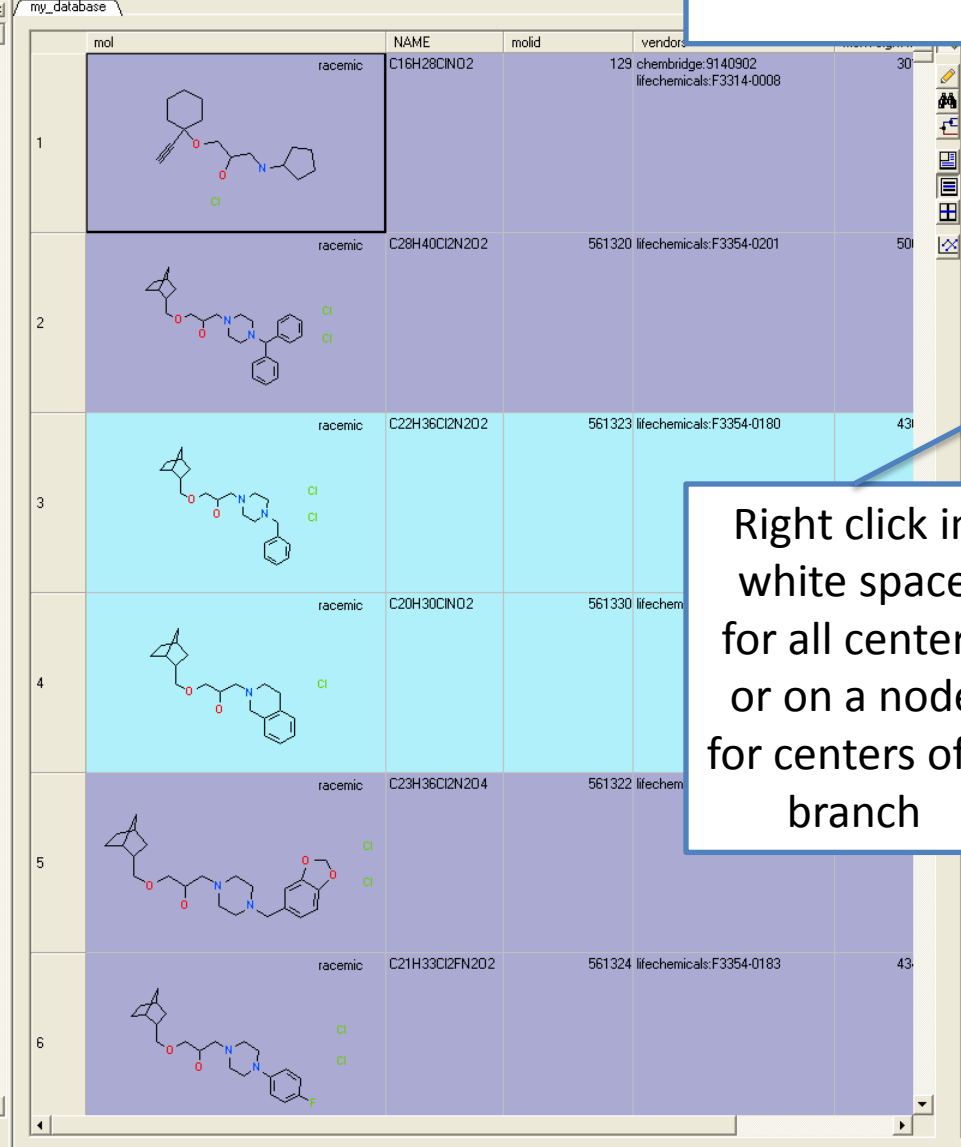
```
icm/def> make tree my_database full "UPGMA" split="c1" label="*NAME_;" name=""  
Info> Column 'ord' (record number in the tree order) has been appended to table my_database.  
Info> Column 'cl' (cluster number) has been appended to table my_database  
Info> Tree 'my_database.cluster[1]' has been successfully created  
icm/def> sort my_database.ord  
icm/def>
```

no selection

tables (1 item)

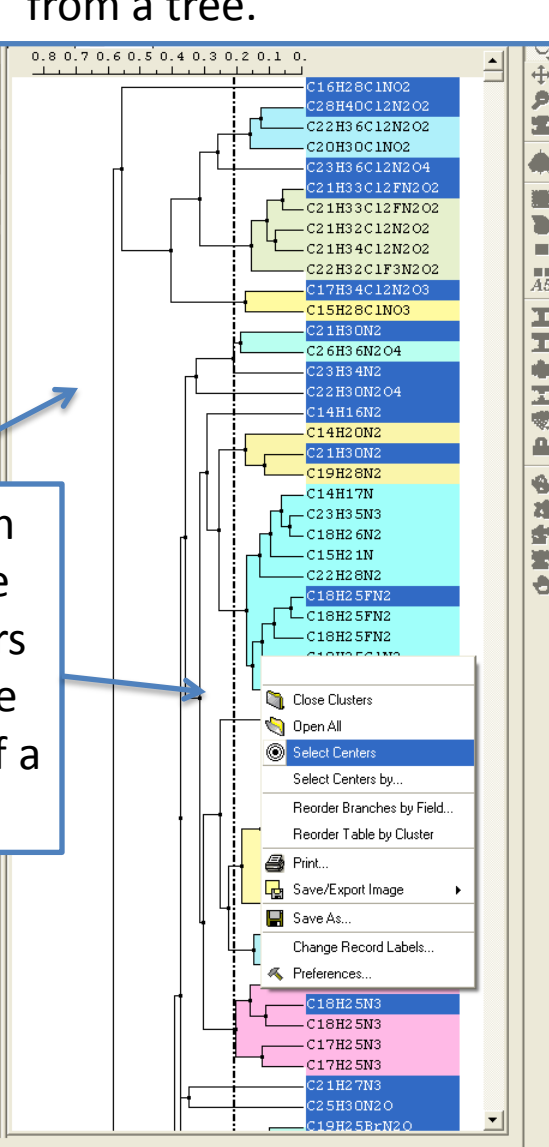
my_database 10001 rows 8 cols 1 head

mol	NAME	molid	vendor
1	racemic C16H28ClNO2	129	chembridge:9140902 lifechemicals:F3314-0008
2	racemic C28H40Cl2N2O2	561320	lifechemicals:F3354-0201
3	racemic C22H36Cl2N2O2	561323	lifechemicals:F3354-0180
4	racemic C20H30ClNO2	561330	lifechem
5	racemic C23H36Cl2N2O4	561322	lifechem
6	racemic C21H33Cl2FN2O2	561324	lifechemicals:F3354-0183



How to select representative centers from a tree.

Right click in white space for all centers or on a node for centers of a branch



```

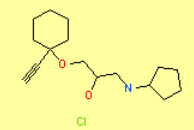
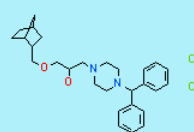
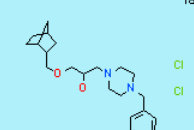
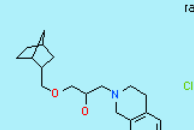
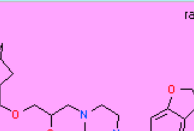
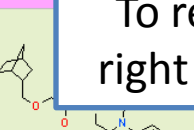
icm/def> make tree my_database full "UPGMA" split="c1" label="*NAME_;" name=""
Info> Column 'ord' (record number in the tree order) has been appended to table my_database.
Info> Column 'c1' (cluster number) has been appended to table my_database
Info> Tree 'my_database.cluster[1]' has been successfully created
icm/def> sort my_database.ord
icm/def>
    
```

How to re-order branches and change distance of tree.

File Edit View Tools Chemistry Windows Help

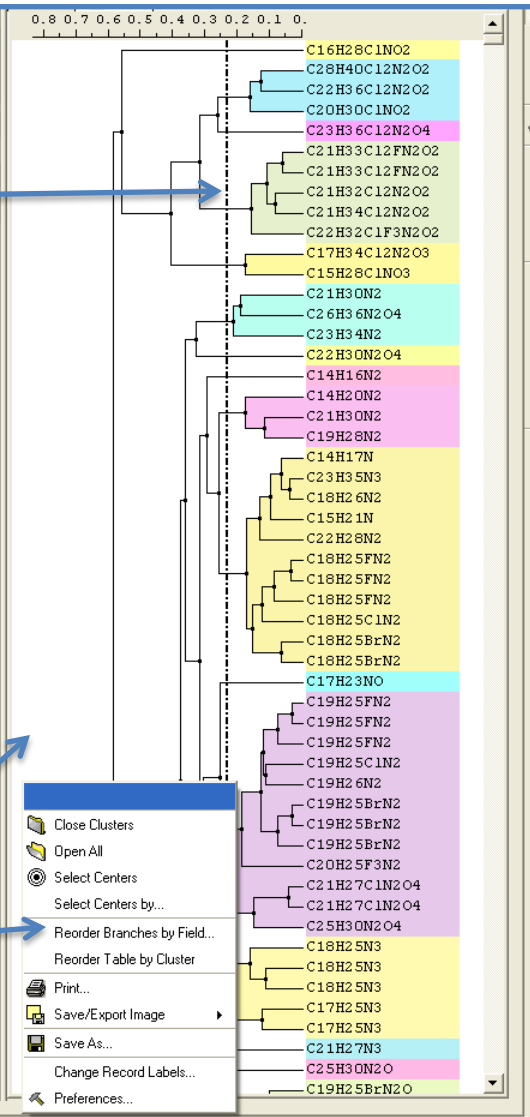


no selection
tables (1 item)
my_database 10001 rows 8 cols 1 head

	mol	NAME	molid	vendor
1		racemic C16H28ClNO2	129	chembridge:9140902 lifechemicals:F3314-0008
2		racemic C28H40Cl2N		
3		racemic C22H36Cl2N2O2	561323	lifechemicals:F3354-0180
4		racemic C20H30ClNO2	561330	lifechemicals:F3354-0198
5		racemic C23H36Cl2N2O4	561322	lifechemicals:F3354-0185
6				

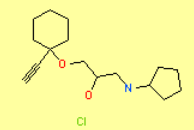
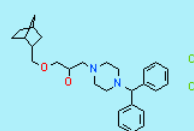
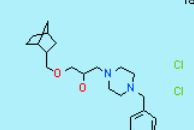
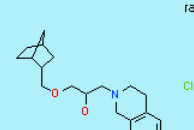
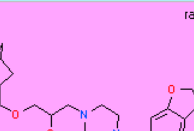
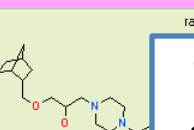
To change distance – click and drag here

To re-order branches – right click in white space



```

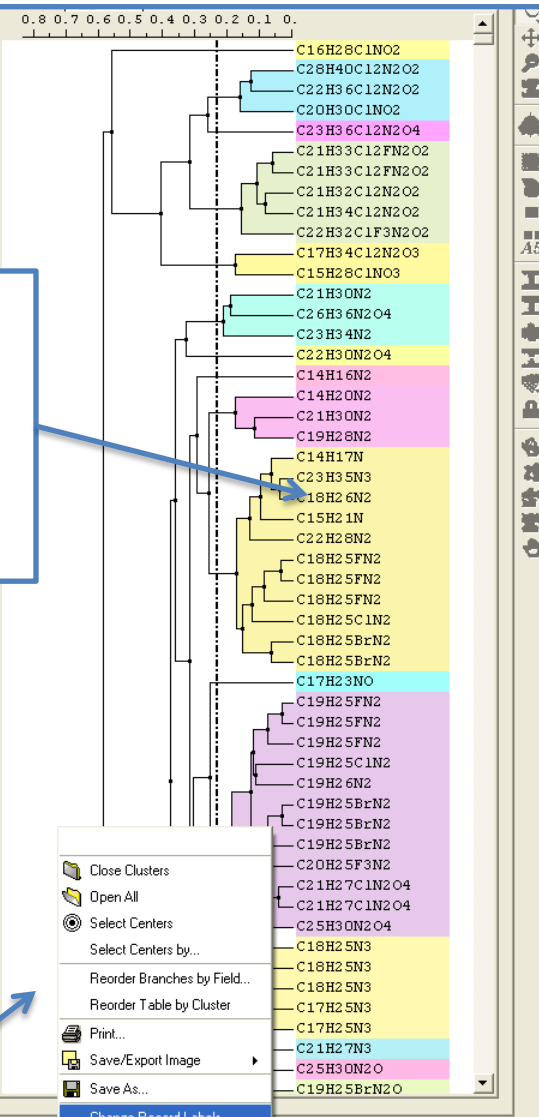
icm/def> make tree my_database full "UPGMA" split="c1" label="*NAME_;" name=""
Info> Column 'ord' (record number in the tree order) has been appended to table my_database.
Info> Column 'cl' (cluster number) has been appended to table my_database
Info> Tree 'my_database.cluster[1]' has been successfully created
icm/def> sort my_database.ord
icm/def>
    
```

	mol	NAME	molid	vendor
1		racemic C16H28ClNO2	129	chembridge:9140902 lifechemicals:F3314-0008
2		racemic C28H40Cl2N2O2	561320	lifechemicals:F3354-0201
3		racemic C22H36Cl2N2O2	561323	lifechemicals:F3354-0185
4		racemic C20H30ClNO2	561330	lifechemicals:F3354-0183
5		racemic C23H36Cl2N2O4	561322	lifechemicals:F3354-0185
6		racemic C21H33Cl2FN2O2	561324	lifechemicals:F3354-0183

How to edit the tree – labels, spacing and coloring.

To edit labels, spacing and coloring: right click on the tree

To change record labels: right click in white space and select "Change Record Labels"



- Close Clusters
- Open All
- Select Centers
- Select Centers by...
- Reorder Branches by Field...
- Reorder Table by Cluster
- Print...
- Save/Export Image
- Save As...
- Change Record Labels...**
- Preferences...

```

icm/def> make tree my_database full "UPGMA" split="c1" label="%NAME"; name
Info> Column 'ord' (record number in the tree order) has been appended to table my_database.
Info> Column 'c1' (cluster number) has been appended to table my_database
Info> Tree 'my_database.cluster[1]' has been successfully created
icm/def> sort my_database.ord
icm/def>
    
```


ICM-Chemist

HOW TO GENERATE STEREOMERS AND TAUTOMERS

no selection

tables (1 it
L_my_databas

- Calculate Properties
- Standardize...
- Annotate by Substructure...
- Predict
- Convert Smiles to 2D...
- Convert Structure to Smiles...
- 2D Depiction...
- Generate Tautomers...
- Convert To Racemic...
- Generate Stereoisomers...**
- Align/Color By 2D Scaffold...
- Cluster Set
- Compare Two Sets...
- Merge Two Sets...
- Sort Table...
- Select Duplicates...
- Create/Modify Markush...
- Enumerate by Scaffold...
- R-Group Decomposition...
- Enumerate by Reaction...

1. Chemistry/Generate Stereoisomers

Choose "Files" for batch mode

2. Enter name of chemical table

Generate Stereoisomers

Local Tables Files


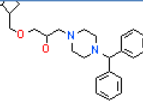

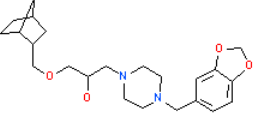
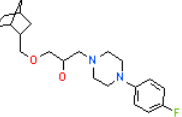
Hint
Enumerates ONLY undefined 'R/S' stereo centers.
Use 'Convert To Racemic' for chiral molecules

Molecular Table my_database

Group Rows With Color

Skip If Number Of Centers Greater Than No limit

Ok Cancel Help

	mol	NAME	molid	vendors	molWeight mol	molLogP mol	ord	cl
1		racemic C16H28ClN02		129 chembridge:9140902 lifechemicals:F3314-0008	301.2	2.807	1	1
2		racemic C22H36Cl2N2O2		561320 lifechemicals:F3354-0201	506.2	4.177	2	2
3					351.2	2.938	4	2
5					474.2	2.97	5	3
6		racemic C21H33Cl2FN2O2		561324 lifechemicals:F3354-0183	434.2	3.284	6	4

```
icm/def> delete hydrogen my_database.mol
Info> 3297 hydrogens removed
icm/def> modify my_database.mol auto
Info> 905 replacements done
icm/def> delete my_database.cluster[1]
icm/def>
```

no selection

tables (1 it
_my_databases

- Calculate Properties
- Standardize...
- Annotate by Substructure...
- Predict
- Convert Smiles to 2D...
- Convert Structure to Smiles...
- 2D Depiction...
- Generate Tautomers...**
- Convert To Racemic...
- Generate Stereoisomers...
- Align/Color By 2D Scaffold...
- Cluster Set
- Compare Two Sets...
- Merge Two Sets...
- Sort Table...
- Select Duplicates...
- Create/Modify Markush...
- Enumerate by Scaffold...
- R-Group Decomposition...
- Enumerate by Reaction...

1. Chemistry/Generate Tautomers

Choose "Files" for batch mode

2. Enter name of chemical table

Generate Tautomers


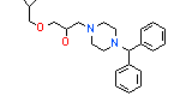
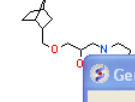
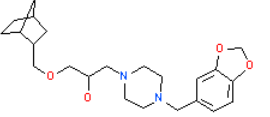
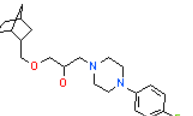
Local Tables Files

Molecular Table my_database

Filter Unwanted Groups Preserve Hybridisation

Group Rows With Color

Ok Cancel Help

	mol	NAME	molid	vendors	molWeight mol	molLogP mol	ord	cl
1		racemic C16H28ClNO2		129 chembridge:9140902 lifechemicals:F3314-0008	301.2	2.807	1	1
2		racemic C22H36Cl2N2O2		561320 lifechemicals:F3354-0201	506.2	4.177	2	2
3								
					351.2	2.938	4	2
5		racemic C23H36Cl2N2O4		561322 lifechemicals:F3354-0185	474.2	2.97	5	3
6		racemic C21H33Cl2FN2O2		561324 lifechemicals:F3354-0183	434.2	3.284	6	4

```
icm/def> delete hydrogen my_database.mol
Info> 3297 hydrogens removed
icm/def> modify my_database.mol auto
Info> 905 replacements done
icm/def> delete my_database.cluster[1]
icm/def>
```

ICM-Chemist

HOW TO GENERATE COMBINATORIAL LIBRARIES

The screenshot shows the Chemist 3.6-1g software interface. The top menu bar includes File, Edit, View, Tools, Chemistry, Windows, and Help. The toolbar contains various icons for file operations and chemical editing. On the left, a tree view shows a project structure with 'no selection' at the top, followed by 'tables (4 items)' containing 'scaffold', 'R1', 'R2', and 'R3', and 'script (2 items)' containing 'Enumerate' and 'SplitR'. The main window displays a chemical structure of a Markush scaffold: a central amide group with a carbonyl oxygen (O) and a nitrogen atom (N) bonded to an R1 group. This nitrogen is further bonded to another nitrogen atom, which is bonded to a carbon atom bonded to an R2 group and another carbonyl group with an oxygen (O) and an R3 group. The structure is labeled 'racemic' and '1'. A blue arrow points from the 'Enumerate' item in the tree view to the '1' label on the structure.

How to enumerate a Markush chemical library. (1)

1. Sketch a Markush structure in the molecule editor and save it as a chemical spreadsheet

The screenshot shows the command line interface of the software. The following commands and their outputs are visible:

```
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R1.sdf
icm/def> write table mol compress R2 "V:/training course/icm-chemist-webinar-1209/R2.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R2.sdf
icm/def> write table mol compress R3 "V:/training course/icm-chemist-webinar-1209/R3.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R3.sdf
icm/def>
```

The status bar at the bottom indicates 'table: 1 rows, 1 columns'.

Remember to add R-groups to your scaffold.

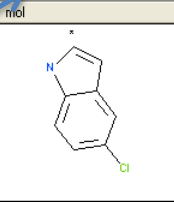
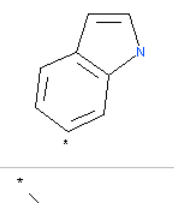
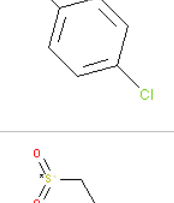
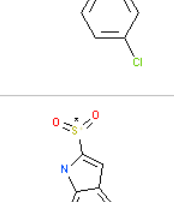
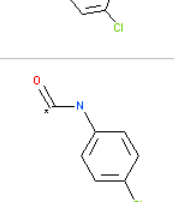
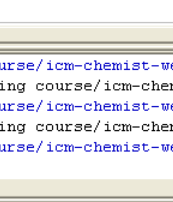
How to enumerate a Markush chemical library. (2)

no selection

tables (4 items)

- scaffold 1 rows 1 cols 0 headers
- R1 11 rows 3 cols 0 headers
- R2 15 rows 3 cols 0 headers
- R3 8 rows 3 cols 0 headers

Read in a set of chemical substituents for each of your R-groups in your Markush scaffold

	mol	ID1	ID
1		ID1	IDD1
2		ID2	IDD2
3		ID3	IDD3
4		ID4	IDD4
5		ID5	IDD5
6		ID6	IDD6

```

Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R1.sdf
icm/def> write table mol compress R2 "V:/training course/icm-chemist-webinar-1209/R2.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R2.sdf
icm/def> write table mol compress R3 "V:/training course/icm-chemist-webinar-1209/R3.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R3.sdf
icm/def>

```

ICM comes with some built in substituents if you want to use those.

How to enumerate a Markush chemical library. (3)

The screenshot shows the Molsoft Chemist interface with a table of chemical structures. The table has columns for 'mol', 'ID1', and 'ID'. The rows contain chemical structures and their corresponding IDs. A menu is open on the left, and a dialog box is shown in the foreground.

mol	ID1	ID
	ID1	IDD1
	ID1	IDD1
	ID3	IDD3
	ID4	IDD4
	ID5	IDD5
	ID6	

1. Chemistry/Enumerate by Scaffold

2. Enter the name of the table and the row number containing your Markush structure (scaffold)

The 'Enumerate by Scaffold' dialog box shows the following options:

- Choose Table With Scaffold (selected) / Draw New Scaffold
- Scaffold: scaffold
- Index: 1

```

Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R1.sdf
icm/def> write table mol compress R2 "V:/training course/icm-chemist-webinar-1209/R2.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R2.sdf
icm/def> write table mol compress R3 "V:/training course/icm-chemist-webinar-1209/R3.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R3.sdf
icm/def>
    
```

How to enumerate a Markush chemical library. (4)

The screenshot shows the Molsoft Chemist 3.6.1g interface. The 'R-Group Enumerate' dialog box is open, with the following configuration:

	R1	R2	R3
Component	R1.mol	R2.mol	R3.mol
Labels A			
Labels B			
Labels C			

The 'Enumerate' button is highlighted with a blue arrow pointing to a callout box.

1. Enter the table names for each R-group

2. Click "Enumerate" and a new table of compounds will be displayed called "enum_result"

```
icm/def> scfld = scaffold.mol[ 1 ]
icm/def> s_out2 = AskG( scfld, enumerate )
icm/def> if ( s_out2 != "" ) enumerate library scfld $s_out2 name = Name( "enum_result" unique )
icm/def> scfld = scaffold.mol[ 1 ]
icm/def> s_out2 = AskG( scfld, enumerate )
```


How to decompose a library based on a Markush structure. (1)

1. Sketch a Markush structure in the molecule editor and save it as a chemical spreadsheet

2. Read in the table you wish to decompose

```
icm/def> if ( s_out2 != "" ) enumerate library scfld $s_out2 name = Name( "enum_result" unique )
icm/def> delete R1
icm/def> delete R3
icm/def> delete R2
icm/def> rename enum_result Name( Name( "binding_data" simple ), unique )
icm/def>
```

How to decompose a library based on a Markush structure. (2)

The screenshot shows the ICM-Pro software interface. On the left, a menu is open with 'R-Group Decomposition...' selected. The main window displays a table with columns R1, R2, R3, and mol. Row 1 is highlighted, and a callout points to the 'T_sar' table name in the top toolbar. A dialog box titled 'R-Group Decomposition' is open, showing 'T_sar' as the scaffold and 'binding_data' as the table for decomposition. The 'mol' column is selected as the structure column. The 'Generate Single SAR Table' and 'Auto Add Missing R-Groups' options are checked. The 'OK' button is highlighted.

1. Chemistry/R-Group Decomposition

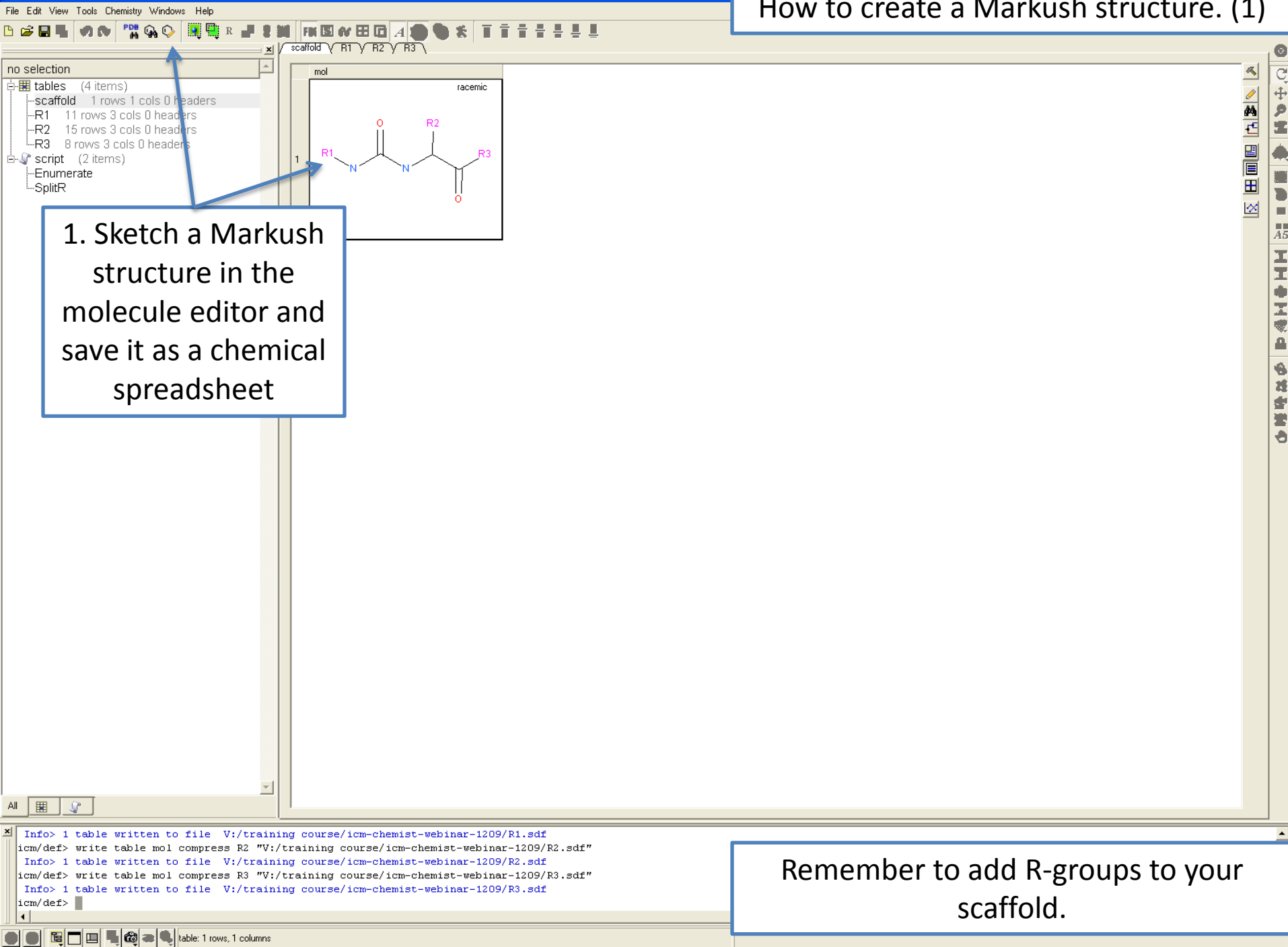
2. Choose table with scaffold and the row number

3. Choose the table for decomposition and the name of the column containing the 2D sketch

4. Click OK and a new table called "T_sar" will be displayed

```

icm/def> delete R2
icm/def> rename enum_result Name(Name("binding_data" simple),unique)
icm/def> scfld = scaffold.mol[ 1 ]
icm/def> make molsar binding_data.mol scfld sort auto append
icm/def> sort T_sar.R1 T_sar.R2 T_sar.R3
icm/def>
    
```



1. Sketch a Markush structure in the molecule editor and save it as a chemical spreadsheet

```
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R1.sdf
icm/def> write table mol compress R2 "V:/training course/icm-chemist-webinar-1209/R2.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R2.sdf
icm/def> write table mol compress R3 "V:/training course/icm-chemist-webinar-1209/R3.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R3.sdf
icm/def>
```

table: 1 rows, 1 columns

Remember to add R-groups to your scaffold.

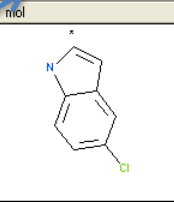
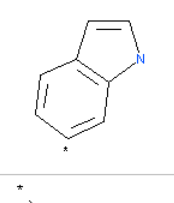
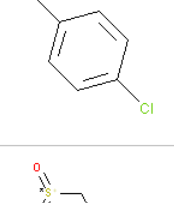
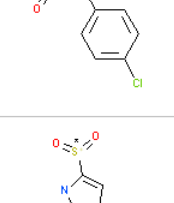
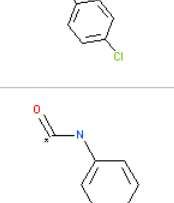
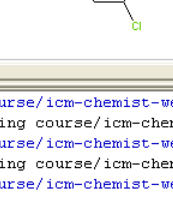


no selection

tables (4 items)

- scaffold 1 rows 1 cols 0 headers
- R1 11 rows 3 cols 0 headers
- R2 15 rows 3 cols 0 headers
- R3 8 rows 3 cols 0 headers

Read in a set of chemical substituents for each of your R-groups in your Markush scaffold

	scaffold	R1	R2	R3
mol				
ID1	ID1	ID1	ID1	ID1
1				
2				
3				
4				
5				
6				

```

Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R1.sdf
icm/def> write table mol compress R2 "V:/training course/icm-chemist-webinar-1209/R2.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R2.sdf
icm/def> write table mol compress R3 "V:/training course/icm-chemist-webinar-1209/R3.sdf"
Info> 1 table written to file V:/training course/icm-chemist-webinar-1209/R3.sdf
icm/def>
  
```

ICM comes with some built in substituents if you want to use those.

- Standardize...
- Annotate by Substructure...
- Predict
- Convert Smiles to 2D...
- Convert Structure to Smiles...
- 2D Depiction...
- Generate Tautomers...
- Convert To Racemic...
- Generate Stereoisomers...
- Align/Color By 2D Scaffold...
- Cluster Set
- Compare Two Sets...
- Merge Two Sets...
- Sort Table...
- Select Duplicates...
- Create/Modify Markush...**
- Enumerate by Scaffold...
- R-Group Decomposition...
- Enumerate by Reaction...

1. Chemistry/Create/Modify Markush

Create/Modify Markush

Scaffold Or Markush scaffold Index 1

Result Name markush

Next Cancel

2. Enter the name of the table and the row number containing your Markush structure (scaffold)

```
Info> table markush (0 headers, 1 array) has been created
Headers:
Arrays : markush.mol
icm/def> delete menuResName
icm/def> delete markush
icm/def>
```

How to create a Markush structure. (4)

1. Enter the table names for each R-group

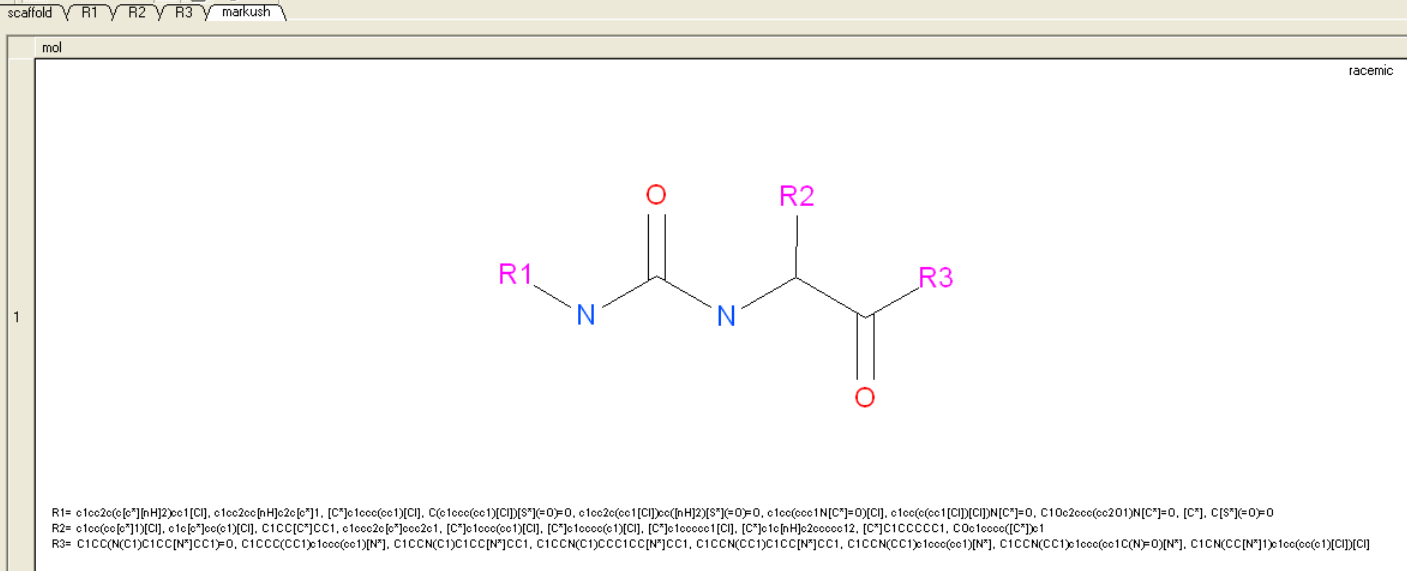
2. Click "Create"

```
icm/def> delete menuResName
icm/def> delete markush
icm/def> scfld = scaffold.mol[ 1 ]
icm/def> menuResName = Name( "markush" unique )
icm/def> s_out2 = askg( scfld, enumerate link )
```



no selection

- tables (5 items)
 - scaffold 1 rows 1 cols 0 headers
 - R1 11 rows 3 cols 0 headers
 - R2 15 rows 3 cols 0 headers
 - R3 8 rows 3 cols 0 headers
 - markush 1 rows 1 cols 0 headers
- script (2 items)
 - Enumerate
 - SplitR



```
icm/def> if ( s_out2 != "" ) group table $menuResName scfld "mol"
Info> table markush (0 headers, 1 array ) has been created
Headers:
Arrays : markush.mol
icm/def> delete menuResName
icm/def>
```



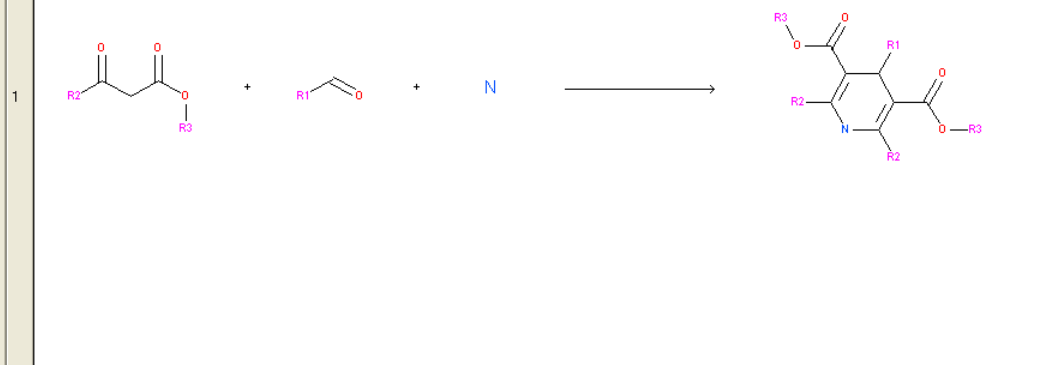
doc1 | r_han_pyr | reactant1 | reactant2

Hantzsch
Dihydropyridine
(Pyr
Syn

This re
prepar
derivat
an aldehy
equivalents of a β -ketoester in
the presence of ammonia.
Subsequent oxidation (or
dehydrogenation) gives
pyridine-3,5-dicarboxylates,
which may also be
decarboxylated to yield the
corresponding pyridines.

[Click here to try a
reaction.](#)

1. Sketch reactants and products in the molecule editor



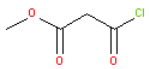
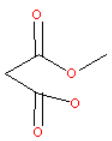
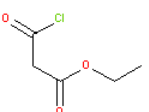
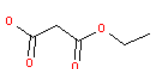
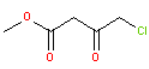
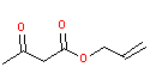
How to enumerate a chemical library by reaction. (1)

```
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb" 1 yes no no no ""
Info> 6 shell objects read (skipped 1) from C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb
icm/def>
```


Hantzsch Dihydropyridine (Pyridine) Synthesis

This reaction allows the preparation of dihydropyridine derivatives by condensation of an aldehyde with two equivalents of a β -ketoester in the presence of ammonia. Subsequent oxidation (or dehydrogenation) gives pyridine-3,5-dicarboxylates, which may also be decarboxylated to yield the corresponding pyridines.

[Click here to try a reaction.](#)

	molid	MolW	mol	ID	vendors
1	87796	136		ID1	apolloscientific:2939 asdi:500006171 aurora:37517-81-0
2	87808	118		ID2	aurora
3	65213	150		ID3	aurora:36239-09-5
4	65250	132		ID4	asdi:500011199
5	87805	150		ID5	asdi:500013383
6	46261	142.1		ID6	asdi:500014867

How to enumerate a chemical library by reaction. (2)

1. Read in a table of your reactants

```
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb" 1 yes no no no ""
Info> 6 shell objects read (skipped 1) from C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb
icm/def>
```

How to enumerate a chemical library by reaction. (3)

File Edit View Tools Chemistry Windows Help

Calculate Properties

Standardize...

Annotate by Substructure...

Predict

Convert Smiles to 2D...

Convert Structure to Smiles...

2D Depiction...

Generate Tautomers...

Convert To Racemic...

Generate Stereoisomers...

Align/Color By 2D Scaffold...

Cluster Set

Compare Two Sets...

Merge Two Sets...

Sort Table...

Select Duplicates...

Create/Modify Markush...

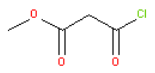
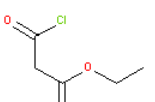
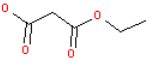
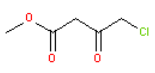
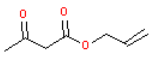
Enumerate by Scaffold...

R-Group Decomposition...

Enumerate by Reaction...

reactant2

Substructure search: Found 88 hits of 'O=C([C,D2]C=

	MoW	mol	ID	vendors
	136		ID1	apolloscientific:2939 asdi:500006171 aurora:37517-81-0
	150		ID3	aurora:36239-09-5
3	65250	132	ID4	asdi:500
4				
5	87805	150	ID5	asdi:
				
6	46261	142.1	ID6	asdi:
				

1. Chemistry/Enumerate by Reaction

Enumerate by Reaction

Choose Table With Reaction Draw New Reaction

Reaction: Index:

Ok Cancel Help

2. Enter the name of the table and the row number containing your reaction sketch (Reaction)

```
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb" 1 yes no no no ""
Info> 6 shell objects read (skipped 1) from C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb
icm/def>
```

How to enumerate a chemical library by reaction. (4)

example_reaction1.icb Molsoft Chemist 3.6-1g [C:\Program Files\Molsoft LLC\ICM-Pro\example_reaction1.icb] (3 tables)

File Edit View Tools Chemistry Windows Help

doc1 r_han_pyr reactant1 reactant2

Substructure search: Found 88 hits of 'O=C([C:D2]C=

molid	MolW	mol	ID	vendors
1				
2				
3				
4				
5				
6				

Hantzsch Dihydropyridine (Pyridine) Synthesis

This reaction allows the preparation of dihydropyridine derivatives by condensation of an aldehyde with two equivalents of a β -ketoester in the presence of ammonia. Subsequent oxidation (or dehydrogenation) gives pyridine-3,5-dicarboxylates, which may also be decarboxylated to yield the corresponding pyridines.

[Click here to try a reaction.](#)

1. Enter the names of the tables with your reactants and a new table called "react_results" will be displayed with your new library

Apply Reaction

Reactant R2&R3: reactant1.mol Reactant R1: reactant2.mol

Compounds: reactant1.mol, reactant2.mol

Labels A: [dropdown]

Filter: [text field]

Mark Unused Reactants: 1

Keep SMARTS attributes in the result

Multiple Matches: Skip First All

Create Cancel

```
icm/def> openFile "C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb" 1 yes no no no ""
Info> 6 shell objects read (skipped 1) from C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb
icm/def> scfld = r_han_pyr.rxn[ 1 ]
icm/def> s_out2 = Askg( scfld, enumerate )
```

ICM-Chemist

HOW TO GENERATE PLOTS AND HISTOGRAMS

my_database Molsoft Chemist 3.6-1g [NewProject *] (1 table)

File Edit View Tools Chemistry Windows Help

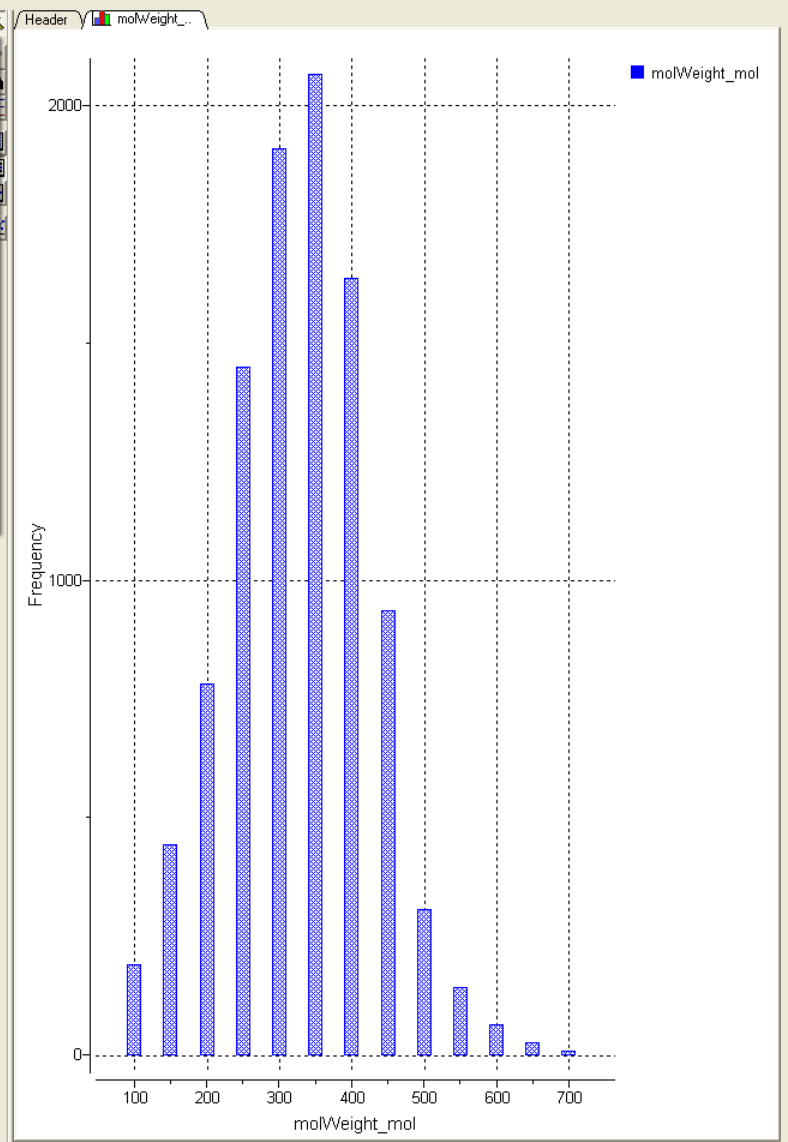
my_database

mol	NAME	molid	vendors	molWeight_mol (real)
1	racemic C16H28ClNO2	129	chembridge:9140902 lifechemicals:F3314-0009	
2	racemic C22H22O	191	ncic:649435	
3	racemic C15H20N2O2	8		561
4	racemic C12H12O4	1380	chembridge:6930118 chemdiv:8010-0947 interchim:A2165/0090947 interchim princeton:DSSK_170995 vitasmilab:STK058509	220.1 0.3767
5	chiral C12H12O4	1483	lscreen:STOCK15-60179 interchim	220.1 0.3767

1. Select a column.
Click on the column header to select.

2. Right click on the column header and select "Column Histogram"

How to make a histogram.



```
icm/def> s_currentProject = ""
icm/def> openFile "V:\\training course\\icm-chemist-webinar-1209\\my_database.sdf"
Info> table 'my_database' ( 0 headers, 5 arrays[10001]) created
icm/def> make plot my_database "x=(molWeight_mol)"
icm/def>
```

How to make a X-Y scatter plot.

my_database

mol	NAME	molid	vendors	molVolume
1	racemic	C16H28ClNO2	129 chembridge:9140902 lifechemicals:F3314-0008	314.3
2	racemic	C16H28FNO2	0	294.5
3	racemic			
4	racemic			
5	chiral			
6				

1. Click here

2. Enter the column names for the axes

3. Add more dimensions to the plots

Plot title

Plot Histogram

Data

X molWeight_mol Logarithmic

Y molVolume Logarithmic

Swap X and Y

Marks

Size 6

Shape

Point labels

Show labels for selection only

Plotting style dots

Color

Source molLogP_mol

Gradient red/orange/gold/green/blue/darkblue/purple

Least squares fitting line

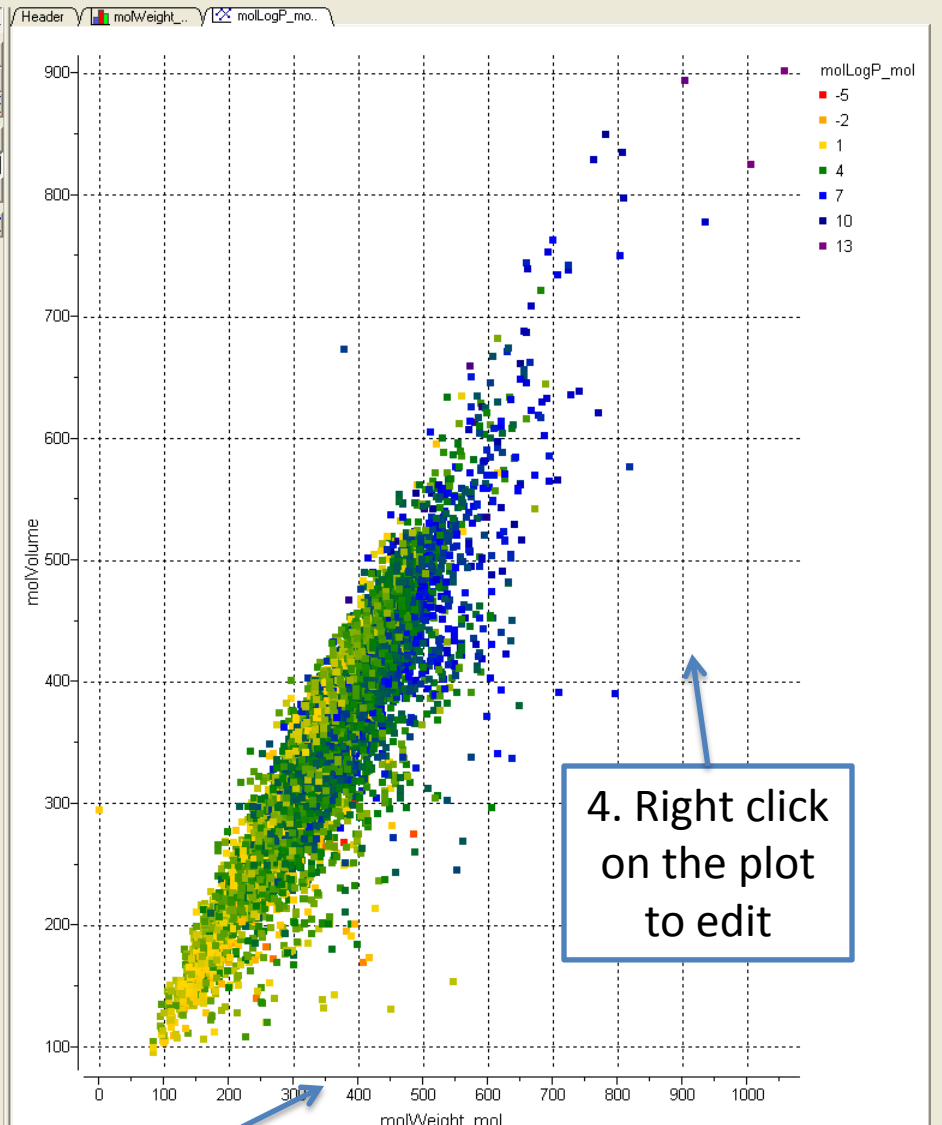
Linear

Logarithmic

Options

Show grid Emphasize axes

OK Close



4. Right click on the plot to edit

5. Click on the axis to edit and zoom

```
icm/def> make plot my_database "x=(molWeight_mol)"
icm/def> make plot my_database "x=molLogP_mol;y=molWeight_mol;size=6;style=dots;";
icm/def> add column my_database function="MolVolume(mol)" index=5 name="molVolume" append
Info> 1 column 'molVolume' added to table 'my_database'
icm/def>
```