ICM-Chemist How-To Guide

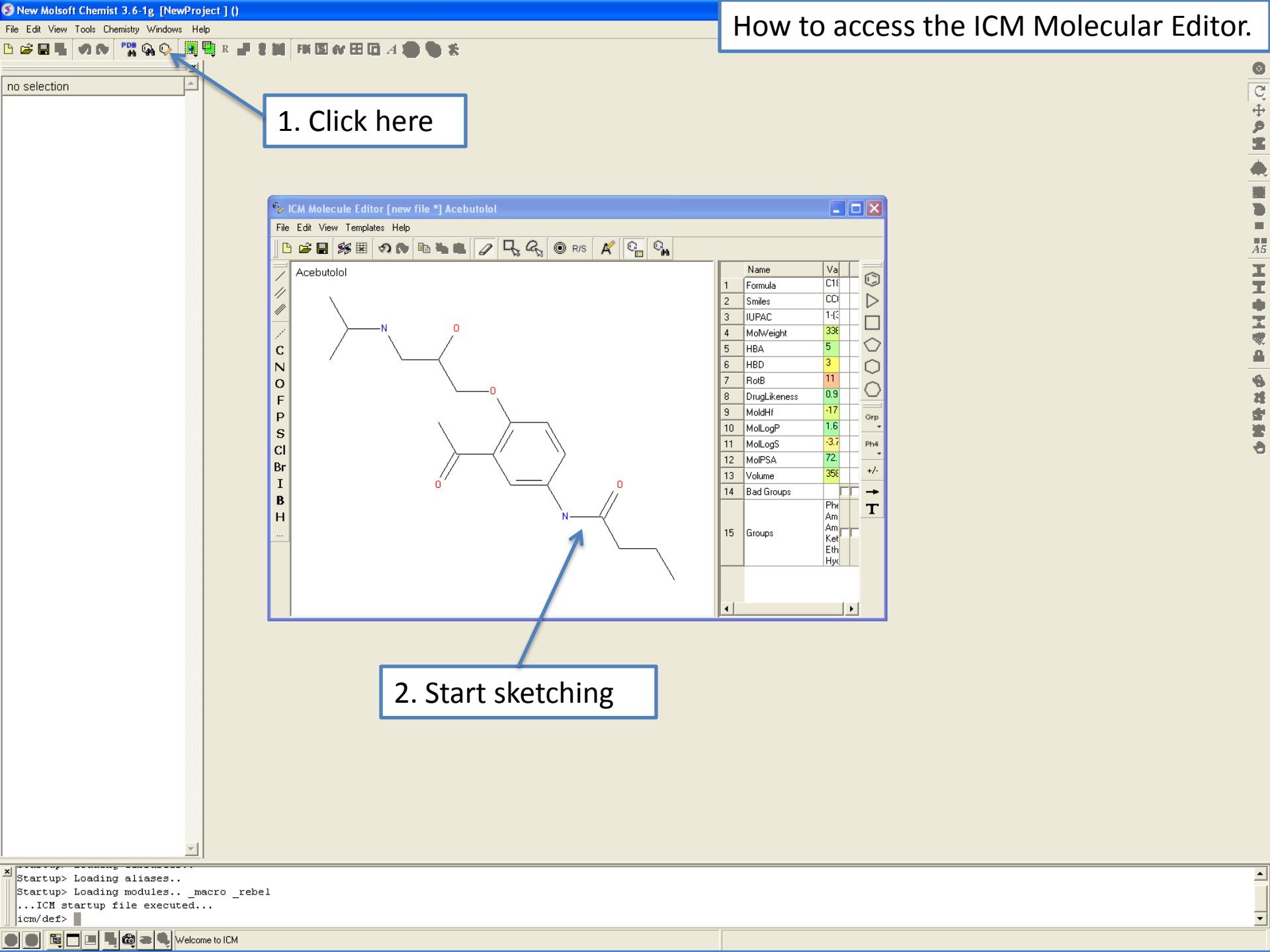
Version 3.6-1g

Last Updated 12/01/2009

ICM-Chemist

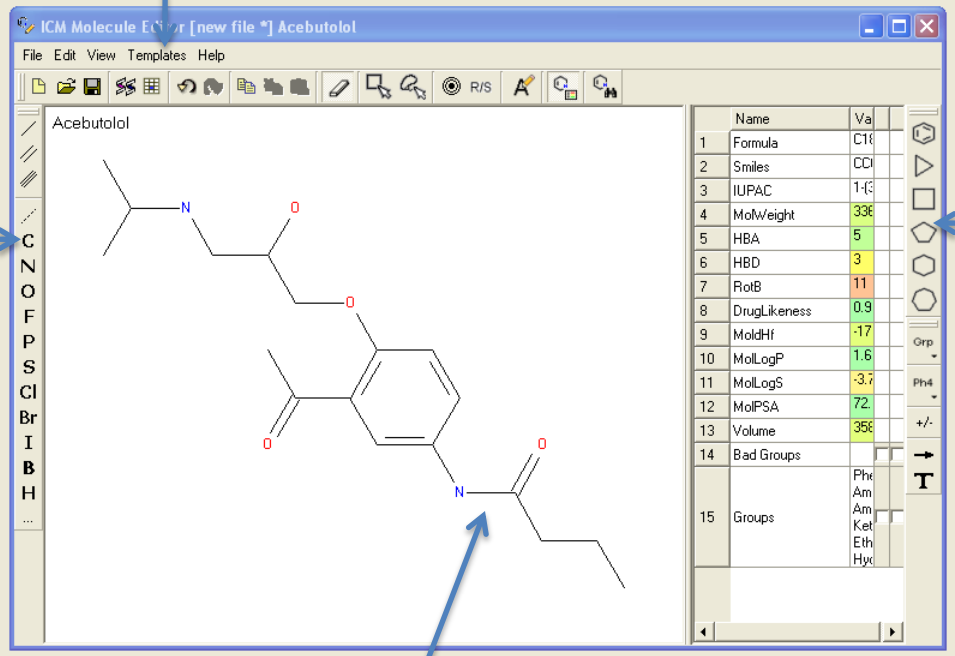
HOW TO IMPORT, SKETCH AND EDIT CHEMICALS

How to access the ICM Molecular Editor.



How to sketch chemicals in the ICM Molecular Editor.

1c. Click Templates menu for even more templates

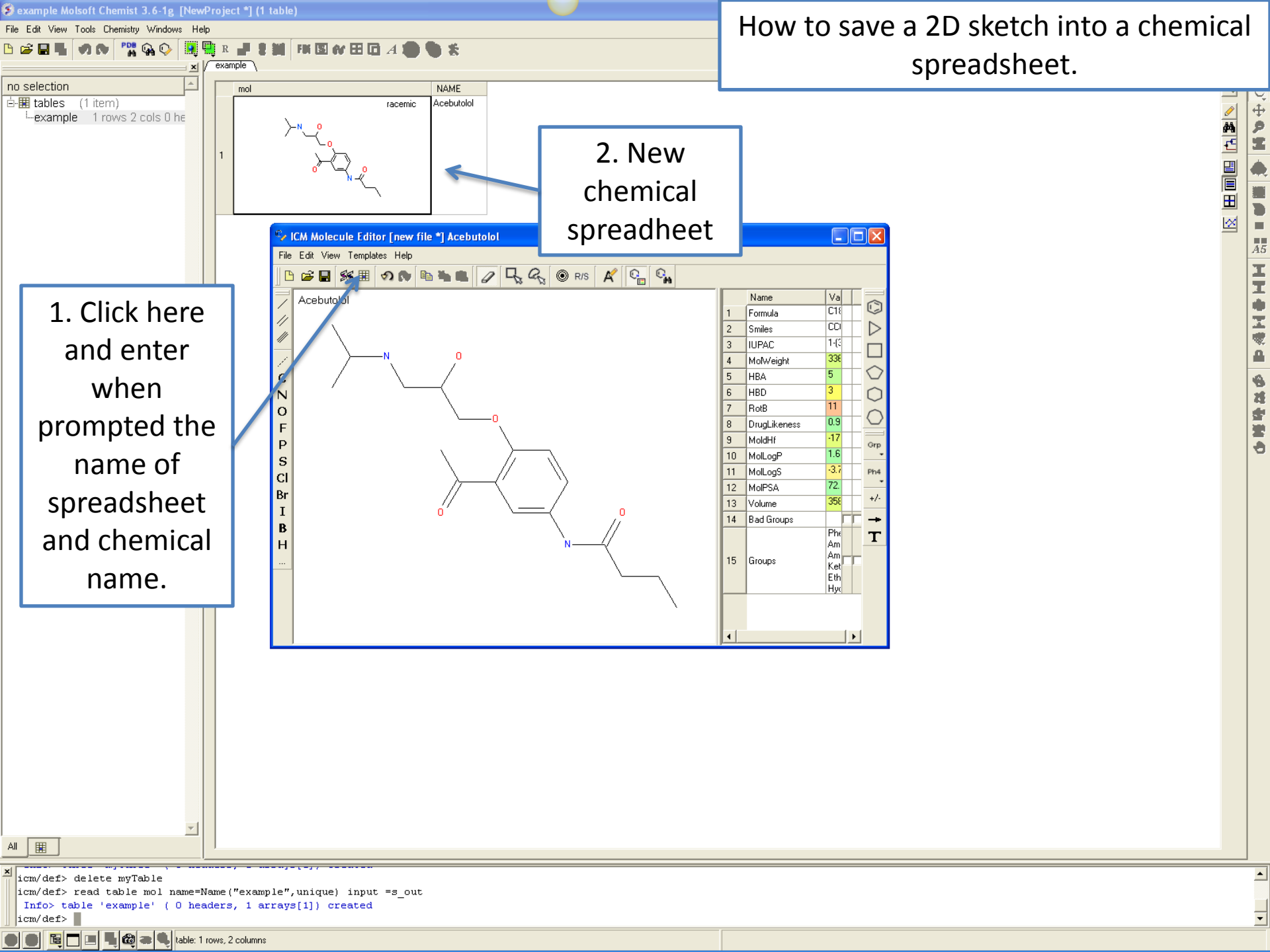


1a. Select atoms and bonds here

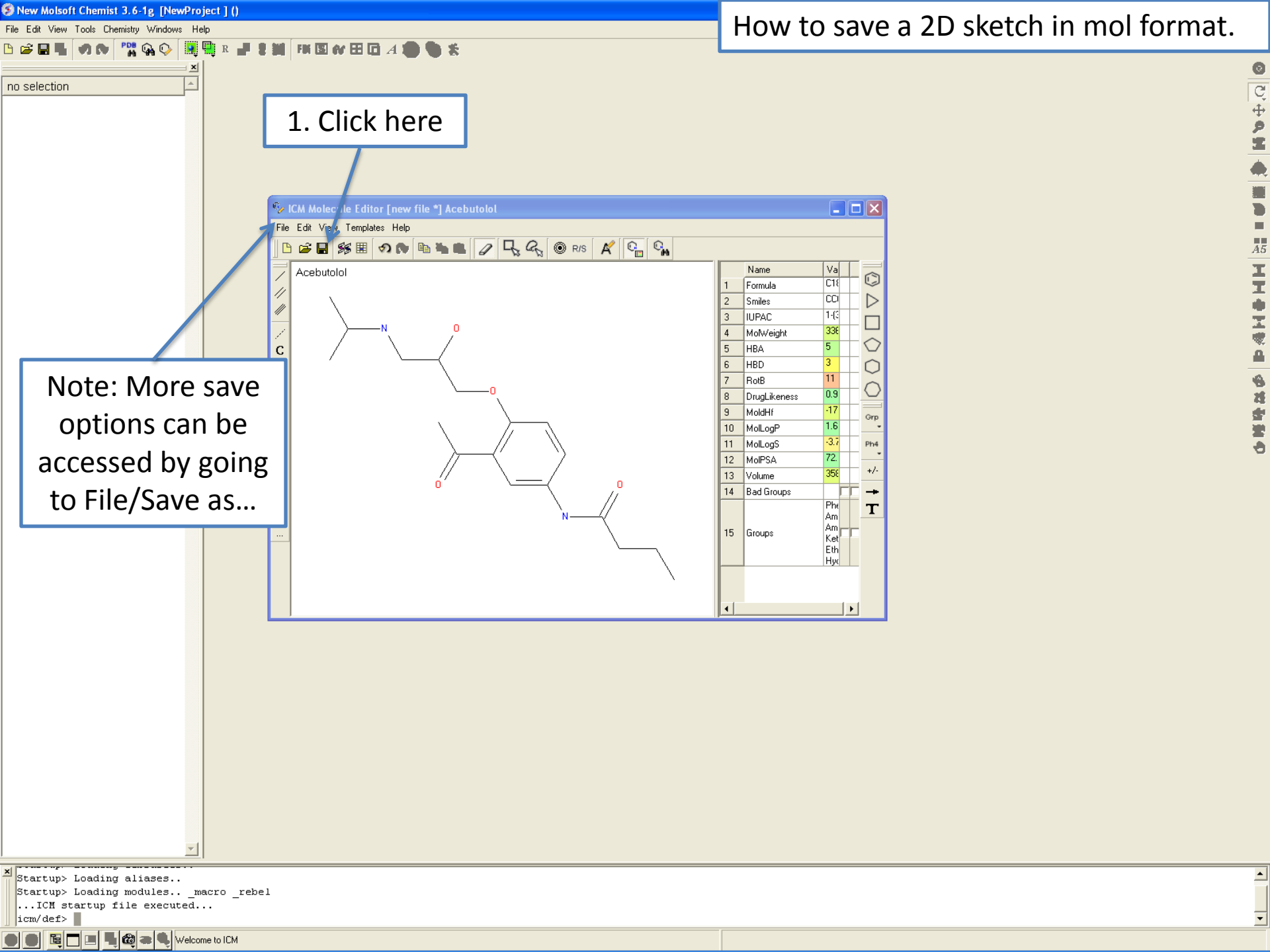
1b. Select rings here

2. Click on the canvas to start sketching

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

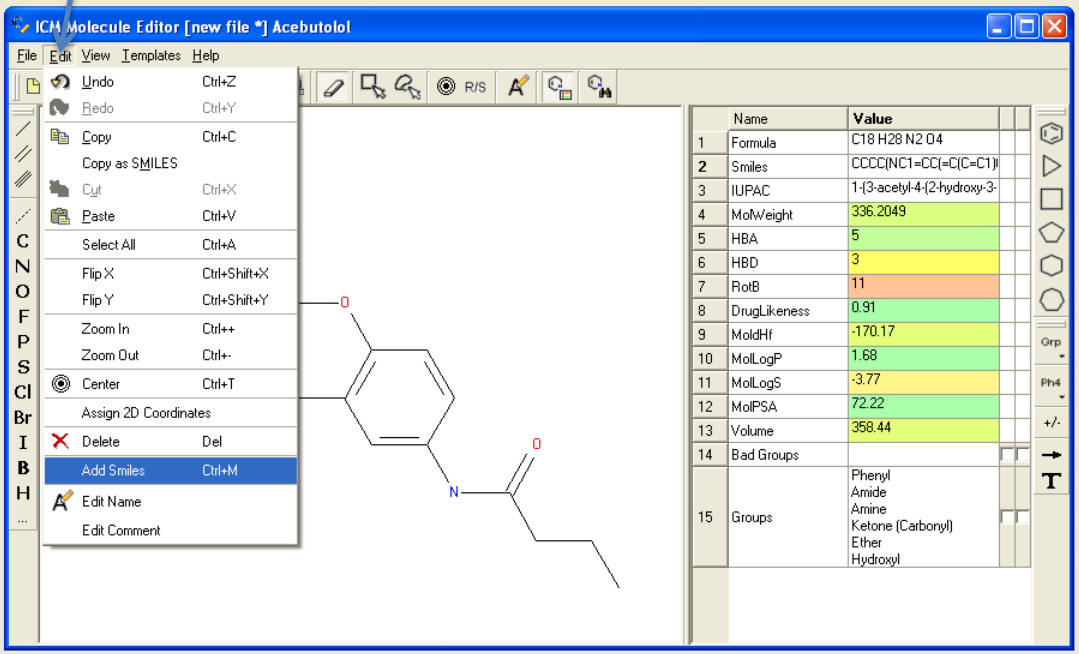


How to save a 2D sketch in mol format.



How to use SMILES strings to sketch a chemical.

Edit Add Smile

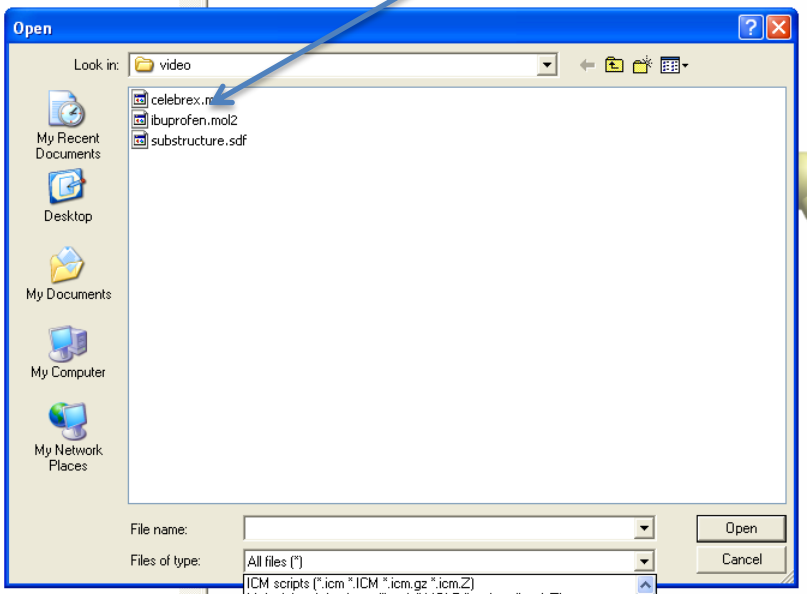


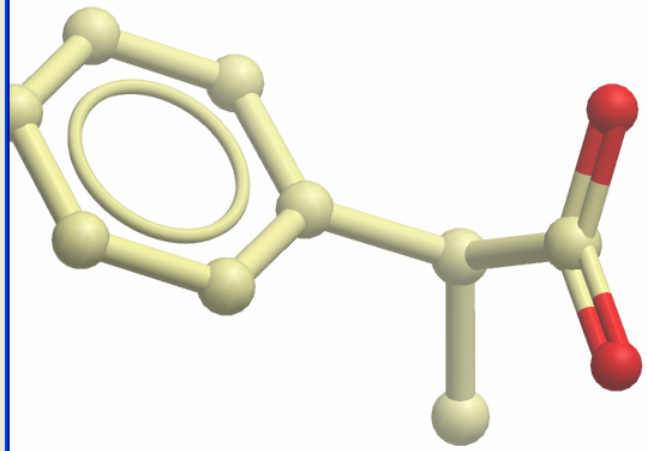
Example of a SMILES string C1C=CC=CC=1

How to load a mol, sdf, or mol2 file.

1. File/Open

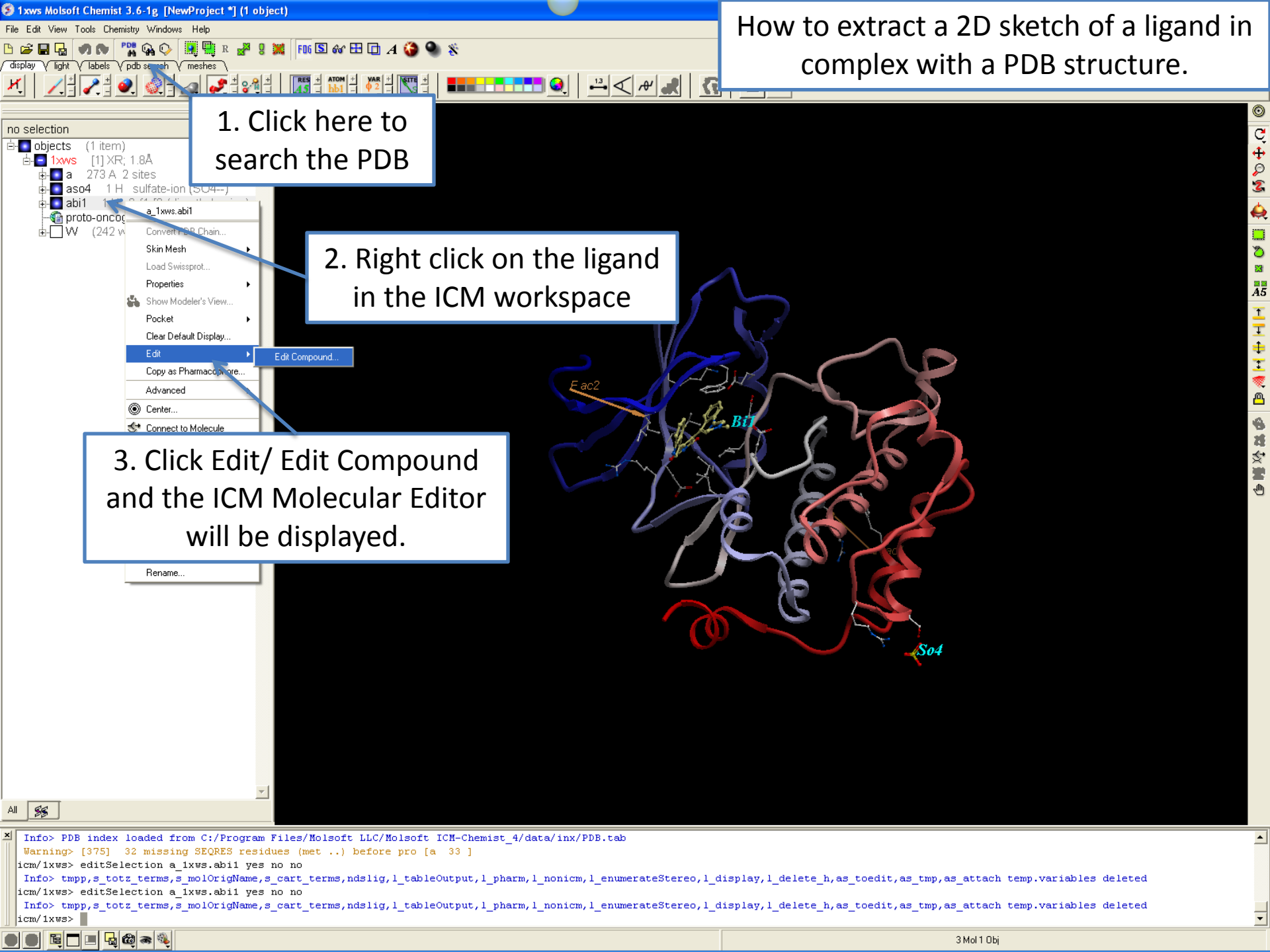
2. Locate file





- 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.



ICM-Chemist

WORKING WITH CHEMICAL SPREADHSHEETS

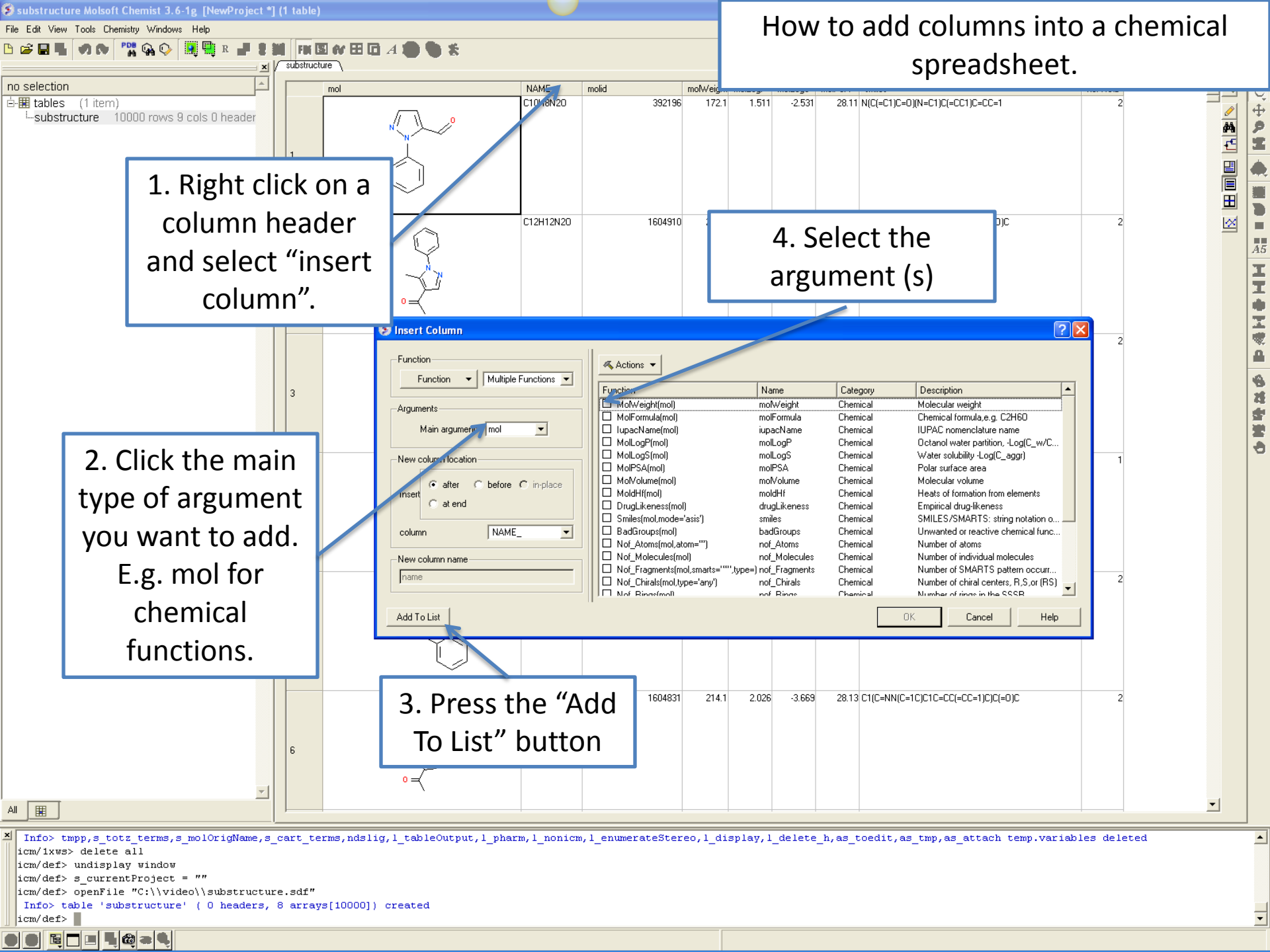
How to add columns into a chemical spreadsheet.

1. Right click on a column header and select “insert column”.

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

3. Press the “Add To List” button

4. Select the argument (s)



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

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

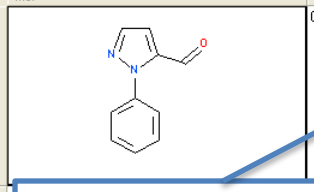
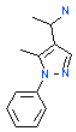
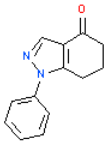
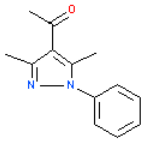
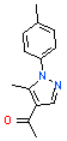
File Edit View Tools Chemistry Windows Help

no selection

tables (1 item)

substructure 10000 rows 9 cols 0 header

substructure

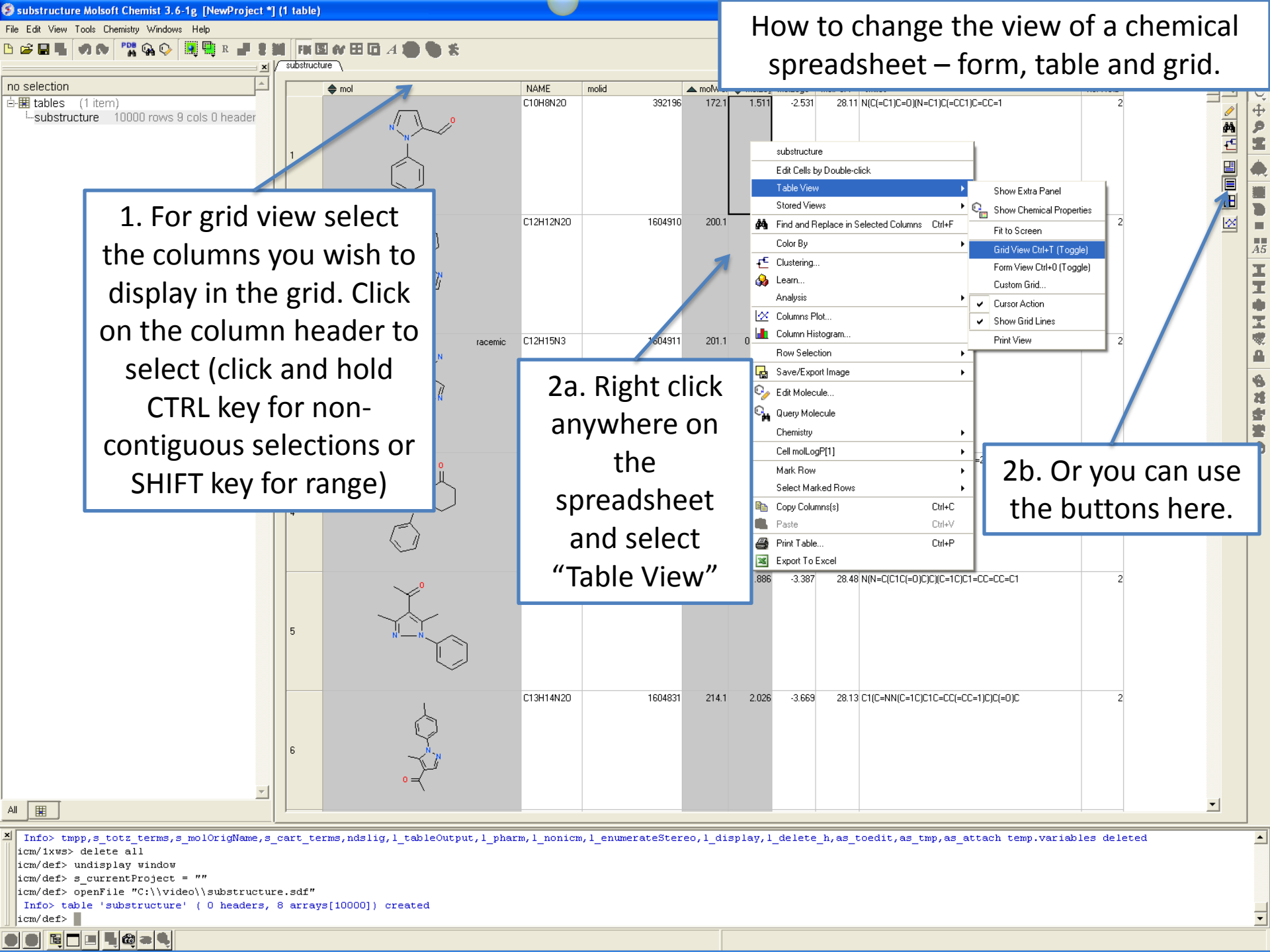
	mol	NAME	molid	molWeight (real)				
1		C10H8N2O	392[illegible]	17				N(C(=C1)C=O)(N=C1)C(=CC1)C=CC=1	2
2			1604910	20				C1(C=NN(C=1C)C1C=CC=CC=1)C(=O)C	2
3		racemic C12H13N3	1604911	20				N(C1C)(N=CC=1C(N)C)C1=CC=CC=C1	2
4		C13H12N2O	510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1C1)C2C=CC=CC=2)C(=O)CC1	1
5		C13H14N2O	1526405	214.1	1.886	-3.387	28.48	N(N=C(C1C(=O)C)C)(C=1C)C1=CC=CC=C1	2
6		C13H14N2O	1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1C)C1C=CC(=CC=1)C)C(=O)C	2

1. Right click on a column header and select “Sort”

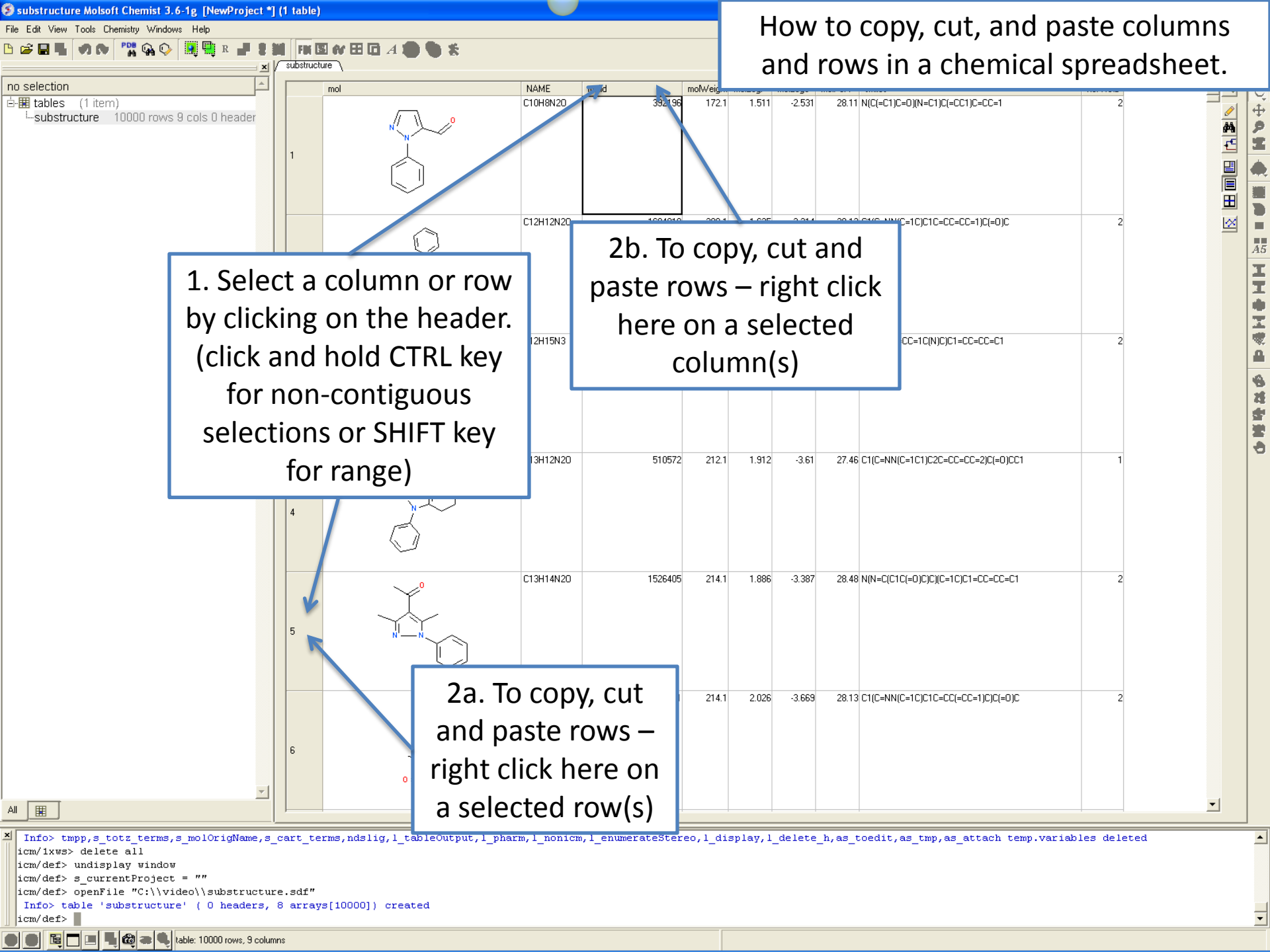
- molWeight (real)
- Hide Column(s)
- Freeze Column
- Paste Column(s) Ctrl+V
- Edit Mode
- Rename Column...
- Delete Column(s)
- Insert Column...
- Add External Columns...
- Column Statistics...
- Sort
- Filter
- Learn...
- Group by Column...
- Format...

```
 Info> tmpp,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/lxws> 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.



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



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)

How to hide rows in a chemical spreadsheet.

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

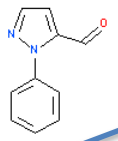
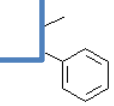
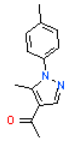
File Edit View Tools Chemistry Windows Help

no selection

tables (1 item)

substructure 10000 rows 9 cols 0 header

substructure

	mol	NAME	molid	moWeig					
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							13	C1(C=NN(C=1C)C1C=CC=CC=1)C(=O)C	2
3		racemic C12H15N3	1604911	201.1	0.5295	-3.096	34.66	N(C1C)(N=CC=1C(N)C)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
6		C13H14N2O	1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1C)C1C=CC(=CC=1)C)C(=O)C	2

Cut Row(s)
Copy Row(s)
Paste Row(s)
Freeze Row(s)
Delete Row(s)
Hide Rows
Insert Empty Row Before
Insert Empty Row After

2. Right click here and select “Hide Rows”

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

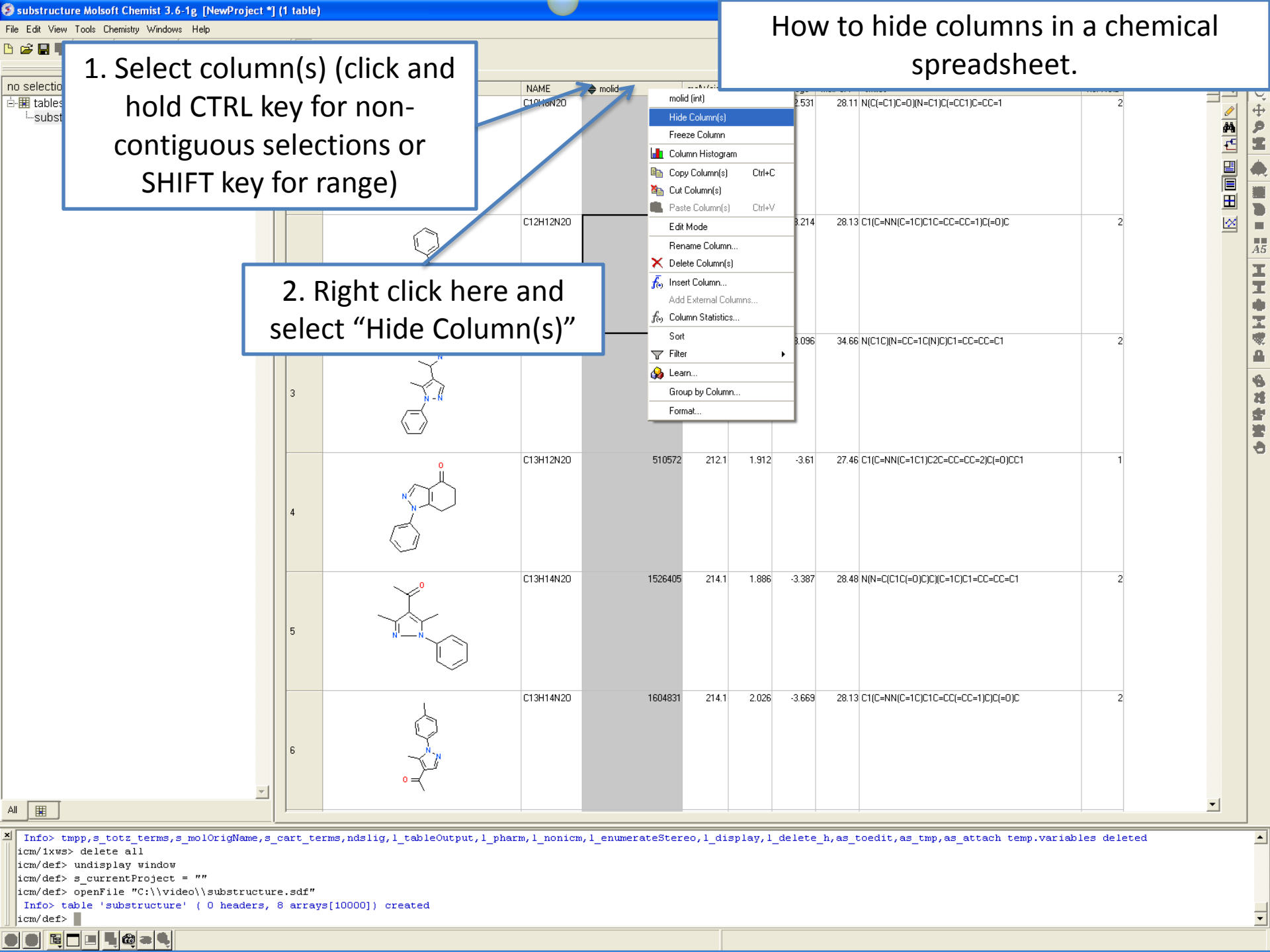
All

```
 Info> tmpp,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/lxws> 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>
```

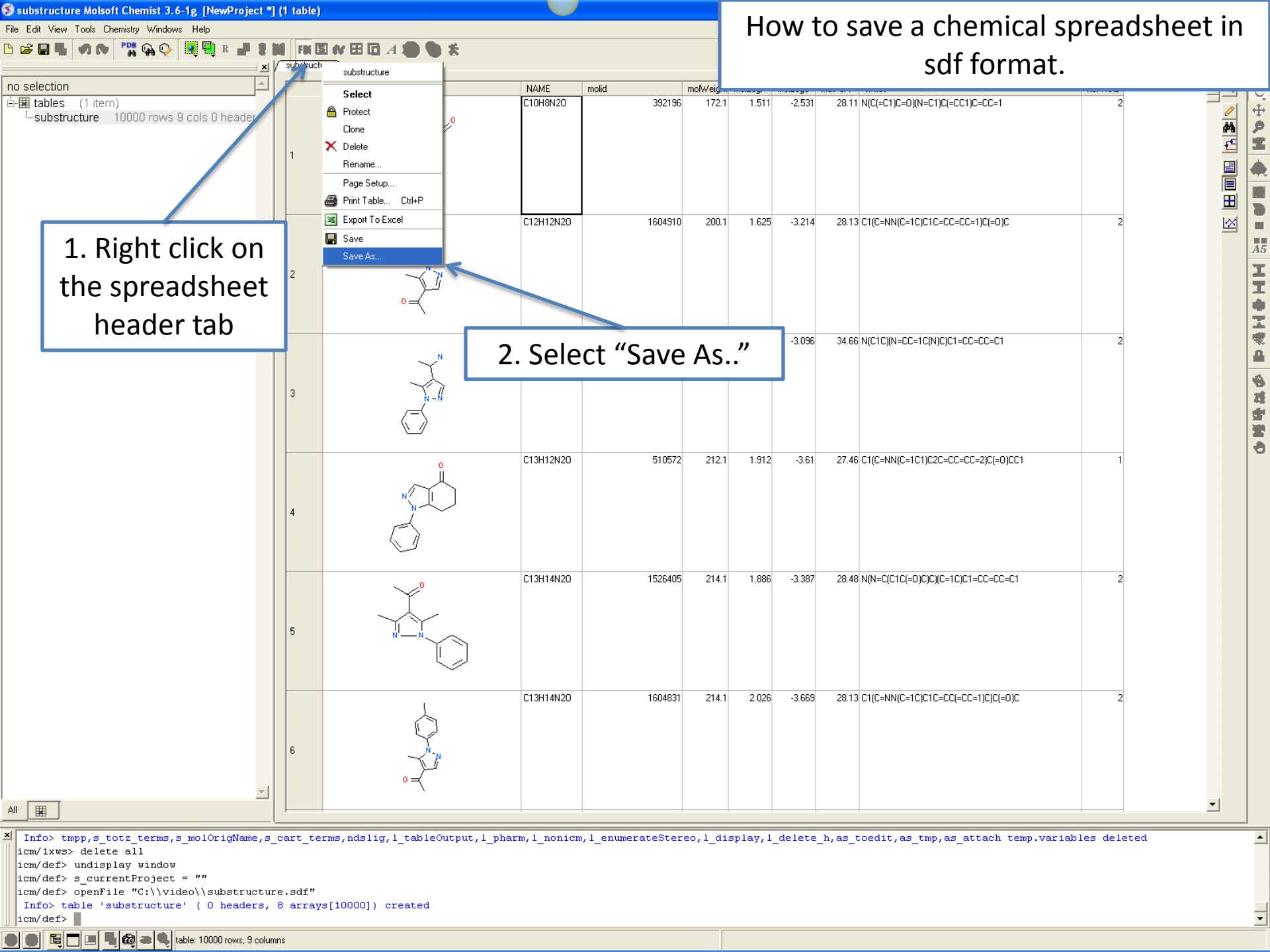
How to hide columns in a chemical spreadsheet.

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

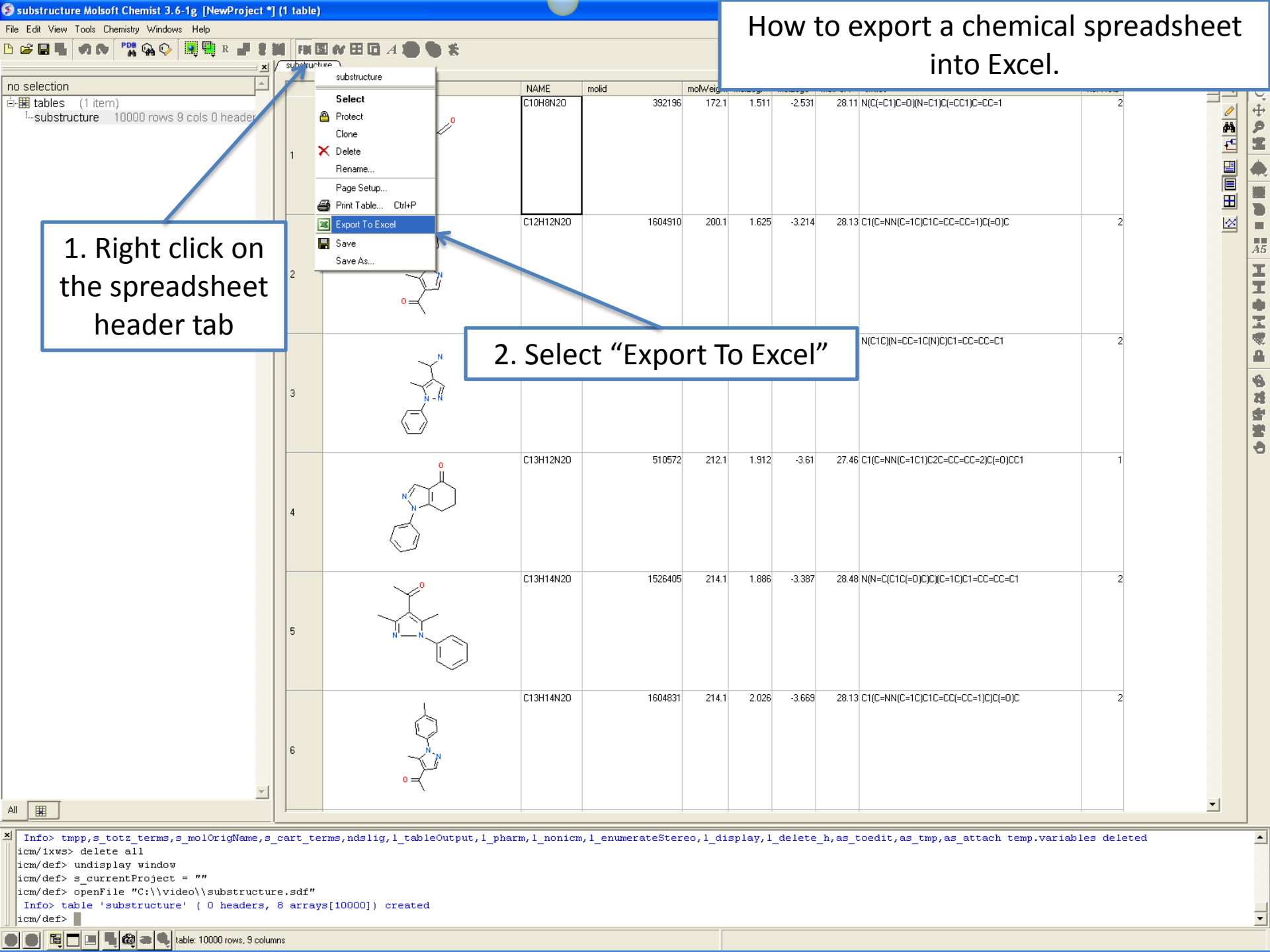
2. Right click here and select “Hide Column(s)”



How to save a chemical spreadsheet in sdf format.



How to export a chemical spreadsheet into Excel.



How to print a chemical spreadsheet.

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

File Edit View Tools Chemistry Windows Help

no selection

tables (1 item)

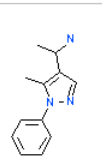
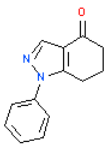
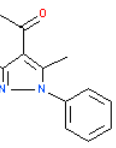
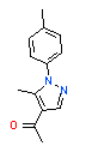
substructure 10000 rows 9 cols 0 header

substructure

Select
Protect
Clone
Delete
Rename...
Page Setup...
Print Table... Ctrl+P
Export To Excel
Save
Save As...

1. Right click on the spreadsheet header tab

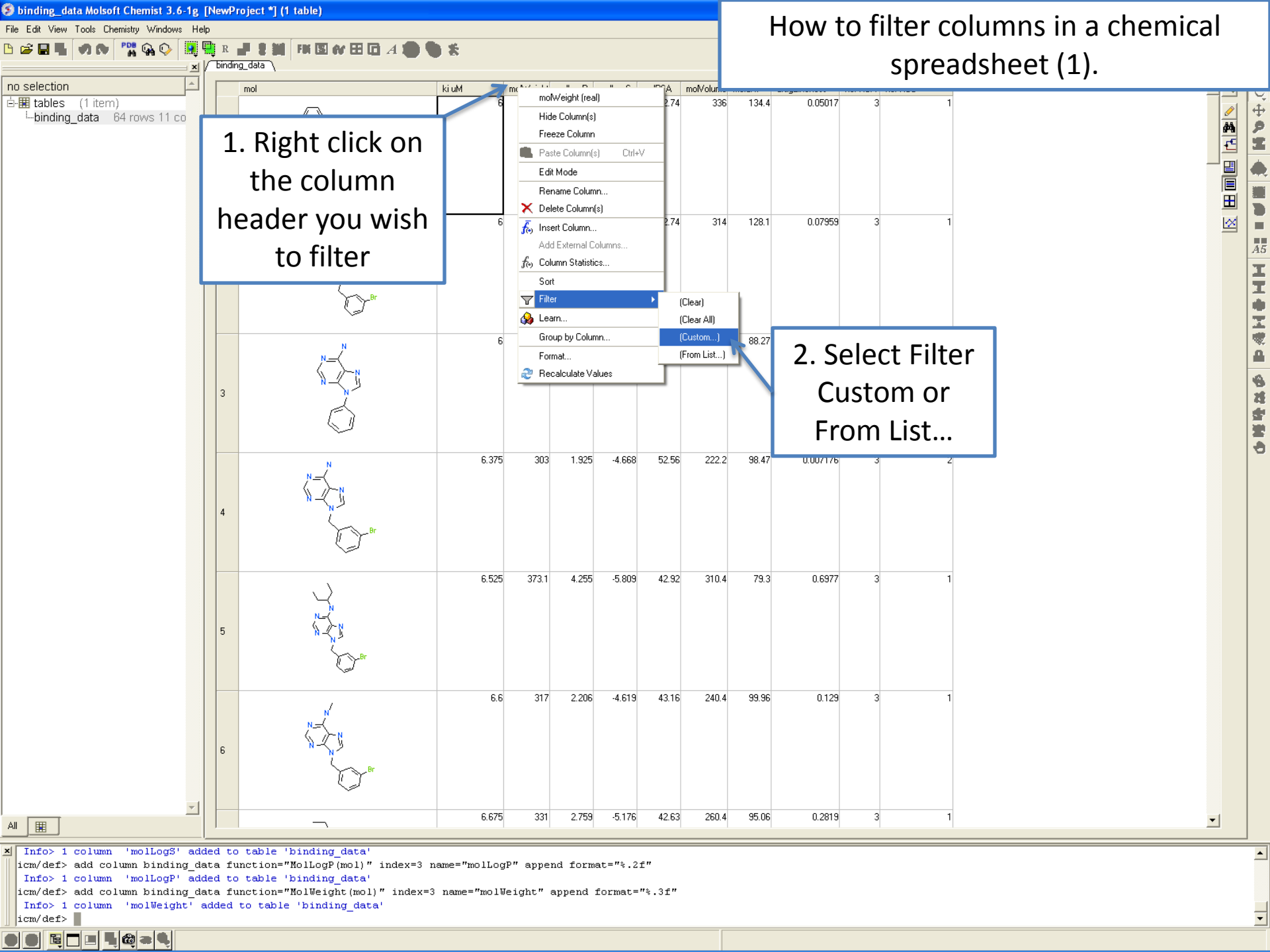
2. Select “Print Table”

		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=1C)C1C=CC=CC=1)C(=O)C	2
3								N(C1C)(N=CC=1C(N)C)C1=CC=CC=C1	2
4		C13H12N2O	510572	212.1	1.912	-3.61	27.46	C1(C=NN(C=1C1)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=1C)C1=CC=CC=C1	2
6		C13H14N2O	1604831	214.1	2.026	-3.669	28.13	C1(C=NN(C=1C)C1C=CC(=CC=1)C)C(=O)C	2

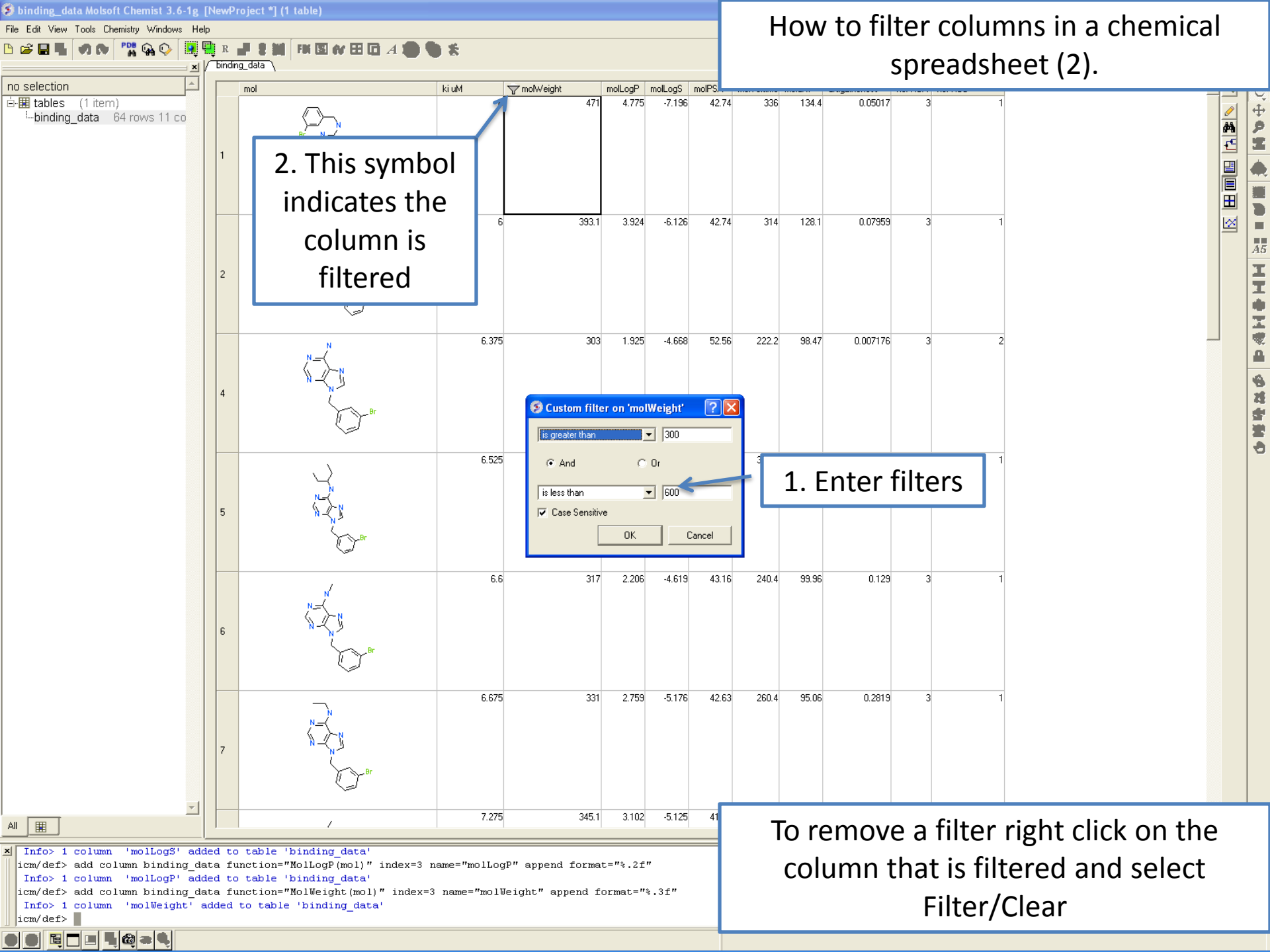
```
 Info> tmpp,s_totz_terms,s_molOrigName,s_cart_terms,ndslig,l_tableOutput,l_pharm,l_nonicm,l_enumerateStereo,l_display,l_delete_h,as_toedit,as_tmp,as_attach temp.variables deleted
icm/lxws> delete all
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\video\\substructure.sdf"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

table: 10000 rows, 9 columns

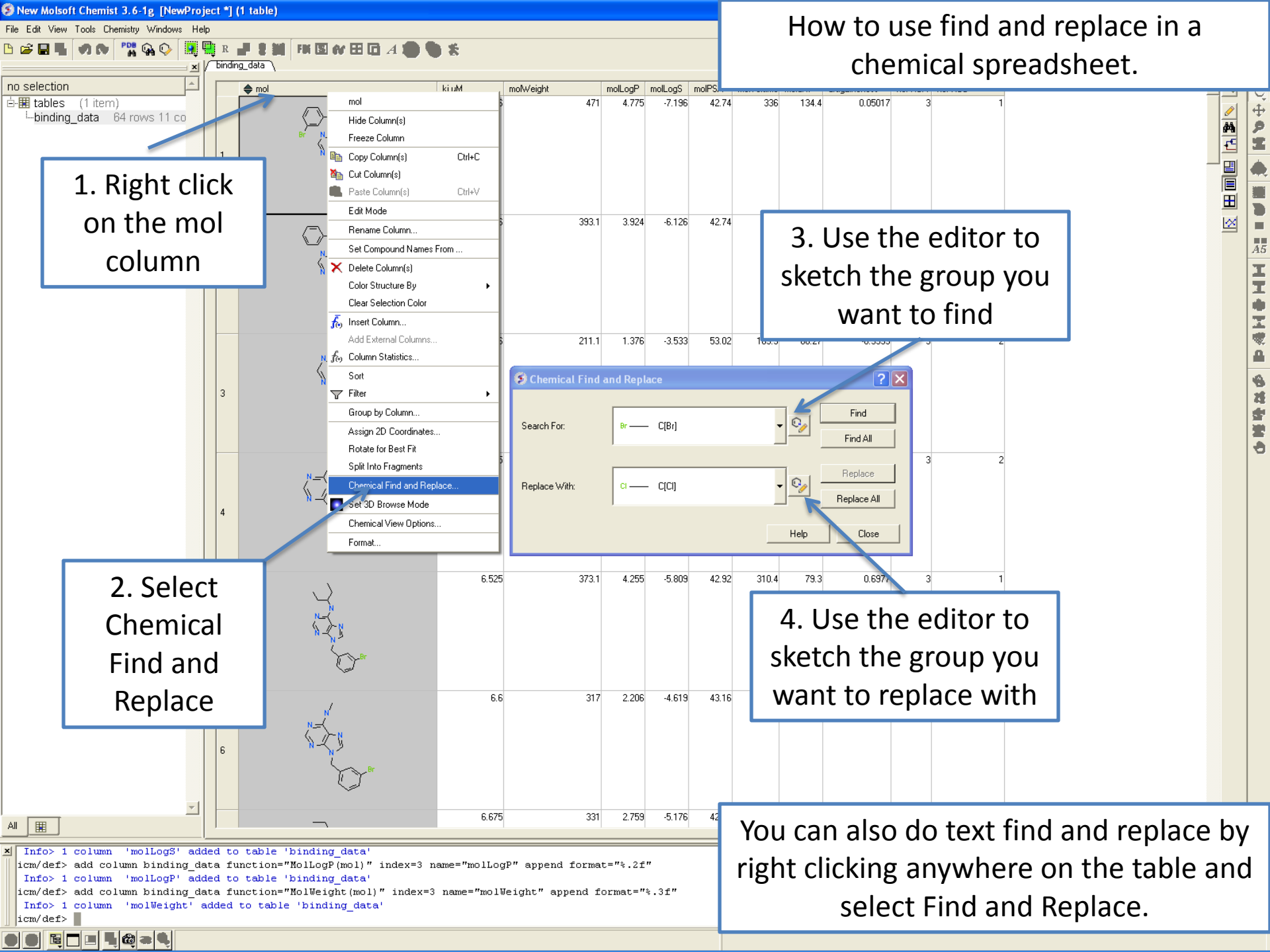
How to filter columns in a chemical spreadsheet (1).



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



How to use find and replace in a chemical spreadsheet.



1. Right click on the mol column

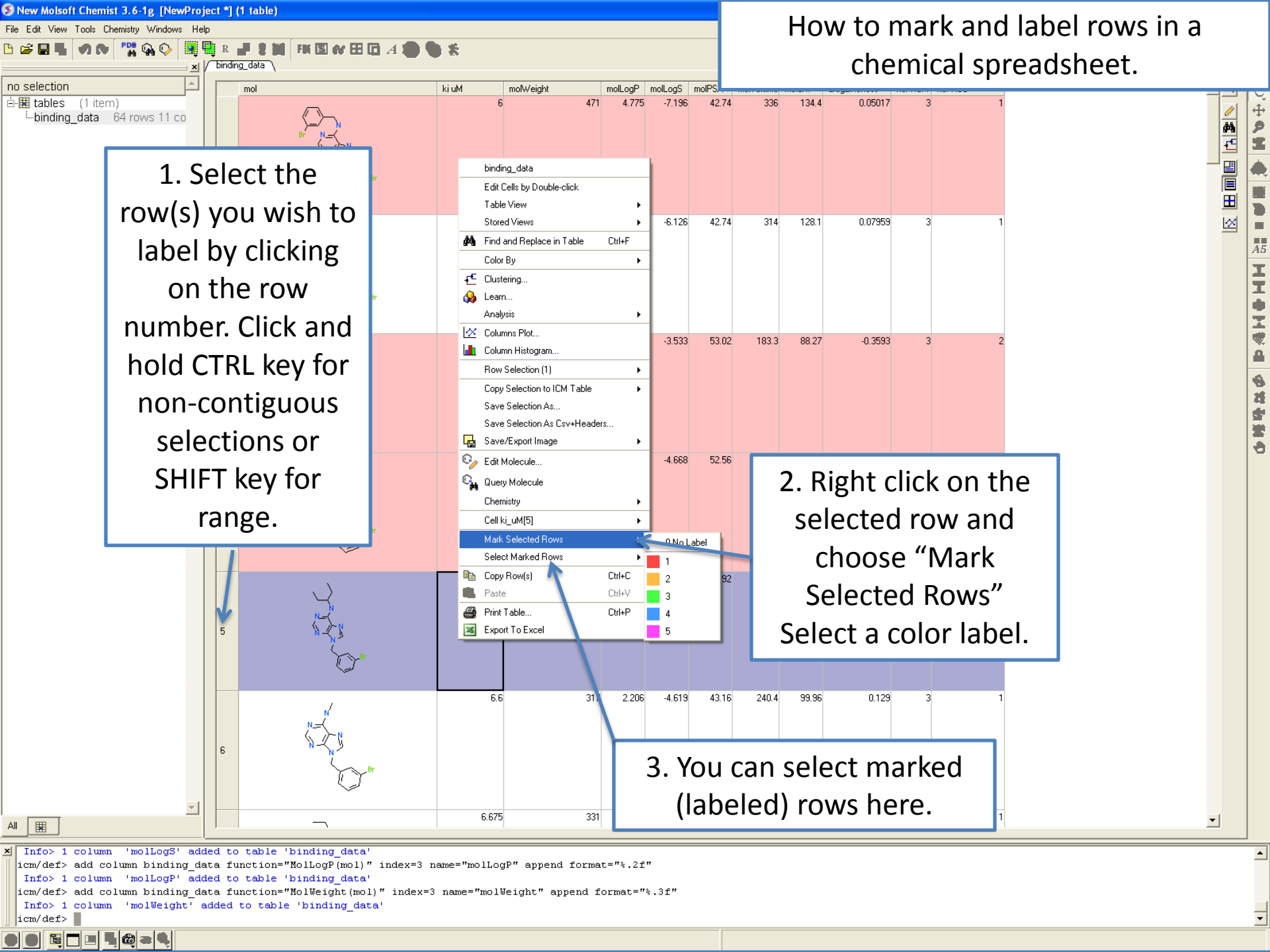
2. Select Chemical Find and Replace

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

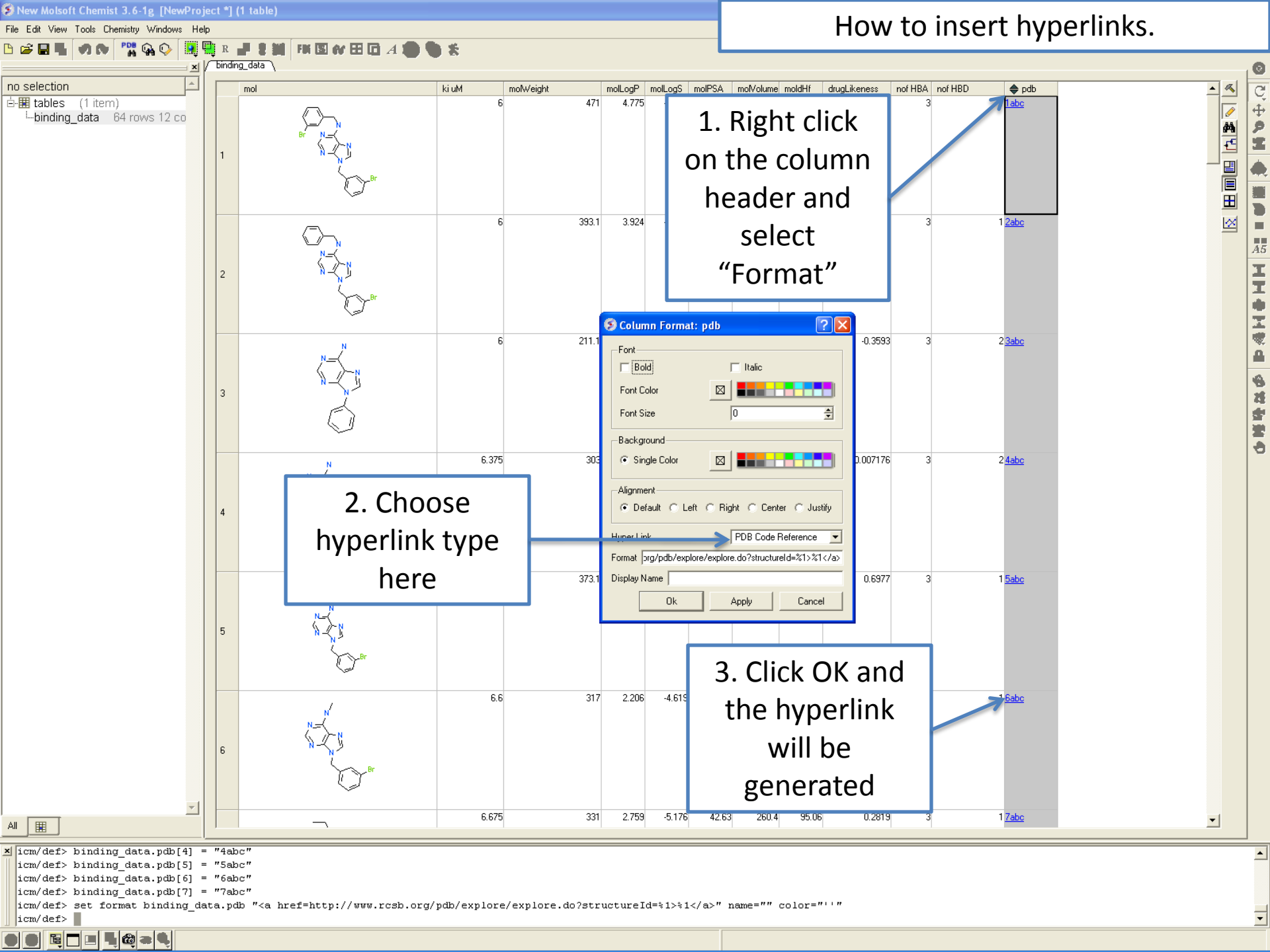
4. Use the editor to sketch the group you want to replace with

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

How to mark and label rows in a chemical spreadsheet.



How to insert hyperlinks.

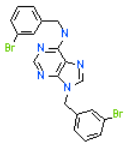
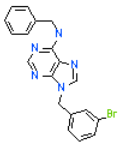
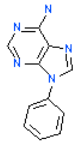
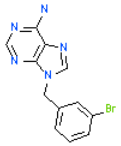
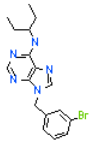
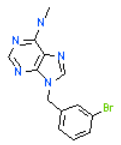


How to copy and paste 2D chemicals.

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

File Edit View Tools Chemistry Windows Help

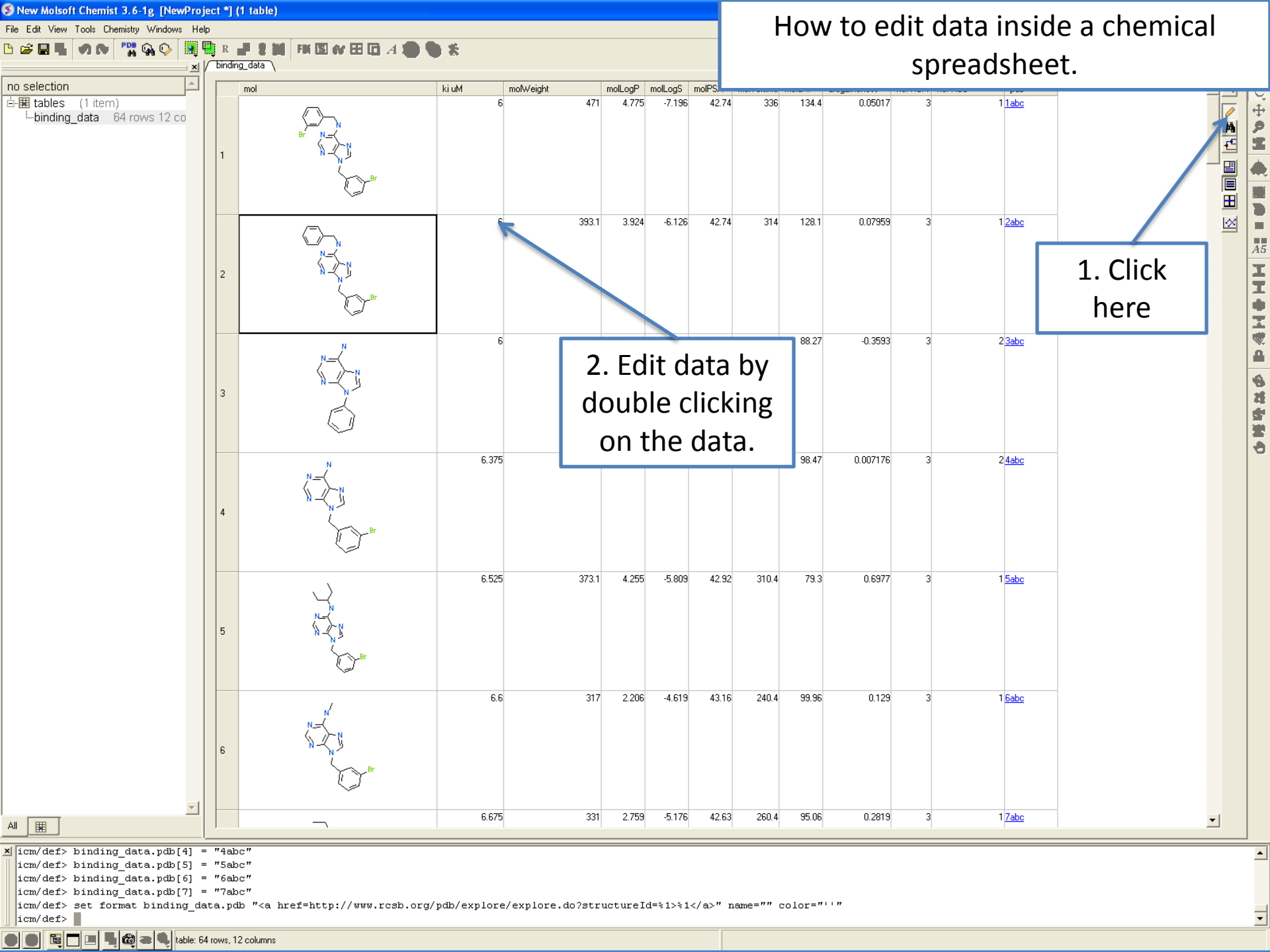
1. Right click on the 2D chemical.

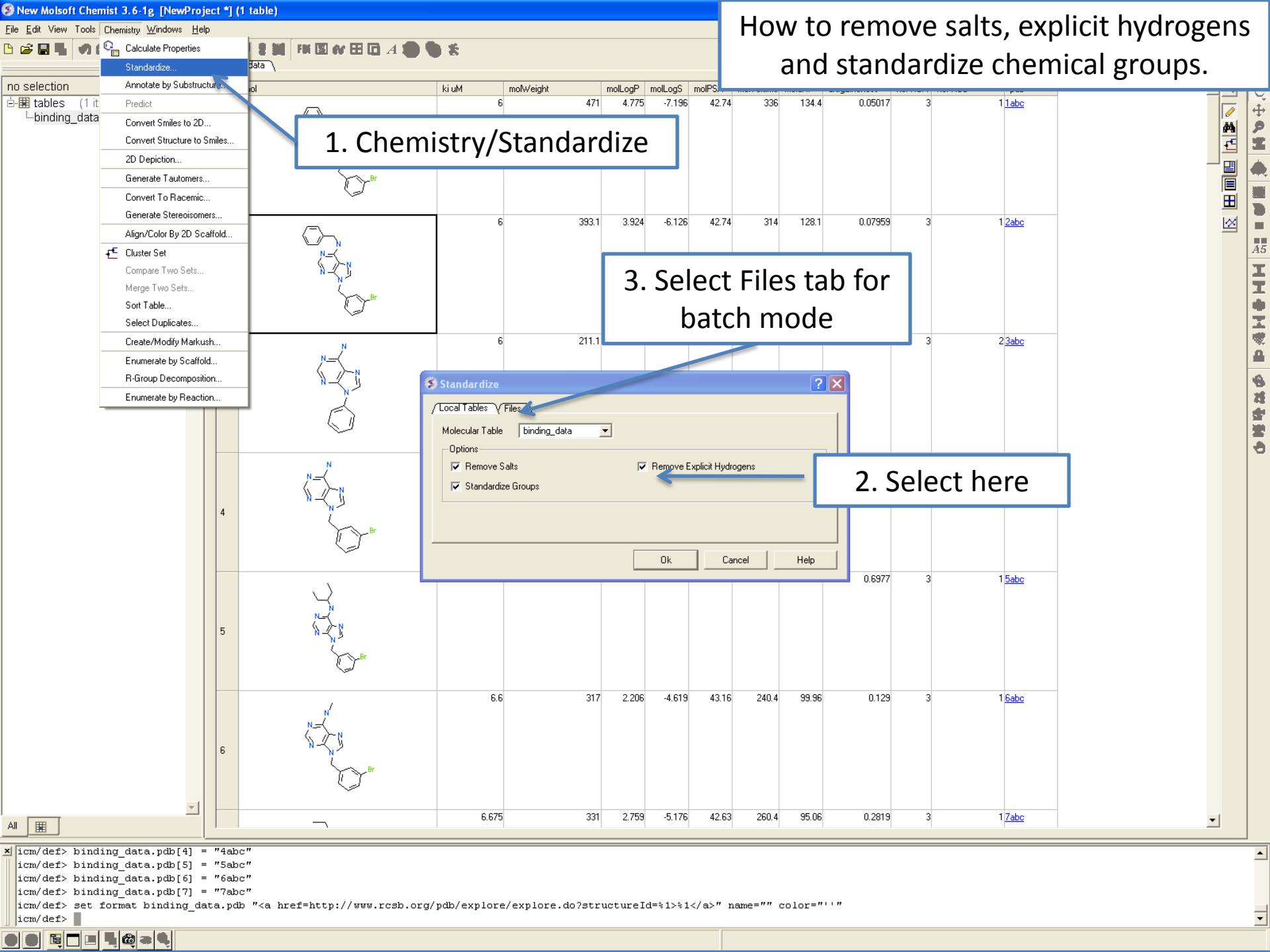
	mol	ki uM	molWeight	molLogP	molLogS	molPSA	molVolume	moldHf	drugLikeness	nof HBA	nof HBD	pdb
1		6	471	4.775	-7.196	42.74	336	134.4	0.05017	3	1	1abc
2		6	393.1	3.924	-6.126	42.74	314	128.1	0.07959	3	1	2abc
3		1.1	1.376	-3.533	53.02	183.3	88.27	-0.3593	3	2	3abc
4		303	1.925	-4.668	52.56	222.2	98.47	0.007176	3	2	4abc
5		73.1	4.255	-5.809	42.92	310.4	79.3	0.6977	3	1	5abc
6		317						0.129	3	1	6abc
		6.675	331	2.759	-5.176	42.63	260.4	95.06	0.2819	3	1	7abc

2. Select “ Copy 2D Molecule”

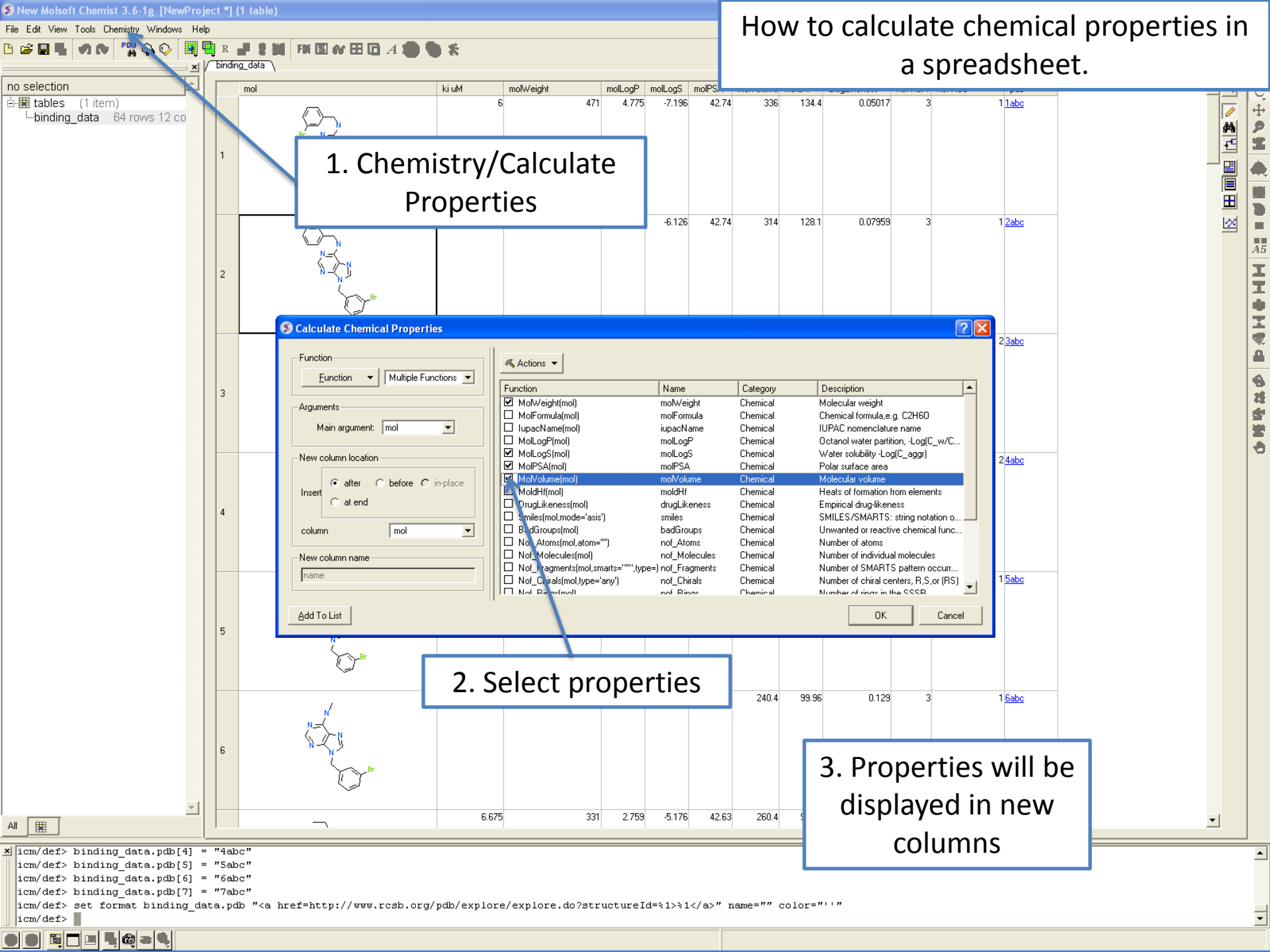
```
icm/def> binding_data.pdb[4] = "4abc"
icm/def> binding_data.pdb[5] = "5abc"
icm/def> binding_data.pdb[6] = "6abc"
icm/def> binding_data.pdb[7] = "7abc"
icm/def> set format binding_data.pdb "<a href=http://www.rcsb.org/pdb/explore/explore.do?structureId=%1>%1</a>" name="" color="''"
icm/def>
```

How to edit data inside a chemical spreadsheet.

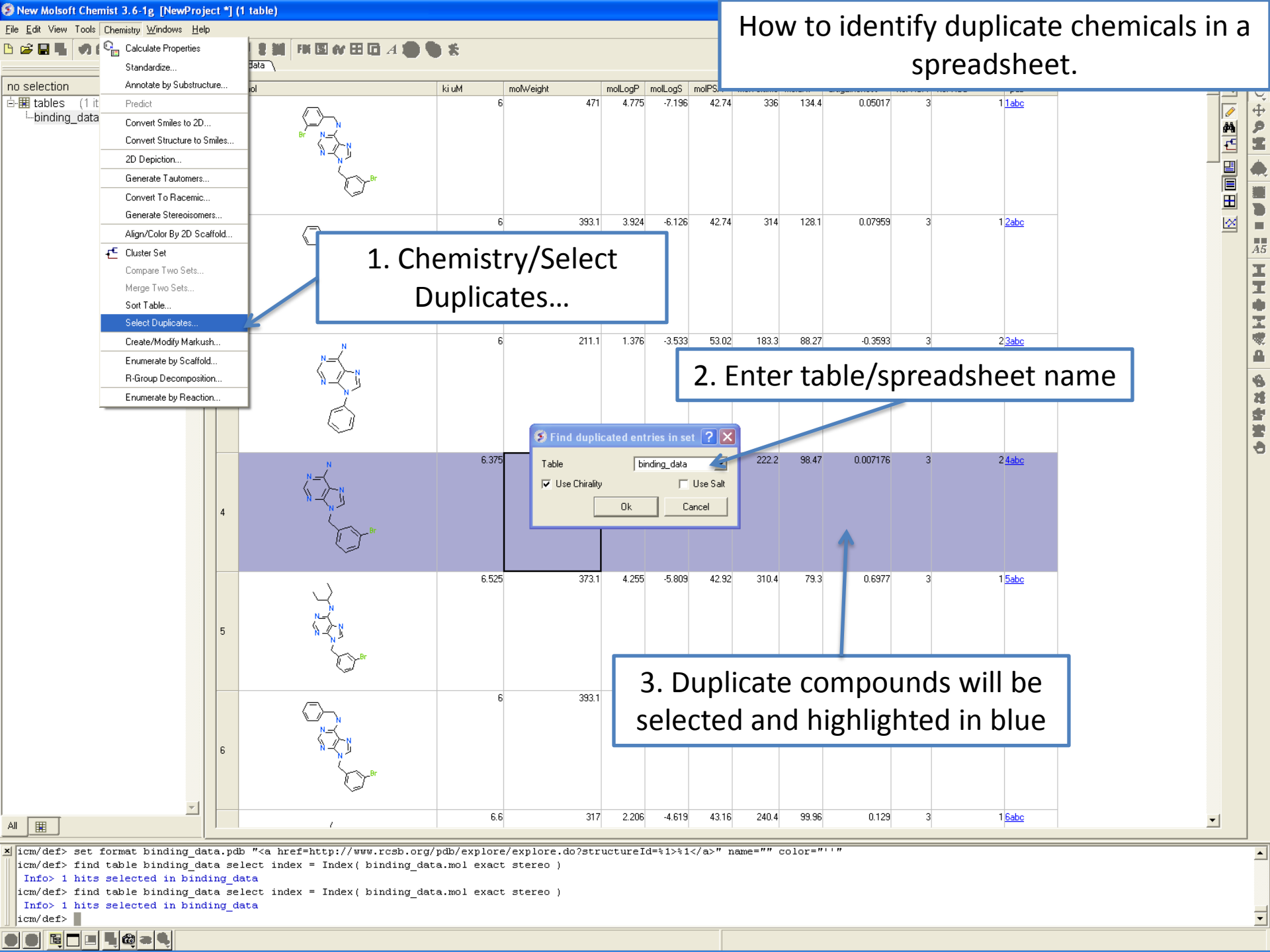



New Molsoft Chemist 3.6-1g [NewProject *] (1 table)
File Edit View Tools Chemistry Windows Help
Calculate Properties
Standardize...
Annotate by Substructure...
Predict
Convert Smiles to 2D...
Convert Structure to Smiles...
2D Depiction...
Generate Tautomers...
Convert To Racemic...
Generate Stereoisomers...
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...
How to remove salts, explicit hydrogens and standardize chemical groups.
1. Chemistry/Standardize
3. Select Files tab for batch mode
2. Select here
Standardize
Local Tables
Files
Molecular Table
binding_data
Options
Remove Salts
Remove Explicit Hydrogens
Standardize Groups
Ok
Cancel
Help
no selection
tables
binding_data
ki uM
molWeight
molLogP
molLogS
molPSA
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 "%1" name="" color="!!"
icm/def>

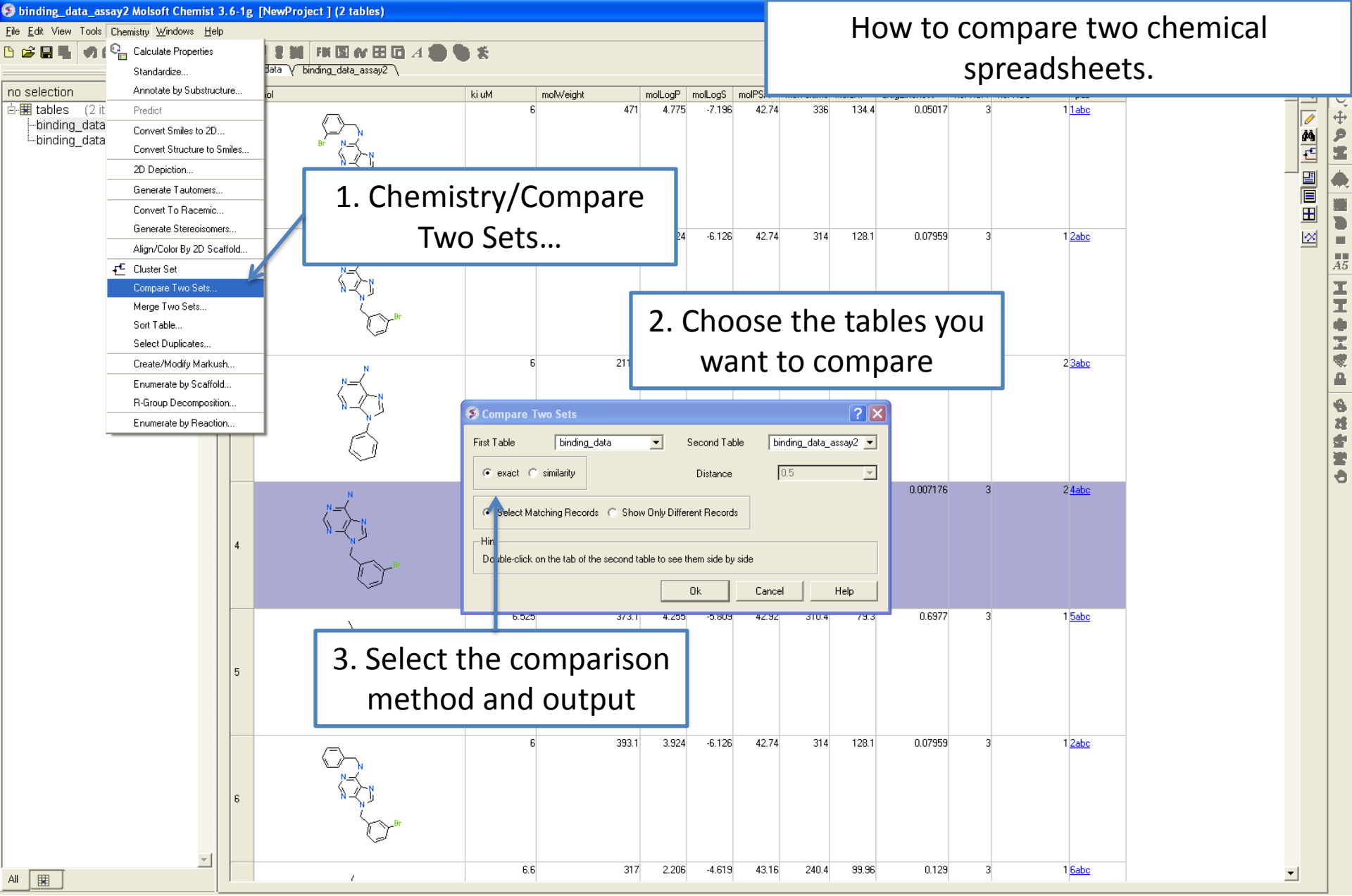
How to calculate chemical properties in a spreadsheet.



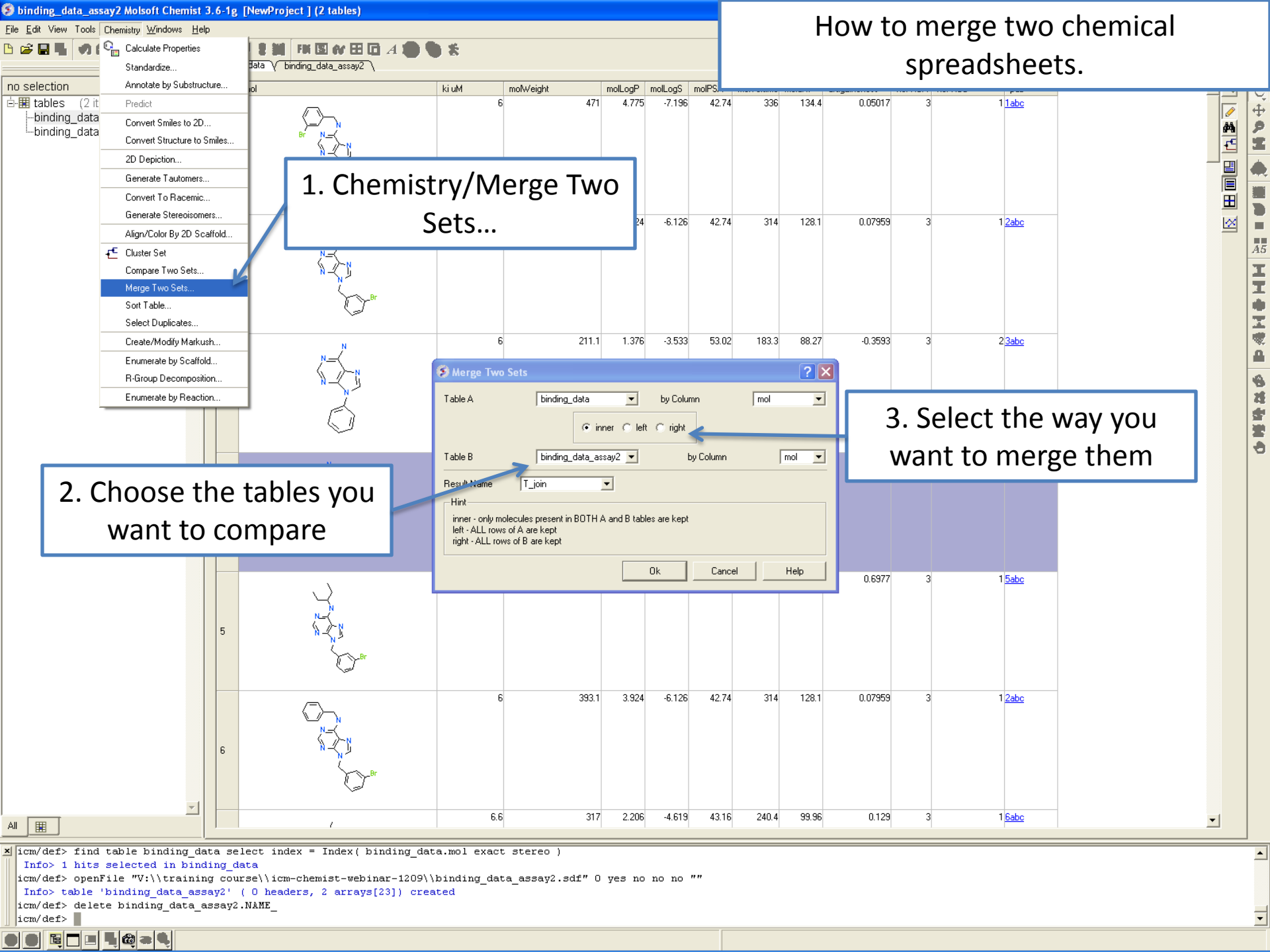
How to identify duplicate chemicals in a spreadsheet.



How to compare two chemical spreadsheets.



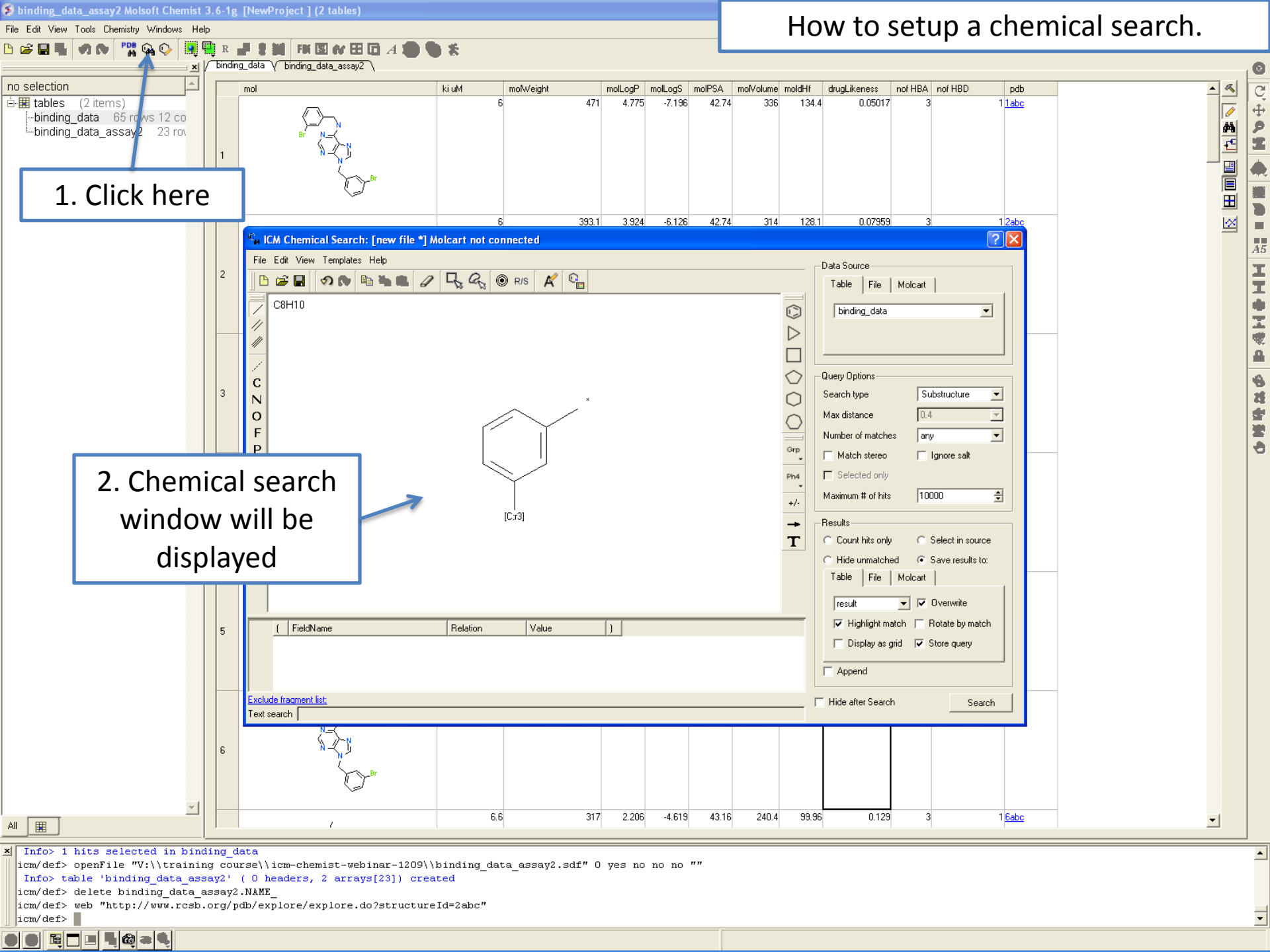
How to merge two chemical spreadsheets.



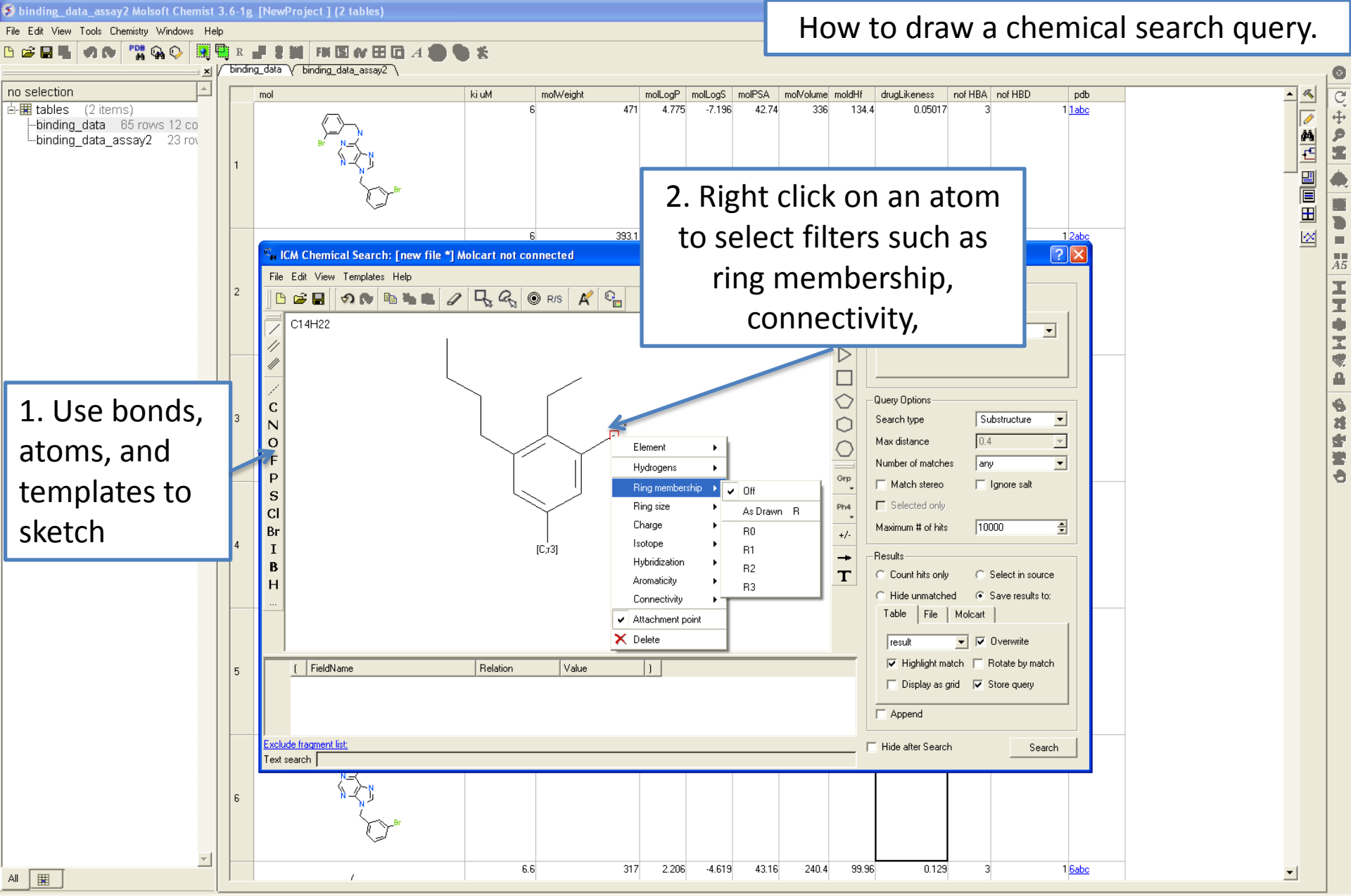
ICM-Chemist

HOW TO PERFORM CHEMICAL SEARCHING

How to setup a chemical search.



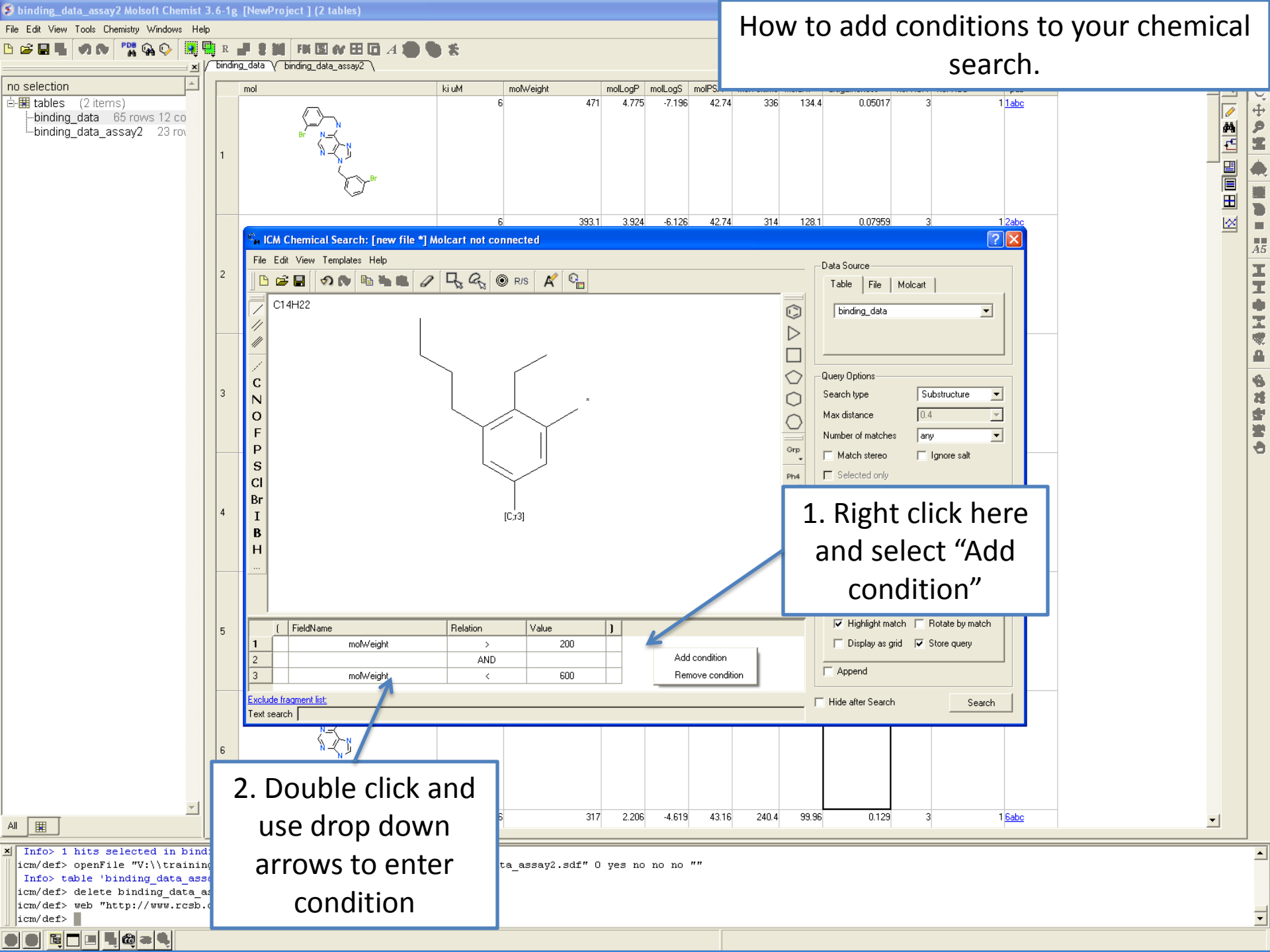
How to draw a chemical search query.



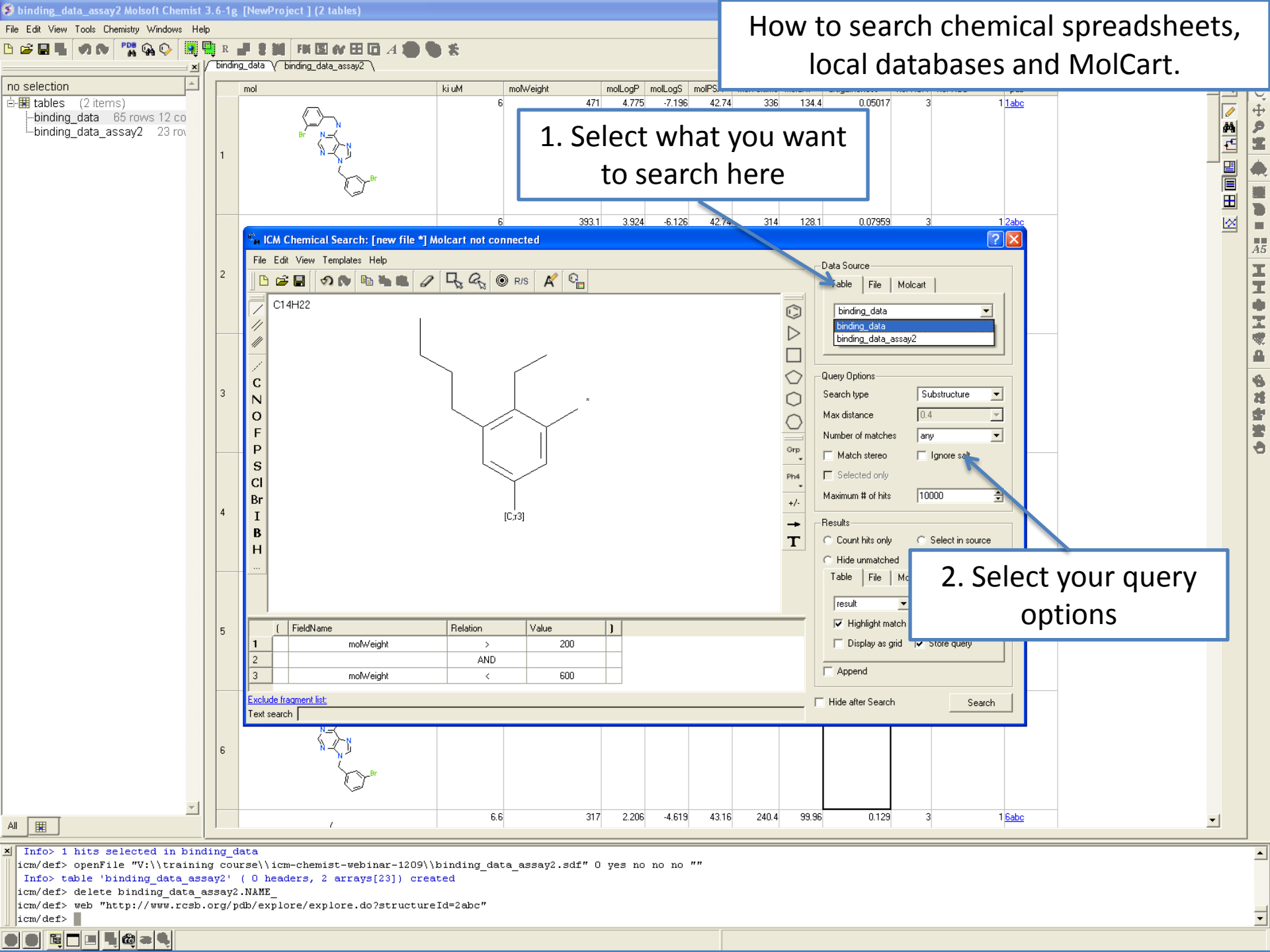
1. Use bonds, atoms, and templates to sketch

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

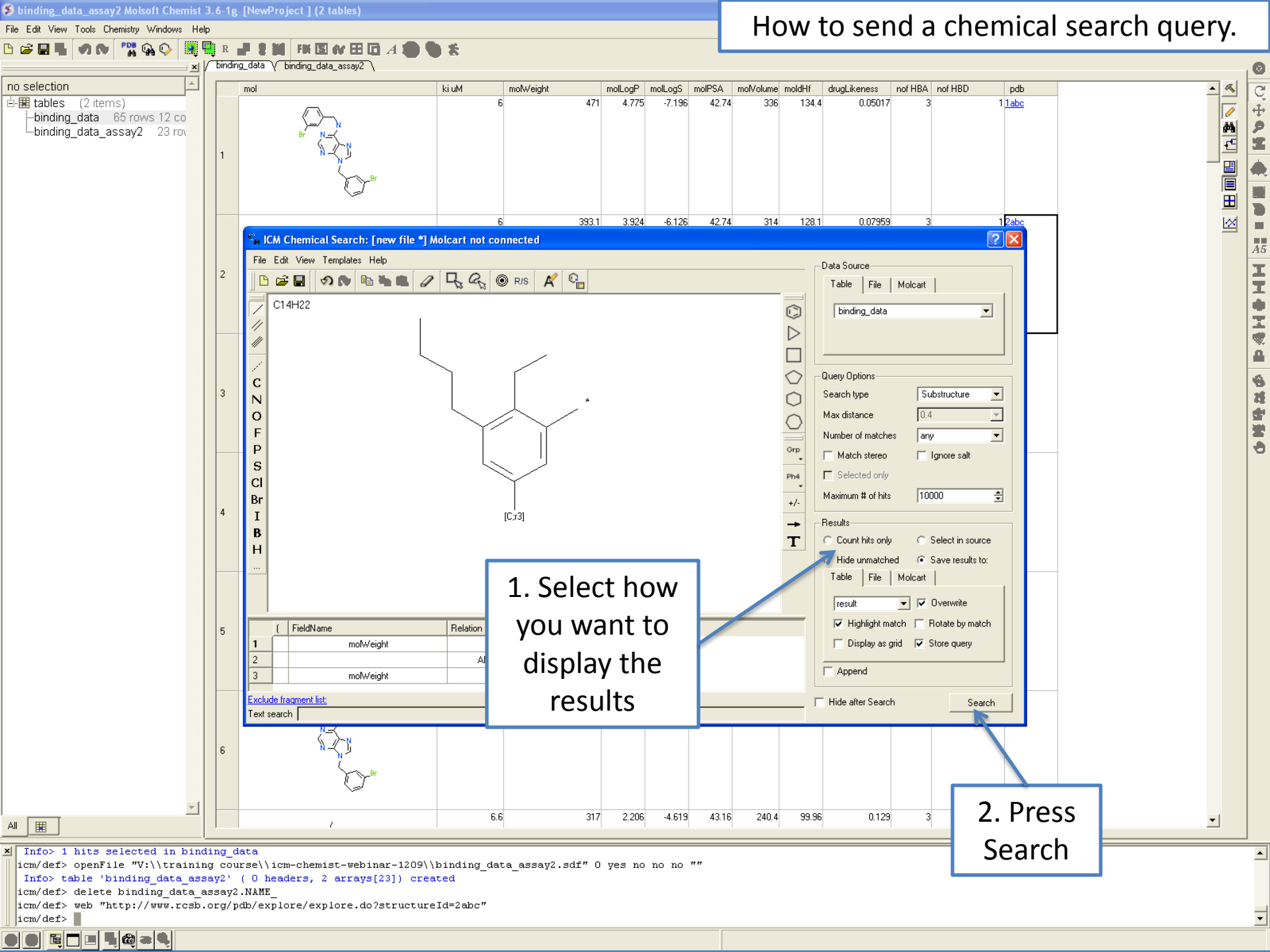
How to add conditions to your chemical search.



How to search chemical spreadsheets, local databases and MolCart.



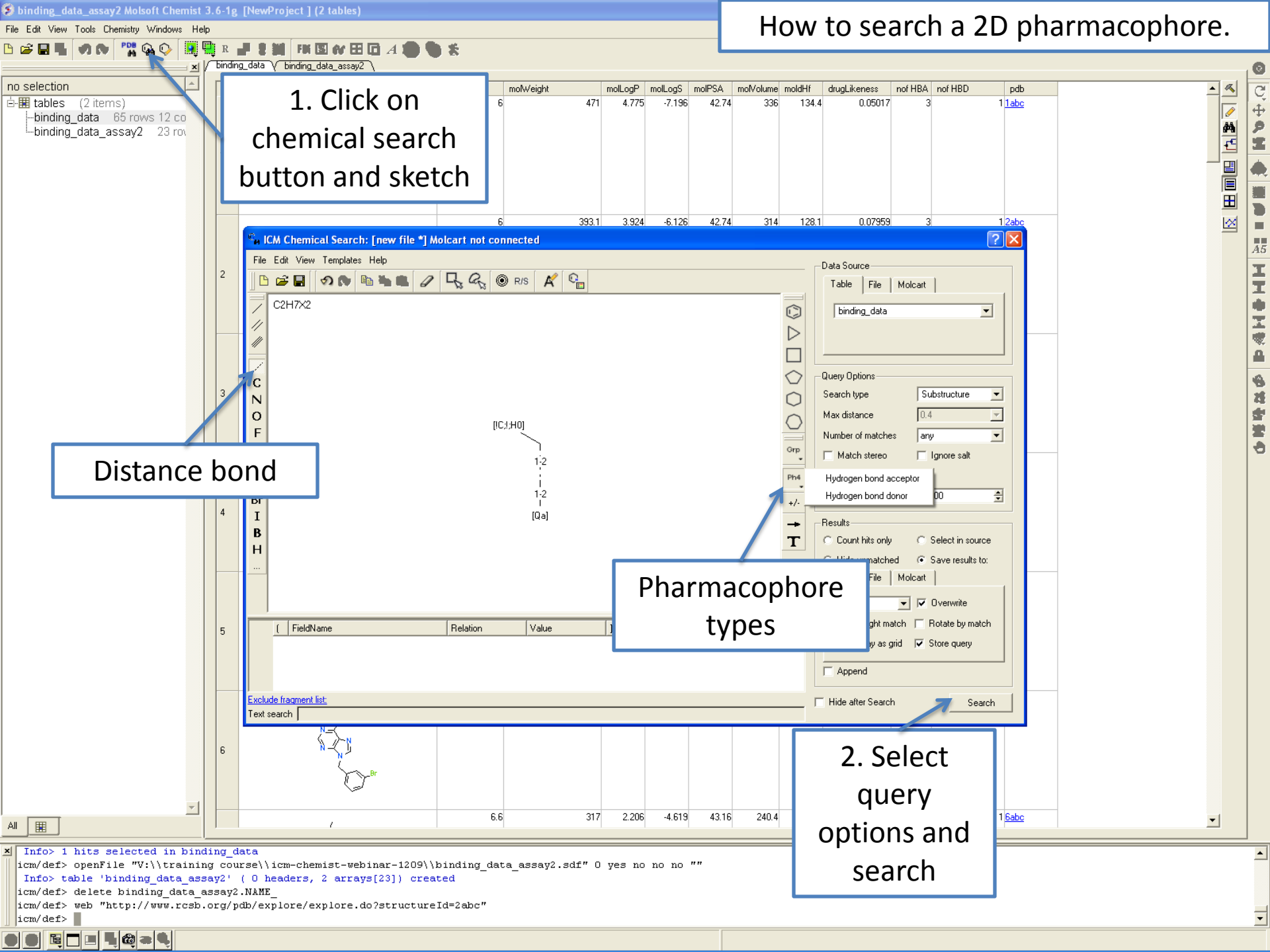
How to send a chemical search query.



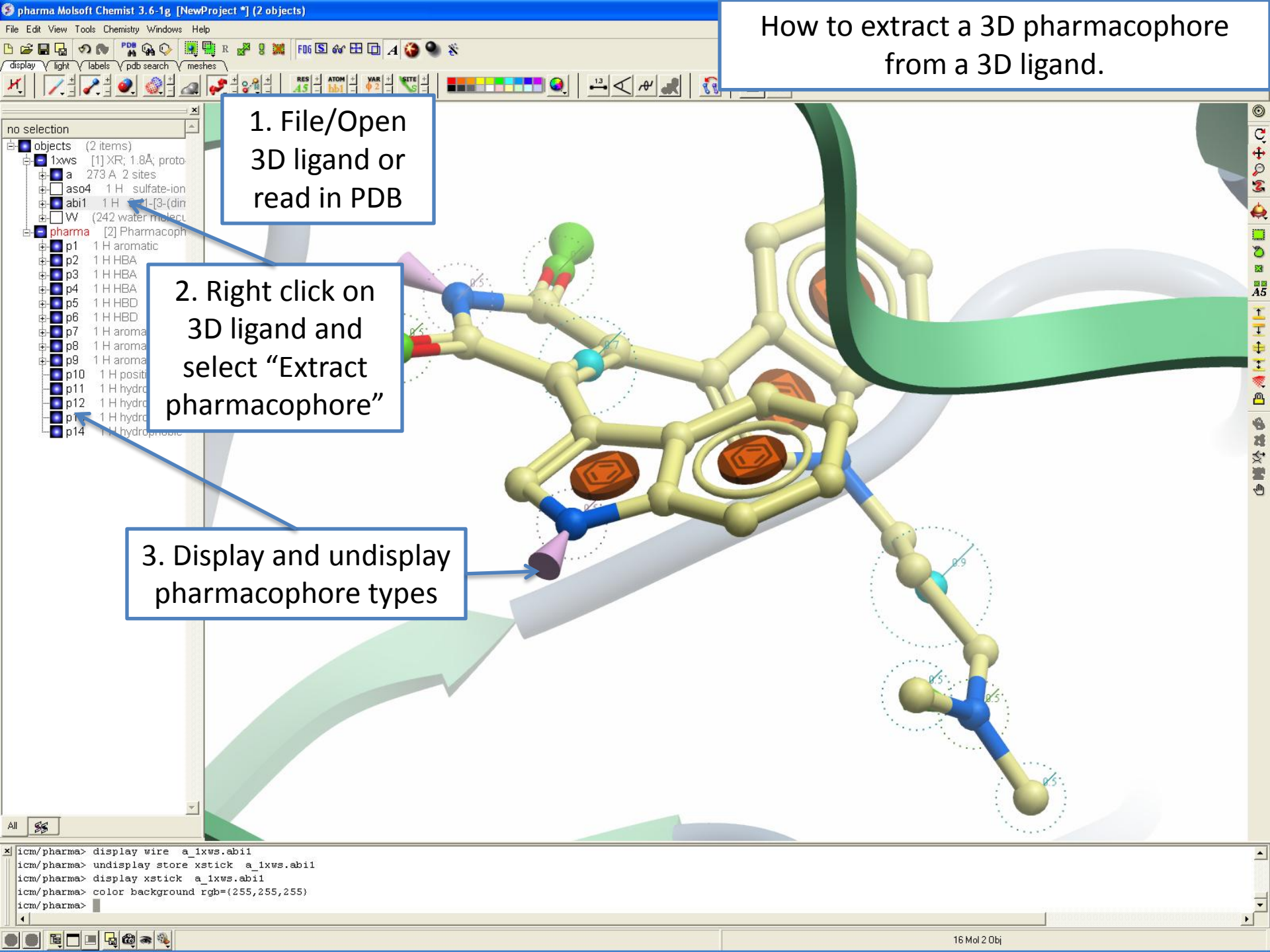
ICM-Chemist

HOW TO WORK WITH PHARMACOPHORES

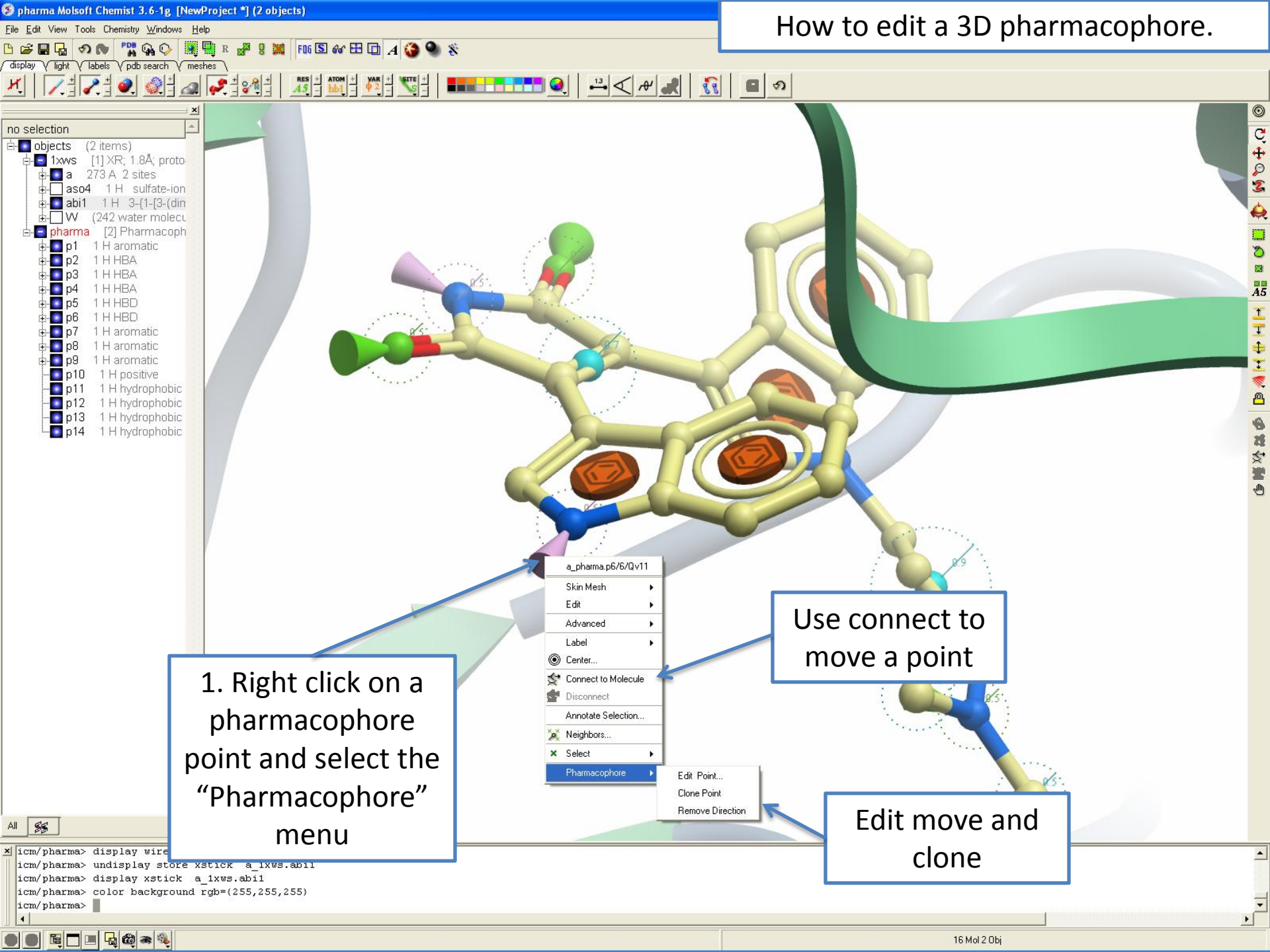
How to search a 2D pharmacophore.



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



How to edit a 3D pharmacophore.

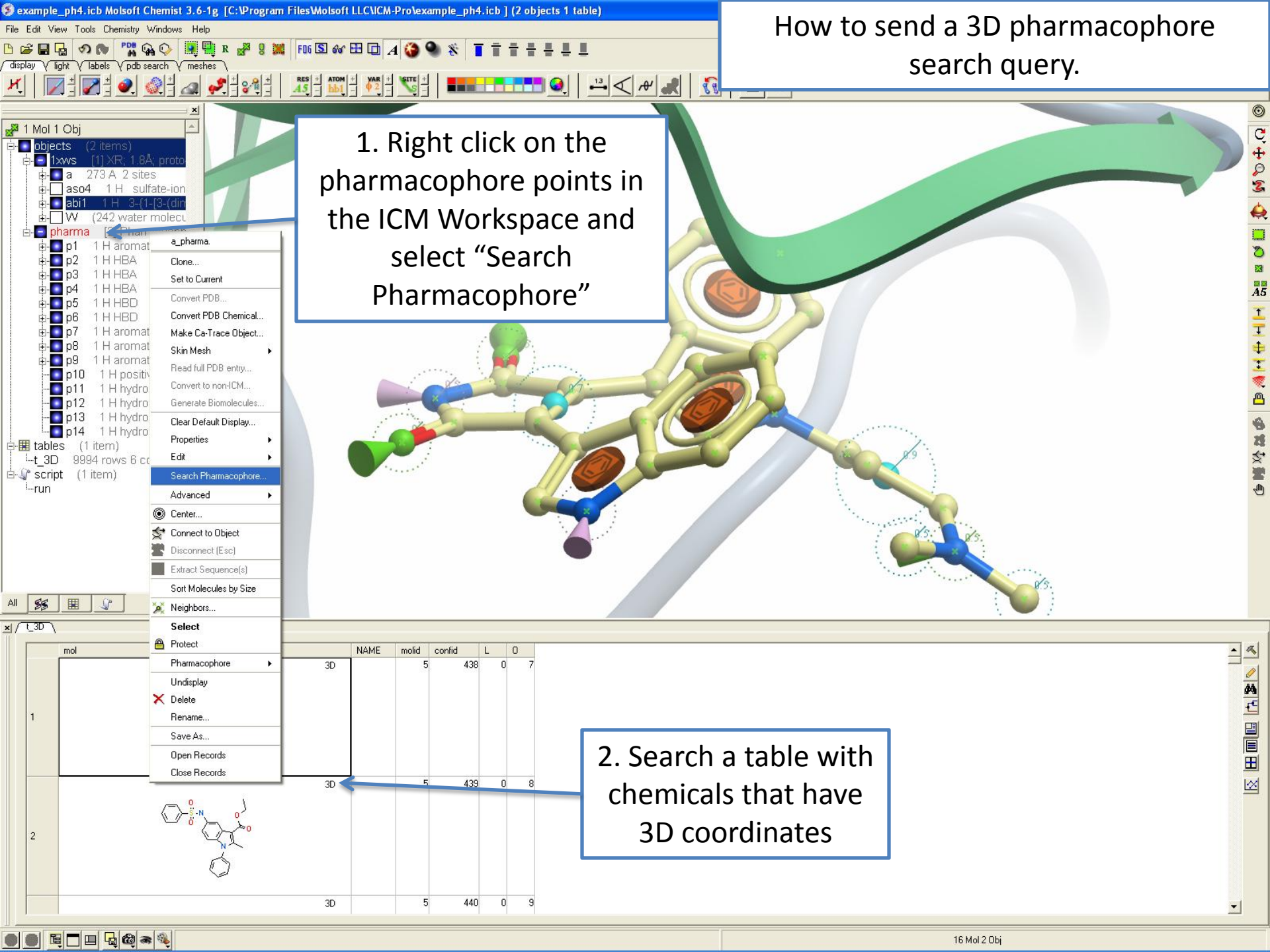


1. Right click on a pharmacophore point and select the “Pharmacophore” menu

Use connect to move a point

Edit move and clone

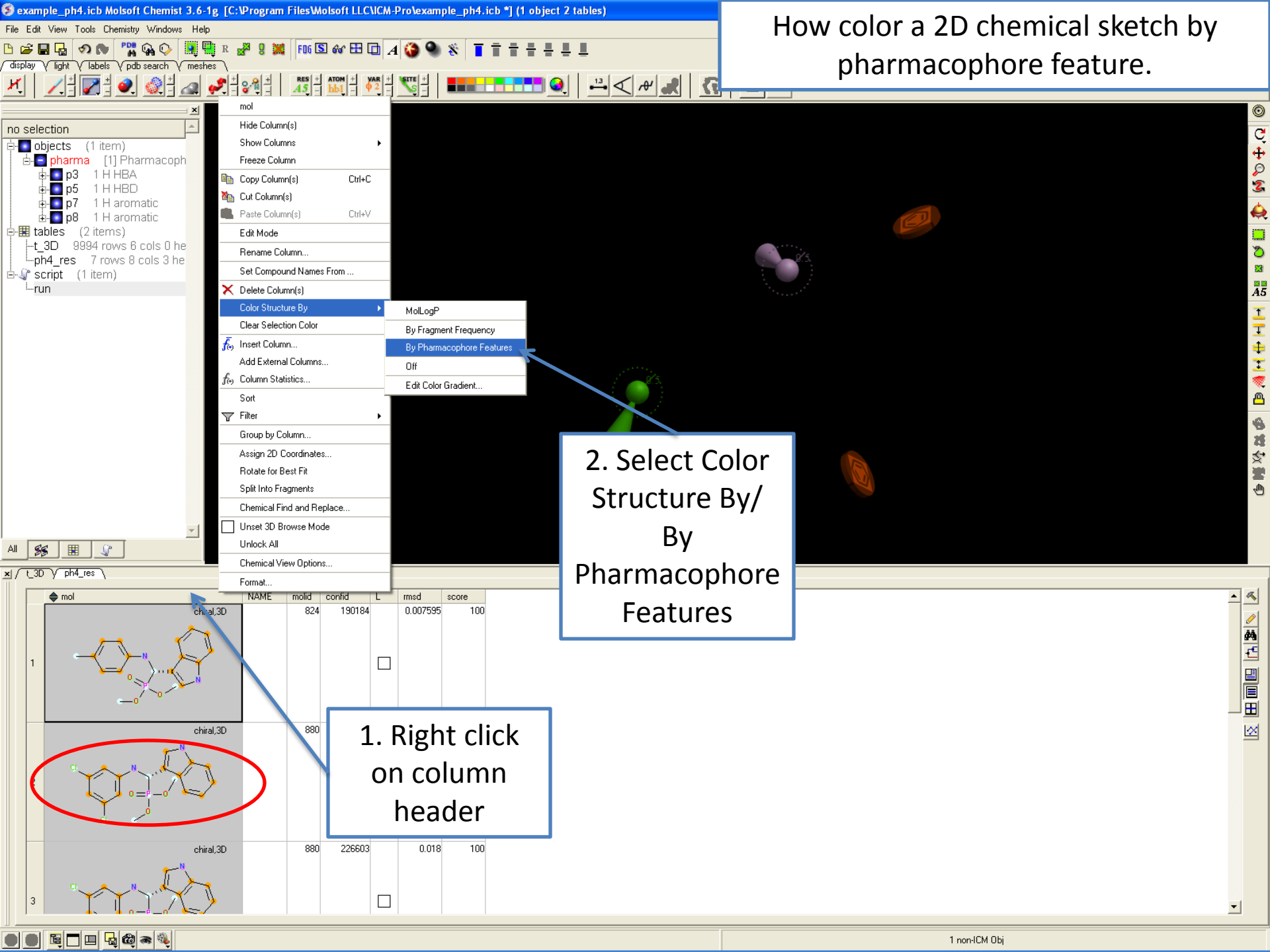
How to send a 3D pharmacophore search query.



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

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

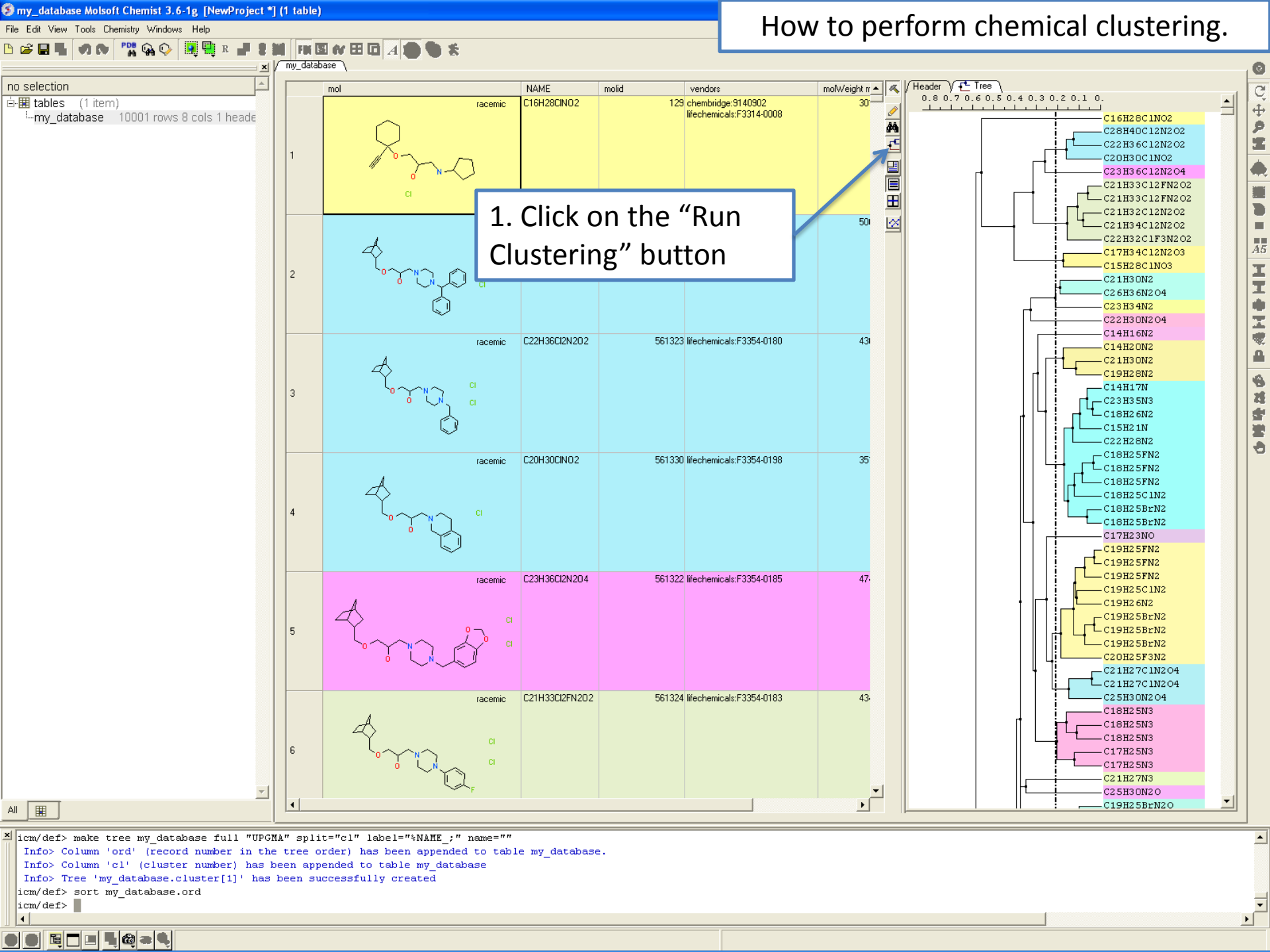
How color a 2D chemical sketch by pharmacophore feature.

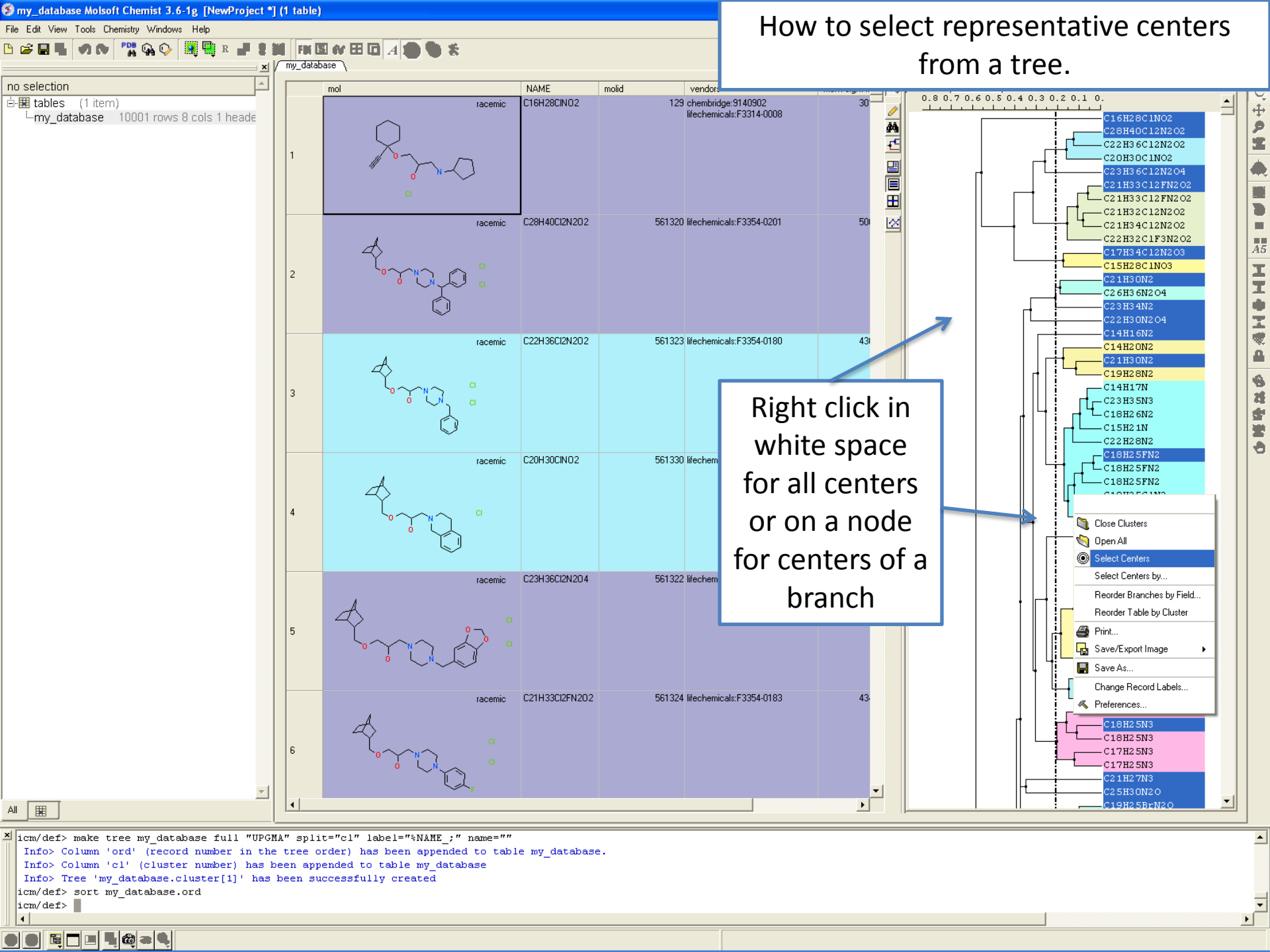


ICM-Chemist

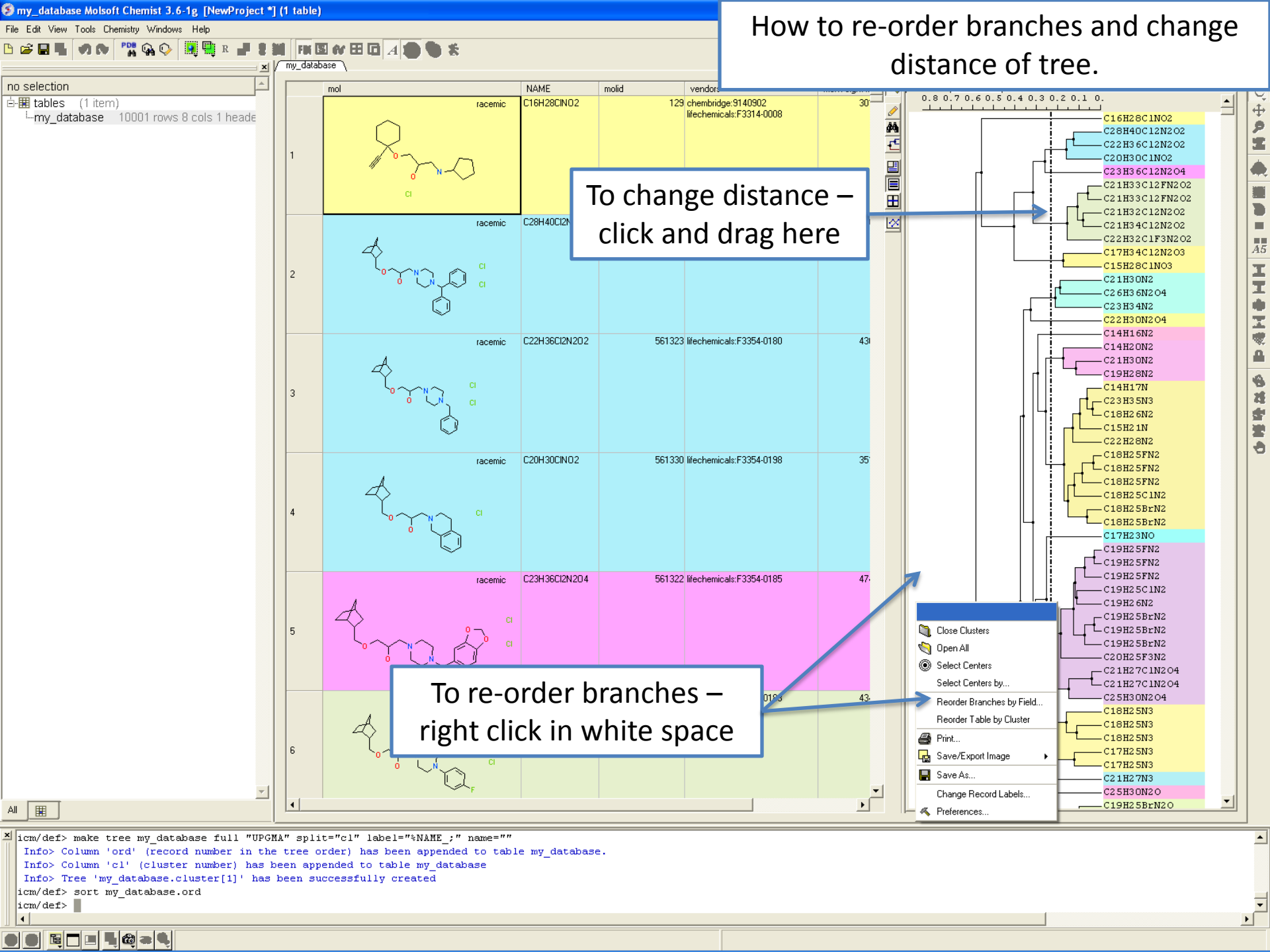
HOW TO PERFORM CHEMICAL CLUSTERING

How to perform chemical clustering.

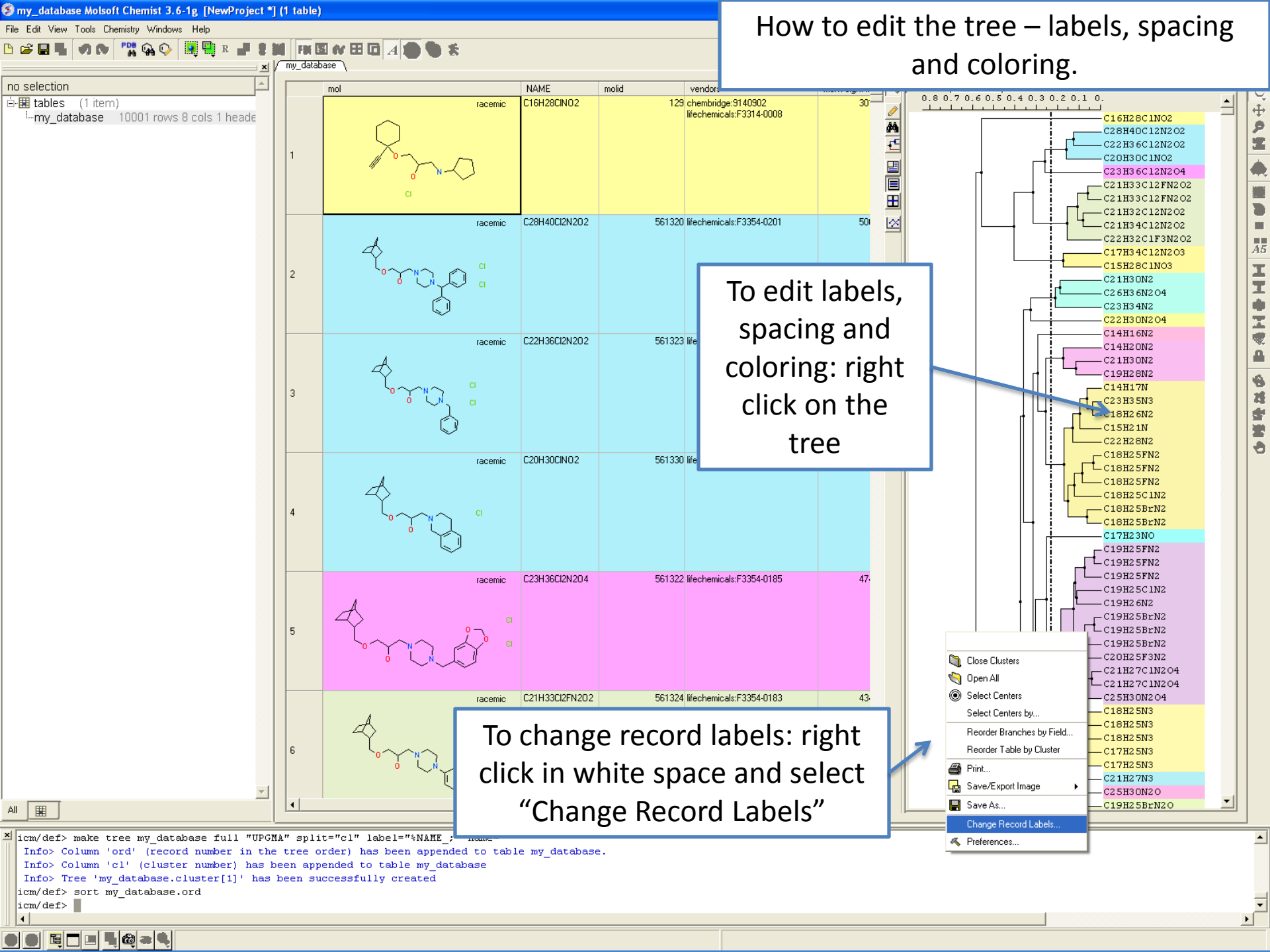



my_database Molsoft Chemist 3.6-1g [NewProject *] (1 table)
File Edit View Tools Chemistry Windows Help
How to select representative centers from a tree.
no selection
tables (1 item)
my_database 10001 rows 8 cols 1 heade
my_database
mol
NAME
molid
vendors
racemic
C16H28ClNO2
129 chembridge:9140902
lifechemicals:F3314-0008
C28H40Cl2N2O2
561320 lifechemicals:F3354-0201
C22H36Cl2N2O2
561323 lifechemicals:F3354-0180
C20H30ClNO2
561330 lifechem
C23H36Cl2N2O4
561322 lifechem
C21H33Cl2FN2O2
561324 lifechemicals:F3354-0183
Right click in white space for all centers or on a node for centers of a branch
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="cl" 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>

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



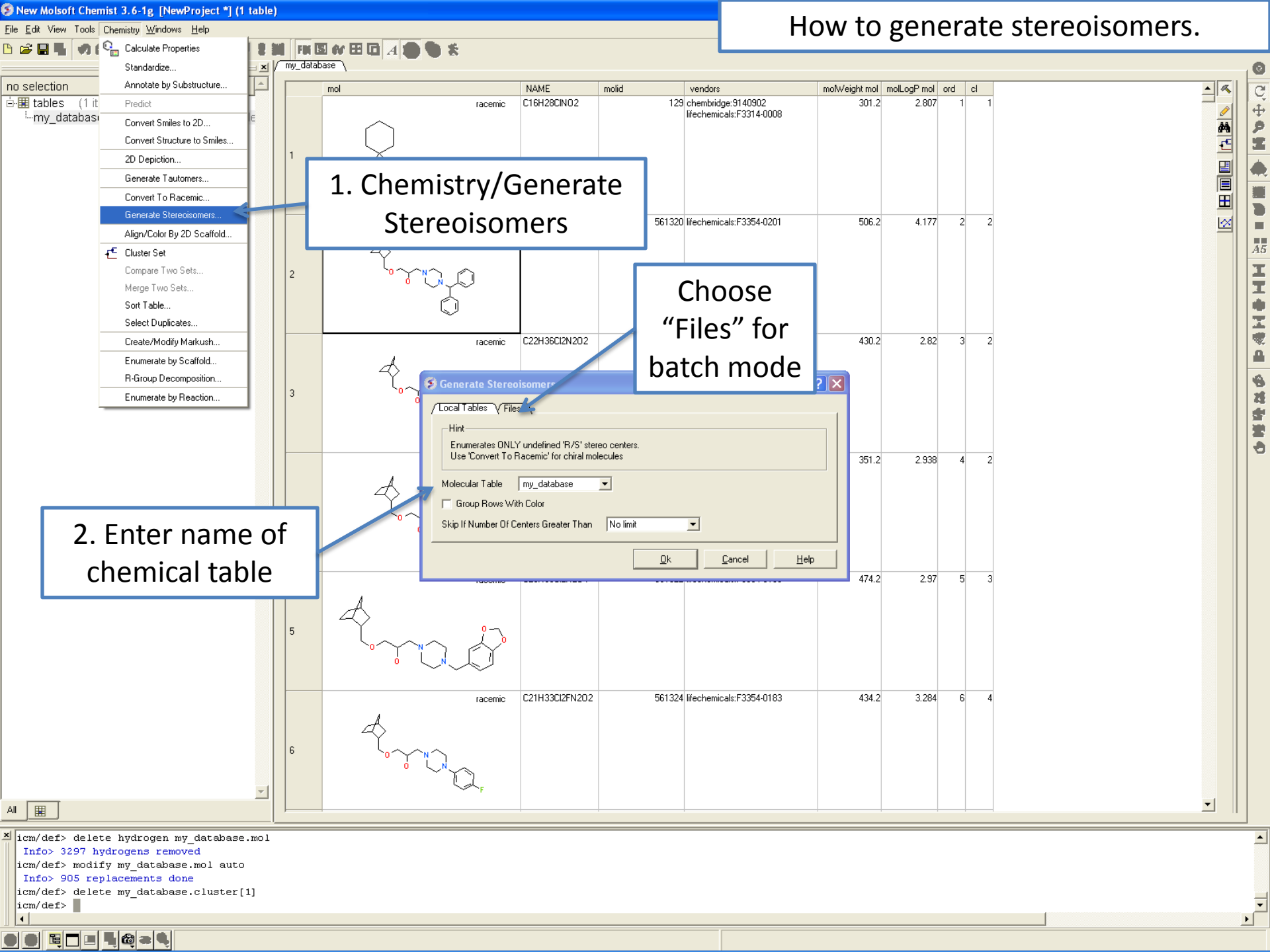
How to edit the tree – labels, spacing and coloring.



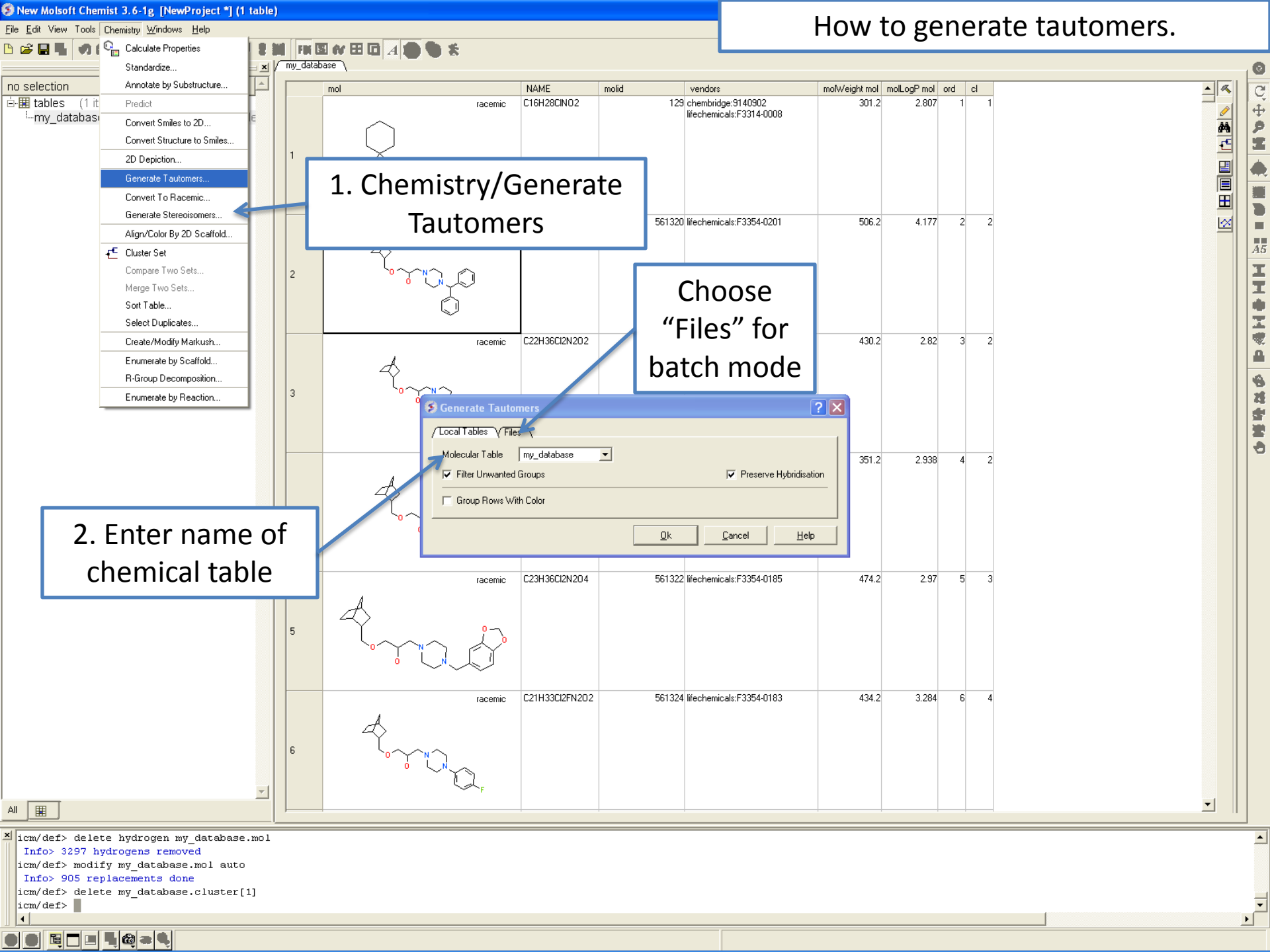
ICM-Chemist

HOW TO GENERATE STEREOISOMERS AND TAUTOMERS

How to generate stereoisomers.



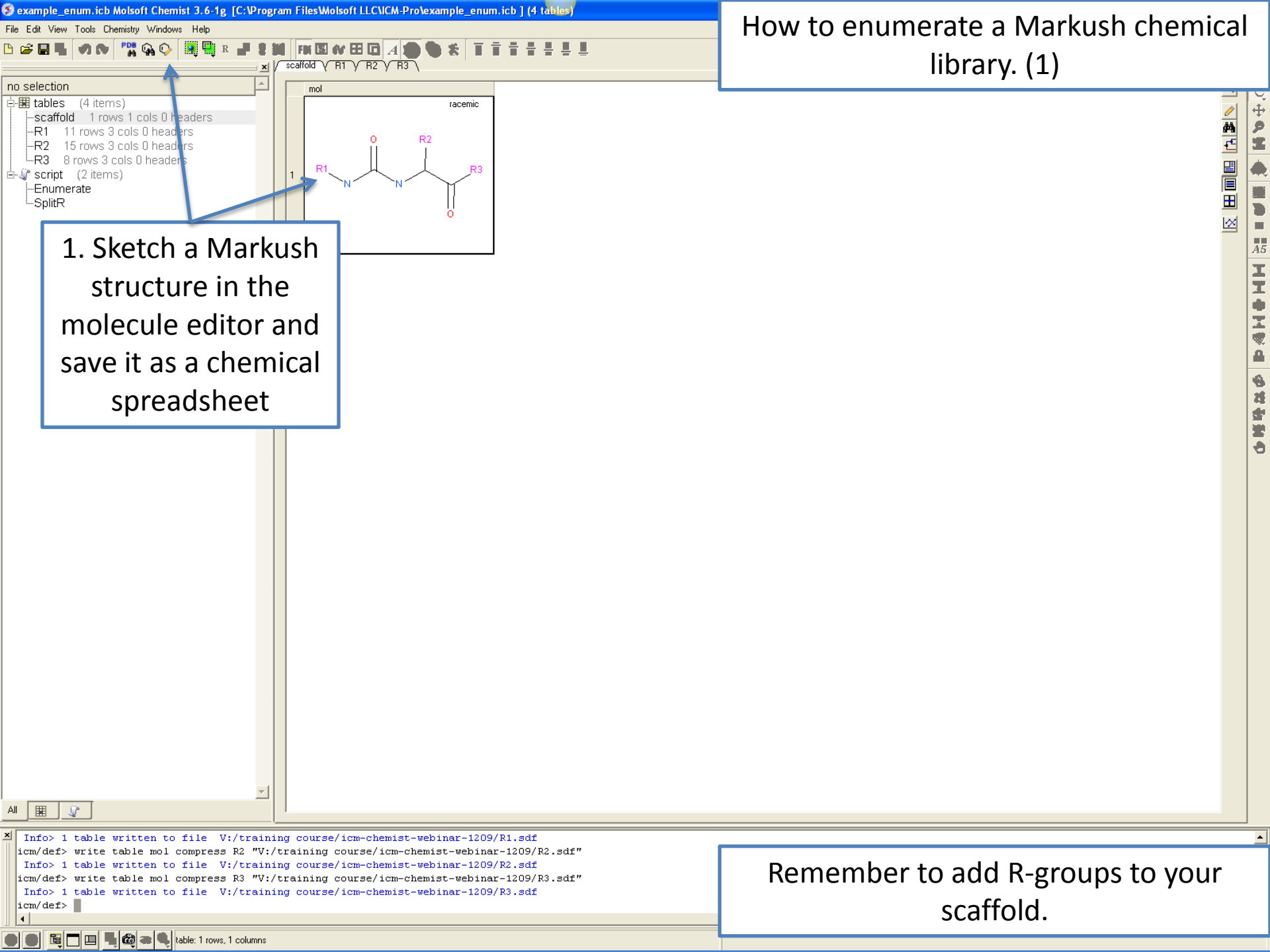
How to generate tautomers.



ICM-Chemist

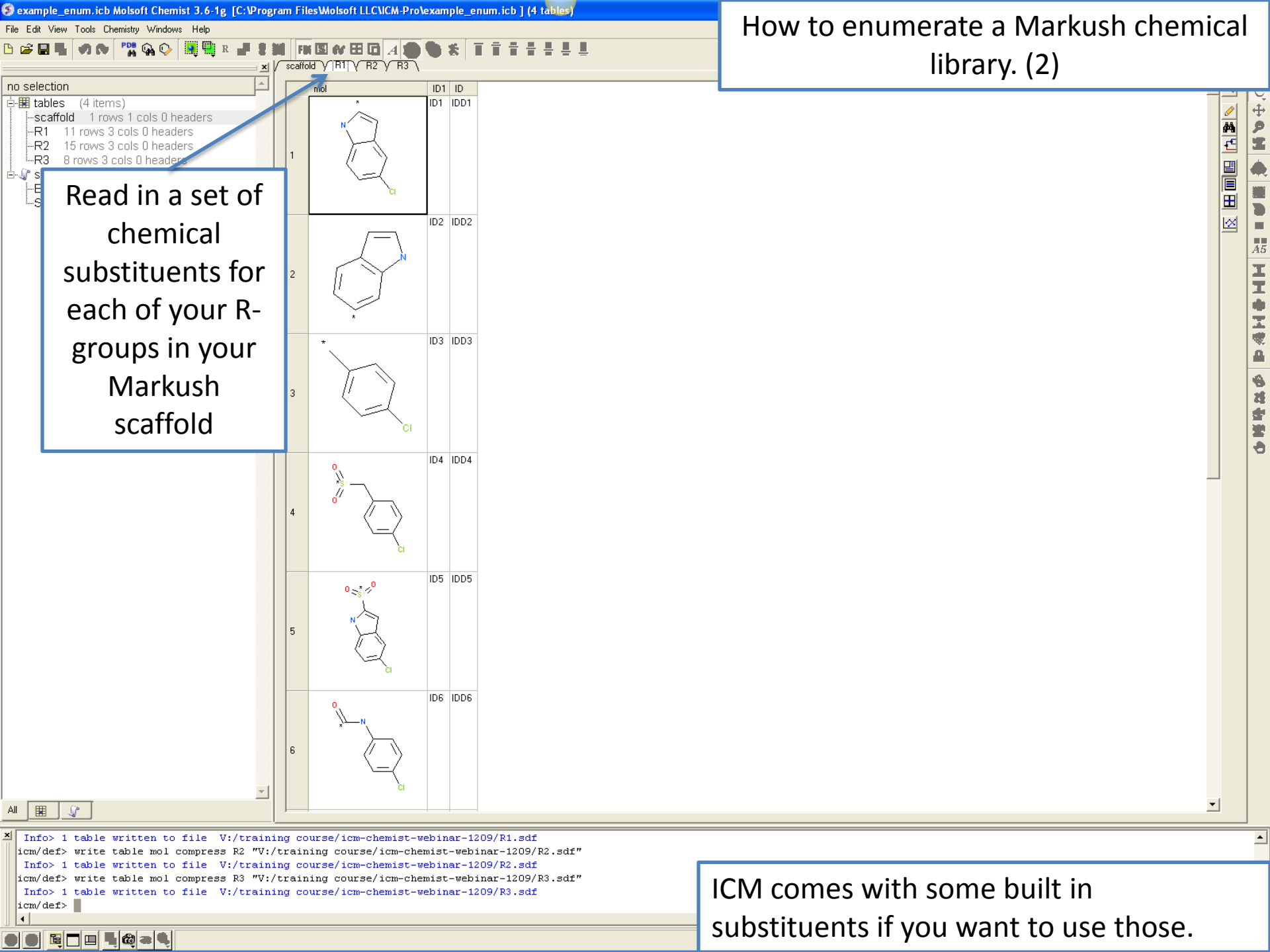
HOW TO GENERATE COMBINATORIAL LIBRARIES

How to enumerate a Markush chemical library. (1)



Remember to add R-groups to your scaffold.

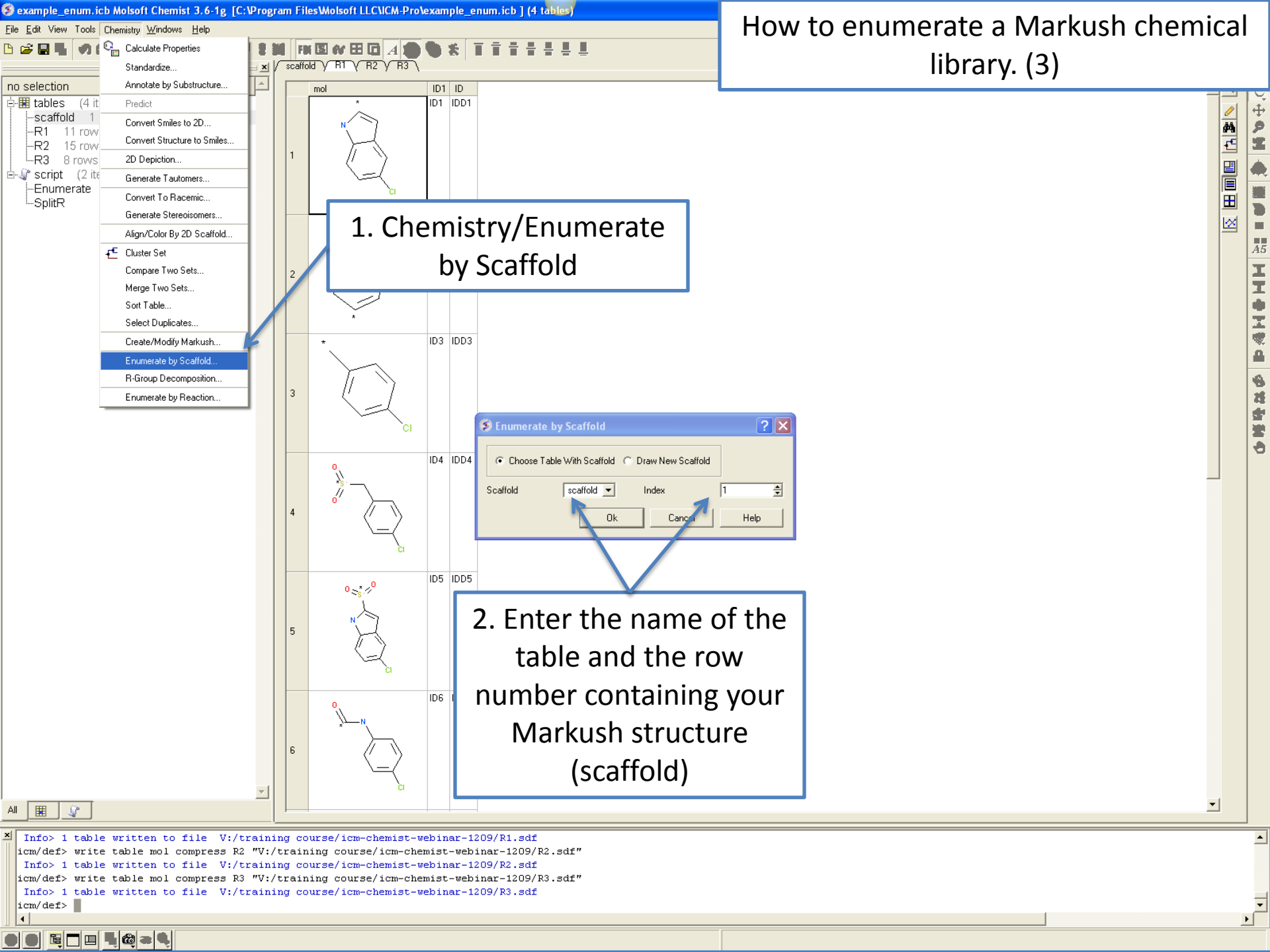
How to enumerate a Markush chemical library. (2)



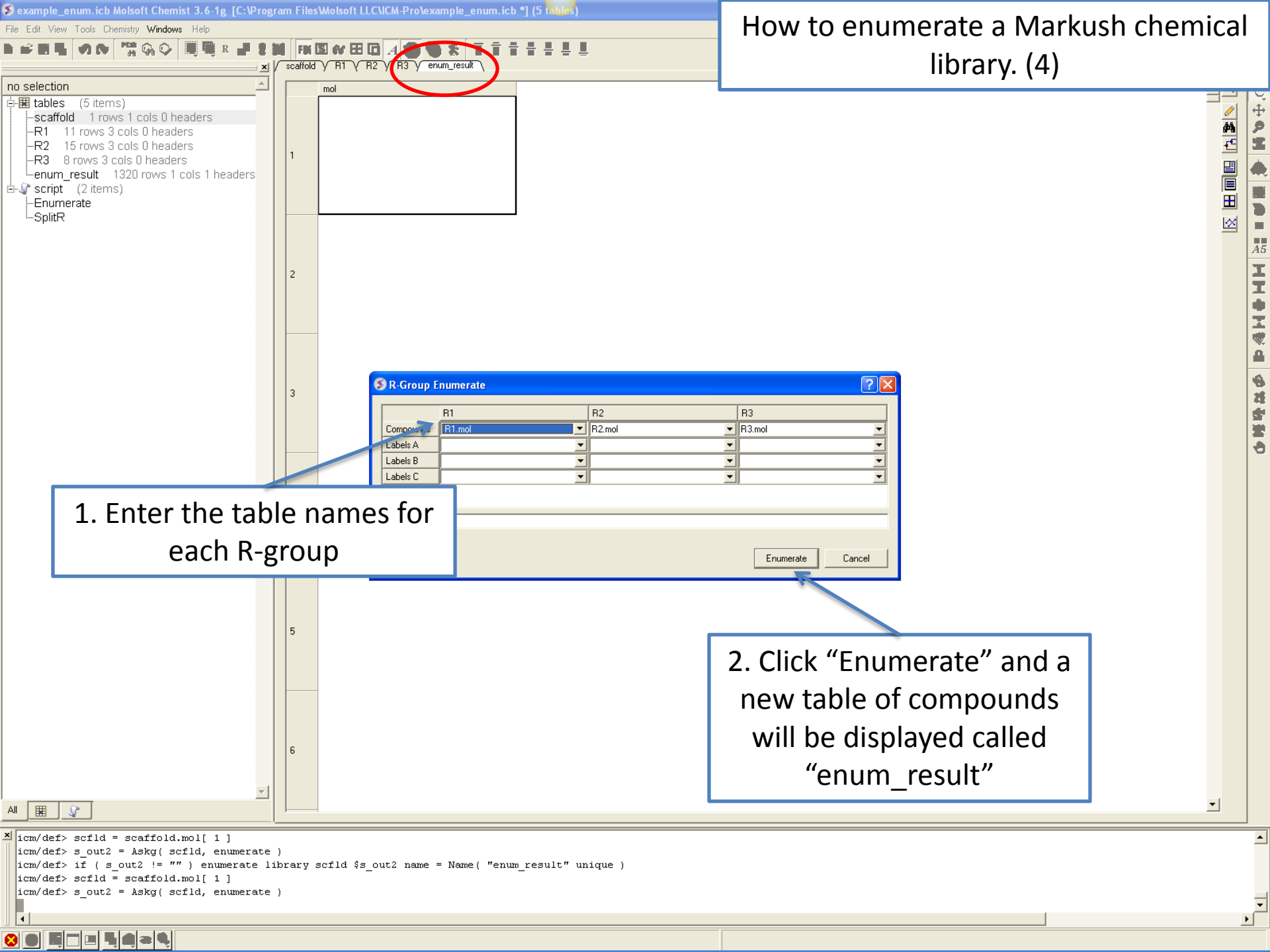
Read in a set of chemical substituents for each of your R-groups in your Markush scaffold

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

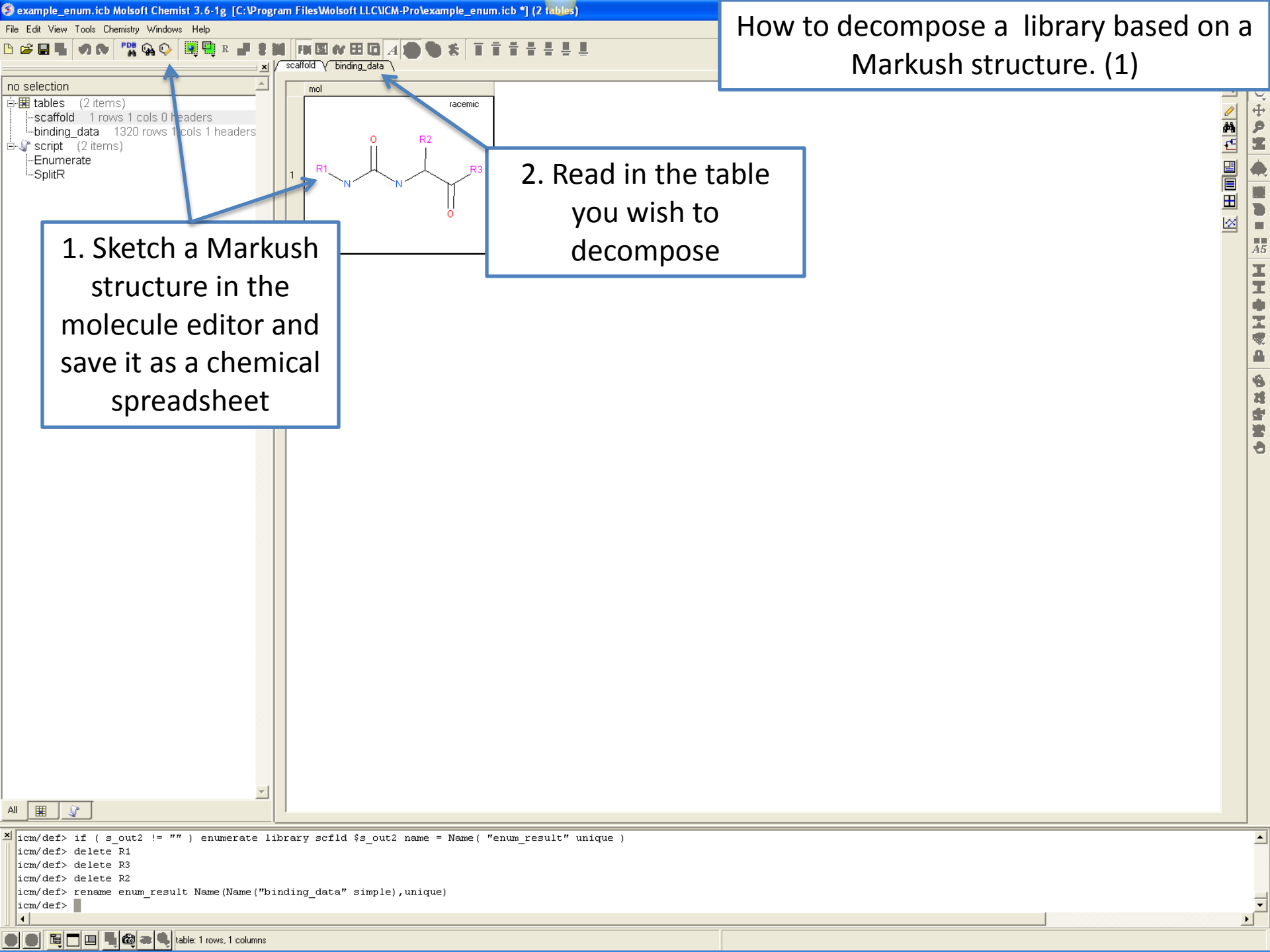
How to enumerate a Markush chemical library. (3)



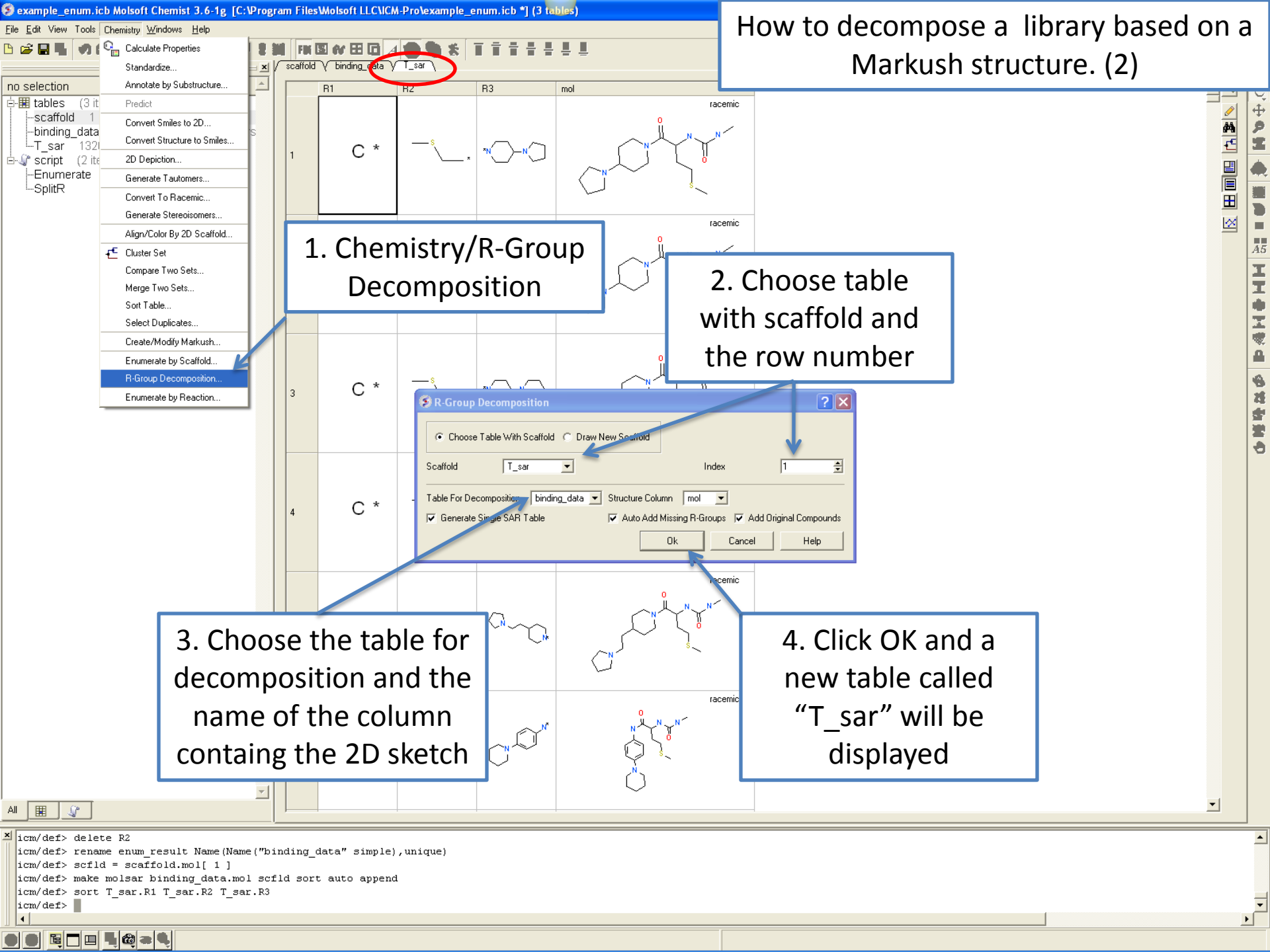
How to enumerate a Markush chemical library. (4)



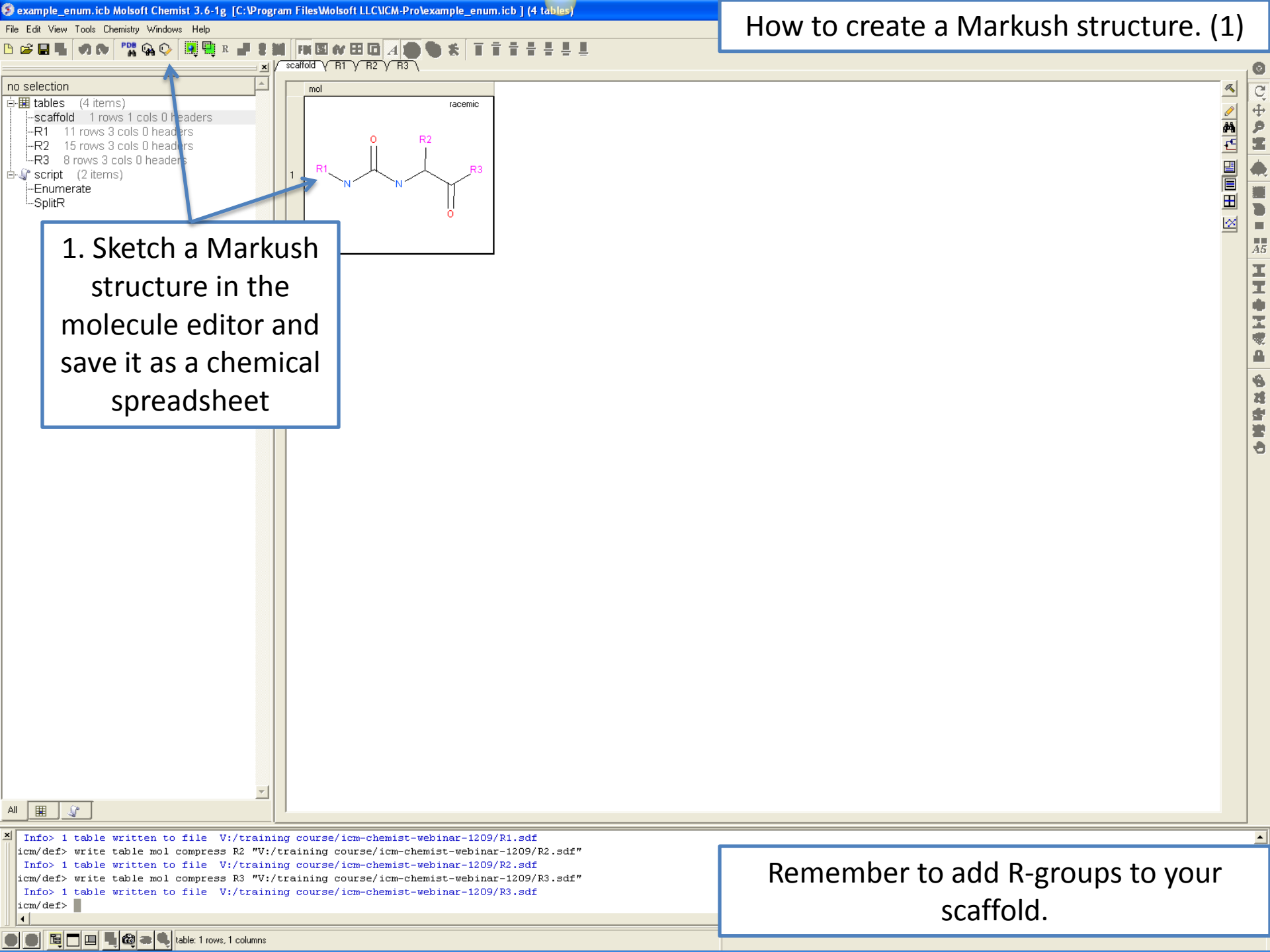
How to decompose a library based on a Markush structure. (1)



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



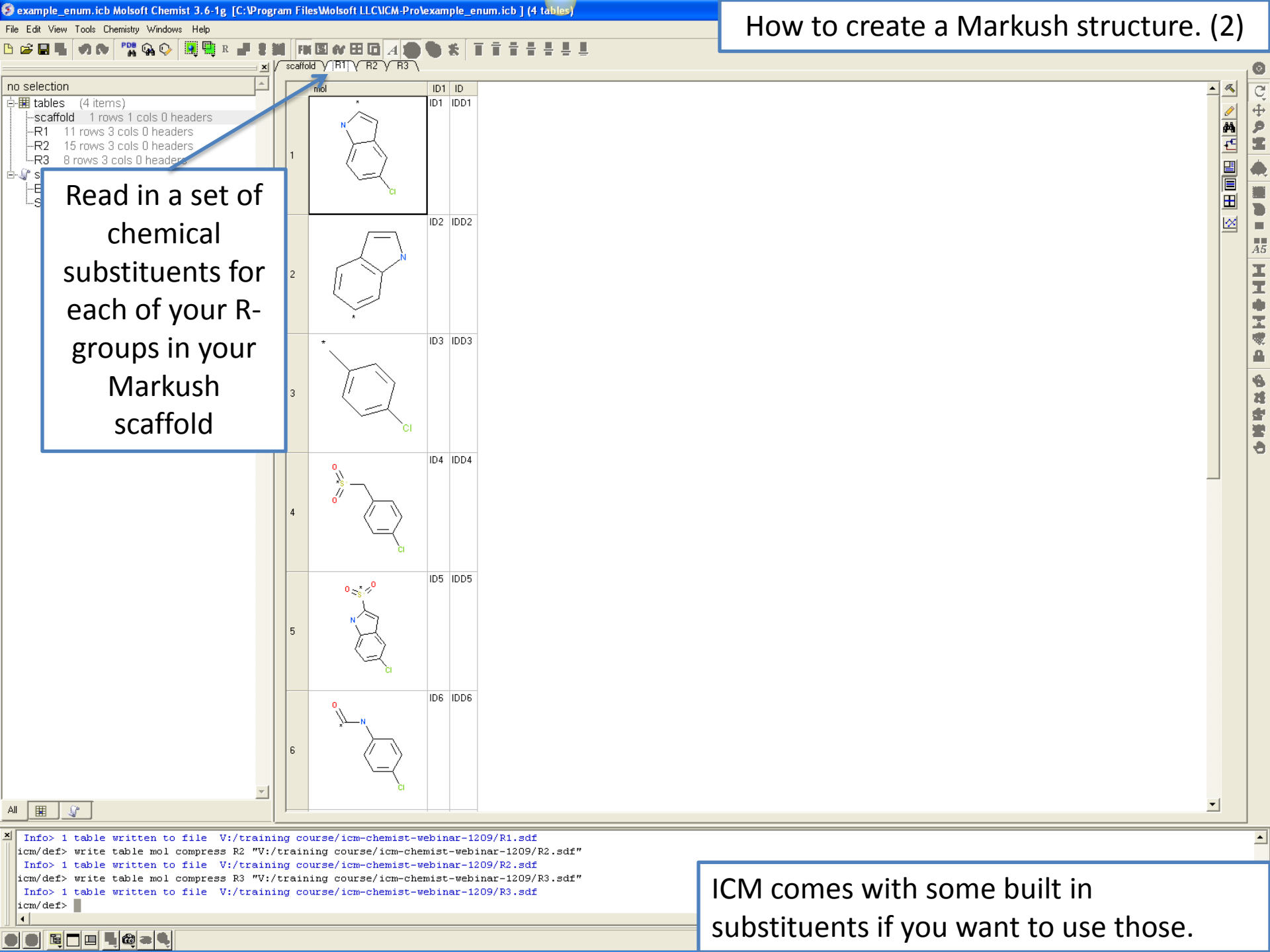
How to create a Markush structure. (1)



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

Remember to add R-groups to your scaffold.

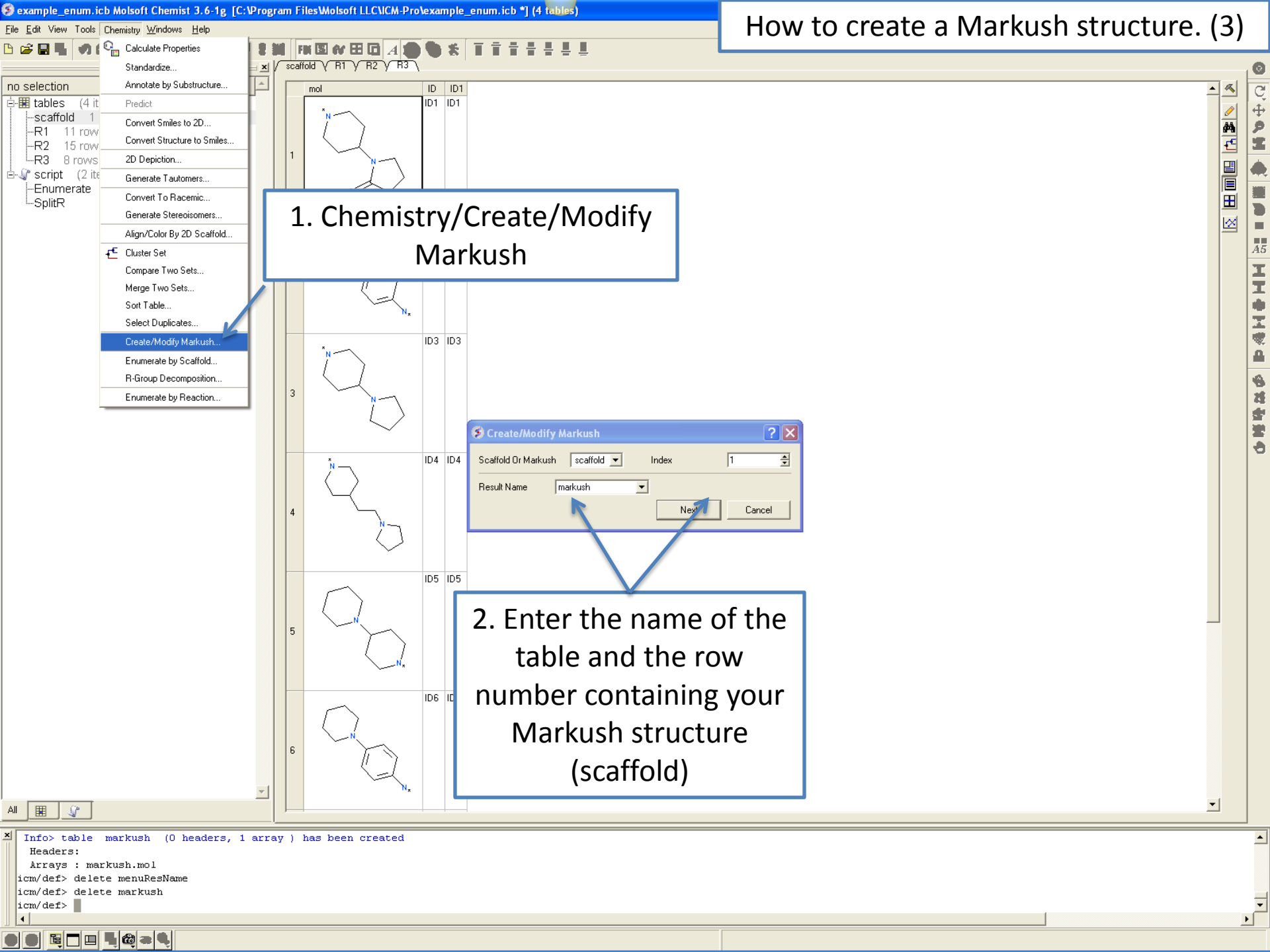
How to create a Markush structure. (2)



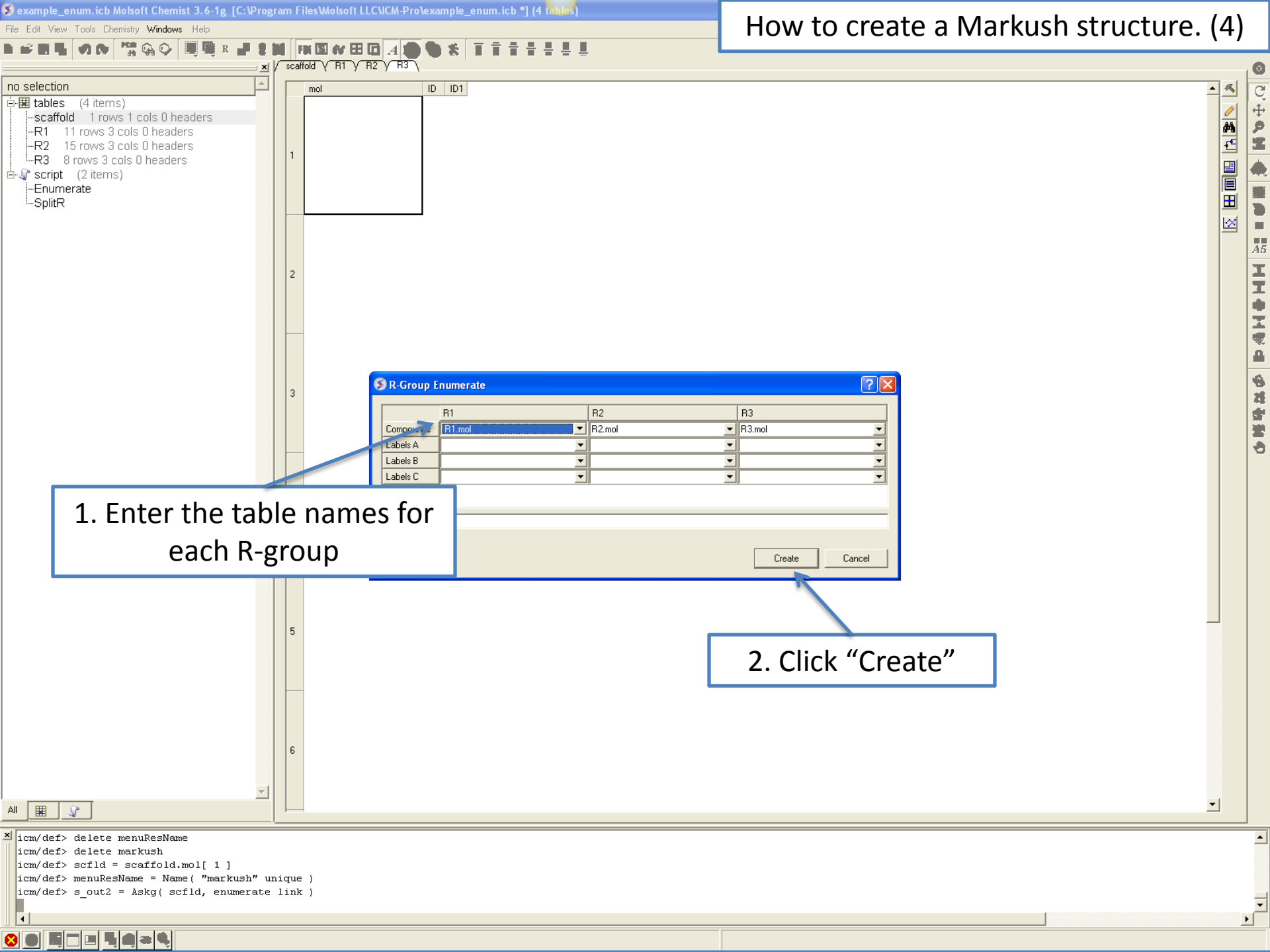
Read in a set of chemical substituents for each of your R-groups in your Markush scaffold

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

How to create a Markush structure. (3)



How to create a Markush structure. (4)



How to create a Markush structure. (5)

example_enum.icb Molsoft Chemist 3.6-1g [C:\Program Files\Molsoft LLC\ICM-Pro\example_enum.icb *] (5 tables)

File Edit View Tools Chemistry Windows Help

scaffold R1 R2 R3 markush

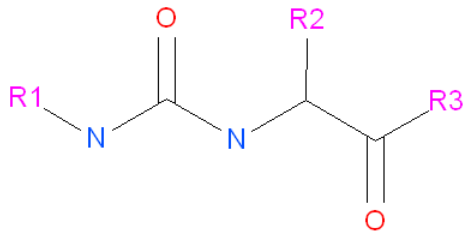
no selection

- 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

All

mol

racemic



1

R1= c1cc2c(c[c*][nH]2)cc1[Cl], c1cc2cc[nH]c2c[c*]1, [C*]c1ccc(cc1)[Cl], C(c1ccc(cc1)[Cl])[S*](=O)=O, c1cc2c(cc1[Cl])cc([nH]2)[S*](=O)=O, c1cc(ccc1N[C*]=O)[Cl], c1cc(c(cc1[Cl])[Cl])N[C*]=O, C1Oc2ccc(cc2O1)N[C*]=O, [C*], C[S*](=O)=O

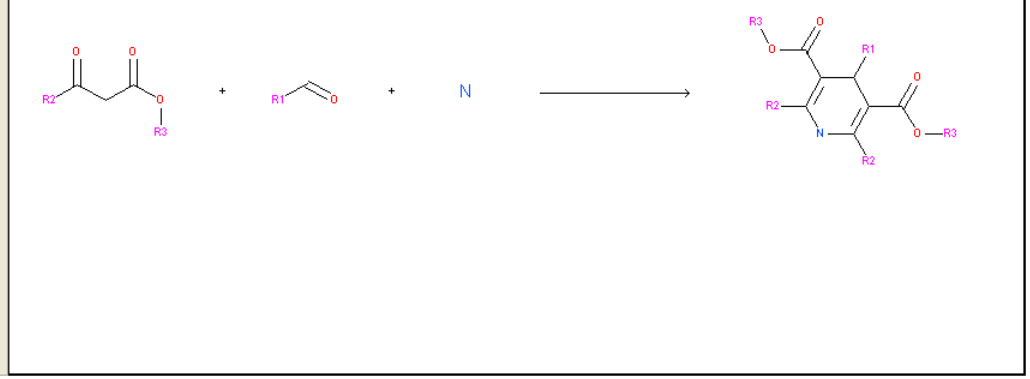
R2= c1cc(cc[c*]1)[Cl], c1c[c*]cc(c1)[Cl], C1CC[C*]CC1, c1ccc2c[c*]ccc2c1, [C*]c1ccc(cc1)[Cl], [C*]c1cccc(c1)[Cl], [C*]c1ccccc1[Cl], [C*]c1c[nH]c2ccccc12, [C*]C1CCCCC1, COc1cccc([C*])c1

R3= C1CC(N(C1)C1CC[N*]CC1)=O, C1CCC(CC1)c1ccc(cc1)[N*], C1CCN(C1)C1CC[N*]CC1, C1CCN(C1)CCC1CC[N*]CC1, C1CCN(CC1)C1CC[N*]CC1, C1CCN(CC1)c1ccc(cc1)[N*], C1CCN(CC1)c1ccc(cc1C(N)=O)[N*], C1CN(CC[N*]1)c1cc(cc(c1)[Cl])[Cl]

```
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>
```

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

1. Sketch reactants and products in the molecule editor



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

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

r_han_pyr | reactant1 | reactant2

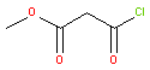
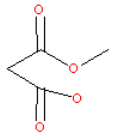
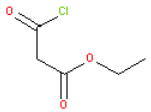
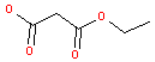
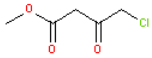
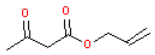
doc1

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.

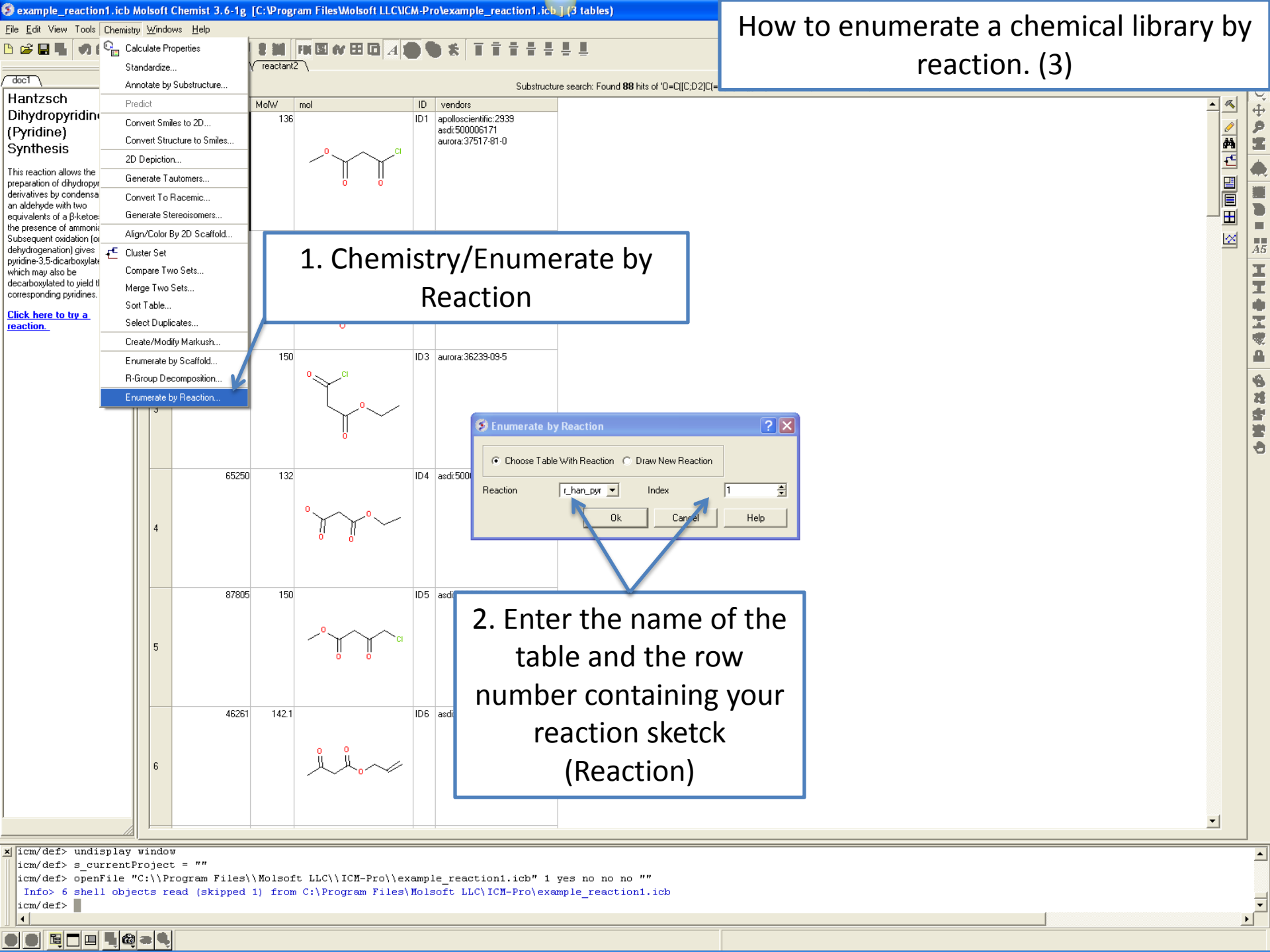
Substructure search: Found **88** hits of 'O=C([C;D2]C(=

	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

1. Read in a table of your reactants

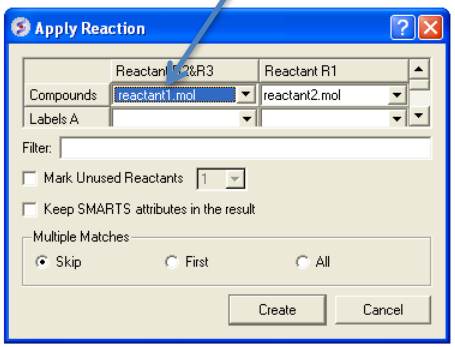
```
icm/def> undisplay window
icm/def> s_currentProject = ""
icm/def> openFile "C:\\Program Files\\Molsoft LLC\\ICM-Pro\\example_reaction1.icb" 1 yes no no no ""
 Info> 6 shell objects read (skipped 1) from C:\Program Files\Molsoft LLC\ICM-Pro\example_reaction1.icb
icm/def>
```

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



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

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



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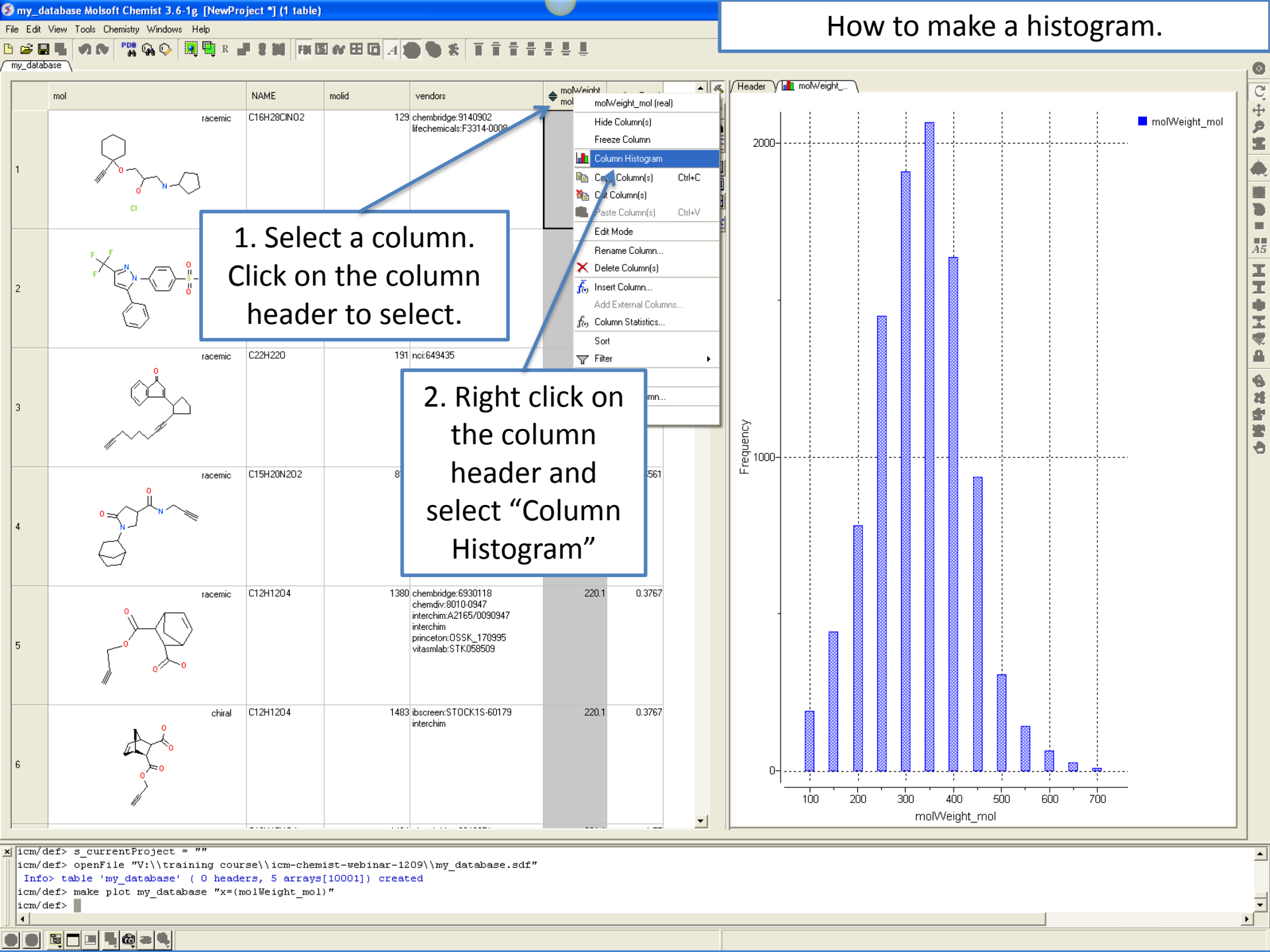
HOW TO GENERATE PLOTS AND HISTOGRAMS

How to make a histogram.



How to make a X-Y scatter plot.