

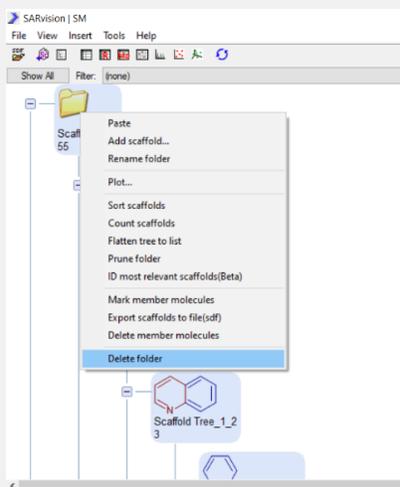
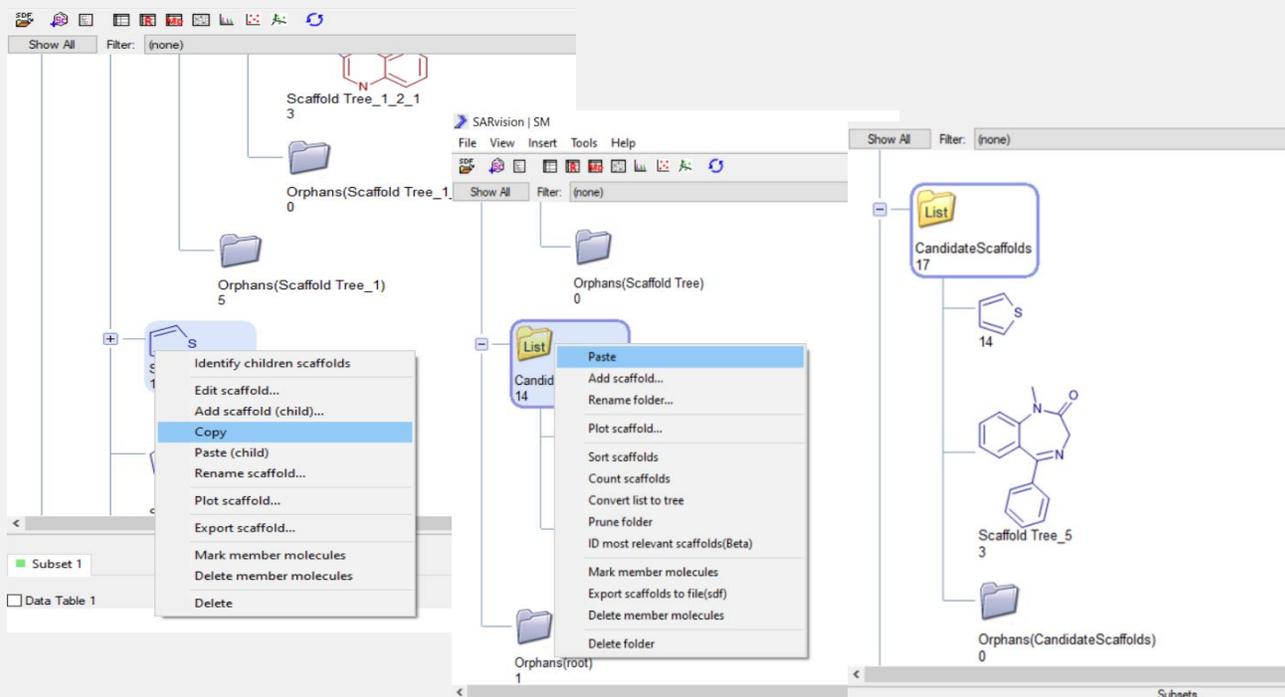
Scanning Catalogs in SARvision|SM

1. Create a list of scaffolds; If you need help with this step, please look at our First Steps quickstart guide: http://www.chemapps.com/wp-content/uploads/2018/05/SVSM_FS.pdf

	Structure	Mol_ID	Name	Activity
1		1	Flunitrazepam	Agonist
2		2	Diazepam	Agonist
3		3	Prazepam	Agonist
4		5	CGS8216	Inverse Agonist
5		6	CGS9895	Antagonist
6		7	CGS9896	Agonist
7		8	RO15-1788	Antagonist
8		9	Cyanocarboline	Antagonist

2. You may want to create a folder where you can collect the scaffolds you are interested in. Right click in the scaffolds working area; once you create it you can rename the folder by right clicking on it and choosing Rename Folder....

3. Select scaffolds of interest and place them into. You have two options, right click on a scaffold and select copy; then paste them in the folder of interesting scaffolds. You can drag and drop the scaffolds into the folder as an alternative to copying and pasting, that works as well. Compile the list of all the scaffolds you care about.

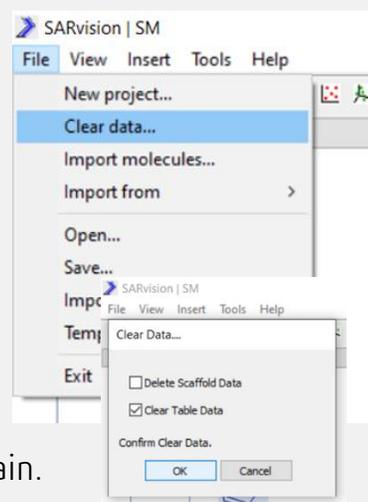


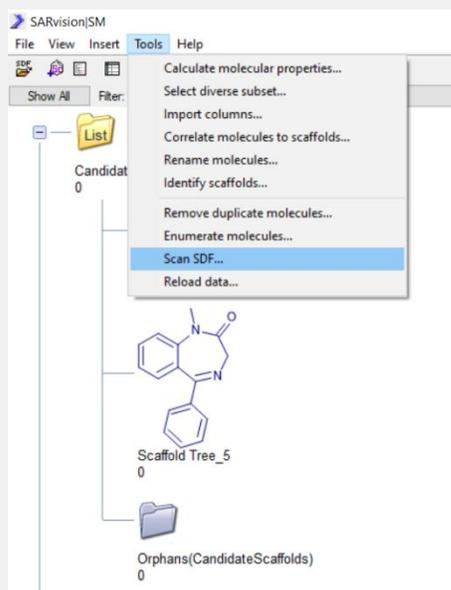
4. Remove the folder with all the scaffolds and retain only the folder with scaffolds of interest. In this way you can have just the list of scaffolds of interest. You could add manually scaffolds to the list, if you want.

Before you start looking for additional compounds, you may want to remove any compounds you have in the table. It is advisable that you save your work at this point, using a new file name.

To remove the compounds in the Table workspace, select Clear Data option in the File Pulldown and in the Clear Data pop-up, make sure that the Delete Scaffold Data is not selected.

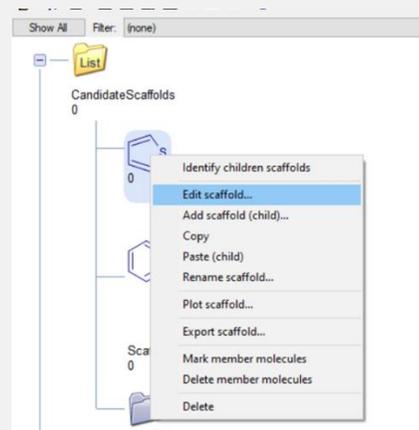
At this point only the folder with the scaffolds of interest will remain.



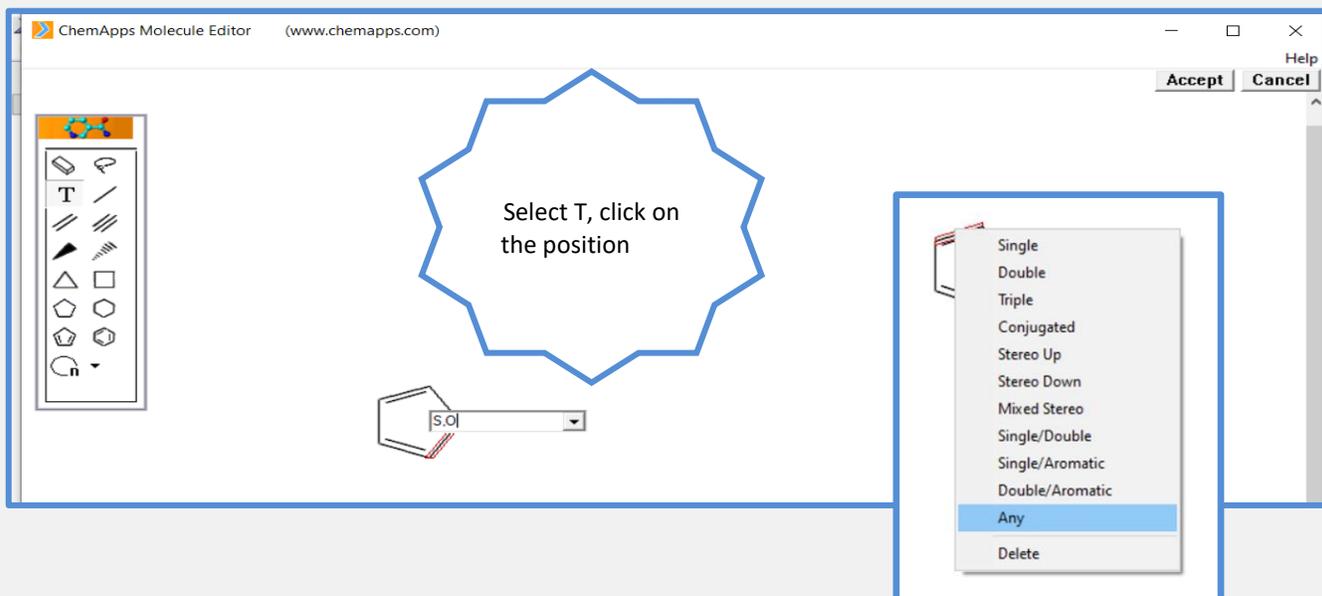


5. Scan vendor catalogs for those scaffolds of interest. The program searches for multiple substructures in parallel rather than one at a time. To scan catalogs, do Tools -> Scan SDF. You will need to select the SD files to scan. The result will be that all compounds that contain any of the scaffolds of interest will be retrieved, together with any other information about them in the catalog. Of course, the SD file you scan does not have to be a vendor catalog, but it could be any other types of file with chemicals, such as PubChem, provided that you have them as an SD File.

6. In some cases, you may want to generalize the scaffolds. That is look for compounds that are similar but not identical to the ones you have in the folder. To that end, you can edit the scaffolds. Select a scaffold, right click on it and select edit scaffold in the pop-up menu. This will open the ChemAppsEditor.



7. Edit the molecules with the editor. The program supports generalized atom types, such as A (any atom, except H), Q (any heteroatom) or lists of atoms separated by comma, e.g. N,S,O. Also with T selected, you can select a bond right click on it and select the bond type



8. The generalized substructure can be used to scan files as shown above.

	Structure	ZINC000000000023
1		ZINC00000001601
2		ZINC000000007546
3		ZINC000000008850
4		ZINC000000026959

9. A feature that it is not always known about SARvision|SM is that users can create trees that are formed by unrelated substructures, in that case the program interprets it as Substructure1 AND Substructure2. For example, we may want to limit a substructure search, to compounds that have a particular functionality functionality. In that case, we will include that functionality of interest as a child of the parent structure
To add a substructure that is unrelated, we right click on the scaffold of interest and select "Add scaffold (child)..."

The screenshot displays the SARVISION|SM interface. On the left, a tree view shows a folder named 'CandidateScaffolds 10715' with a context menu open. The menu options include: Identify children scaffolds, Edit scaffold..., Add scaffold (child)..., Copy, Paste (child), Rename scaffold..., Plot scaffold..., Export scaffold..., Mark member molecules, Delete member molecules, and Delete. The main workspace shows a hierarchical view of scaffolds, including 'CandidateScaffolds 10715', a sub-scaffold '[S,O] 10709', and a molecule '2582'. A 'Data Table 1' is visible on the right, containing five rows of chemical structures and their corresponding ZINC IDs (all 'ZINC00').

Structure	ZINC ID
	ZINC00

Notice how the parent and the child are unrelated, a Thiophene or Furan-like structure should contain a carboxylic acid.

This screenshot shows the same SARVISION|SM interface, but with a different context menu open over the 'CandidateScaffolds 10715' folder. The menu options are: Paste, Add scaffold..., Rename folder, Plot..., Sort scaffolds, Count scaffolds, Flatten tree to list, Prune folder, ID most relevant scaffolds(Beta), Mark member molecules, Export scaffolds to file(sdf), Delete member molecules (highlighted), and Delete folder.

10. At this point a number of options are possible, such as exporting the compound lists as SD files. You can also upload a second set of scaffolds, such as a set of undesirable chemotypes. Then molecules containing any of those scaffolds can be eliminated by right clicking on the folder that contains the undesirable molecules and select Delete member molecules. This would eliminate any of the molecules that contain scaffolds in that folder. This can be done for individual scaffolds as well.