



Building R-Group Tables

A product of



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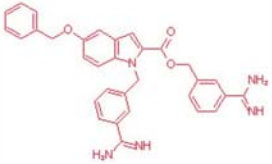
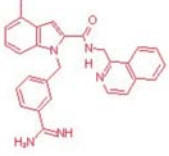
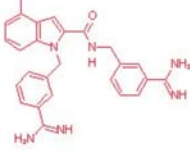
Welcome to SARvision

SARvision2.2 is a Chemistry Reporting tool developed to analyze medium to large datasets, group molecules within datasets intuitively into families, and enable facile SAR table generation and reporting. This product is the result of several years of development based on the valuable feedback from many Medicinal Chemists in the Pharmaceutical Industry. Please contact us (support@chemapps.com) to share any recommendations that you may have for future releases or to report any bugs that you may encounter. We want to hear from you.

1. Load Molecule DataSet.

To get started, import an sd file into **SARvision** under **File:Import: Molecule Dataset(sdf)**. This file format is the most common format employed for sharing molecule datasets between programs. It should be available for download from your database. If not contact your informatics group. For this example, we use a dataset of 139 factor Xa inhibitors.



The screenshot displays the SARvision 2.2 interface with the 'File' menu open, highlighting 'Import' > 'Molecule Dataset(sdf)...'. A callout box points to the 'File' menu with the text '1. Open SD file FFsar_fXA.sdf'. The main window shows a table with three rows of data, each with a chemical structure, a 'cmd' value, and a 'Ki(FXA)(nM)' value. A callout box points to the table with the text 'Molecules and All Data is Displayed in Table.'

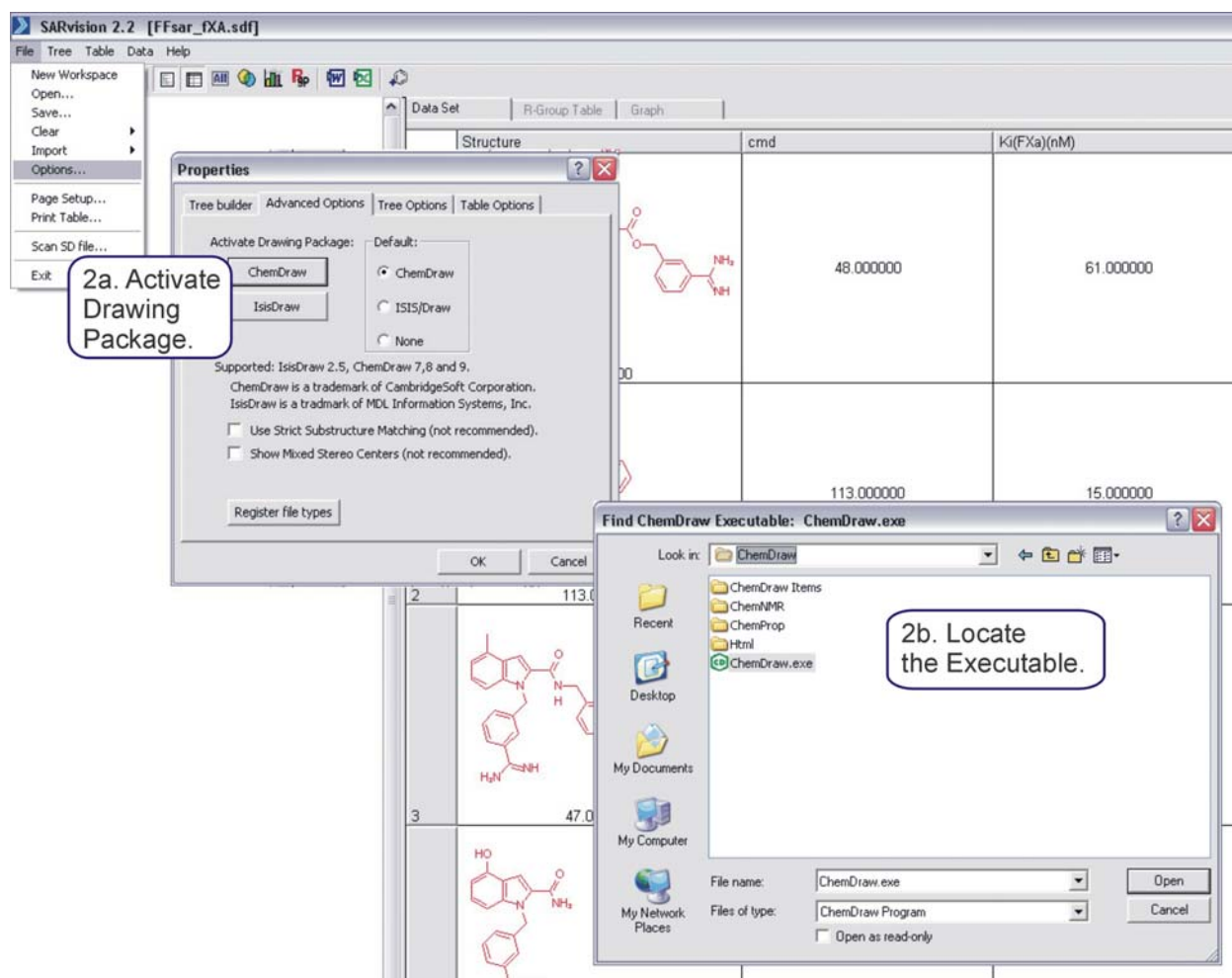
	Structure	cmd	Ki(FXA)(nM)
1	 48.000000	48.000000	61.000000
2	 113.000000	113.000000	15.000000
3	 47.000000	47.000000	7.000000

Molecules and associated data are shown in the table on the right. Under the menu **Table: Display Options**, the color of the displayed molecules can be changed. By right clicking on individual columns, the data can be formatted, sorted or deleted. The columns can be 'drag and dropped' in any order you desire and by double clicking the column header, locked to the left-hand side of the table.

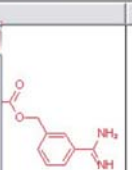
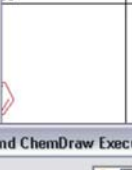


The molecule table is designed to have as many as 3000 columns of data and up to 10,000 molecules in **SARvision** and 100,000 molecules in **SARvisionPlus** if enough memory is available.

2. Interactivity with Chemistry Drawing Programs


To use either ChemDraw (CambridgeSoft) or IsisDraw (Elsevier MDL) chemistry drawing packages, activate the desired program under **File: Options**. A dialogue will popup that will allow you to tell SARvision where the executables for these programs are installed. Click the 'ChemDraw' button on the dialogue and locate the 'ChemDraw.exe' program on the disk. IsisDraw is activated similarly by clicking the 'IsisDraw' button. In this case, the user must identify two executables, IsisDraw.exe and cs32.exe. The 'Default' radial buttons to the right allow the user to toggle between drawing packages. The add 'Scaffold Button' () and the 'Add Molecule' button () can now be used to draw scaffolds and molecules respectively. Note that a drawing package is not a requirement to use **SARvision**.

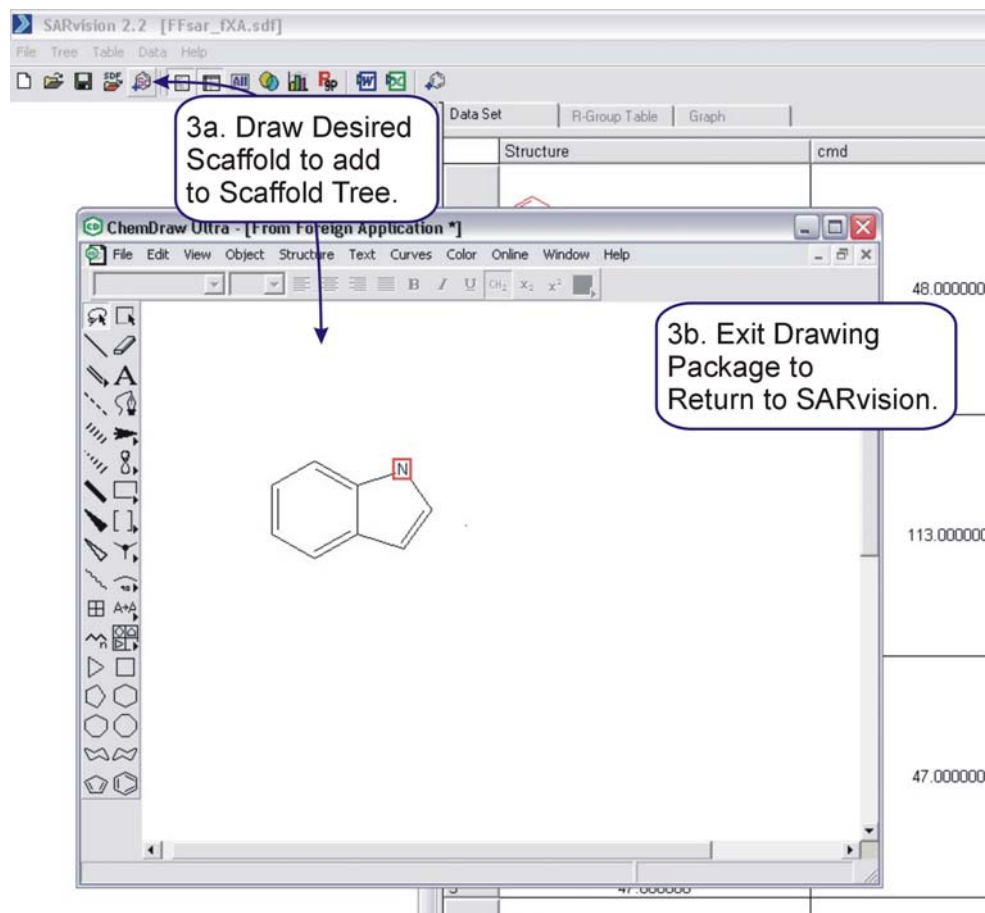


The screenshot displays the SARvision 2.2 interface with two dialog boxes open. The 'Properties' dialog box is titled '2a. Activate Drawing Package.' and shows the 'Activate Drawing Package' section with 'ChemDraw' selected. The 'Find ChemDraw Executable: ChemDraw.exe' dialog box is titled '2b. Locate the Executable.' and shows the 'ChemDraw' folder containing 'ChemDraw.exe'.

Structure	cmd	Ki(FXa)(nM)
	48.000000	61.000000
	113.000000	15.000000
	113.0	
	47.0	

3. Add a Scaffold

Now that a drawing package has been activated, click the 'Draw Scaffold' button () and draw a scaffold. When done **completely exit** Drawing Package to return back to SARvision.



Upon exit of the drawing package, the scaffold will appear in the Scaffold space on the left hand side of SARvision. The number below the scaffold indicates the number of molecules in the table that contain this scaffold as a substructure.

4. Align Molecules to a Scaffold and Build a Table

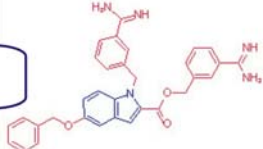
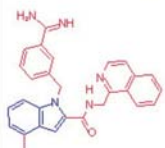
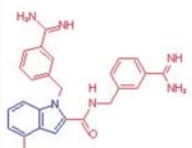
Double click on the scaffold to identify all the molecules in the table that contain this motif and to color and align these molecules according to the drawn scaffold. Under [Tree: Display Options](#), is a check box ([show singleton folders](#)) that will enable singleton folder generation. If this box is checked then a grey folder will appear under the scaffold that will contain all of the molecules that do not contain any of the scaffolds as substructures, in this case 0. By double clicking on this folder, these molecules can be similarly displayed.

number of molecules

139

4. Double Click on Scaffold to Identify Member Molecules in the Table.

Molecules in Table are Aligned and Colored by Scaffold Motif.

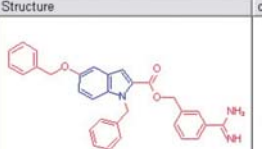
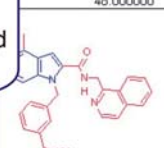

Structure	cmd	Ki(Fxa)(nM)	Ki(Thr)(nM)
 48.000000	48.000000	61.000000	
 113.000000	113.000000	15.000000	200.000000
 47.000000	47.000000	7.000000	2390.000000

The color coding of the scaffolds can be changed under [Table: Display Options](#). By right clicking on the scaffold, the user can [edit scaffold](#) to change the structure or its orientation using the selected drawing package. Double click the scaffold again to rebuild the Molecule Table and redisplay the new molecule set in the new orientation (see below: scaffold is flipped 180°).

5. Create a Scaffold Tree

Right clicking on any scaffold pops up a menu that allows the user to manipulate them within a hierarchical framework. The scaffold can be deleted, edited in a drawing program or named. In addition, 'children scaffolds' can be generated using this 'parent' scaffold as a seed under the [Expand Scaffold](#) menu item.

5. Right Click on Scaffold To Identify Additional Motifs by Building a Scaffold Tree (Expand Scaffold).

Structure	cn
 48.000000	4
 113.000000	11
 113.000000	2

The result is a series of scaffolds generated in a tree structure, each child being more complex than the parent. Each Scaffold in the tree is color coded to illustrate the parent-child relationships and oriented similarly. Double clicking on any scaffold builds a molecule dataset in the table for that scaffold.

6. Create an R-Group Table

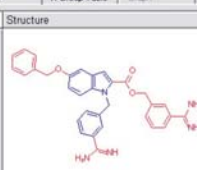
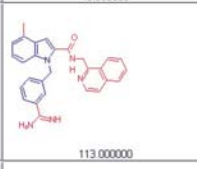
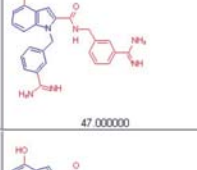
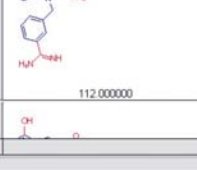
To view the molecules in R-group table format, click the R-Group Table button (R). This activates the R-Group Table tab at the top of the table. The user can now visualize the molecules in either the Molecule table or broken down as R-groups in an R-Group table.

6. Click the Rgp Button to view Molecule Family in Rgp Table Format.

Scaffolds Are Organized into a Hierarchical Scaffold Tree.

Double Click on any Scaffold to Build a Molecule Table with this Family of Molecules.

Drill down into the Tree to Identify interesting Scaffolds.

Structure	cmd	Ki(Fxa)(nM)	Ki(Thr)(nM)
 46.000000	48.000000	61.000000	
 113.000000	113.000000	15.000000	200.000000
 47.000000	47.000000	7.000000	2390.000000
 112.000000	112.000000	7160.000000	

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7. Name R-Group Fragments

In the R-Group tables, the columns behave similarly and can be moved, locked, sorted and deleted. An R-Group naming library can be constructed to associate names with substructures in the table by right clicking on the R-group. Typing a name into the box creates an alias name for the structure in all instances in the table. The Alias library is maintained throughout the table and between instances of the program.

7a. Right Click on Any Column to sort or edit it.

7b. Right Click on Rgroup To Start a Library of Rgp Aliases.

	R1	R2	R3	R4	R5	R6	R7	cmd	Ki(FX ₀)
1		H	H		H	H		48.000000	6
2		H	CH3	H	H	H		113.000000	1
3		H	CH3	H	H	H		47.000000	2
4		H	OH	H	H	H		112.000000	71
5		H	CH3	H	H	H		46.000000	1
6		H	CH3	H	H	H		111.000000	79

8. Export Table to Microsoft Word or Excel

To export, simply click on the Export to Excel () or Export to Word () buttons.

8. Finally, Export your Data to Excel or to Word.

	R1	R2	R3	R4	R5	R6	R7	cmd	Ki(FX ₀)(nM)
1		H	H		H	H		48.000000	61.000000
2		H	CH3	H	H	H		113.000000	15.000000
3		H	CH3	H	H	H		47.000000	7.000000