



Integrating SARvision into a PipelinePilot Protocol

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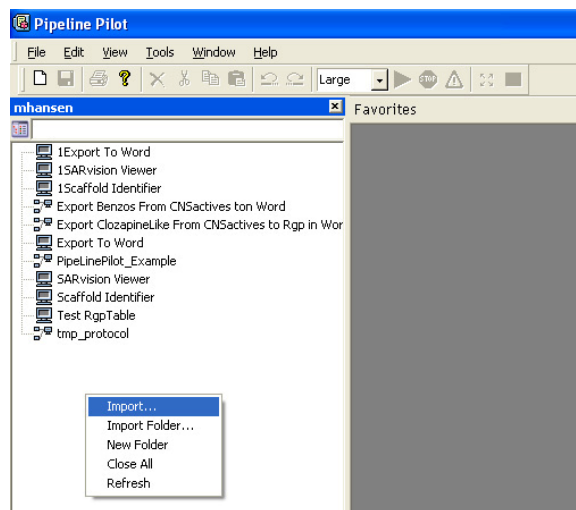
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Welcome to *SARvision*

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.

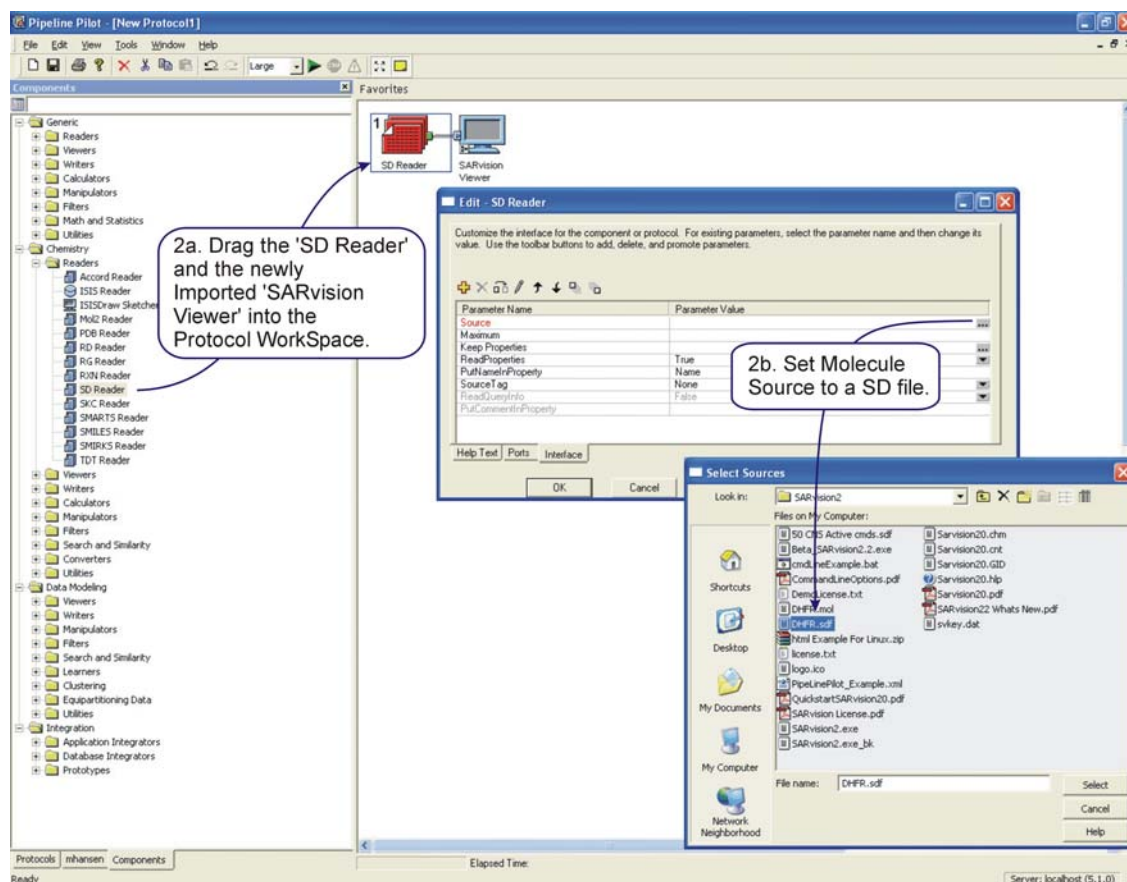
1. Open Pipeline Pilot and Import a *SARvision* Module

To get started, open **Pipeline Pilot** and import the SARvision Viewer from the SARvision install directory (`C:\Program Files\ChemApps\SARvision2\SARvision Viewer.xml`). This will add an example module into the Module panel call 'SARvision Viewer'.



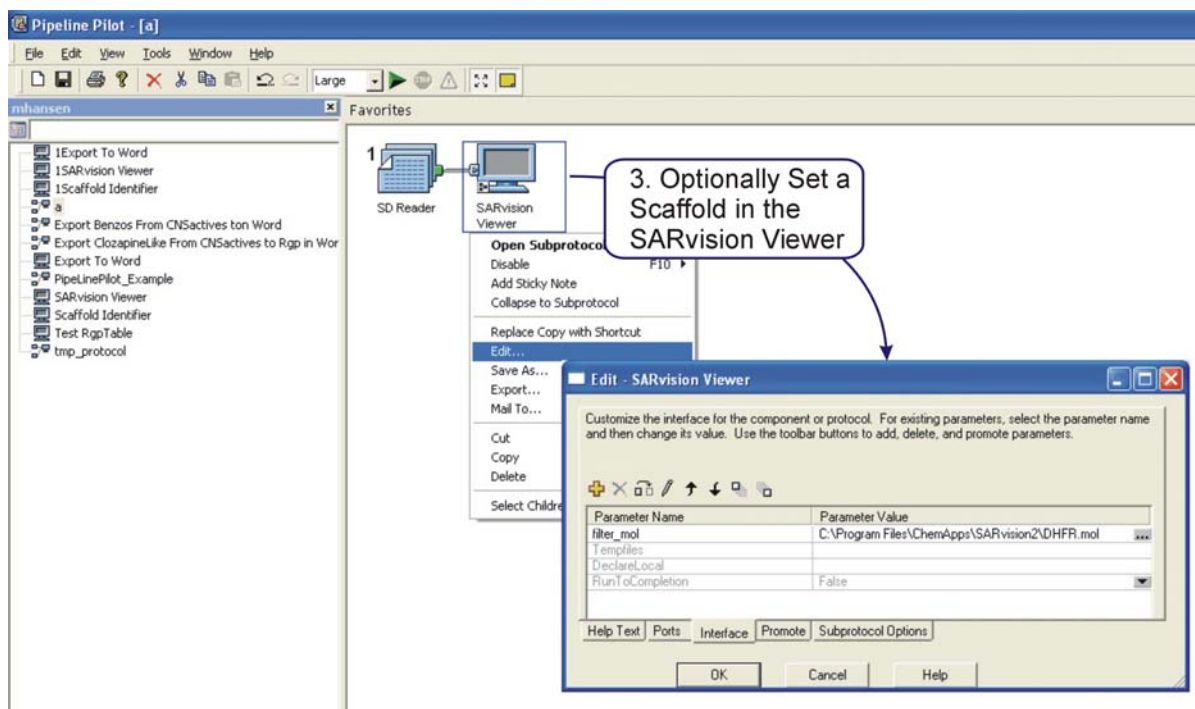
2. Create a Simple Protocol that Utilizes *SARvision*

This *SARvision Viewer* module accepts a molecule stream from other Pipeline pilot chemistry modules and loads and processes these molecules in *SARvision*. From the Chemoinformatics group, drag the *SD Reader* over in to Pipeline Pilot workspace. Under the right-click menu: *edit* set this component to read an sd file. For this example, the sd file located in the SARvision install directory is read (`C:\Program Files\ChemApps\SARvision2\DHFR.sdf`). This file contains a number of Dihydrofolate reductase inhibitors.



3. Set the Scaffold in the Protocol

Next, under the right-click menu: edit for SARvision Viewer, set the 'filter mol' (or scaffold) to relevant chemical motif contained within the dataset. For this example, use the mol file located in the SARvision install directory (C:\Program Files\ChemApps\SARvision2\DHFR.mol). This file should be in MDL-mol file format and can be generated using ChemDraw, IsisDraw or any number of chemistry drawing applications.



4. Execute the Protocol

By clicking on the green arrow at the top of Pipeline Pilot executes this simple protocol. The molecule dataset is read by the **SD Reader** and passed into the **SARvision Viewer** which will launch **SARvision**. The Scaffold is read by the **SARvision Viewer** and used by SARvision to align molecules in the **SARvision** table. Alternatively it can also be used to create Rgp-Tables for **SARvision**.

	R1	R2	R3	R4	R5	R6	R7	Name	CMD	MA
1	CH3	H	Cl	H	H	CH3	H	16.000000	16.000000	
2	Et	H	OCH3	H	H	CF3	H	48.000000	48.000000	
3	CH3	H	CH3	H	H	CH3	H	15.000000	15.000000	
4	CH3	H	OCH3	H	H	CF3	H	47.000000	47.000000	
5	CH3	H	OCH3	H		H	H	14.000000	14.000000	
6	CH3	H	F	H	H	CF3	H	46.000000	46.000000	
7	CH3	H		H	H		H	78.000000	78.000000	
8	CH3	H	F	H	H	F	H	13.000000	13.000000	
9		H	H	OCH3	OCH3	H	H	45.000000	45.000000	
10	Et	H	OCH3	H	H	CH3	H	12.000000	12.000000	

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5. Command Line Options

A number of command line options have been added specifically to call SARvision directly from other application such as Pipeline Pilot. These command lines allow the user to automatically launch **SARvision**, load a molecule dataset, manipulate, generate any reports and/or export the data directly to text, Word or Excel.

The command line options are:

- d "dataset.sdf" open a data set of molecules (sd format). Can be multiple.
- s "scaffold.mol" open a scaffold molecule file (mol format).
- a auto align molecules in dataset.sdf to scaffold in scaffold.mol.
- id identify scaffolds in dataset.sdf.
- r display table in default R group mode.
- ew export table to word document.
- ex export table to excel.
- ets "file.sdf" export tree to sd file.
- etx export tree to excel.
- tn name tree nodes.
- tx expand all nodes in tree.
- cp calculate all properties.
- cs correlate molecules to scaffold.
- wo "workspace.sarv" open workspace.
- ws "Workspace.sarv" save workspace.

An example of a MS-DOS command line function.

Example: SARvision.exe -d "C:\My Documents\dataset.sdf" -s ".\scaffold.mol" -a -r -ew

This command launches **SARvision**, reads in the molecule set *dataset.sdf*, reads in the scaffold *scaffold.mol*, aligns the molecules in *dataset.sdf* to *scaffold.mol*, displays them in the Rgp table format and automatically exports this table to Microsoft Word.

6. Creating Advance SARvision Modules

The Command line in the **SARvision Viewer** can be broken down into its components and the 'Run Program (Client)' module which launches **SARvision** can be changed to incorporate any of the above command line options. The molecule stream that enters this component is saved as `$(tmpfile)` and the scaffold molecule as `$(filter_mol)`.

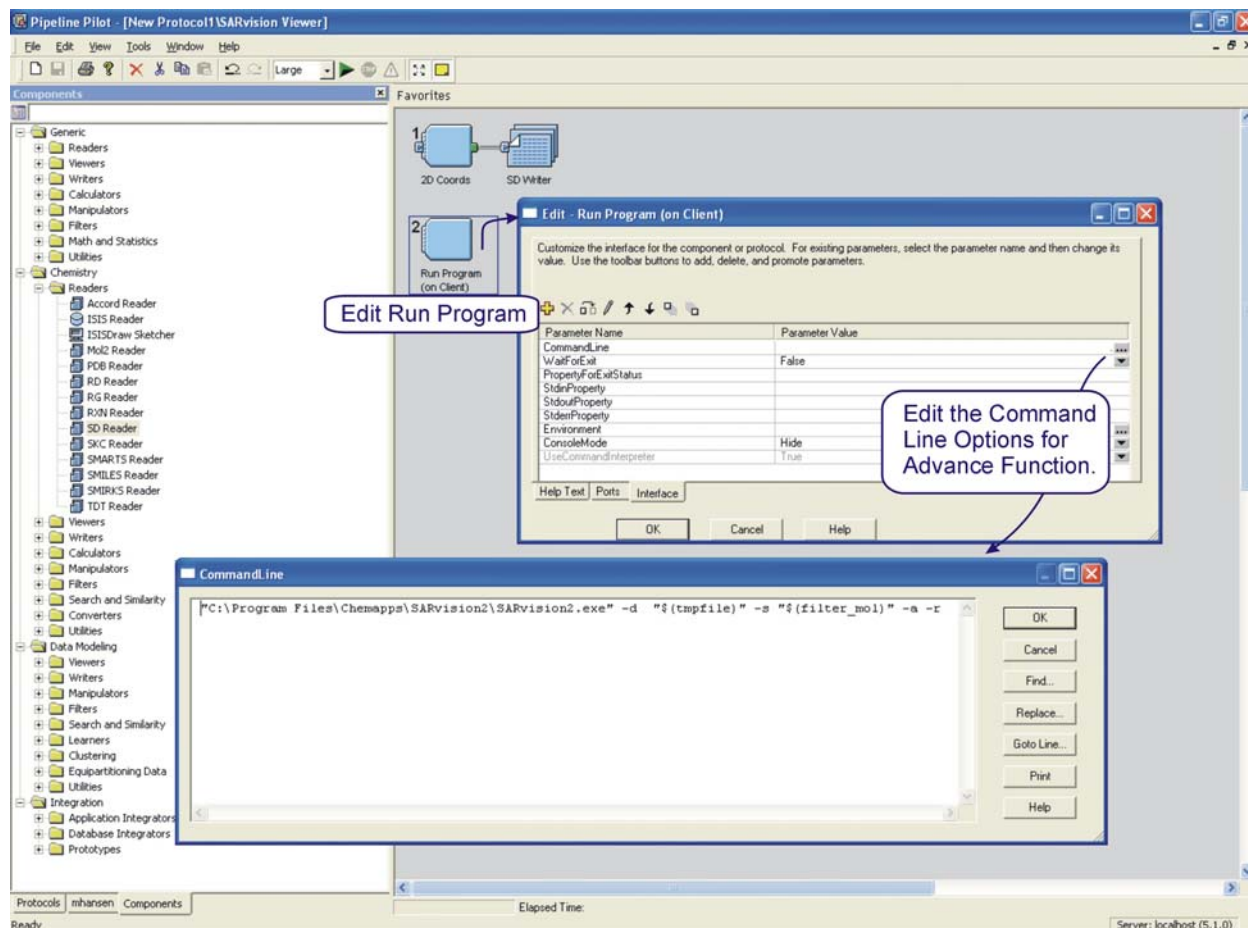
The simplest is to merely load an sd file into the SARvision Table:

```
"C:\Program Files\Chemapps\SARvision2\SARvision2.exe" -d "$(tmpfile)"
```

Whereas a more complex version would be:

```
"C:\Program Files\Chemapps\SARvision2\SARvision2.exe" -d "$(tmpfile)" -s  
"$(filter_mol)" -a -r
```

where an sd file is imported, a scaffold is imported, the molecules in the sd file are aligned to the scaffold and an R-group table is generated.



7. Server-Side SARvision Applications

Currently, **SARvision** has been only released as a client side application for viewing and manipulating data as a last step. Future server side versions of **SARvision** are being developed for Linux, Solaris, Irix and Windows. These applications will be command line driven and have similar command line functionality. Please contact us if you would like to beta test these applications.