

CERF CHEMISTRY FUNCTIONALITY

The CERF Electronic Laboratory Notebook is unique in that the notebook page display engine supports plugins that can provide additional functionality. Out of the box, CERF includes plugin viewers that allow users to display several scientific data types inline without requiring the native applications for these files. As a separate option, customers may purchase the CERF Chemistry Search Module, which adds structural search capabilities.

Standard CERF Chemistry Plugins

Standard CERF installs include plugin viewers that can display scientific data types inline in the CERF Notebook. Examples include .ab1, .mol, .pdb, .txt, .rtf, .gbk, .gb, .svg and many others. For displaying chemistry structure files, CERF comes with both **JMol Molecular Structure Viewer** and **JChemBase software suite from ChemAxon**, which includes MarvinView™, MarvinSketch™. The Chemaxon tools viewer plugin is used by default unless your organization requests that JMol be used as the default instead.

JMol Molecular Structure Viewer

This plugin renders a variety of molecular structure file-types (including .mol and .pdb) as inline 3D views, which the user can interact with by clicking and dragging to rotate the display.



Figure 1. A CERF entry displayed in JMol using a 3D view.

MarvinView™ by ChemAxon

CERF also includes the JChemBase software suite from ChemAxon, which includes MarvinView™, MarvinSketch™, and also JChemBase™ for searching. Current license from chemaxon is required to activate the search functionality. Lab-Ally can provide these for an additional fee if your organization does not have one. Please ask your customer account manager for information about additional tools from [ChemAxon](#) such as JChem for Excel, Reactor, Metabolizer, and others, which are available to CERF users at a significant discount.

MarvinView provides a dynamic display of chemical structures and reaction equations - including dynamic rendering of 2D and 3D structures in a variety of styles (ball and stick, space-filling, etc.).

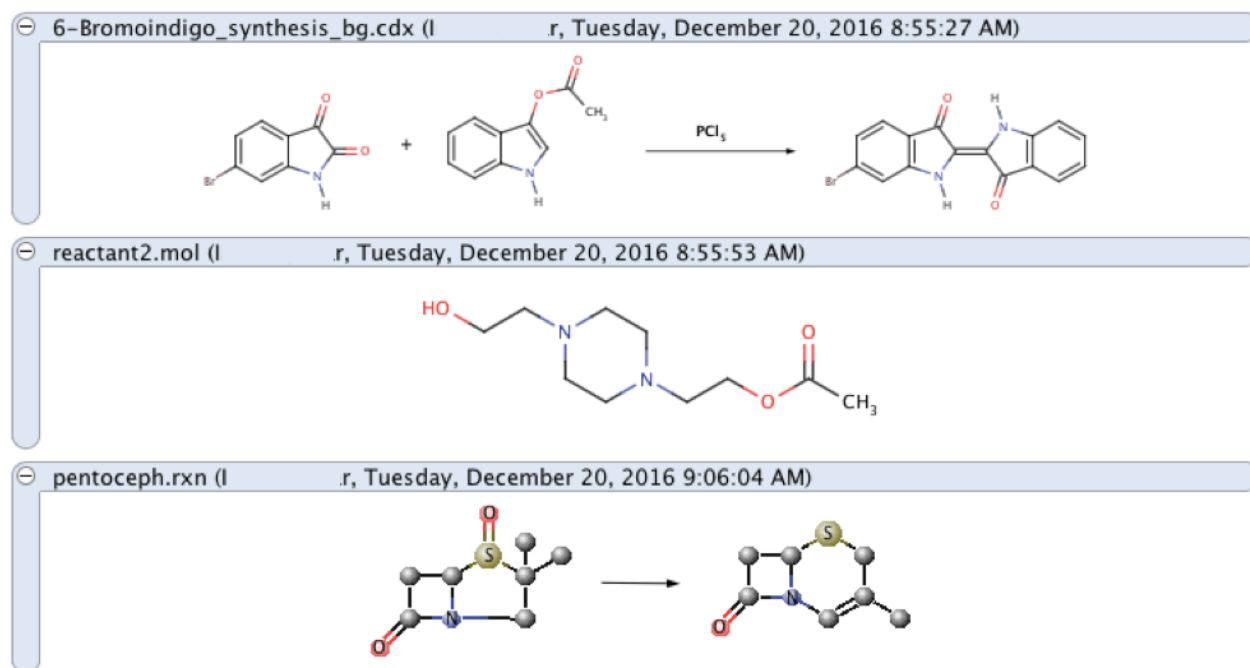


Figure 2. Display of molecular structures and chemical reactions with the Extended *CERF Chemistry Structure module*.

Right-clicking on the entry allows users to access various in-line view and animation options, or users can right-click and choose “Window” to manipulate the file in a new separate window. Naturally, as with any other type of data placed within CERF, chemical structures and reactions can be edited and modified using your default chemistry editing and authoring tools by choosing checkout and edit.

MarvinSketch™ by ChemAxon

MarvinSketch™ is an advanced chemical editor for drawing chemical structures, queries and reactions. When the user selects a chemical reaction or molecule displayed in the CERF Notebook and selects the “View” action, the structure opens in the MarvinSketch application or your default application for that file type. To create new chemistry structures on your local computer, go to the main CERF menu and choose Search > Chemical Structure Search. This will open MarvinSketch. Once you have created a structure you can choose File > Save As to save the structure to your local computer. From there you can add this file to CERF.

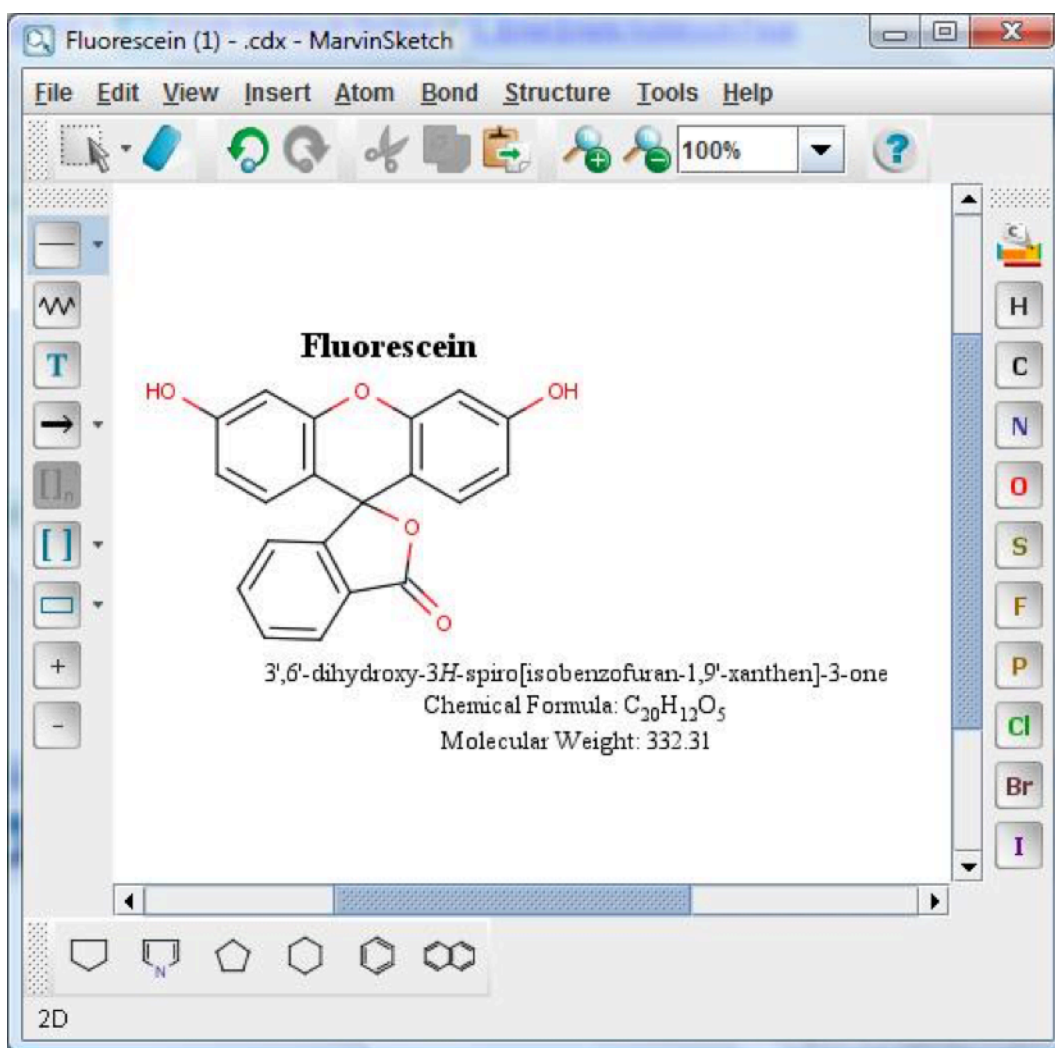


Figure 3. A MarvinSketch™ view of a fluorescein.cdx file.

Chemical Structure Searching

Chemical structure files and/or reaction files in the CERF system are indexed for intelligent searching. Structures can be searched in their entirety, by sub-structure, or by similarity. Any experiment that includes chemical information can easily be found using this chemistry search tool. This is a powerful tool, especially when used in conjunction with the standard CERF search, which allows users to search the entire system using text or metadata.

To search, go to the main CERF menu and choose Search > Chemical Structure Search to launch the Chemical Structure Search dialog. The user simply selects the basic structure from the toolbar and then adds bonds and chemicals using the drawing tools. The search results are returned in the standard CERF format, with the usual CERF functionality that allows users to “View Info” and “Locate” the resource in its CERF context. If a ChemAxon license is not installed the search returns an error.

The screenshot displays the 'Chemical Structure Search' window. On the left, a chemical structure is drawn in the center pane. Below it, the 'Structure' field contains the SMILES string S1C=NC2=CC=CC=C12 and the 'Search Type' is set to 'Substructure'. On the right, the 'Results' table lists the following data:

Title /	Contrib	Creatio...	Last Up...	Resour...	Content...
nci500.....	Wo	Jan 14, 2.....	Jan 14, 2.....	Document	Smiles
nci100.....	Wo	Jan 14, 2.....	Jan 14, 2.....	Document	MDL Stru...
nci100.....	Wo	Jan 14, 2.....	Jan 14, 2.....	Document	Smiles
opt-bet.....	Wo	Jan 14, 2.....	Jan 14, 2.....	Document	Smiles
stat-nc.....	Wo	Jan 14, 2.....	Jan 14, 2.....	Document	Smiles
valid-b.....	Wo	Jan 14, 2.....	Jan 14, 2.....	Document	Smiles
valid-b.....	Ba	Jan 19, 2.....	Jan 19, 2.....	Document	Smiles

Buttons at the bottom include 'View', 'Locate', 'View Info', 'Search', and 'Close'.

Figure 4. A substructure search using the Chemical Structure Search tools. Results are returned that contain this substructure.

Results

Title / Cont...	Crea...	Last...	Res...	Cont...
nci... Wo... Jan 1... Jan 1... Docu... Smiles				
nci... Wo... Jan 1... Jan 1... Docu... MDL S...				
nci... Wo... Jan 1... Jan 1... Docu... Smiles				
opt... Wo... Jan 1... Jan 1... Docu... Smiles				
sta... Wo... Jan 1... Jan 1... Docu... Smiles				
vali... Wo... Jan 1... Jan 1... Docu... Smiles				
vali... Ba... Jan 1... Jan 1... Docu... Smiles				

View

Locate

Hide Info

Title: valid-beta2-target.smiles

Status ?

Edit Status: Versionable
Owner: ba
My Role: Notebook Creator
Closed: No
Checked Out: No
Visibility: Shared

Thumbnail

Metadata ?

Title: valid-beta2-target.smiles

Submission/Modification

Resource Type: Document
Creation Date: Jan 19, 2010 3:38:02 PM
Last Update: Jan 19, 2010 3:38:02 PM
Contributor: Ba
File Size: 24760 Bytes

Search

Close

Figure 5. When the user selects a result, more information is readily available in CERF. “View Info” shows the Status, Thumbnail, and Metadata. This info also shows Version History, Annotations, and Digital Signatures when these are a part of the record.

Supported File Types

Below is a list of file types/formats supported by standard CERF installs. Please note that if your favorite file type is *not* listed below, it may still be viewable inline by one of our other plugins - and if not, you can still add the file to CERF as a non-displayed file which can be edited and modified using the default external application of your choice!

CDX, CDXML
CML
CSD
CSMOL
CSRDF
CSRXN
CXSMARTS
CXSMILES
INCHI
MOL, MOL2
MRV
PDB
RDF
RXN
SD
SDF
SMARTS
SMI, SMILES, SMIRKS
SYB, SYBYL
XYZ