

SigmaCERF Electronic Laboratory Notebook is unique in that the notebook page display engine supports plugins that can provide additional functionality. Right out of the box, SIGMACERF includes plugin viewers that allow users to display several scientific data types inline, including chemical structures, without requiring the native applications for these files. Leveraging this novel plug-in architecture, Rescentris offers an add-on module enabling chemical structure viewing and editing, with both full structure and substructure search capabilities.

Standard SigmaCERF Chemistry Plugin

Standard SigmaCERF installations include plugin viewers that display several scientific data types including – .ab1, .mol, .pdb, .txt, .rtf, .gbk, .gb, and .svg files – inline in the SigmaCERF Notebook. The files are stored in SigmaCERF, searchable metadata can be added, and screen captures can be printed as Official Printed Copies on the Notebook Page. One of the standard plugins included with every SigmaCERF purchase is the 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.

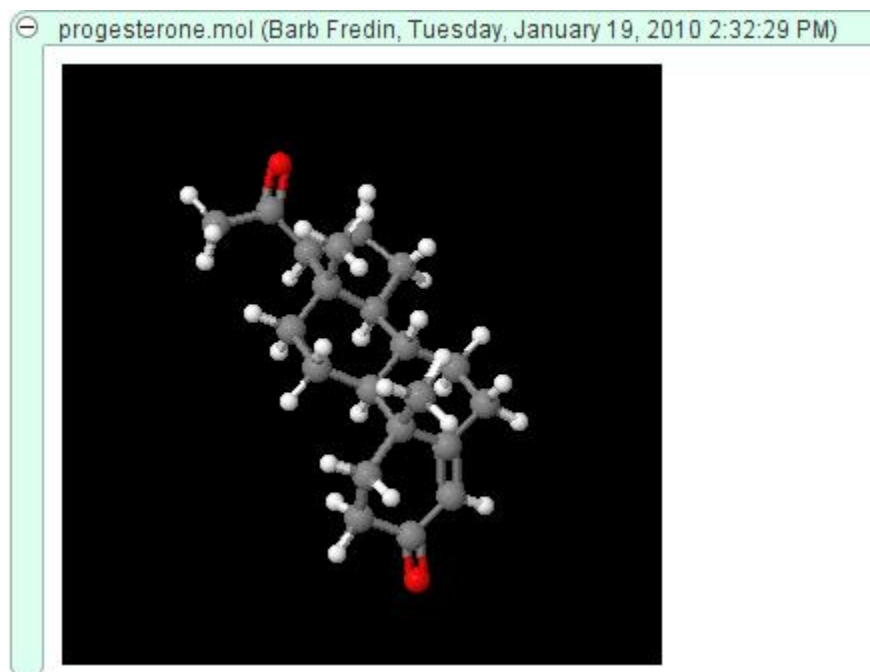


Figure 1. Display of molecular structure with the Standard SIGMASIGMACERF Chemistry Plugin.

The SigmaCERF Chemistry Module

With the purchase of the SigmaCERF Chemistry Module, SigmaCERF integrates functionality licensed from ChemAxon Ltd. to deliver a robust chemistry platform providing inline structure viewing, creation, editing and searching to store your chemical intellectual property. The SigmaCERF Chemistry Module can be expanded further with the addition of virtual synthesis and metabolite analysis enterprise components. Please ask your Customer Account Manager for more details on these exciting additions available to Chemistry Module subscribers at significant discounts.

Inline Viewing

The SigmaCERF Chemistry Module 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.).

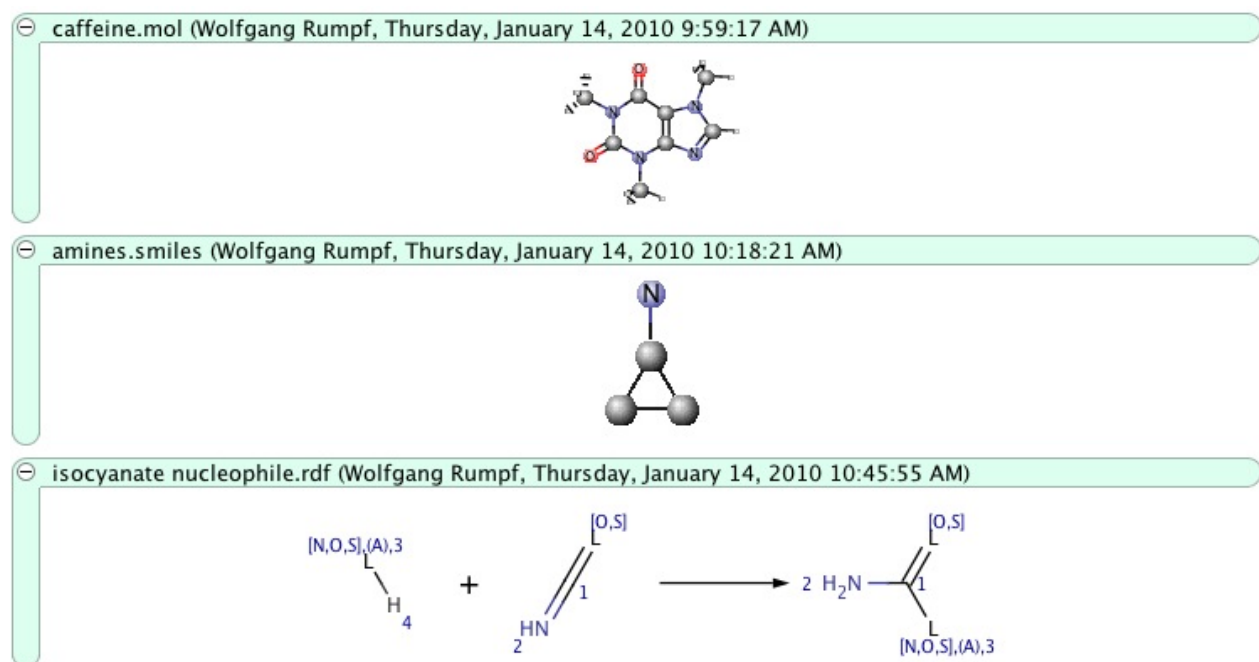


Figure 2. Sample images showing molecular structures and chemical reactions viewed within the SigmaCERF Chemistry Module.

Animation of structures and equations is also supported directly inline. And naturally, as with any other type of data placed within SIGMASIGMACERF, chemical structures and reactions can be edited and modified using your default chemistry editing and authoring tools.

SigmaCERF Chemistry Editor

The SigmaCERF Chemistry Module provides an advanced chemical editor for drawing chemical structures and reactions. Use the Chemistry Module to create both structures and reactions as well to draw structures for structure and substructure queries. When a user selects a chemical reaction or molecule displayed in the SigmaCERF Notebook and selects the "View" action, the structure opens in the chemical editor application.

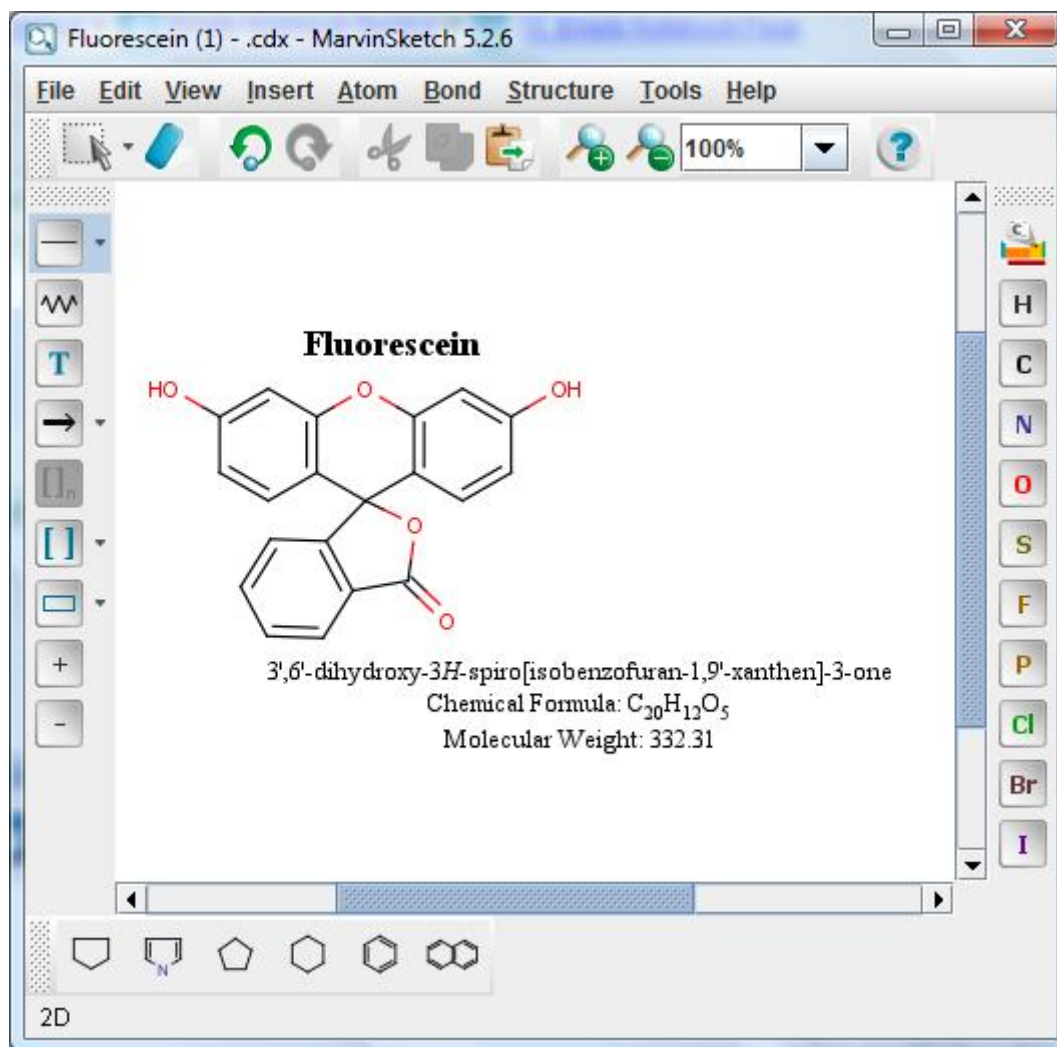


Figure 3. The SigmaCERF Chemistry Editor View of a fluorescein.cdx file.

The SigmaCERF Chemistry Editor can also perform useful calculations including elemental analysis, IUPAC naming, isoelectric point and stereoisomer determinations, polar and molecular surface areas and Huckel Analysis, with a complete list below.

<p><i>Elemental Analysis</i></p> <ul style="list-style-type: none"> • Elemental Analysis <p><i>IUPAC Name</i></p> <ul style="list-style-type: none"> • Structure to Name <p><i>Protonation</i></p> <ul style="list-style-type: none"> • pKa • Microspecies • Isoelectric Point <p><i>Partitioning</i></p> <ul style="list-style-type: none"> • logP • logD 	<p><i>Charge</i></p> <ul style="list-style-type: none"> • Charge • Polarizability • Orbital Electronegativity <p><i>Isomers</i></p> <ul style="list-style-type: none"> • Tautomerization • Stereoisomer <p><i>Conformation</i></p> <ul style="list-style-type: none"> • Conformer • Flexible 3D-Alignment • Molecular Dynamics 	<p><i>Geometry</i></p> <ul style="list-style-type: none"> • Topology Analysis • Geometry • Polar Surface Area (2D) • Molecular Surface Area (3D) <p><i>Markush</i></p> <ul style="list-style-type: none"> • Markush Enumeration <p><i>Other</i></p> <ul style="list-style-type: none"> • Hydrogen Bond Donor-Acceptor • Huckel Analysis • Refractivity • Structural Framework • Resonance
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Table 1. SigmaCERF Chemistry Editor – supported calculations.

Chemical Structure Searching

Any chemical structure and/or reaction in the SigmaCERF system is 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 SigmaCERF search, which allows users to search the entire system using text or metadata.

A chemical structure search in SigmaCERF launches the Chemical Structure Search dialog. The user simply draws the desired target molecule by selecting basic ring structures, modifying bonds and adding atoms as necessary, using the included drawing tools. The search results are returned in the standard SigmaCERF format, with the usual SigmaCERF functionality that allows users to “View” and “Locate” the resource in its SigmaCERF context.

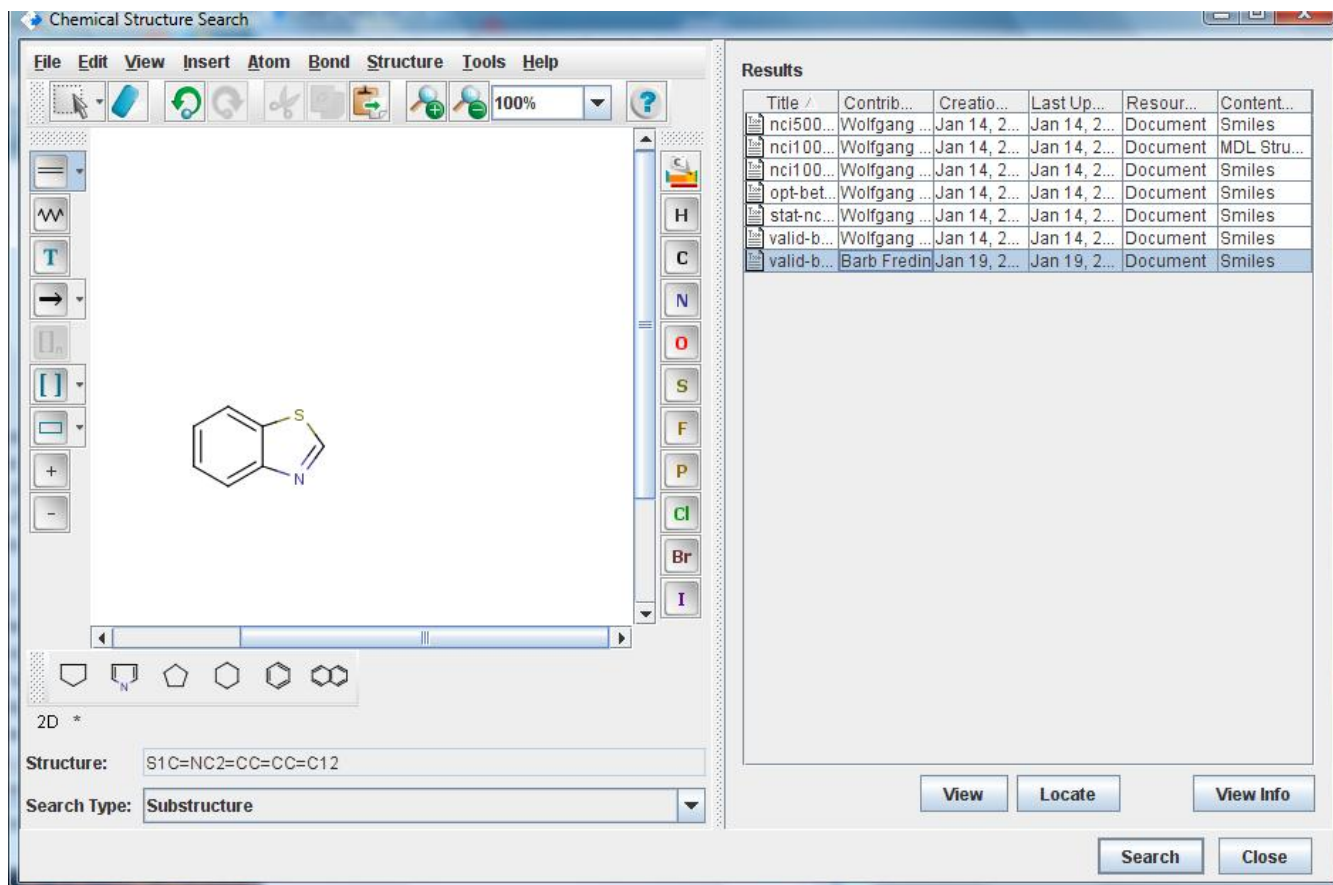


Figure 4. A substructure search using the Chemical Structure Search tools. Results are returned that contain this substructure.

Additionally, the "View Info" function provides a thumbnail of the potential target molecule for easier identification and confirmation of the desired target molecule.


Results

Title	Cont...	Crea...	Last ...	Res...	Cont...
nci...	Wolfg...	Jan 1...	Jan 1...	Docu...	Smiles
nci...	Wolfg...	Jan 1...	Jan 1...	Docu...	MDL S...
nci...	Wolfg...	Jan 1...	Jan 1...	Docu...	Smiles
opt...	Wolfg...	Jan 1...	Jan 1...	Docu...	Smiles
sta...	Wolfg...	Jan 1...	Jan 1...	Docu...	Smiles
vali...	Wolfg...	Jan 1...	Jan 1...	Docu...	Smiles
vali...	Barb F...	Jan 1...	Jan 1...	Docu...	Smiles

Title: valid-beta2-target.smiles

Status ?

Edit Status: Versionable

Owner:  [barb](#)

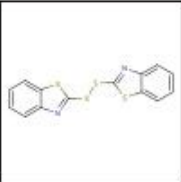
My Role: Notebook Creator

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:  [Barb Fredin](#)

File Size: 24760 Bytes

View **Locate** **Hide Info**

Search **Close**

Figure 5. When the user selects a result, more information is readily available in SigmaCERF. "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

The SigmaCERF Chemistry Module supports the files types and formats listed below. 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 SigmaCERF as a non-displayed file which can be edited and modified using the default external application of your choice!

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

Table 2. SigmaCERF Chemistry Module – supported file types and formats.