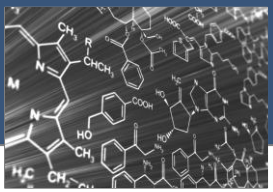
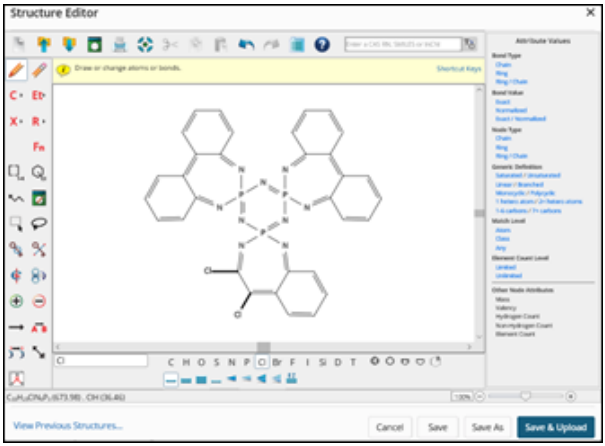
Structure Searching in

CAS STNext

Drawing and modifying structures for comprehensive retrieval

- Variables
- Shortcuts
- Templates





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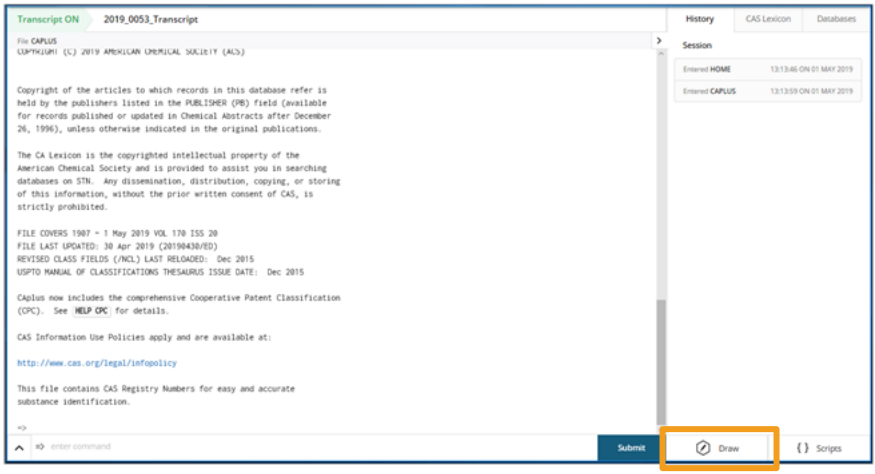
Structure Editor in STNext

STNext allows you to use chemical structure drawings as part of your search process. Drawing compounds, using templates, modifying known substance structures or converting text to a drawing are a few of the options we discuss in this booklet.

Using substance structure drawings allows you to search CAS REGISTRY[SM] and other substance searchable databases to identify relevant substances.

Login to STNext to get started. Use your STN login credentials at next.stn.org (Contact your STN helpdesk if you need assistance.)



Open the Structure Editor by clicking the Draw button in the lower, right-hand corner of STNext.

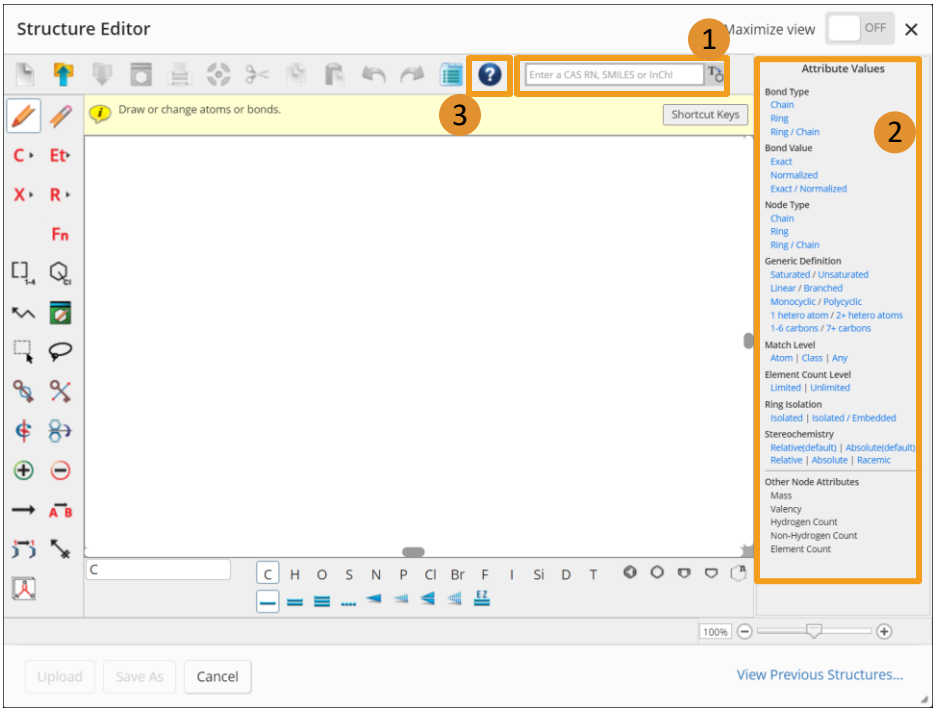
The STNext structure editor contains the latest options for generating complex structure and reaction schemes. It has easy to use file naming, file saving, and retrieval options.

Features available in STNext include:

1. Structure modeling from CAS Registry Numbers®, SMILE strings, or InCHi codes

2. Constantly visible Attributes panel for easy verification and modification of structures

3. Structure Editor help



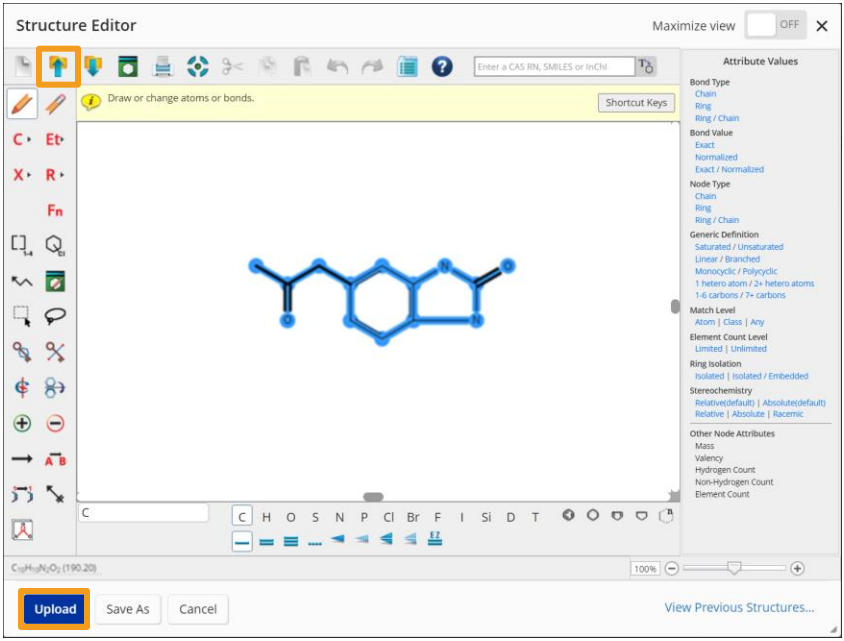
Import and Export Structures

STNext supports structure drawings in .cxf, .mol, or .str file formats. You can import drawings into the Structure Editor to use as the basis of your search strategy.

1. Click the **Import** button.

2. Edit the structure drawing (if desired) by adding, changing or removing atoms, bonds, rings, etc.

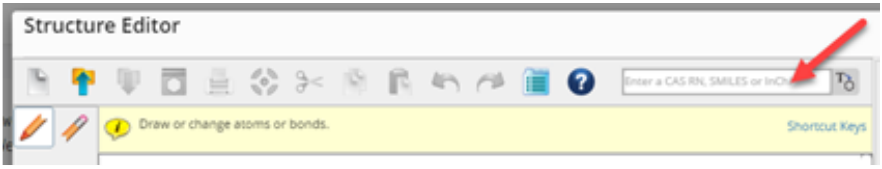
3. Click the **Upload** button to make the structure available in STNext.



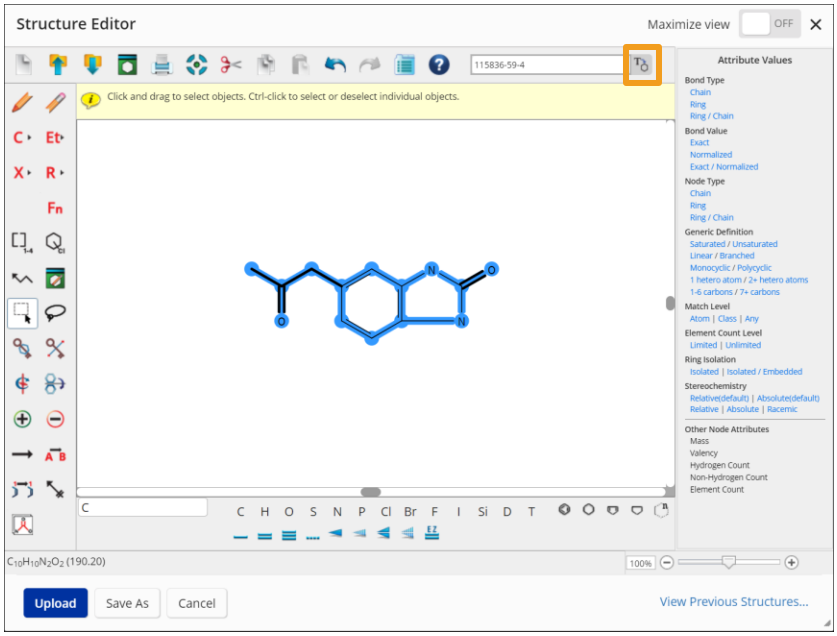
Export drawings from the Structure Editor as .cxf, .mol or .str files by clicking the **Export** button.

Text to Structure

The Add to Editor feature allows structures to be modeled directly from CAS Registry Numbers, SMILES strings, and InCHi codes. (NOTE: InCHiKey is not supported.)



1. Enter the text descriptor and click the **Text to Structure** button.
   The chemical structure will be displayed on the editing canvas.



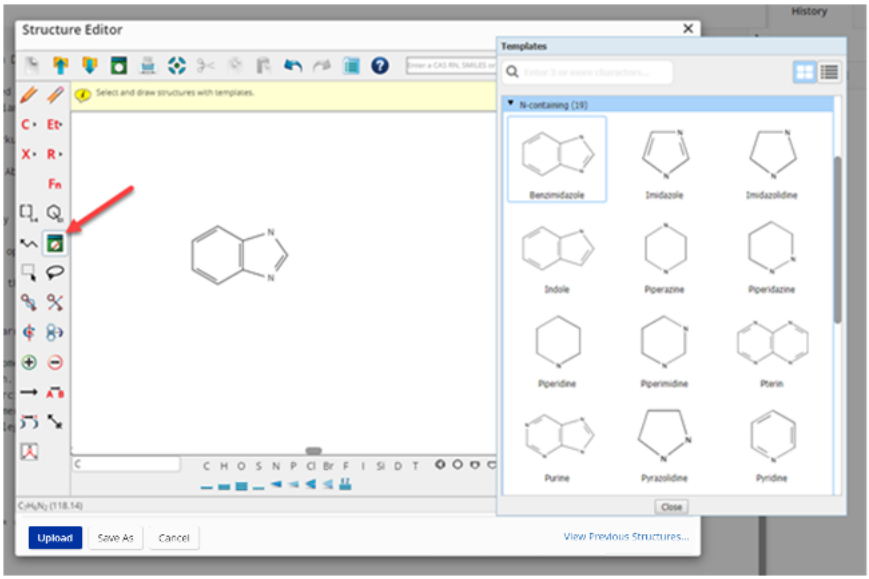
   You can edit the structure as desired.

2. Click the **Upload** button to make the structure available in STNext.

Templates

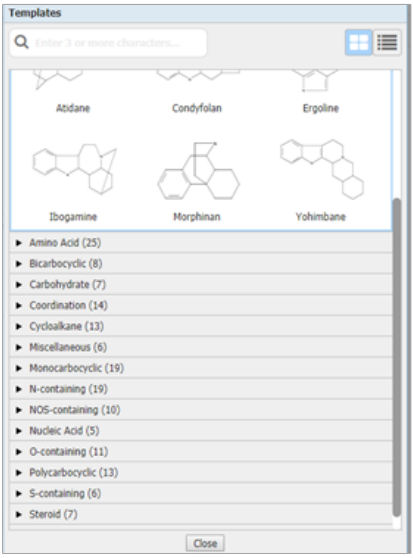
The STNext Structure Editor provides access to a collection of chemical structure templates that can be used as the basis for your drawing.

1. Click the **Templates** button on side toolbar.
   A panel displays the available structures.



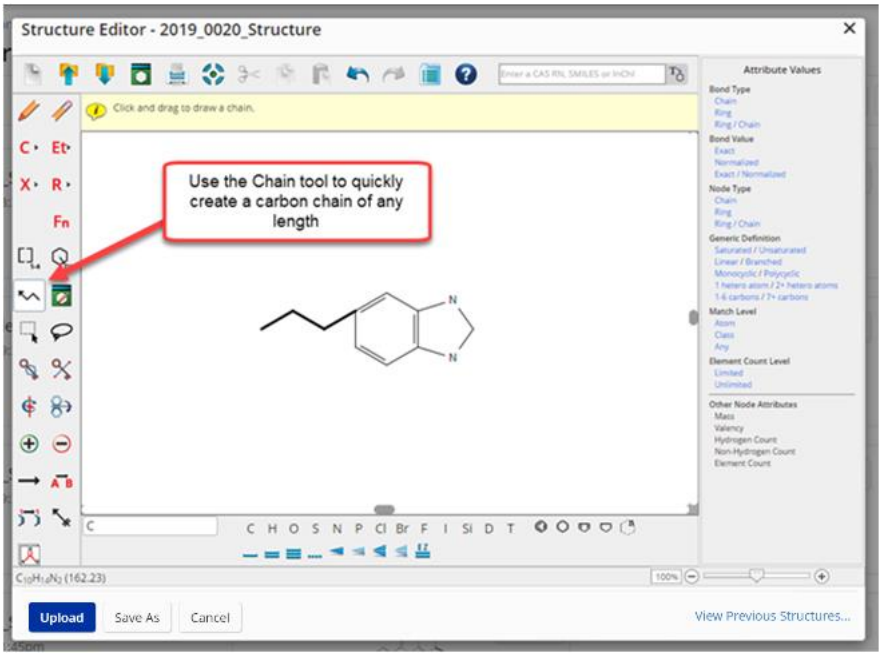
2. Explore the collection and click on the structure you want to use.

3. Click on the drawing canvas to place the selected template onto your structure drawing.



Carbon Chains

Carbon chains can be created or attached to a structure in several ways. One quick option is to use the Chain tool. Here we are attaching a three carbon chain to a ring system:



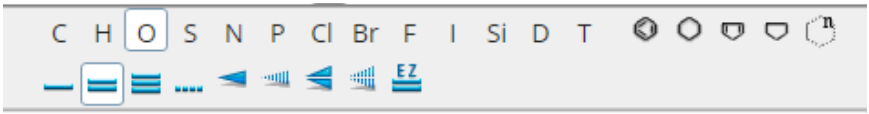
1. Select the **Chain** button.

2. Hover over the ring system to highlight the node where you wish to attach a carbon chain.

3. Click on the drawing canvas and drag the mouse to create the carbon chain.

Adding Atoms and Bonds

Common atoms can be added to a structure using the Atoms Palette at the bottom of the editor window. (Note: D refers to Deuterium, and T to Tritium.)

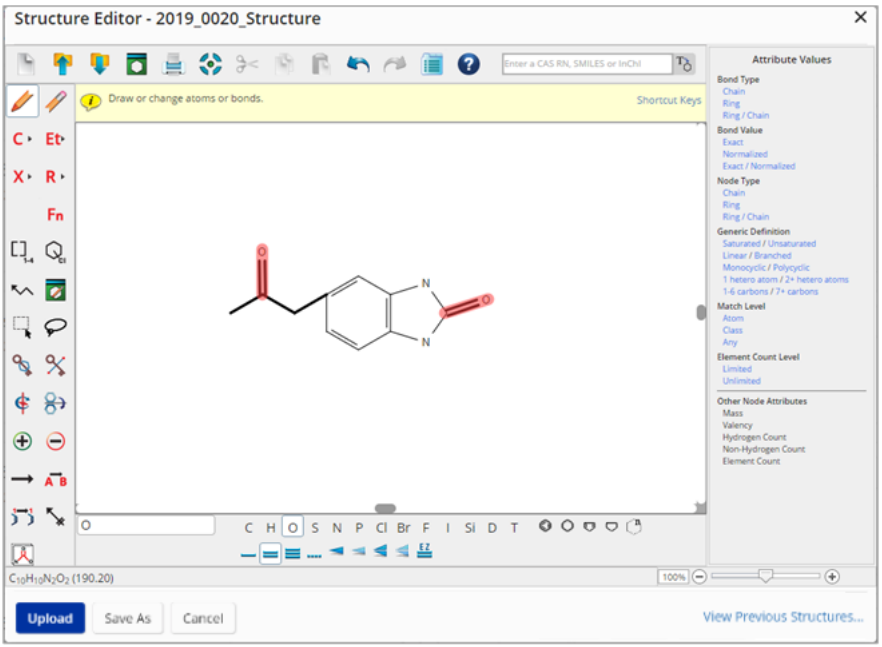


Bond types can also be selected here, on the Bonds Palette. Bonds can be drawn or changed using these symbols, including single and double stereo bonds.

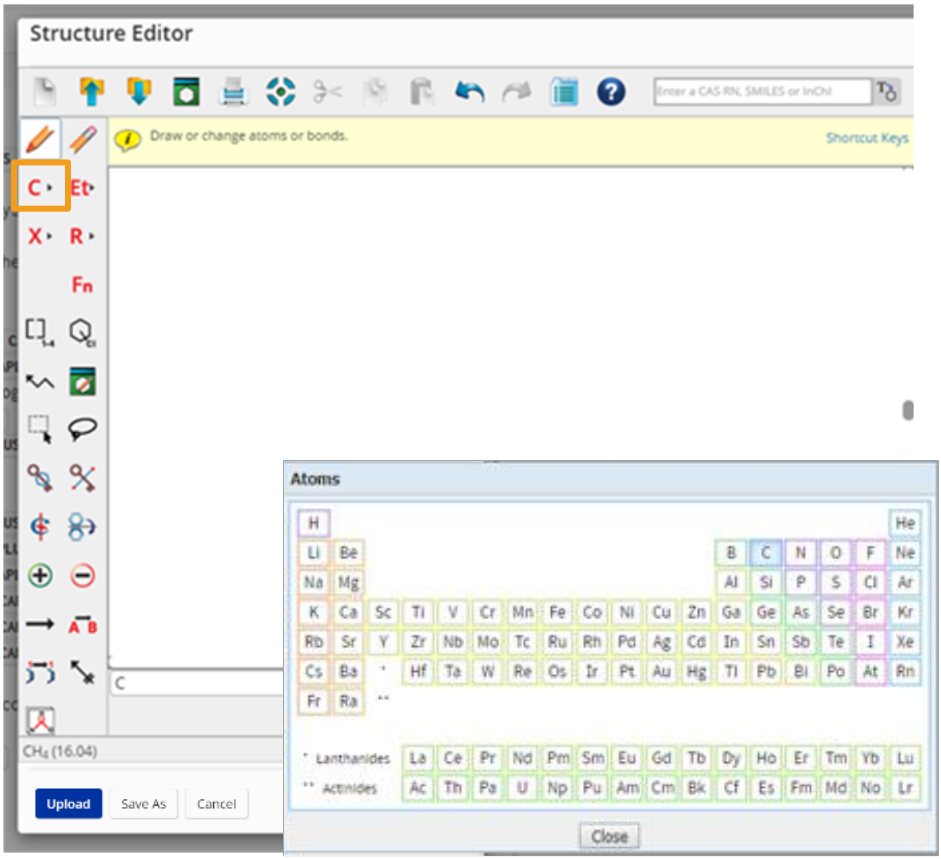
1. Select an Atom and Bond Type.

2. Hover over the structure to highlight the node where you wish to attach the atom using the selected bond type.

3. Click on the drawing canvas and drag the mouse to attach the atom.



To access atoms not shown on the Atoms Palette, click the **Atom** button on the side toolbar.



A panel of the periodic table will allow you to select any atom. Then click on the drawing canvas to place the atom.

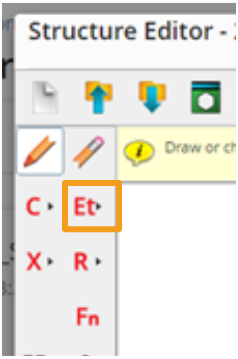
NOTE: You cannot attach a template to an existing atom or bond, but you can attach atoms and bonds to a template. If you want to use templates, be sure to start your drawing with the template.

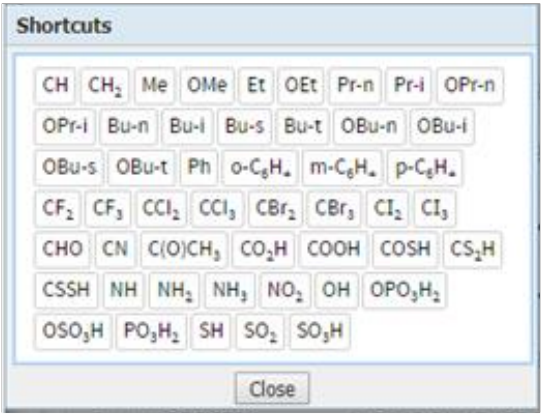
Shortcuts, Variables and R-groups

Common functional groups can be added to a drawing quickly by using the Shortcuts feature.

1. Click the **Shortcuts** button to display a list of common functional groups.

2. Select a functional group.





3. Hover over the drawing where you want to place the functional group.

4. Click on the drawing canvas to place the group.

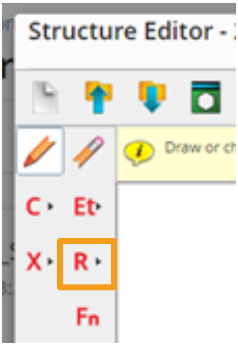
The R-group feature enables you to define a list of allowed substituents at an attachment point.

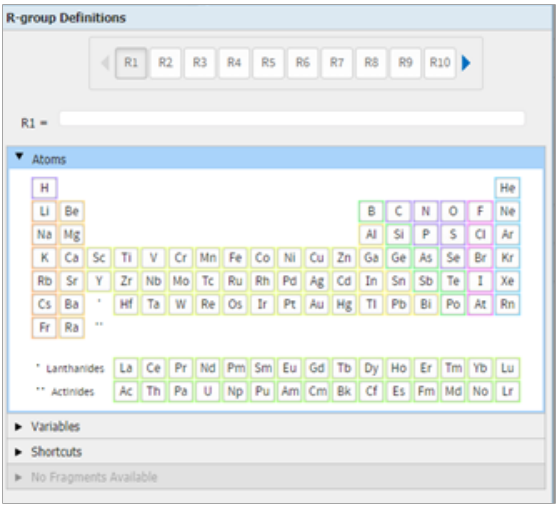
1. Click the **R-group** button.

2. Choose the R-group number you want to define (Example: R1, R5).

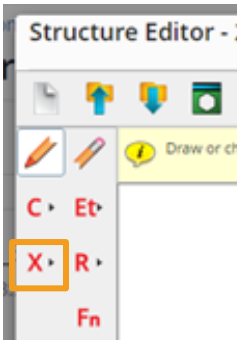
3. Select at least two atoms, variables or shortcuts from the lists.

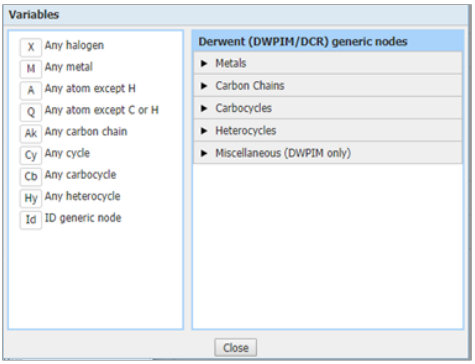
4. Apply the defined R-group to the structure by clicking on the drawing canvas.





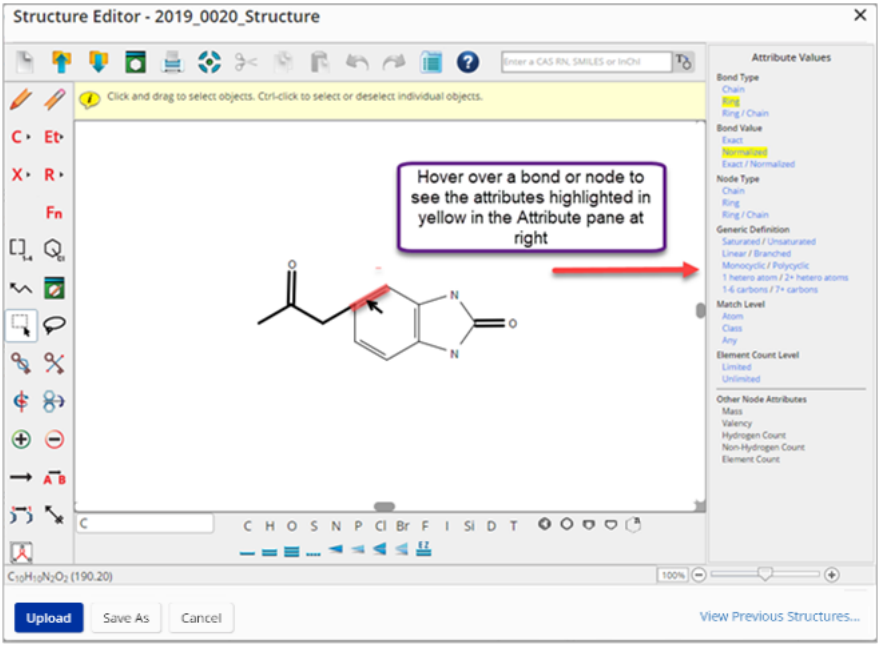
For substructure searches, you can use variable atoms. Use the **Variables** feature to select a variable atom or generic nodes for use in Derwent file searches.





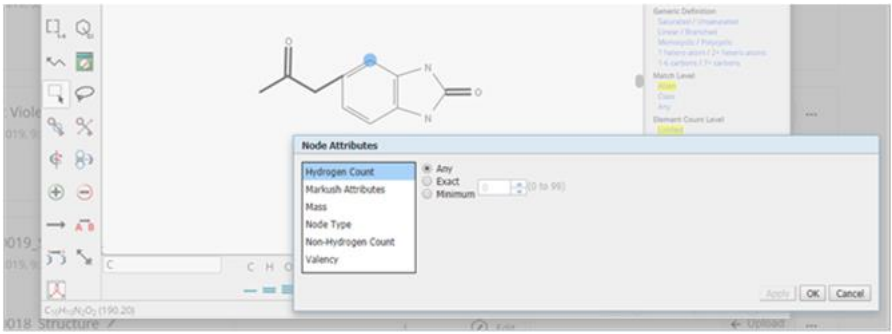
Attribute Panel

After the structure is drawn, the Attributes for each bond and node in the structure are easy to see in the Attribute Panel on the right side of the Editor.



The assigned attributes highlight in the panel when the mouse hovers over a portion of the drawing. Similarly, portions of the drawing will highlight when the mouse hovers over a value in the attribute panel.

View additional attribute information by right-clicking on the bond or node of interest. Edit as needed.

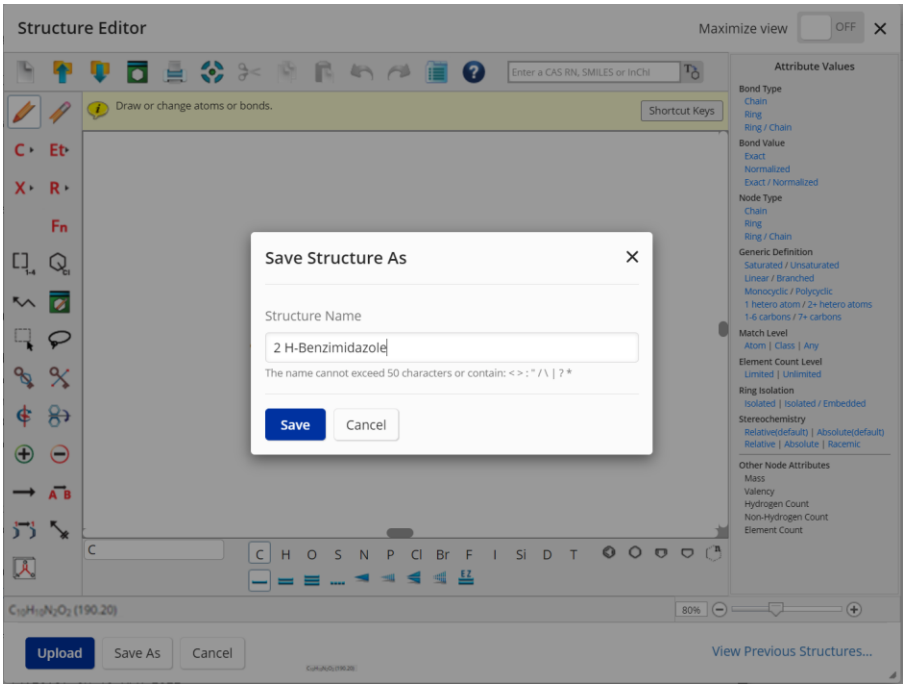


Saving & Uploading Structures

To save the drawing file into STNext, choose one of the following options:

Click the **Upload** button to directly upload the structure. The structure will be automatically saved with a sequential number name, e.g., 2019_0020_Structure. If you are not searching in a structure searchable database, the structure will not upload, but will be saved to the Structures page.

Click the **Save As** button to save the structure query with your unique preferred name to the Structures page under My Files. You can then upload the query as a second step.

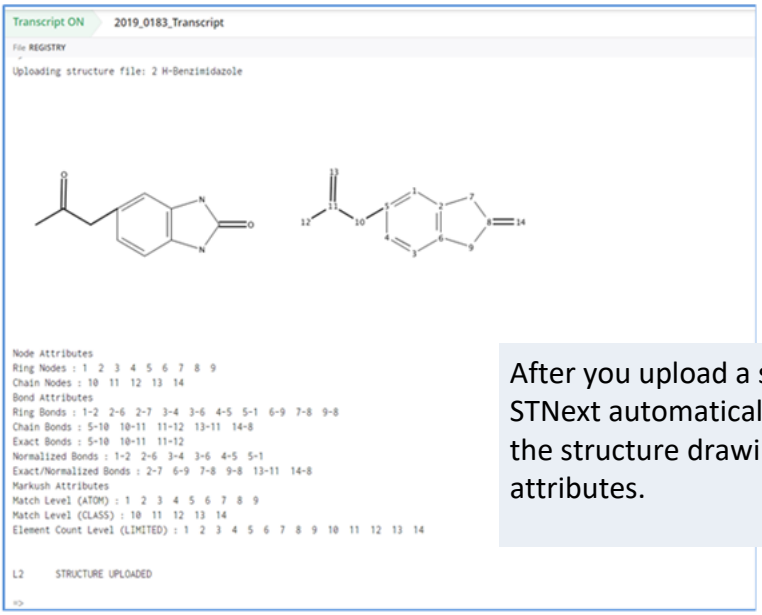


The Structure Editor window will stay active until you click the **Cancel** button, save to **My Files** > **Structures**, or **Upload** your structure.

Saving & Uploading Structures, continued

After saving a drawing, your structure will now be saved on the Structures page in STNext, under the My Files menu. This page is where you can manage all the structures you use to conduct searches in STNext.

From the Structures page, you can edit the structure name, delete structure files, open a structure in the Editor, and upload structure files into your search session.



After you upload a structure, STNext automatically displays the structure drawing and attributes.

Search with Structure

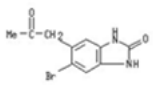
After you have uploaded the structure into your STNext session, you are ready to run your search.

1. Run a sample search (e.g., in REGISTRY) using the L-number created when you uploaded the structure.

Transcript ON 2019_0183_Transcript

File REGISTRY

```
=> s l2 sss sam

SAMPLE SEARCH INITIATED 13:06:53
SAMPLE SCREEN SEARCH COMPLETED -      260 TO ITERATE

100.0% PROCESSED       260 ITERATIONS                          7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         4233 TO     6167
PROJECTED ANSWERS:               7 TO      298

L4             7 SEA SSS SAM L2

=> d scan


L4   7 ANSWERS   REGISTRY  COPYRIGHT 2019 ACS on STN
IN   2H-Benzimidazol-2-one, 5-bromo-1,3-dihydro-6-(2-oxopropyl)-
MF   C10 H9 Br N2 O2
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
```

2. Random answers from the search results set can be displayed for review using the SCAN display format (D SCAN).

3. Proceed with your search strategy.

For more information...

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help@cas.org

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www.cas.org/support

FIZ Karlsruhe
helpdesk@fiz-karlsruhe.de

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