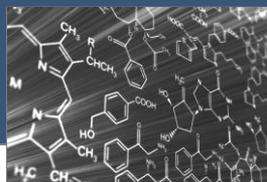
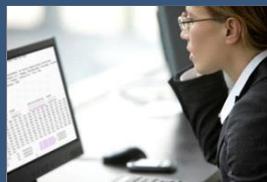


Structure Searching in

CAS  STNext

Drawing and modifying structures for comprehensive retrieval

- Variables
- Shortcuts
- Templates



Structure Editor

Draw or change atoms or bonds.

Chemical Editor

Chemical Formula: C12C3N4C5C6C7C8C9C10C11C12

View Previous Structures...

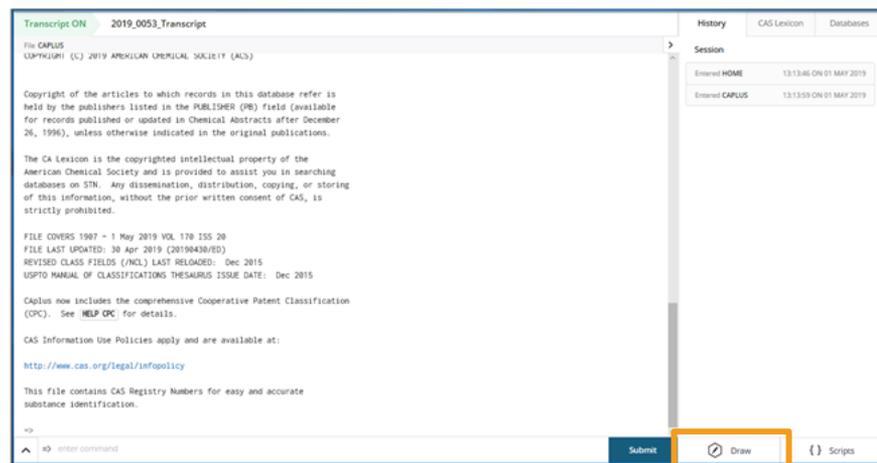
Cancel Save Save All Save & Upload

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 REGISTRYSM 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.)



The screenshot shows the STNext interface. The main content area displays a transcript for '2019_0053_Transcript' from CAPLUS. The transcript text includes copyright information for the American Chemical Society, a notice about the CAS Lexicon, and file details such as 'FILE COVERS 1907 - 1 May 2019 VOL 170 ISS 20'. At the bottom of the transcript area, there is a command prompt with the text 'enter command'. To the right of the transcript area is a 'History' panel with tabs for 'CAS Lexicon' and 'Databases'. Below the transcript area, there is a 'Submit' button and a 'Draw' button, which is highlighted with an orange box. To the right of the 'Draw' button is a 'Scripts' button.

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

The screenshot displays the STNext Structure Editor interface. The window title is "Structure Editor". At the top right, there is a "Maximize view" checkbox labeled "1" which is currently turned "OFF". Below the title bar is a toolbar with various icons, including a question mark icon labeled "3" and a search box labeled "1" containing the text "Enter a CAS RN, SMILES or InChI". The main workspace is a large white area with a yellow banner at the top that says "Draw or change atoms or bonds." and "Shortcut Keys". On the left side, there is a vertical toolbar with icons for drawing atoms (C, Et, X, R, Fn), rings, and other structures. At the bottom of the workspace, there is a horizontal toolbar with element symbols (C, H, O, S, N, P, Cl, Br, F, I, Si, D, T) and other drawing tools. On the right side, there is a panel titled "Attribute Values" labeled "2", which lists various attributes such as Bond Type, Bond Value, Node Type, Generic Definition, Match Level, Element Count Level, Ring Isolation, Stereochemistry, and Other Node Attributes. At the bottom of the window, there are buttons for "Upload", "Save As", and "Cancel", and a "View Previous Structures..." link.

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.

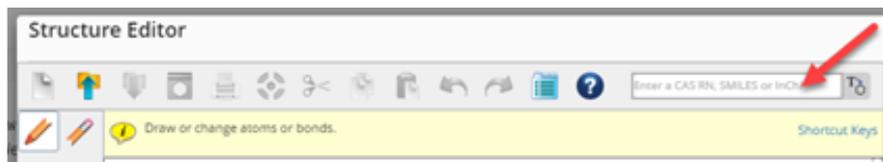
The screenshot displays the Structure Editor window. At the top, there is a title bar with 'Structure Editor' and a 'Maximize view' button set to 'OFF'. Below the title bar is a toolbar with various icons, including a highlighted 'Import' button (a blue square with a white arrow pointing down). A search bar contains the text 'Enter a CAS RN, SMILES or InChI'. The main workspace shows a chemical structure of a fused ring system with a carbonyl group. To the left is a vertical toolbar with icons for drawing atoms and bonds, and a list of elements (C, Et, X, R, Fn). Below the workspace is a text input field containing 'C' and a periodic table with highlighted elements. On the right side, there is a 'Attribute Values' panel with various settings for Bond Type, Bond Value, Node Type, Generic Definition, Match Level, Ring Isolation, Stereochemistry, and Other Node Attributes. At the bottom, there are 'Upload', 'Save As', and 'Cancel' buttons, and a 'View Previous Structures...' link.

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

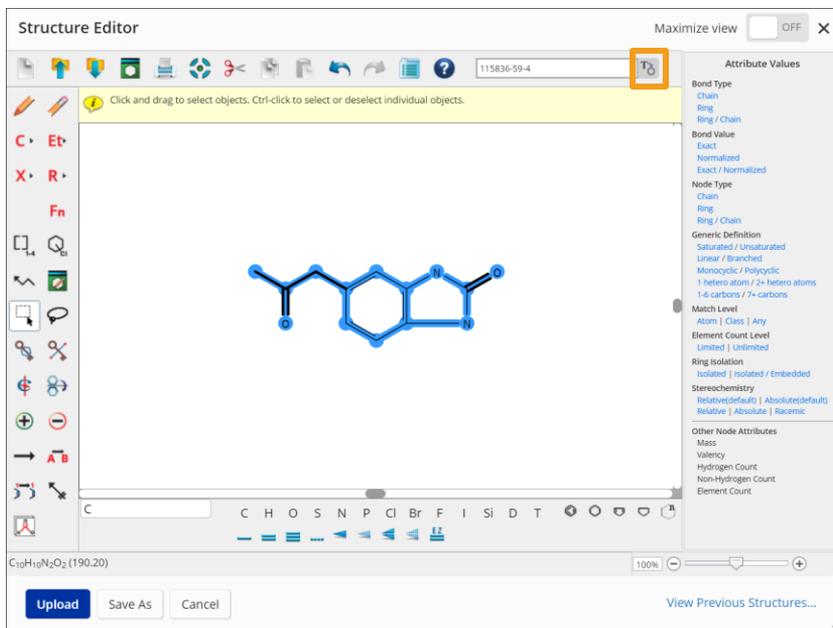


Text to Structure

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.



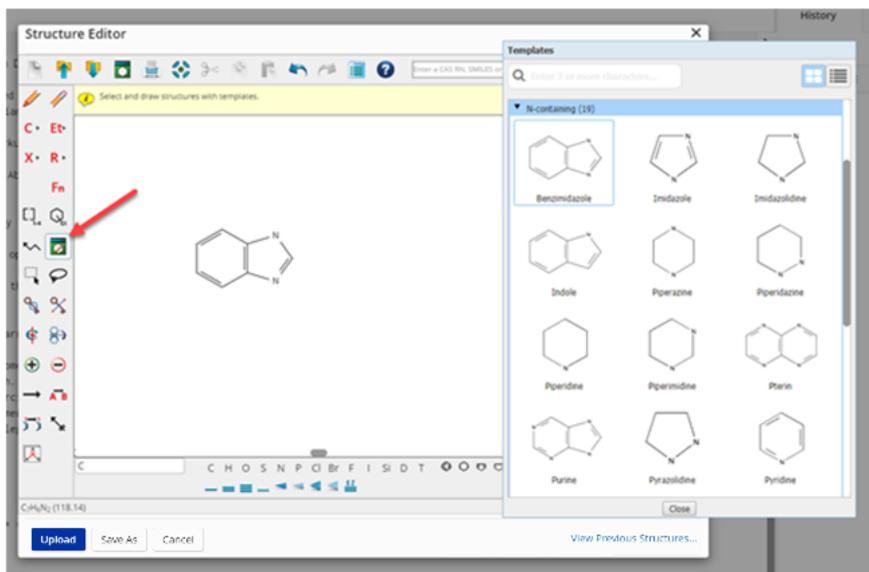
You can edit the structure as desired.

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

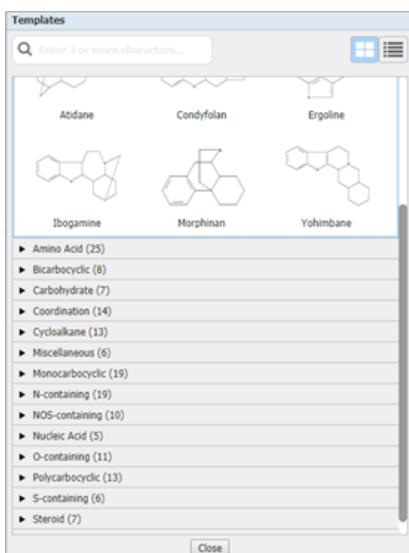
Templates

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

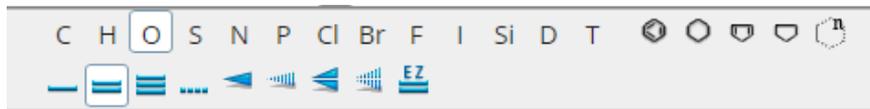
Carbon chains can be created or attached to a structure in several ways. One quick option is to use the Chain tool. Here we are attaching a three carbon chain to a ring system:

The screenshot shows the 'Structure Editor - 2019_0020_Structure' window. The main canvas displays a chemical structure of a benzimidazole ring system with a three-carbon chain attached to one of the ring carbons. A red box highlights the 'Chain' tool icon in the left-hand toolbar, with a red arrow pointing to it. A text box above the arrow reads: 'Use the Chain tool to quickly create a carbon chain of any length'. The right-hand panel shows 'Attribute Values' for the selected tool, including 'Bond Type' (Chain), 'Bond Value' (Exact), and 'Node Type' (Chain). The bottom status bar shows the molecular formula $C_{10}H_{10}N_2$ (162.23) and a zoom level of 100%.

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.

Structure Editor - 2019_0020_Structure

Draw or change atoms or bonds. Shortcut Keys

Attribute Values

- Bond Type
 - Chain
 - Ring / Chain
- Bond Value
 - Exact
 - Normalized
 - Exact / Normalized
- Node Type
 - Chain
 - Ring / Chain
- Generic Definition
 - Saturated / Unsaturated
 - Linear / Branched
 - Monocyclic / Polycyclic
 - 1 hetero atom / 2+ hetero atoms
 - 1-6 carbons / 7+ carbons
- Match Level
 - Atom
 - Class
 - Any
- Element Count Level
 - Limited
 - Unlimited
- Other Node Attributes
 - Mass
 - Valency
 - Hydrogen Count
 - Non-Hydrogen Count
 - Element Count

C10H10N2O2 (190.20) 100% View Previous Structures...

Upload Save As Cancel

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

The screenshot shows the Structure Editor interface. The top toolbar contains various drawing tools. The side toolbar on the left has a button labeled 'C' with a red dot, which is highlighted with a red box. Below it are buttons for 'Et', 'X', 'R', and 'Fn'. The main drawing canvas is empty. An 'Atoms' palette is open, displaying a periodic table of elements. The elements are color-coded: H (blue), He (light blue), Li (orange), Be (yellow), B (green), C (light green), N (purple), O (pink), F (light purple), Ne (light blue), Na (orange), Mg (yellow), Al (green), Si (light green), P (purple), S (pink), Cl (light purple), Ar (light blue), K (orange), Ca (yellow), Sc (green), Ti (light green), V (purple), Cr (pink), Mn (light purple), Fe (light blue), Co (orange), Ni (yellow), Cu (green), Zn (light green), Ga (purple), Ge (pink), As (light purple), Se (light blue), Br (orange), Kr (yellow), Rb (orange), Sr (yellow), Y (green), Zr (light green), Nb (purple), Mo (pink), Tc (light purple), Ru (light blue), Rh (orange), Pd (yellow), Ag (green), Cd (light green), In (purple), Sn (pink), Sb (light purple), Te (light blue), I (orange), Xe (yellow), Cs (orange), Ba (yellow), Hf (green), Ta (light green), W (purple), Re (pink), Os (light purple), Ir (light blue), Pt (orange), Au (yellow), Hg (green), Tl (light green), Pb (purple), Bi (pink), Po (light purple), At (light blue), Rn (orange), Fr (orange), Ra (yellow), and ** (green). Below the main table are sections for Lanthanides (La to Lu) and Actinides (Ac to Lr). The 'Atoms' palette has a 'Close' button at the bottom.

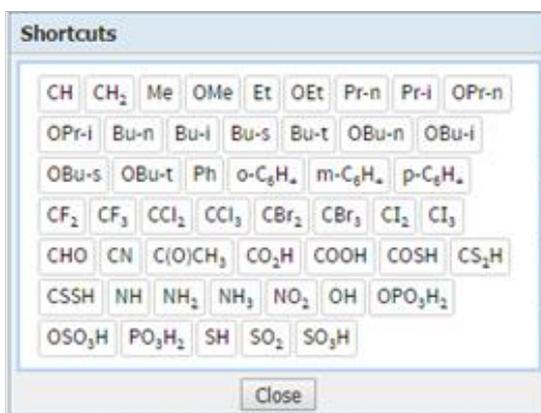
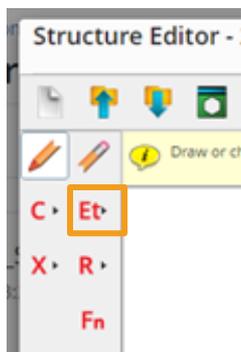
A panel of the periodic table will allow you to select any atom. Then click on the drawing canvas to place the atom.

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.

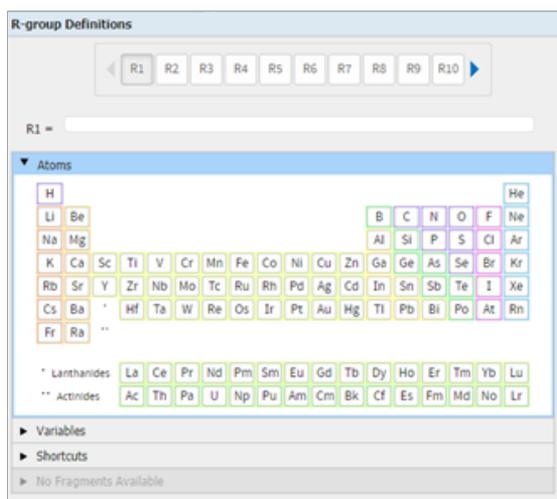
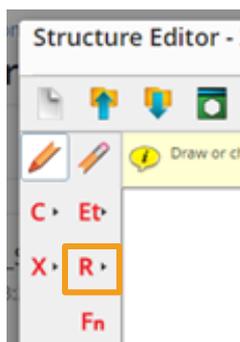
1. Click the **Shortcuts** button to display a list of common functional groups.
2. Select a functional group.



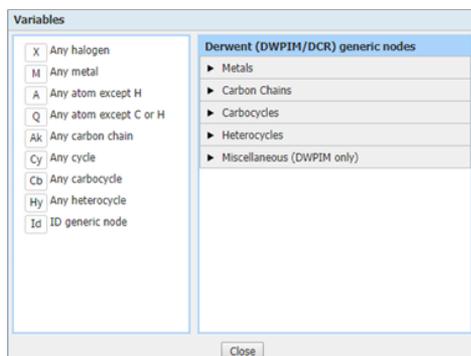
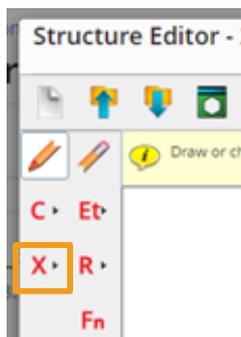
3. Hover over the drawing where you want to place the functional group.
4. Click on the drawing canvas to place the group.

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 screenshot shows the 'Structure Editor - 2019_0020_Structure' window. On the left is a toolbar with various drawing tools. The main canvas displays a chemical structure of a benzimidazole derivative with a propyl group. A red arrow points from a callout box to the Attribute Values panel on the right. The callout box contains the text: 'Hover over a bond or node to see the attributes highlighted in yellow in the Attribute pane at right'. The Attribute Values panel lists various properties such as Bond Type, Bond Value, Node Type, Generic Definition, Match Level, Element Count Level, and Other Node Attributes. Several values in this panel are highlighted in yellow.

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.

This screenshot shows the same chemical structure as the previous image, but with a 'Node Attributes' dialog box open. The dialog box has a list of attributes: Hydrogen Count, Markush Attributes, Mass, Node Type, Non-Hydrogen Count, and Valency. The 'Hydrogen Count' attribute is selected, and its value is set to 'Any'. There are also radio buttons for 'Exact' and 'Minimum', and a range input field showing '0 to 99'. The dialog box has 'Apply', 'OK', and 'Cancel' buttons.

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.

The screenshot shows the 'Structures' page interface. At the top, there are buttons for 'Import Biosequence' and 'Import Structure'. Below this is a list of three structures:

- 2 H-Benzimidazole** (May 1, 2019, 12:41pm): Includes an 'Edit structure name' button and an 'Edit structure' button.
- 2019_0020_Structure** (May 1, 2019, 12:03pm): Includes an 'Edit' button, a 'Delete structure' button, and a dropdown menu with 'Move' and 'Delete' options.
- 2019_0019_Structure** (Apr 16, 2019, 9:24am): Includes an 'Edit' button and an 'Upload structure' button.

The screenshot shows the 'Transcript ON' interface for file '2019_0183_Transcript'. It displays the upload progress for the structure '2 H-Benzimidazole' and shows two chemical structure drawings. Below the drawings, the following attributes are listed:

```
Node Attributes
Ring Nodes : 1 2 3 4 5 6 7 8 9
Chain Nodes : 10 11 12 13 14
Bond Attributes
Ring Bonds : 1-2 2-6 2-7 3-4 3-6 4-5 5-1 6-9 7-8 9-8
Chain Bonds : 5-10 10-11 11-12 13-11 14-8
Exact Bonds : 5-10 10-11 11-12
Normalized Bonds : 1-2 2-6 3-4 3-6 4-5 5-1
Exact/Normalized Bonds : 2-7 6-9 7-8 9-8 13-11 14-8
Markush Attributes
Match Level (ATOM) : 1 2 3 4 5 6 7 8 9
Match Level (CLASS) : 10 11 12 13 14
Element Count Level (LIMITED) : 1 2 3 4 5 6 7 8 9 10 11 12 13 14
```

At the bottom, a status message reads: 'L2 STRUCTURE UPLOADED'.

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

Search with Structure

After you have uploaded the structure into your STNnext 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 12 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

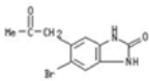
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

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...

CAS

help@cas.org

Support & Training:

www.cas.org/support

FIZ Karlsruhe

helpdesk@fiz-karlsruhe.de

Support & Training:

www.stn-international.de