



## How to get the best from a Structure Search

I know the structure of Codeine, how can I find what information is available?

### STEP 1

Select the **Search** option from the top toolbar and choose **Structure Search** from the side navigation menu. Click on the structure picture to activate the structure editor.

### STEP 2

There are three ways to enter a chemical structure:

1. From a chemical name you can auto-generate a structure by typing in the name and selecting **Convert**.

The screenshot displays the ChemSpider web interface. At the top, a navigation bar contains 'About', 'Search', 'Browse', 'Services', and 'Help'. Below this, the 'Search' section is active, with 'Simple', 'Structure', and 'Advanced' tabs. The 'Structure' tab is selected, showing a chemical structure of codeine. A dialog box titled 'Convert from String (Name, SMILES, InChI, etc)' is open, with 'codeine' entered in the input field and the 'Convert' button highlighted. The dialog box also has 'Accept' and 'Cancel' buttons at the bottom. In the background, the 'Search Options' section shows 'Exact Match' selected.

Click **Accept** to accept the structure or **Draw** or **Edit** to change features of the structure. For example you might want to change the pre-defined stereochemistry of the bonds.

2. Alternatively, you can draw the structure in your favourite drawing package and save as a mol, sdf, cdx or skc file to your desktop. Upload the file to ChemSpider using the **Load** button. This is also the way to use any existing structure files you have in a ChemSpider search.

There are also options to Load a structure from a JPEG or GIF image, which will run an OCR process and let you correct any errors before accepting the structure.

3. You can also draw the structure using one of the two Java-based structure drawing applets available in ChemSpider: ACD/Labs SDA and Symyx JDraw. Use the **Draw** or **Edit** to select and activate the applets.

### STEP 3

Once the structure is submitted, CLICK on search and display the record view.



1 hit(s) found in 0.05 seconds  
Search term: SEARCH\_BY\_MOLECULE Exact AND SingleComponent AND NonIsotopic

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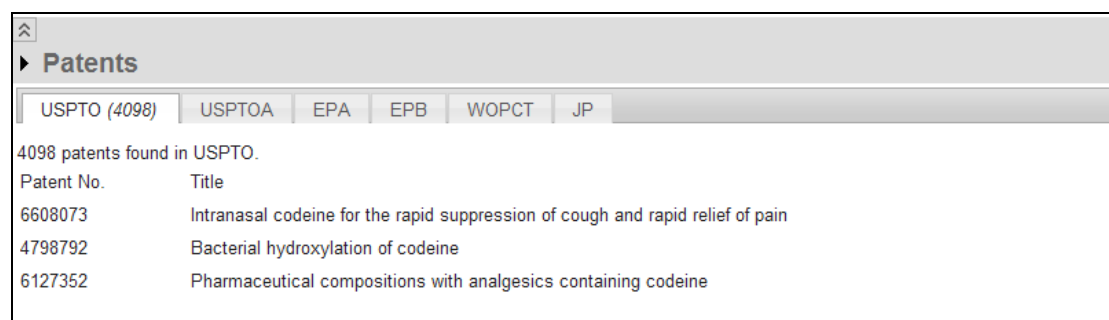
**(5 $\alpha$ ,6 $\alpha$ )-3-methoxy-17-methyl-7,8-didehydro-4,5-epoxymorphinan-6-ol**

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Patent information can be available for many substances in ChemSpider. Click on the title to link to the full record in SureChem.



**Patents**

USPTO (4098) USPTOA EPA EPB WOPCT JP

4098 patents found in USPTO.

Patent No.	Title
6608073	Intranasal codeine for the rapid suppression of cough and rapid relief of pain
4798792	Bacterial hydroxylation of codeine
6127352	Pharmaceutical compositions with analgesics containing codeine

Other links can take you to literature references, RSC journals & databases, property data and spectra.

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The synthesis of some 6,7-annulated codeines. Maxson Liu, Malcolm Sainsbury, Neil Carter, *J. Chem. Soc., Perkin Trans. 1*, 1999, 241

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An efficient preparation of isocodeine from codeine. G. W. Kirby, S. R. Massey, *J. Chem. Soc. C*, 1971, 3047

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Biosynthesis of unnatural morphine derivatives in *Papaver somniferum*. G. W. Kirby, S. R. Massey, P. Steinreich, *J. Chem. Soc., Perkin Trans. 1*, 1972, 1642

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Electrogenerated chemiluminescent determination of codeine and related alkaloids and pharmaceuticals with tris(2,2'-bipyridine)ruthenium (II). Gillian M. Greenway, Andrew W. Knight, Paul J. Knight, *Analyst*, 1995, **120**, 2549

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Chemiluminescence determination of codeine by permanganate oxidation. Tony J. Christie, Rosalind H. Hanway, David A. Paulls, Alan Townshend, *Anal. Proc.*, 1995, **32**, 91

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Mass Spectrometry Bulletin (61) Laboratory Hazards Bulletin Methods in Organic Synthesis Catalysts & Catalysed Reactions  
 Natural Product Updates Analytical Abstracts (1039)

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Determination of codeine methyl ether in commercial codeine.

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Analysis and stability of codeine phosphate. I. Detection and determination of codeine in the presence of decomposition products.

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High-performance liquid-chromatographic assay of codeine in acetaminophen [paracetamol] with codeine dosage forms.