

**Chemistry Add-in for**

**Microsoft Word**

**User Guide**

**Version 3.0**

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# Introduction

The Chemistry add-in for Microsoft Word

# Converting documents from the previous version of the Chemistry Add-in for Microsoft Word

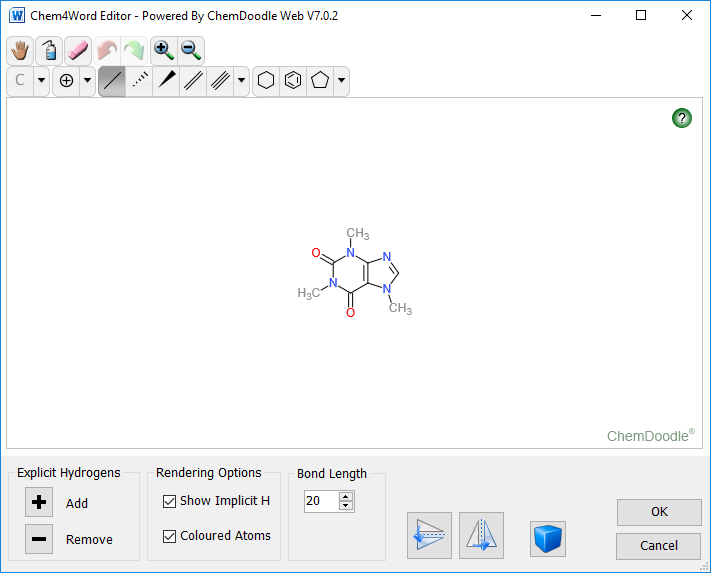
Documents created with the previous version of the add-in will be automatically converted to the new format. Once this conversion has completed, the old version of the add-in will not function correctly.

# How to add a chemical structure to a document

Chemical structures can be added to a Microsoft Word document in many ways. Structures can be drawn using the Chem4Word Editor tool. Structures can also be added from PubChem[[1]](#endnote-1) and ChEBI (Chemical Entities of Biological Interest[[2]](#endnote-2),[[3]](#endnote-3)) searches as well as using the name-to-structure tool, OPSIN (Open Parser for Systematic IUPAC nomenclature[[4]](#endnote-4),[[5]](#endnote-5))

## Draw a structure

To draw a structure in a document, click the Draw button on the Chemistry Ribbon. This will activate the Chem4Word Editor tool.



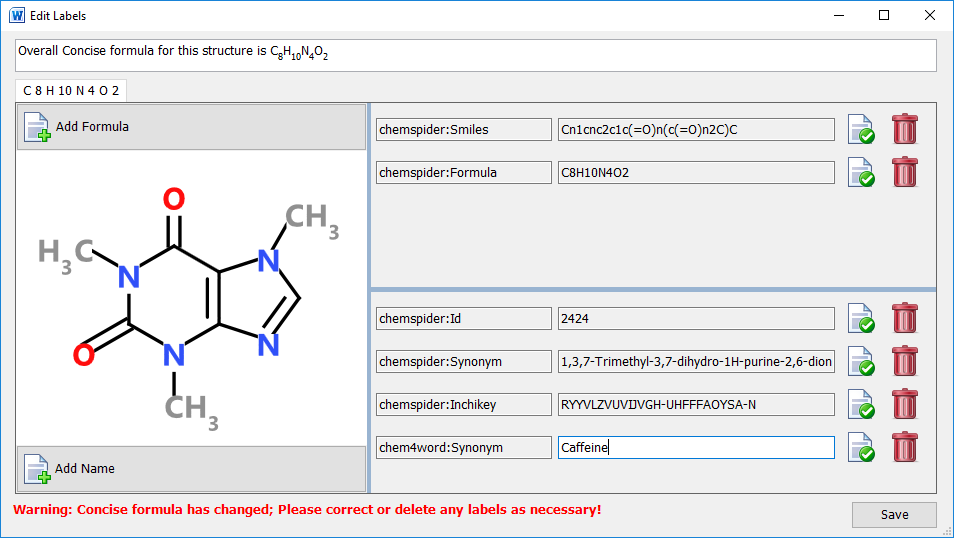
Use the bonds, rings and atoms tools to create a structure; at present, radicals and lone pairs are not supported in Chem4Word.

It is possible to change the default bond length in the drawing tool. Explicit hydrogen atoms can be added or removed from a structure by clicking the + and – buttons in this tool. There are also buttons to flip the structure horizontally or vertically.

|  |  |
| --- | --- |
|  | With the drawing tool, it is also possible to draw multiple structures in the same window. Clicking this button changes the drawing mode to multiple molecules. |

The final option in the drawing tool allows the drawing of explicit atoms with specific colours. Checking the “Coloured atoms” box will show atoms with coloured labels; without this option, all bonds and atoms will be drawn in black.

On clicking the OK button, the add-in runs a ChemSpider search to see if this chemistry is known. Labels such as names and synonyms will be returned. At this point, you have the option to add/edit/delete labels as you may need.



The image above shows the information retrieved when caffeine is drawn using the Chem4Word Editor. In addition to the retrieved information, an additional synonym, Caffeine, has been added.

## Import a structure from a file

The Chemistry Add-in for Microsoft Word supports importing chemistry from three file formats, CML, MolFile and SDFile.

The Import button allows you to browse to a folder containing supported file formats, to select a file and then import that file as a chemical structure into the current document. The structure will be displayed exactly as it was stored in the imported file. Further editing can be done, once the structure is added to the document

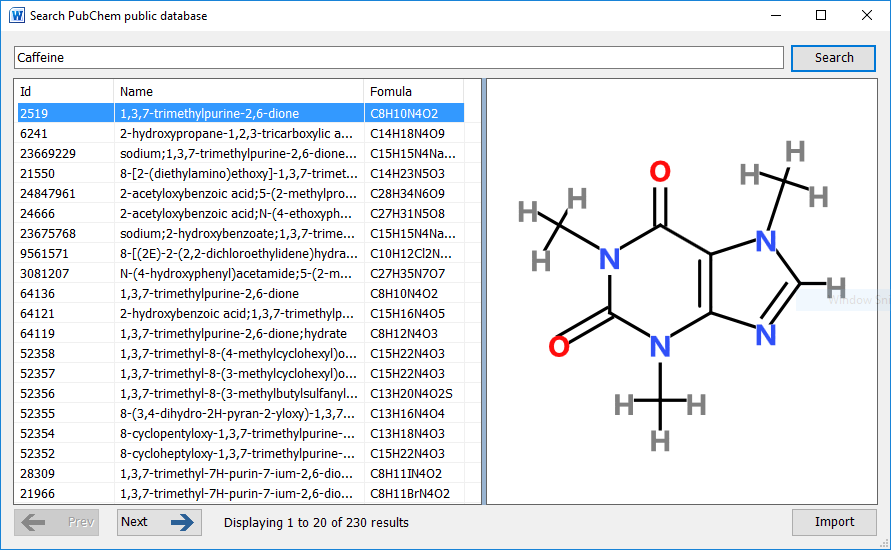
## Add a structure from a web-search

There are three options for importing a structure from web searches.

|  |  |
| --- | --- |
| PubChem Logo | PubChem is a public repository of chemical structures and biological data maintained by National Center for Biotechnology Information (NCBI). |
| ChEBI logo ChEBI | Chemical Entities of Biological Interest (ChEBI) is a freely available dictionary of molecular entities focused on ‘small’ chemical compounds maintained by the European Molecular Biology Laboratory (EMBL). |
| University of CambridgeOPSIN | OPSIN is a tool developed at the University of Cambridge that converts chemical names into chemical structures |

## PubChem search

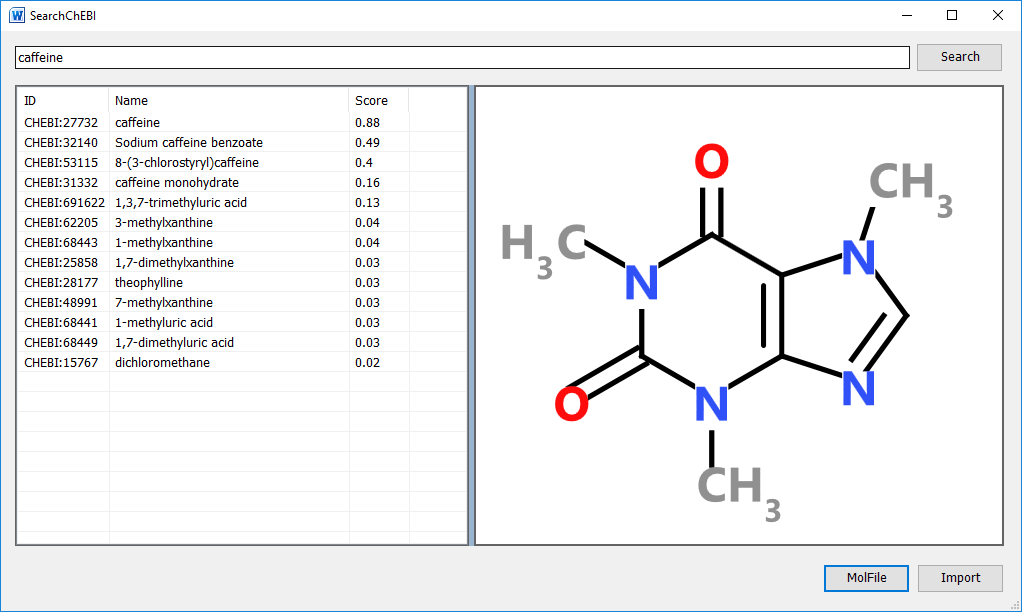
The PubChem search allows you to search by name or formula for structures in the PubChem database. Multiple records can be retrieved by such searches and are sorted by relevance.



Selecting an entry in the returned results displays a structure as stored in the PubChem database. You can navigate forwards and backwards through all of the results and the selected result can be added to the document at the current position by clicking the Import button.

## ChEBI Search

The ChEBI search allows you to search by name for structures in the ChEBI database. Fewer results are returned by this search tool than the PubChem search as a scoring algorithm limits the number of possible structures returned.



It is possible that there are entries in this database where no chemical structure is available. A message indicating this will be shown at the bottom of this window.

The MolFile button can be used to show you how this structure is stored in the ChEBI database.

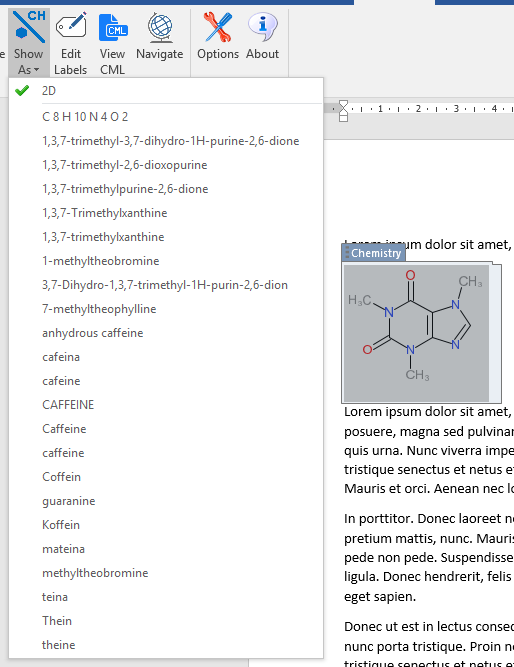
Clicking the Import button adds the displayed structure to the current document.

# How to edit a chemical structure

When you select a chemistry object in a document, you can edit the contents by clicking the edit button. Double-clicking a chemistry object also allows you to edit a structure.

If the chemistry object is changed by your edits, the add-in automatically runs a ChemSpider search to see if the new structure is known. You will be given the opportunity to add/change/delete labels associated with the new structure.

# Display options for Chemistry

The Chemistry Add-in for Microsoft Word allows chemistry to be represented in multiple formats. For structures imported from files and web sources, chemistry objects may have associated names and synonyms as well as formulae.

When you draw a structure in a document, the add-in searched ChemSpider to see if the structure is known, and any known names and synonyms are retrieved.

You can also add your own synonyms and formulae to any structure using the Edit Labels button.

The example on the right shows all of the depiction options for caffeine that available when this chemistry object is inserted from ChEBI. The currently displayed chemistry object can be changed to show any one of these alternative depictions.

By adding other chemistry objects to the document that are linked to another chemistry object will allow the editing of any one of them to be reflected in an automatic change to the automatically created formula label and those imported from ChemSpider. The Edit Labels button also allows you to delete labels and create your own labels.

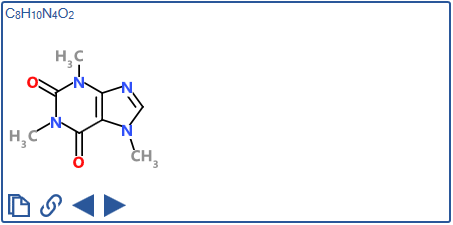
# The Library

The library is a store of re-usable chemical structures.

NEED TO FINISH THIS WHEN WE HAVE MORE STRUCTURES IN THE LIBRARY

# The Navigator

The Navigator shows all the chemical structures in the document and allows you to find the location of chemistry objects throughout the document.

The Navigator will contain one window for each unique structure in the current document. Each window in the Navigator shows the chemical structure and formula of each molecule. At the bottom of each window there are four buttons that are used to add structures to the document by either creating a linked copy or pasting a new copy of an existing structure at the current position in the document.

The Navigator buttons allow you to find individual and linked structures in the document by moving backwards or forwards through the current document.

|  |  |
| --- | --- |
|  | Duplicate the structure and add it to the document at the currently selected position. |
|  | Add a linked copy of the structure to the document at the currently selected position. |
|  | Move to the previous linked structure in the document. |
|  | Move to the next linked structure in the document. |

# Exporting chemistry files

1. Details about the PubChem search tool is available at <https://pubchem.ncbi.nlm.nih.gov/search/>. [↑](#endnote-ref-1)
2. Further information about ChEBI searching is can be found here <https://www.ebi.ac.uk/chebi/>. [↑](#endnote-ref-2)
3. Hastings, J., de Matos, P., Dekker, A., Ennis, M., Harsha, B., Kale, N., Muthukrishnan, V., Owen, G., Turner, S., Williams, M., and Steinbeck, C. (2013) The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. [Nucleic Acids Res.](http://dx.doi.org/10.1093/nar/gks1146) [↑](#endnote-ref-3)
4. More information about OPSIN available from <http://opsin.ch.cam.ac.uk/>. [↑](#endnote-ref-4)
5. [Daniel M. Lowe](http://pubs.acs.org/author/Lowe%2C+Daniel+M), [Peter T. Corbett](http://pubs.acs.org/author/Corbett%2C+Peter+T), [Peter Murray-Rust](http://pubs.acs.org/author/Murray-Rust%2C+Peter), and [Robert C. Glen](http://pubs.acs.org/author/Glen%2C+Robert+C), J. Chem. Inf. Model., 2011, 51 (3), pp 739–753 [↑](#endnote-ref-5)