



## Uploading Spectra into ChemSpider

In order to upload spectra to [ChemSpider](#) and associate them to a chemical compound of interest you need to be a registered user and logged in to the website. You then need to navigate to the appropriate record by conducting either a structure or chemical name search. When you have located the structure of interest then click on **Add Spectrum** to deposit spectra.

If you wish to deposit spectra for a compound which is new to the database then you need to deposit the structure onto [ChemSpider](#) first. See “Quick Card – How do I deposit a single structure” for details of the steps involved.

The screenshot shows the ChemSpider interface with a navigation bar (About, Search, Browse, Services, Help) and a record for 8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine. The record includes a chemical structure, the name, the ChemSpider ID (2034), the molecular formula (C<sub>17</sub>H<sub>13</sub>ClN<sub>4</sub>), and various interactive options like 'Add Spectrum', 'Image', 'CIF', 'Identifier', 'Description', 'Data source', 'Publication', 'DOI', 'PubMed ID', and 'URL'.

Various types of spectra are supported. These include H1 NMR, C13 NMR, IR and Mass Spectra.

Please enter spectrum information here

Spectrum Type:

Spectrum File:  Browse...

Associated Hyperlink:

Comments:

Please check this box if you agree with the policies of Open Data. Please read here if you want to know more about Open Data policies.

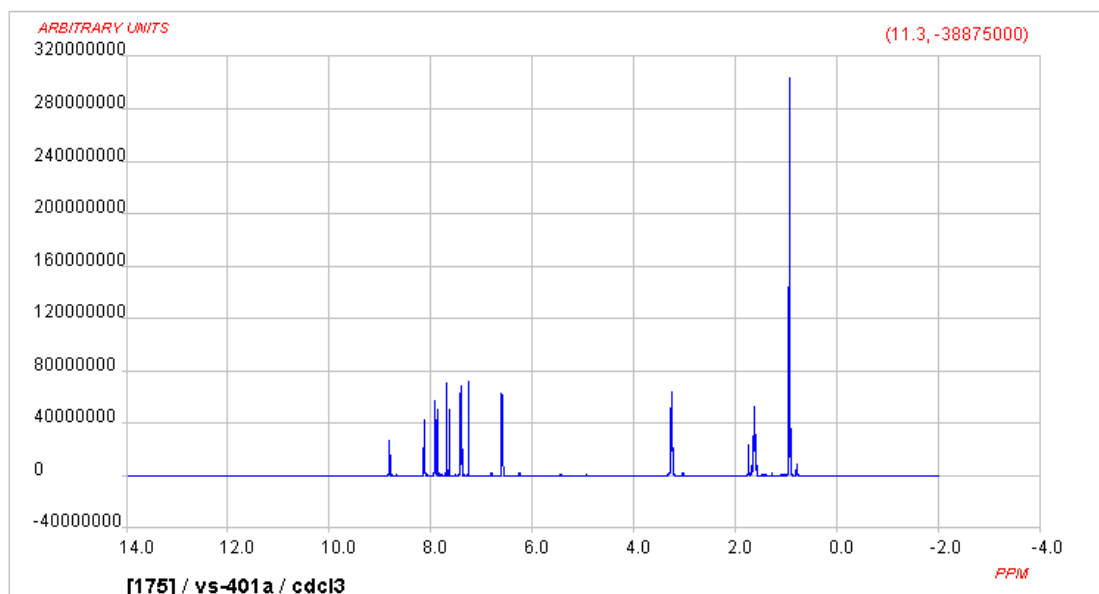
2D NMR 1H-13C Direct correlation  
 2D NMR 1H-13C Long-range correlation  
 2D NMR 1H-1H COSY  
 2D NMR 1H-1H Long range correlation  
 2D NMR 1H-1H NOESY/ROESY  
 APCI+ Mass Spectrum  
 APCI- Mass Spectrum  
 APPI+ Mass Spectrum  
 APPI- Mass Spectrum  
 Chemical Ionization +ve  
 Chemical Ionization -ve  
 CNMR  
 Electron Impact  
 ESI+ Mass Spectrum  
 ESI- Mass Spectrum  
 FNMR  
 HNMR  
 Infrared  
 MALDI+ Mass Spectrum  
 MALDI- Mass Spectrum

[Privacy](#)   [Advertising](#)   [Help](#)

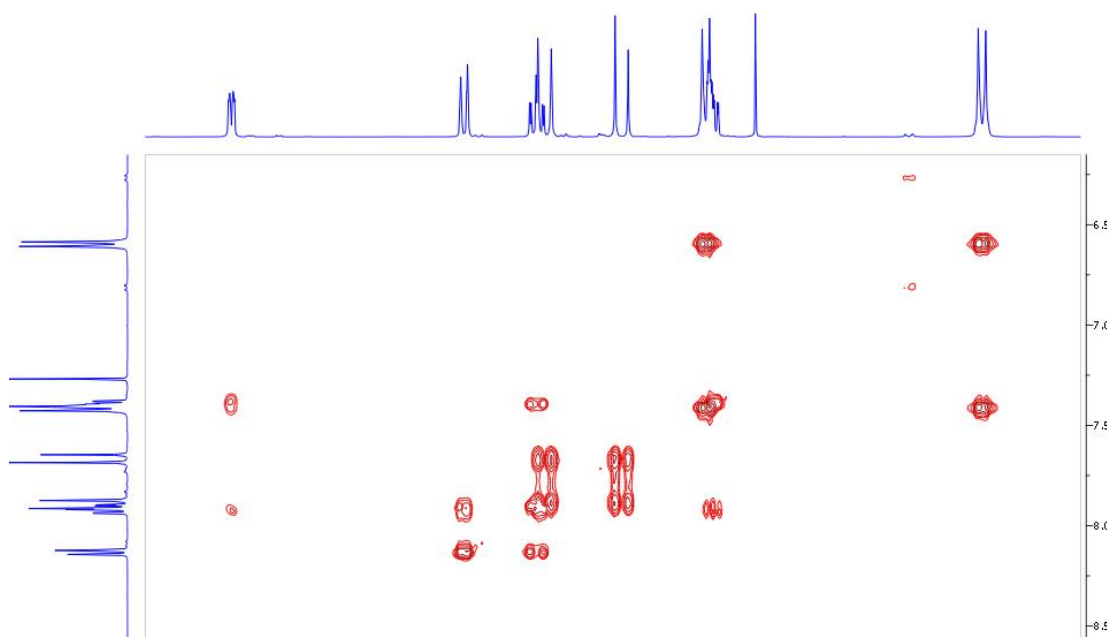
Browse your computer for the location of your files which MUST be in JCAMP format (.DX or .JDX file extensions) for the majority of spectra. 2D NMR spectra can only be supported as image files and need to be uploaded as JPEG images or web-based image formats such as PNG.

Examples of the different types of spectra which have been uploaded and can be viewed in the spectrum viewing applet are shown below.

For ChemSpider ID 24528095 this is the H1 NMR spectrum



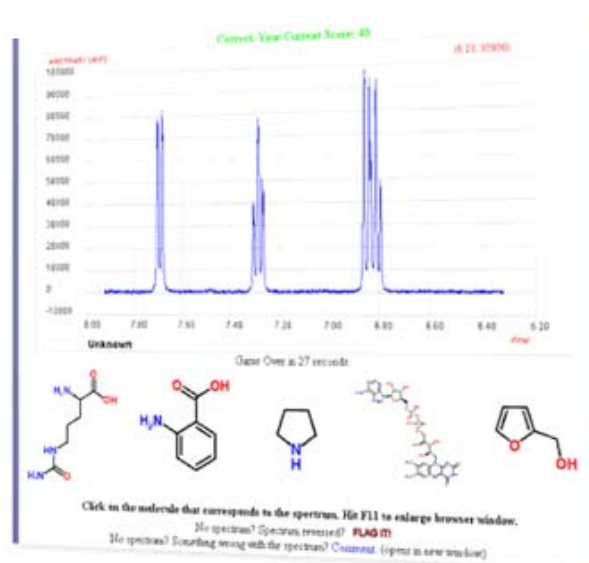
For ChemSpider ID 24528095 this is the 2D1H1HCOSY



If you would like to associate the spectrum with a hyperlink back to an associated webpage insert it in the hyperlink field. In the comments section add any information you feel would be of interest to the viewer of the spectrum. For example, this could include details experimental parameters, colour of solution, liquid or solid state, or details of the sample.

The [ChemSpider](#) database grows as a result of these depositions. In addition, the spectra that you deposit will also contribute to the growing number of spectra in the online spectral game ([www.spectralgame.com](http://www.spectralgame.com)).

# SPECTRAL GAME



The game, which can be used as a teaching aid, is played using a Web browser interface and the spectra from [ChemSpider](#) are displayed in an interactive page.

Players of the game provide both active and passive feedback regarding the quality of the spectral data resulting in crowd sourced curation and validation.

More information about the game can be found in the publication - The Spectral Game: leveraging Open Data and crowdsourcing for education

Journal of Cheminformatics 2009, 1:9doi:10.1186/1758-2946-1-9.

We encourage you to try this game for yourself.