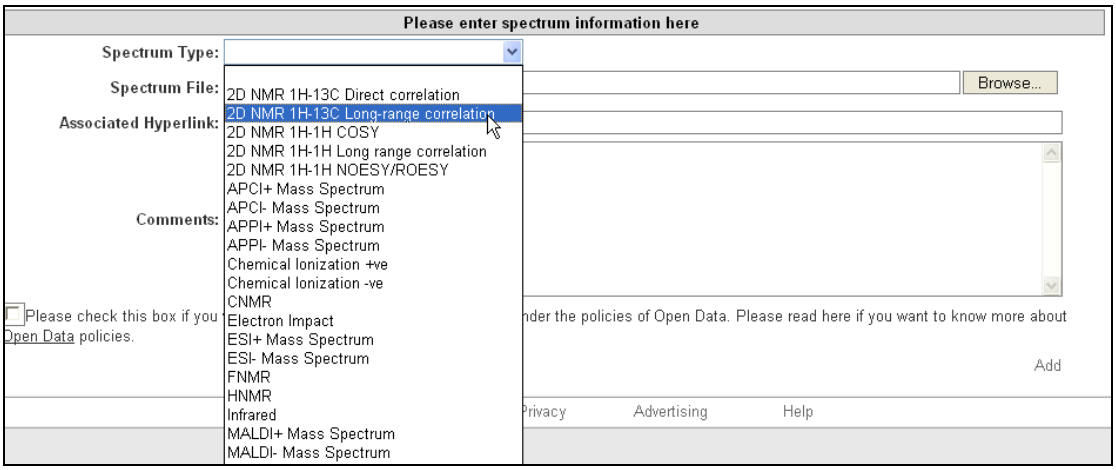
Uploading Spectra into ChemSpider

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.

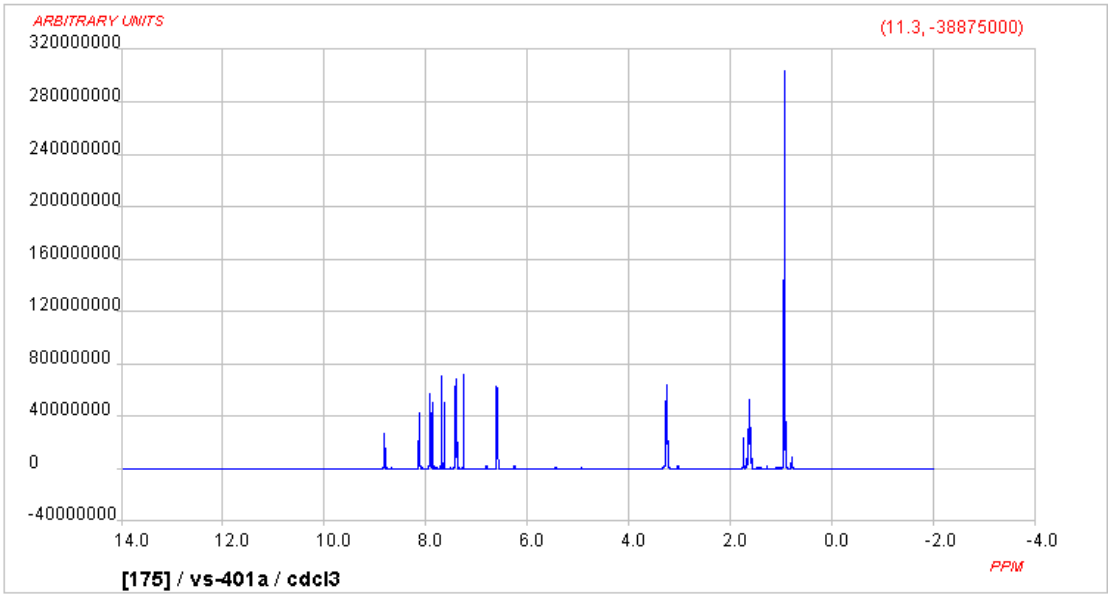
Various types of spectra are supported. These include H1 NMR, C13 NMR, IR and Mass Spectra.



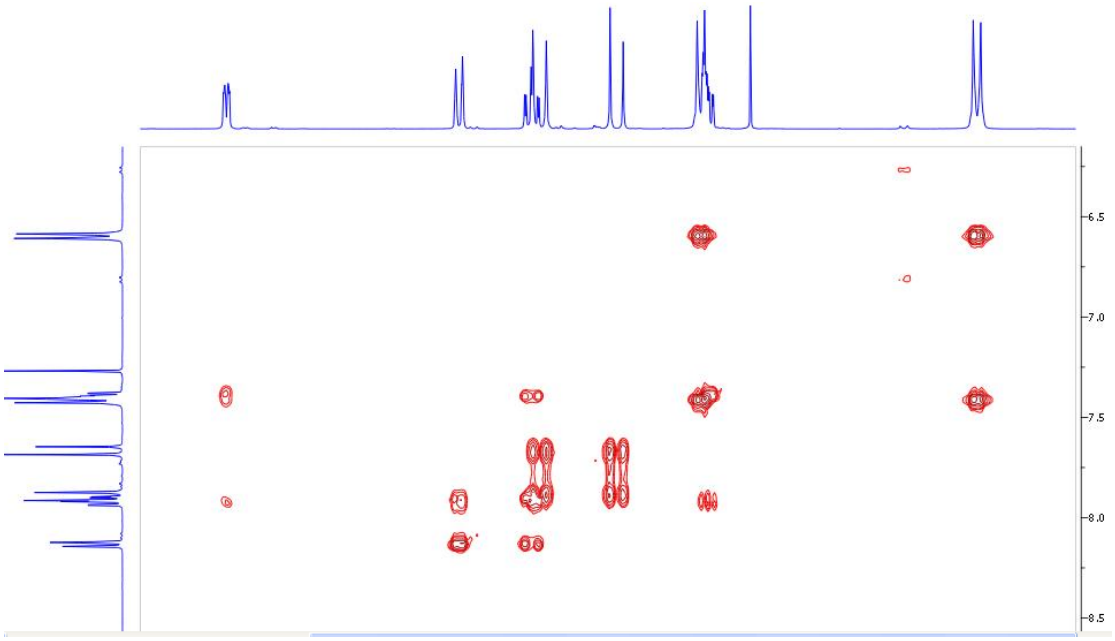
Browse your computer for the location of your files which MUST be in JCAMP format (.DX or . JDX file extensions) for the majority of spectra. 2D NMR spectra can only be supported as image files and need to be uploaded as JPEG images or web-based image formats such as PNG.

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

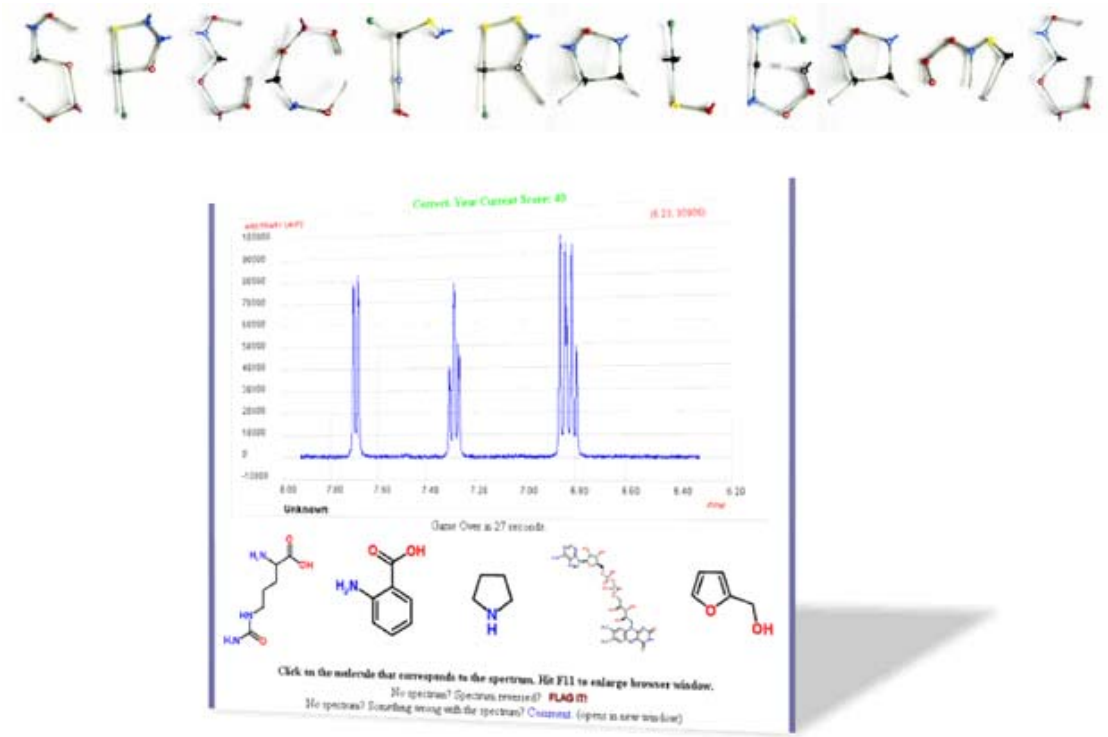


For ChemSpider ID 24528095 this is the 2D1H1HCOSY



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).



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.