

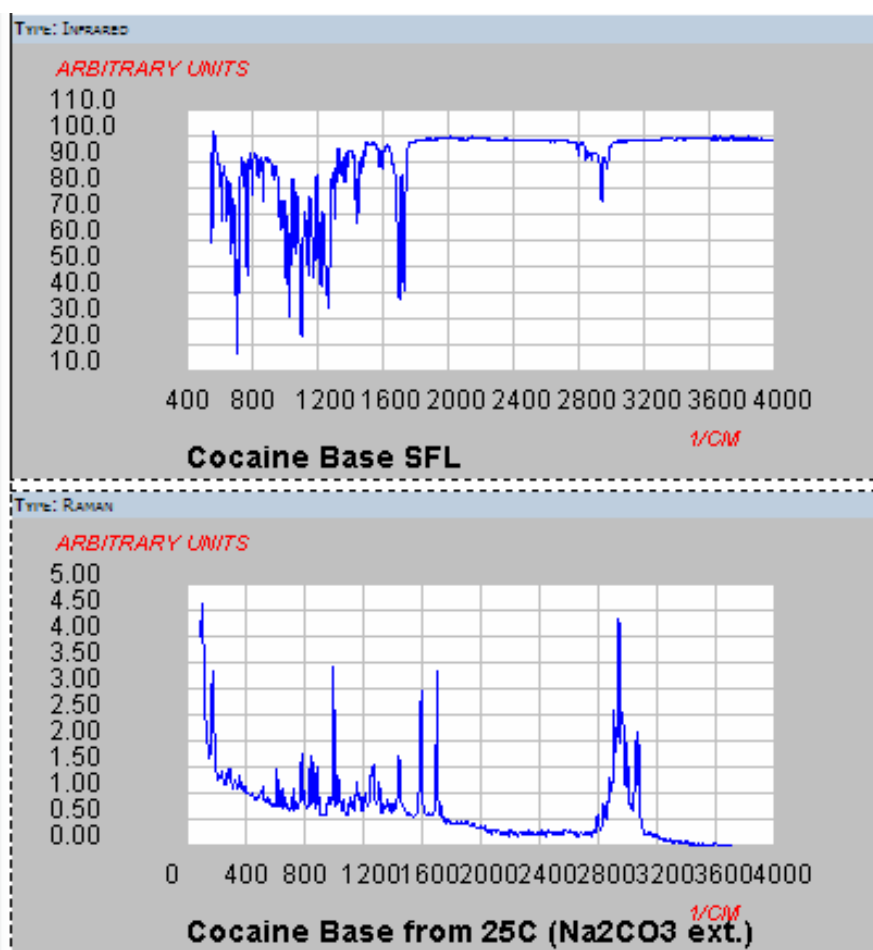
Uploading Spectra Onto ChemSpider

Uploading Spectra to Allow Public Access Online

Antony Williams

Introduction

ChemSpider initially went online with the ability to display structures and associated alphanumeric text information (properties and links to data sources primarily). Our integration of an Open Source spectral viewing component, JSpecView, has allowed us to provide viewing of integrated analytical data on the system as a Proof of Concept (<http://www.chemspider.com/blog/?p=93>). JSpecView is developed by Bob Lancashire and his team at the University of West Indies and, while still in its early development stages, is already a valuable tool for the viewing of multiple forms of spectral data. Already ChemSpider has online NMR, MS, IR and Raman data for viewing. An example can be found at <http://www.chemspider.com/RecordView.aspx?id=5557> with two of the spectra displayed below.



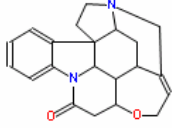


Uploading Spectra

In order to upload spectra to the ChemSpider system you need to be a registered user of the ChemSpider system as described elsewhere. As a registered user should you wish to associate and upload a spectrum to ChemSpider it is first necessary to navigate to the appropriate record by searching on the structure (via text or structure). When that record is located, and assuming you are already logged in, you will see Add Spectrum displayed as shown below and highlighted in the image with a callout box.

[Help](#) [Curate Data](#) [Add Spectrum](#)

INHERENT PROPERTIES, IDENTIFIERS AND REFERENCES

 load save zoom jmol	ChemSpider ID:	5113
	Empirical Formula:	C ₂₁ H ₂₂ N ₂ O ₂
	Molecular Weight:	334.4116
	Nominal Mass:	334 Da
	Average Mass:	334.4116 Da
	Monoisotopic Mass:	334.168128 Da

**Add Spectrum
Hyperlink**

When the hyperlink is selected then the following inputs will be shown above the record details.

[Help](#) [Curate Data](#)

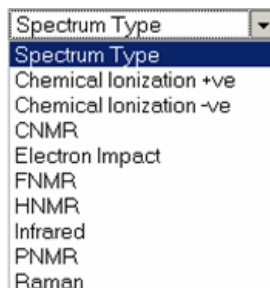
Spectrum Type:

Spectrum File:

Associated Hyperlink:

Comments:

Uploading spectra is easy. Simply select the spectrum type from the drop down list. This list is presently limited as shown below:



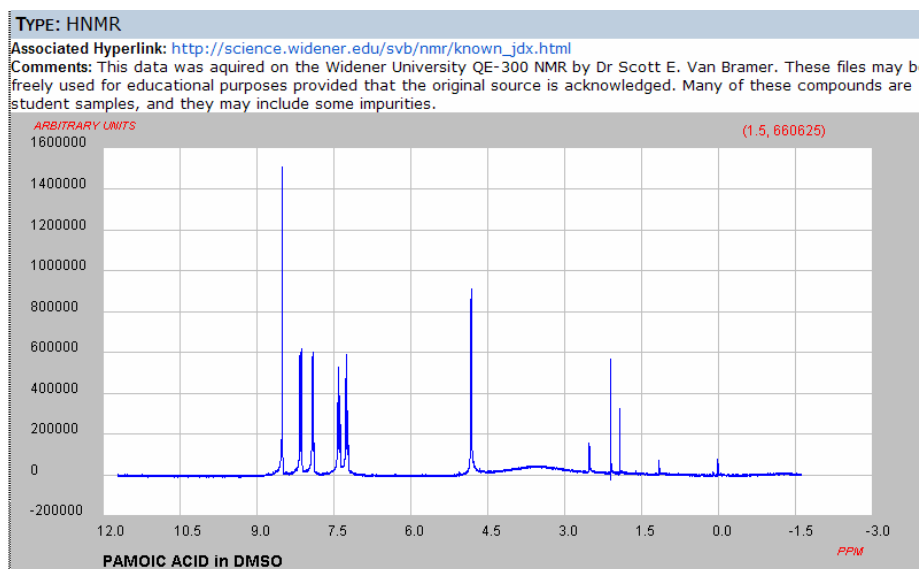


Select the appropriate spectrum for association (if you have any suggestions of others to add please write to us at feedback@chemspider.com with suggestions).

Browse your computer to find the appropriate file to upload to the ChemSpider database. At present ChemSpider only supports JCAMP spectra of the DX or JDX format extension as JSpecView only support JCAMP spectra.

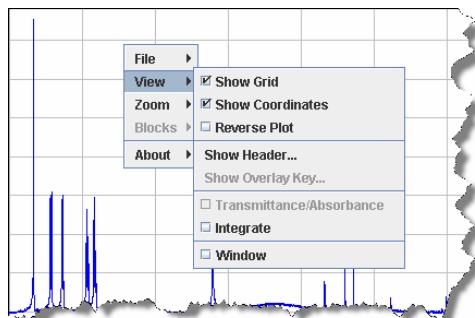
If you would like to associate the spectrum with a hyperlink back to an associated webpage insert it in the hyperlink field. In the comments section add any information you feel would be of interest to a viewer of the spectrum. Example information includes: color of solution, liquid or solid state, details of sample, details of experimental/acquisition parameters.

When all necessary fields have been filled in simply click on **Add Spectrum** and the spectrum should be loaded and displayed in the JSpecView applet as shown below. Note the hyperlink and the comments input during the upload process.



Display Options in the Viewing Applet

A number of display options are available by right-clicking on the spectrum applet. The menu is shown below and should be self-explanatory.





Technical Note

The Header file from the JCAMP spectrum is likely of most interest since it shows a number of the experimental parameters as displayed below.

Label	Description
##TITLE	PAMOIC ACID in DMSO
##JCAMP-DX	5.00
##DATA TYPE	NMR SPECTRUM
##DATA CLASS	XYDATA
##ORIGIN	Processor
##OWNER	Antony Williams
##ZEROFILL	0
##SPECTROMETERDATASYSTEM	??
##SOLVENTNAME	DMSO-d6
##OBSERVEFREQUENCY	300.14951
##ACQUISITIONTIME	4.09600
##ACQUISITIONMODE	SIMULTANEOUS
##OBSERVENUCLEUS	¹ H
##XUNITS	HZ
##YUNITS	ARBITRARY UNITS
##FIRSTX	3513.7028166684245
##LASTX	-486.062116494
##XFACTOR	1.0
##YFACTOR	0.01
##NPOINTS	16384
##FIRSTY	176.23

OK

Java Applet Window

Conclusion

The association of spectral data with chemical structures on ChemSpider has been enabled and this technical note describes the present process by which spectra are uploaded to the database. We welcome your feedback and comments.