EXPORTING DOSY DATA FROM DELTA

In order to export DOSY data from Delta 5.x to third party software such as DOSYToolbox it is necessary to export it in JEOL generic format (as of November 2017). This document provides an explanation on how we can export raw data in generic format once it has been acquired. It is possible to export all data from a certain type of experiments automatically in generic format, but that is beyond the scope of this document. Contact JEOL for further information.

UNDERSTANDING DELTA DATA

JEOL spectrometers from the latest generations store all raw data in the console. This can be accessed through the Delta File Browser under Data Servers from a Delta workstation connected to the console.

🙆 File Browser				
File Options Go 🛞 Recent ☆ Favorite Files				
adolfo-pc				
✓ PLACES	s adolfo-pc - Authenticated as Botana Disconnect			
🧑 Local	► Group by Dimension			
🌍 Global	Group by Node Group by Type			
😂 Data	Group by Project All Files			
Desktop	sample1_Proton_Presentation Botana 491.4 KB 26-APF sample1 Proton ft 1D Botana 280.9 KB 26-APF			
Documents	sample1_Proton 1D Botana 280.9 KB 26-APF			
▼ DEVICES	sample1_Proton_ft 1D Botana 280.9 KB 26-APF			
🦛 Disk Drives	sample1_Proton 1D Botana 280.9 KB 26-APF sample1 Carbon ft 1D Botana 542.3 KB 25-APF			
🥃 Data Servers				
Spectrometers	1D - 16384 - Botana @ DELTA2_NMR Creation:26-APR-2017 08:45:44			
▼ FAVORITES	single_pulse			
	File Filter: *			

From this window, the data can be opened using the 🗹 button and its parameters can be read using the 🗊 button. It can be downloaded to another location through the menu File> Download File...



Whenever a file is downloaded via this method, automated backup or "deliver data" option, its filename incorporates numbers at the end of the filename to indicate the data and processing version. For example, the 2 in ethylindanone_proton-2-1.jdf indicates that this is the second ethylindanone_proton dataset saved and the 1 indicated that this is the raw data (processing version 1). If the data were ethylindanone_proton-1-4.jdf we would be dealing with the first ethylindanone_proton dataset and with the 3rd processing version (processing version 4). Note that Delta uses these numbers when reading data, so if the filename is modified by removing these numbers, Delta may not be able to read it anymore.

In Delta File browser we can choose between the different processing versions of a dataset using a second column that appears in the browser.



When we open DOSY raw data, we should encounter a window like the following one, where we can see a processing list for each of the two axes.

🖉 nD Processor : UTB5_bpp_led_dosy_pfg-1-1.jdf	×		
File Options PreTransform Window Transform PostTransform Display Analyze Tools			
	2		
Axes X Y			
X (>sexp(0.2[Hz], 0.0[s]) ([transpose]			
Y U + Capezoli (1) >zerofil (1) >fft(1, TRUE, TRUE)			
z D ppm [transpose]			
в			
View			
4			
Levels			

If we now save the data via menu File> Save as, what we are saving is the data obtained after the current processing, i.e. in this case we would be exporting the interferogram, not the raw data. If we had added the dosy processing to the y axis we would be exporting the dosy plot.

1) Remove all processing steps by selecting each column and clicking the clear processing list button The processing lists must look like this:



2) Go to menu File > Save as...

We need to choose "JEOL : Generic" as the export format

a) In Delta versions up to 2017, the export format is selecting in menu File>Export Format



b) In later Delta versions, the export format can be selected from the Format drop down field at the bottom of the window.

💋 Save Data File			
File Options Go			
Desktop			
✓ PLACES	> 2017_06_28_2017_HFX - Ashok		
	▶ Delta_520		
	▶ delta_521		
👔 Global	► GMP		
😂 Data	► HFX examples		
	▶ home		
Deskton	▶ JEOL		
Speaktop	▶ newJEOL		
Documents	▶ NOAH		
	▶ Peakdale		
DEVICES	▶ pureshift		
🧼 Disk Drives	V		
🥃 Data Servers			
Spectrometers	Filename: UTB1_gHSQCAD-1		
▼ FAVORITES	Format: JEOL : Generic		
	File Filter: *.jdf		

Choose the location and filename where the data should be saved and click on the 🗹 button. If successful this should have generated two files, an .hdr file containing the data parameters and a .bin file containing the FIDs.