NMDT\_0073



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### How to convert data from/to nmrpipe format

Nmrpipe software provides a command for conversion of NMR data from Delta format to nmrpipe format (delta2pipe). The same conversion as well as the reverse one can be done within Delta as easily as saving/opening a file.

#### From Delta to nmrpipe format

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'Save as' from DataSlate

1. Open FID data or processed data with Data Slate

2. Select File—Save — Save as and in the File Browser that appears select a folder, edit the

#### filename and set format at "NMR Pipe"

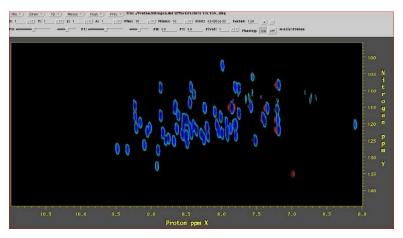
 $\star$  For (n>2)D data, the output would be a series of files. An increasing number index would automatically be added to the filename



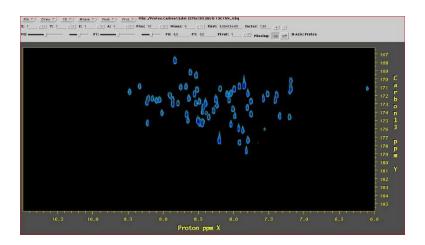
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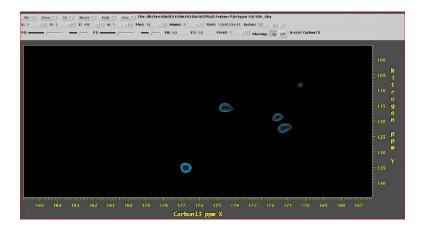
#### Data were saved in nmrpipe format and opened with nmrpipe software (nmrDraw)



#### <sup>1</sup>H<sup>N</sup>-<sup>15</sup>N projection



<sup>1</sup>H<sup>N</sup>–<sup>13</sup>CO projection

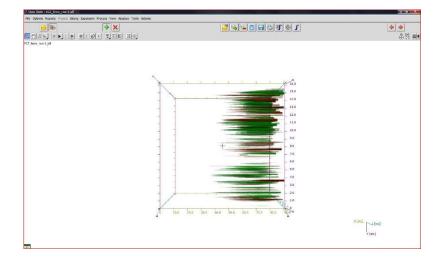


<sup>13</sup>CO –<sup>15</sup>N 2D slice at <sup>1</sup>H<sup>N</sup> = 7.014ppm





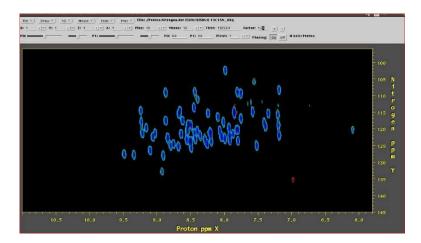
In the same way, preprocessed data (FID data) can be saved in nmrpipe format and then processed within nmrpipe with standard scripts.



'Save as' for 3D FID data from DataSlate

Within nmrpipe and before any processing, you can read the header of the file to confirm that information regarding the original data is correctly preserved

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		3 PM TITLE: 13	
COMMENT: h	nco		
	X-Axis	Y-Axis	Z-Axis
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APOD SIZE:	1024	50	25
SW Hz:	11261.261719	3018.594482	3041.362549
SW PPM:	18.763	20.002	50.010
Hz/POINT:	10.997	30.186	60.827
AQTIME SEC:	0.090931	0.016564	0.008220
OBS MHz:	600.172302	150.913437	60.814930
ORIG Hz:	-2821.206055	25051.466797	5777.110352
DOMAIN:	Time	Time	Time
MODE:	Complex	Complex	Complex
NAME :	Proton	Carbon13	Nitrogen



<sup>1</sup>H<sup>N</sup>–<sup>15</sup>N projection after processing with standard nmrpipe script





#### From nmrpipe to Delta format

The reverse conversion from nmrpipe to Delta format is trivial too:

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**Open \*.fid file with Delta File Browser** 

1. Save data in nmrpipe format using the extension ".fid"

2. Using the Delta File Browser select the above file and open it. Delta will automatically

execute conversion from nmrpipe to Delta format

 $\star$  The \*.fid file should be a single file. If nmrpipe data are in the form of a series of files then combine them into a single file

The aforementioned FID data processed with nmrpipe, were then saved as \*.fid file and opened with Delta.

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