

Delta Tips

NMDT_0073

NMR data processing software

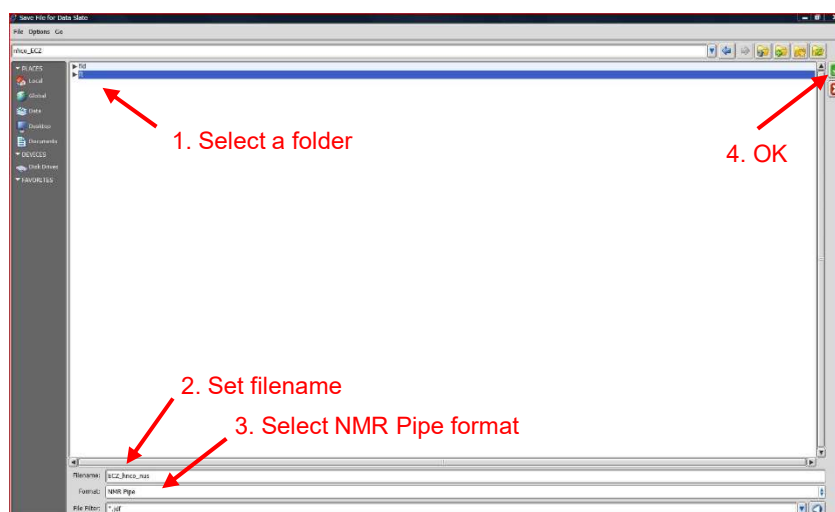
Delta
NMR Software



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

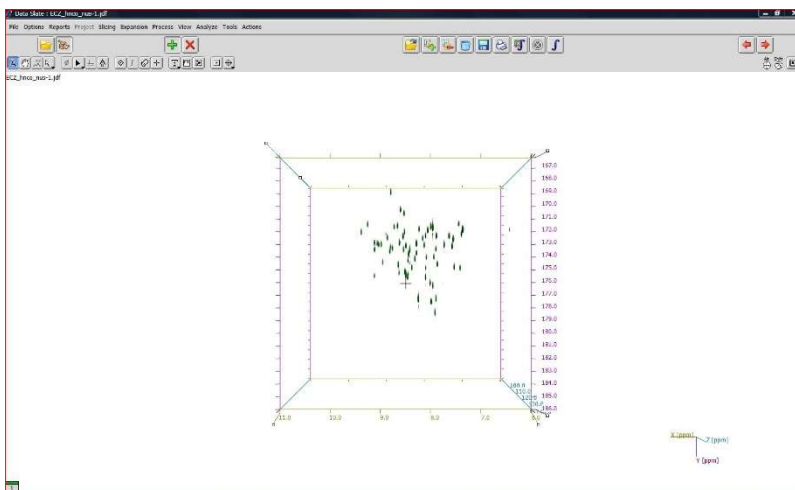


'Save as' from DataSlate

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"

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

The above conversion is demonstrated with processed 3D NMR data (3D HNCOS data).



'Save as' for 3D processed data in DataSlate

1/4

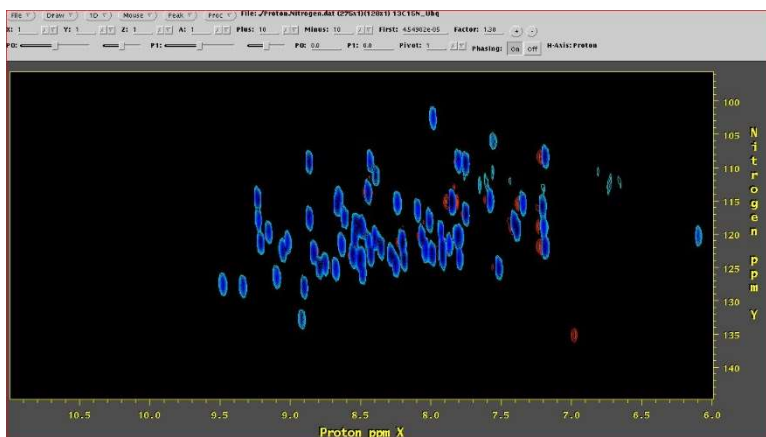
Delta Tips

NMR data processing software

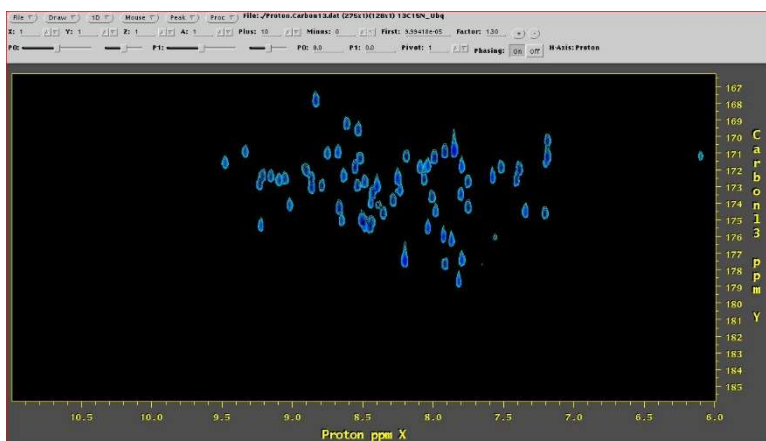
Delta
NMR Software



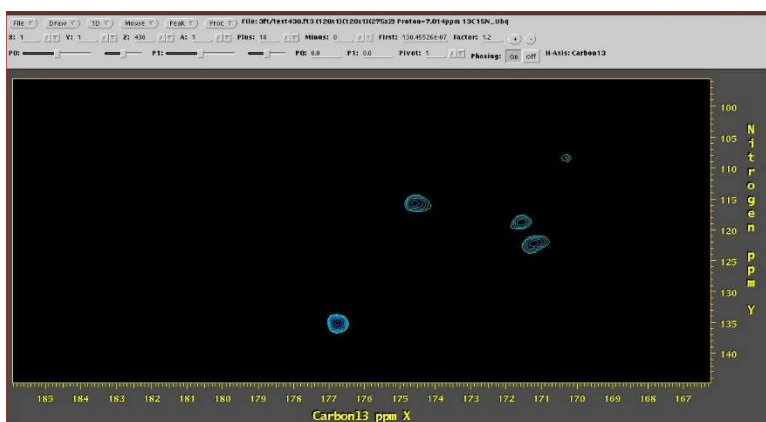
Data were saved in nmrpipe format and opened with nmrpipe software (nmrDraw)



^1H - ^{15}N projection



^1H - ^{13}C projection



^{13}C - ^{15}N 2D slice at ^1H = 7.014ppm

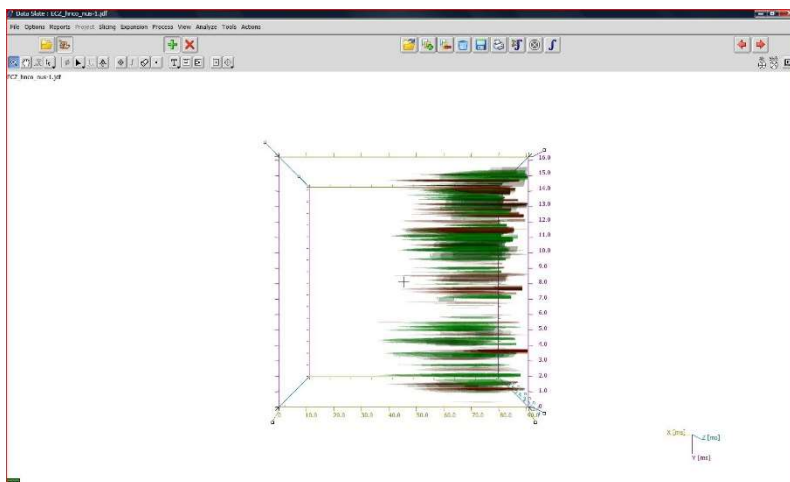
Delta Tips

NMR data processing software

Delta
NMR Software



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

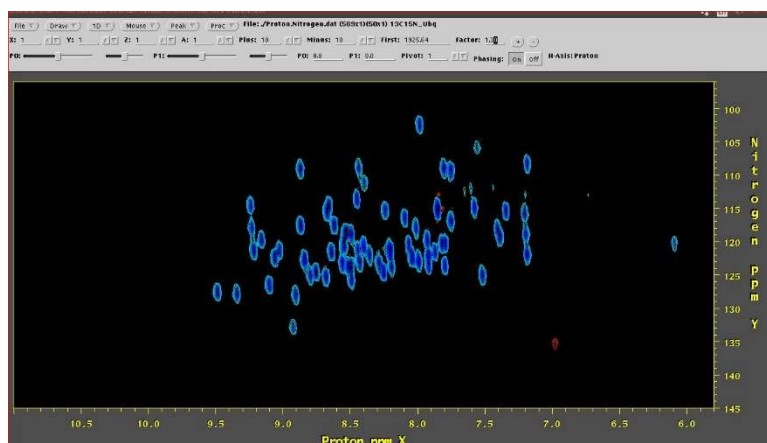


'Save as' for 3D FID data from DataSlate

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

```
FILE: ./zfid/tdata_001.fid DIM: 3 QUAD: Complex 2DMODE: States
BYTES: 821248 PRED: 821248 MIN: 0 MAX: 0 VALID: 0
ORDER: 2 1 3 PIPE: 0 PLANES: 50 1024x100x2 Not Transposed
CONVERTED: 3/26/2015 5:13 PM TITLE: 13C15N_Ubq
COMMENT: hnc0

      X-Axis      Y-Axis      Z-Axis
DATA SIZE:      1024      100      50
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  67.814930
ORIG Hz:      -2821.206055  25051.466797  5777.110352
DOMAIN:      Time      Time      Time
MODE:      Complex      Complex      Complex
NAME:      Proton      Carbon13      Nitrogen
APOD NAME:      None      None      None
```



^1H - ^{15}N projection after processing with standard nmrpipe script

Delta Tips

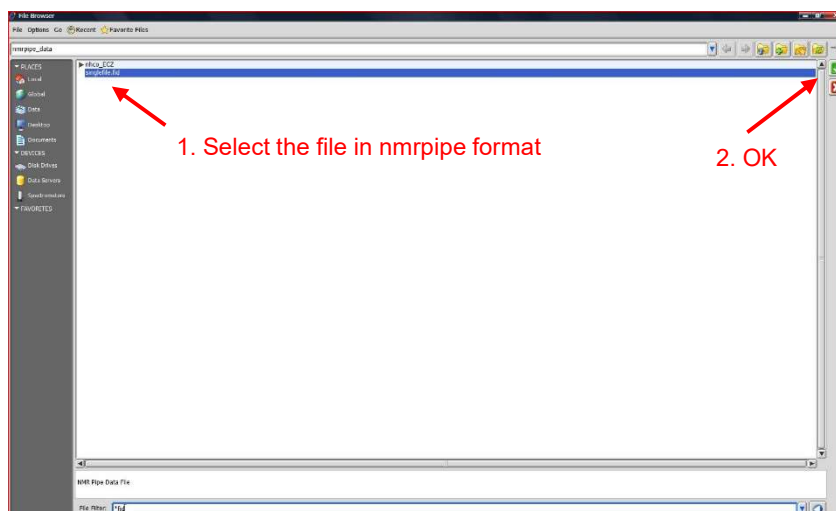
NMR data processing software

Delta
NMR Software



From nmrpipe to Delta format

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



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

★ 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.

