

NOE Difference on AC-300 Spectrometer

Sign in on the logbook.

Sample in and acquire only as many scans as needed. If you know that you do not have any peaks past 10 ppm, then use “.JOBP” so that processing is faster on spectrometer. Transform the FID, phase, and set reference. With cursor determine “O2” values for peaks that you will irradiate & a location absent of peaks for control. You may want to adjust “O1” so that quad images do not occur on top of important peaks.

“filenames MYSAMPLE.*, MY1.*, MY2.*, MYSPC.* are example filenames. You may choose your own filenames for these files.”

```
FL  rt.  FQLIST.001  rt.          1   37555.06      ( example would be for irradiating 2 peaks plus a control)
                                     2   38307.74      ( if you plan to use Nuts macros to process, control should be last value)
                                     3   38835.67
                                     4   END
```

```
VC  rt.  VCLIST.001  rt.          1   3   (= number of frequency values in FQLIST.001)
                                     2   END
```

NE = number of times to interleave (minimum of 4)

D1 = 5

D2 = 10

D3 = 0.1 (AQ + D1 + D2 + D3) x (NS + DS) x VC x NE /3600 = hrs for ACQ to finish

S3 = 23L

NS = 16 (4.1 + 5 + 10 + 0.1) x (16 + 2) x 3 x 4 / 3600 = 1 hour 9 minutes

DS = 2 (4.1 + 5 + 10 + 0.1) x (16 + 2) x 4 x 8 / 3600 = 3 hours 5 minutes

AU NOEDIFF.AUR

Define FID filename #1?

MYSAMPLE

Enter in name to save data as. Do not enter an extension.

Define FREQLIST filename #2?

FQLIST

Enter in frequency list from above without the .001 extension.

If you need to HALT the Acquisition, do so while spectrometer is working on .001 to ensure all FIDs have same number of scans.

If you want to do “Difference” on spectrometer, then:

CNTRL X

COPY MYSAMPLE.*/MY1.*

COPY MYSAMPLE.*/MY2.* 2nd copy in case you make a mistake with 1st copy.

CNTRL X

RE MY1.003 read in control FID

Transform and phase and reference if needed.

RE MY1.003

AI = 1 This command tells spectrometer to be sure to scale all FIDs & Spectra the same.

DC = -1 This value is so you can subtract the FIDs.

AT MY1.003 MY1.001/MY1.001

RE MY1.003

AT MY1.003 MY1.002/MY1.002

RE MY1.001

EFP Irradiated peak will be negative. Positive NOE peaks will be positive. Anti-phase peaks are just cancellation errors.

RE MY1.002

EFP

You can transfer FIDs “MY1.*” via NMRNET and plot difference spectra. In Felix-for-Windows, write down the phase values used for control spectra & type in phase values in box at bottom of screen in phase routine.

If you want a peak listing of intensities for % calculation then:

RE MYSAMPLE.003

Set NE = to number of FIDs

AU EFPNE.PROC

Filename #1? MYSAMPLE do not enter in extension number

Filename #2? MYSPC

RE MYSPC.001

EP Display on screen area you want to peak pick. Move cursor so it sits on the lower part of a peak and type "M" to define a minimum intensity. Type "U" to define region to peak pick. Return to exit EP mode.

Turn on Printing

AU PPNE.PROC

Filename #1? MYSPC do not enter in extension number

If intensity numbers are say 0.678 and you would like a larger numeric value – set CY = 1000 & au ppne.proc

AI = 0 to return intensity scaling back to normal

To plot up data with Felix-for-Windows, import the control & write down phase values. Read in 1 of the difference FIDs & type in the phase values to use.

To plot up data with NUTS, you have to run a couple of macros on the original FIDS. First you run macro to convert 1D FIDs into a 2D matrix, then you define phase values for control, set DC value, then run macro to do the Subtraction. You need to run "_COPY_2D.MAC" and then run "_DIFFSPC.MAC".

You may need to run the 5.02 vers. of Nuts.

Some of the NUTS commands to use:

RU _copy_2d.mac

Open ____.001

Save as ~temp2.2d

Yes replace?

Process & phase control spectra

AS parameter = -1

RU _diffspc.mac

Output will be "!_diffspc.2d"