18. NOESY

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In NOESY, a "magnitude" 2D spectrum is often obtained, but "phase sensitive" data are nearly always preferred. Sensitivity and resolution are both improved with the phase sensitive data set. For quick runs on simple compounds, magnitude data can be successful, and processing is easier with this type of data set. NOESY data requires some approximate understanding of the T_1 times involved for the protons of interest (see the chapter for T_1 measurements). Measuring T_1 usually takes only 15-30 mins, and can preceed the NOESY setup and acquisition. The data acquisition times for NOESY vary widely, from 1 h to multiple days (only on the Unity 500). You should not attempt obtaining NOESY data unless you are willing to invest the time needed to correctly setup and interpret the data!

I. Quick Summary for Acquiring and Plotting NOESY Spectra

[see section II for more detailed discussion]

A. Obtain a high-resolution spectrum

- use normal 1D jobfile, and set reference using **EP-G**
- write down SR
- optimize SW using **EP-<cntl>O**
- retake spectrum with new SW; set SR and CY (=15 for 8.5×11, 19 for 11×17) and **WR *filename*.001**
- write down **DW** , then **TR** [to another job]

B. Setup 2D paramters:

C. Check 2D parameters

D. Process 2D file

1. goto step 5 if you have just taken the data; if coming back later proceed with step 2
2. goto job1, **RE *filename*.001**
   PJ *filename*.001
3. check that SR and CY are set as in step A above (if not, correct them and
   WR <ret> <ret> Y to rewrite spectrum
5. enter: **RE *filename*.SER <ret> ST2D <ret> XFB <ret> SYM <ret>**
   or if already XFB: **RE *filename*.SMX <ret> ST2D <ret>**

6. check that SR=SR2=SR1 and CY are set as in step A above (if not, correct them)

7. enter: **AP2D** (AC's) or **EP2D** (AM's and DataStation)

   • set contour level, and expand region if desired

   enter **<ESC>-X** to exit

8. enter: **CP2P <ret>**

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FILENAME IN F1:  filename.001
FILENAME IN F2:  filename.001
NO. OF PENS:  1 (or 2 if have red pen)
NO. OF CONTOUR LEVELS:  4 (1-7 levels)
OUTLINE BOX:  Y
GRID:  N
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