

NCSU NMR Facility

Using 500 MHz spectrometers

Bruker On-Line Manual

Basic ¹H Acquisition and Processing

I. Inserting the Sample

- A. On the BSMS panel, turn the Lock off
- B. Press Lift to eject
- C. Place the sample in the probe
- D. Press Lift to lower the sample
- E. When the sample is down, press Field and adjust the field until the sweep signals intersect in the middle of the screen.
- F. Turn the Lock on

II. Spectrometer and Acquisition Parameters

System can be operated by using the pull-down menu or by typing in the command line

- A. Type "edc" to create a new data set from the template
- B. Type "edasp" and set the following parameters:

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NUC1    1H
NUC2    OFF
NUC3    OFF
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- C. Exit edasp by clicking "SAVE"
- D. Type "eda" to set the acquisition parameters (see Table 3 in desk manual)
- E. Type "stop" to ensure no acquisition is in progress
- F. To start tuning the probe, type "acqu" to enter acquisition window
- G. Start the frequency sweep by typing "wobb"
 - a. At the magnet turn the blue knob until the "V" on the screen is as low as possible
 - b. Turn the red knob until the "V" is centered on the vertical line
- H. Type "stop"
- I. Type "ii"

III. Locking and Shimming

- A. To display the lock signal, click "lockdisp" with left mouse button
- B. Type "lock" and select the appropriate solvent
- C. Type "rsh" to read shims
- D. Adjust the Z and Z² shims while viewing the lock signal (the best shims correspond to the highest amplitude of the lock signal in the window)

IV. Acquisition

- A. Type "acqu" to enter the acquisition window
- B. Type "zg" to clear previous and start the experiment
- C. Type "rga" to automatically perform several acquisitions and set a suitable value for the receiver gain (rg)

- D. Type "td" to set the time domain digital resolution (approximately 16k)
- E. Type "zg"
- F. To increase the number of scans, type "ns #" (where # is any multiple of 4)
- G. Type "zg"

V. Processing

- A. Type "edp" to display and edit processing parameters
- B. Type "si" to set the number of points used to form the resulting spectrum (approximately 32K)
- C. To execute Fourier Transform type "efp"
- D. Click on "phase" to enter the phase correction submenu
- E. Click and hold the left mouse button on "0" to adjust the 0th order phase by rolling the mouse until the reference peak is positive and the baseline on either side of it is as flat as possible
- F. Click and hold the left mouse button on "1" to adjust the 1st order phase by rolling the mouse until the peaks far from the reference point are positive
- G. Click "store" to save the phase corrections and exit

VI. Plotting Spectra

- A. To select the spectral region, make sure the spectrum appears as desired on the screen, and then click "dpl 1 2 3" and hit return to the three questions that appear
 - B. Type "abs" to perform an automatic baseline correction and to automatically define the integral range.
 - C. To create a title, type "setti"
 - D. To select the desired printer, type "edo"
 - E. Type "plot" to print the spectrum
 - F. To select the desired printing parameters type "edg"
 - G. Type "xwinplot" to get spectra editor program
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