Nuts via Network

Nuts is a powerful, full-featured, one- and two-dimensional NMR data processing program. It is available in four places:

1) On the NMR workstation located in Keck 2337.
2) On machines located in the PChem computational lab.
3) On Charlie, in Windows 2000 format in the directory
   `Charlie.Courses.Chemistry.PC.Nuts`
4) On Charlie, in Macintosh Power PC format in the folder
   `Charlie.Courses.Chemistry.Mac.MacNUTS_PPC`

NMR Workstation (in Jacobs 2337)

Launch Nuts by double-clicking on the icon on the desktop.

Windows 9x/Windows 2000

Launch Nuts by finding the program at
`Charlie.Courses.Chemistry.PC.Nuts`

Macintosh Power PC

Find the Nuts program directory at
`Charlie.Courses.Chemistry.Mac.MacNUTS_PPC`

Launch Nuts by double-clicking on its icon.

Existing Nuts Data Set

`GA` will open an existing Nuts file in the data directory. Files from dpx400 need to be imported with the `IM` command (see below).

Importing a dpx400 Data Set

`IM` will open an XWinNMR data file in the data directory.

You will need to remove the data offset present in all dpx400 data by typing `RD` then <RET>.

^{13}C Data

Type `LB` to set the line broadening parameter. `EM` applies exponential multiplication with this value.

Fourier Transformation

`FT` applies the Fourier transformation.

You will need to reverse the spectrum with `SR` *on all data acquired with the dpx400.*

Phasing

^{1}H data can be phased automatically with `QP` whereas ^{13}C data often requries `AP`. The phase constants from a previous spectrum can be applied via `PS`.

Manual phasing can be done by first selecting the pivot point: Click and hold the left mouse button on the pivot point. Continue to hold the left mouse button down

and type `M`. Don't be alarmed if the computer beeps. Type PH to begin phasing. Moving the mouse to the left or right while holding down the left mouse button adjusts the zeroth order phase constant. Moving the mouse to the left or right while holding down the right mouse button adjusts the first order phase constant. (Macintosh users need to hold down the <SHIFT> key while holding down the mouse button to access right mouse button features.) When you are satisfied with the phasing, press the <ENTER> key.

Manual phasing using two regions is the most sensitive technique. Set the pivot point as described in the previous paragraph. Type `^F` (hold down the <CTRL> key while typing F) to display the full spectrum. Double-click the left mouse button to enter ZOOM mode. Hold down the left mouse button and drag the cursor across the region containing the pivot point. Type `1`. Hold down the left mouse button and drag the cursor across the region containing a peak far removed from the pivot point. Type `2`. Type `PE` (for Phase Expansion). Moving the mouse to the left or right while holding down the left mouse button adjusts the zeroth order phase constant while displaying region 1. Moving the mouse to the left or right while holding down the right mouse button adjusts the first order phase constant while displaying region 2. (Macintosh users need to hold down the <SHIFT> key while holding down the mouse button to access right mouse button features.) When you are satisfied with the phasing, press the <ENTER> key.

Reference

Hold the left mouse button down and place the cross-hairs on the peak to be referenced. Type `O` while holding the button down. Enter the chemical shift of the peak.

Spectral Range

Double-click the left mouse button to enter ZOOM mode. Hold down the left mouse button and drag the cursor across the region to be expanded. Double-clicking the right mouse button will toggle between the expanded region and the full spectrum. (Macintosh users need to hold down the <SHIFT> key while holding down the mouse button to access right mouse button features.) `^E` will expand the selected region, `^F` will return to the full spectrum.

Vertical Scaling

The vertical scale can be changed with the PAGE UP and PAGE DOWN keys, the < and > keys, or by using the scroll bar at the right of the screen. `^Y` or `MF` will scale the spectrum such that the largest peak is shown without clipping.

Baseline Offset

For ^{13}C DEPT spectra and other spectra with negative peaks, you will want to move the baseline upwards. Use `DC` and the slider at the left of the screen to move the baseline. Type <RET> when finished.

Integration

Integration should be preceeded by baseline correction. Use `BF` or `FB` to correct the baseline.

Automatic integration is accomplished with `AI`.

Manual integration is started with `ID`. Clicking with the left mouse button makes the cursor active. Click a second time to start an integral. Click a third time to end

an integral. You can delete an integral by clicking once with the left mouse button to activate the cursor, moving the cursor over the integral, then typing `D`. The value of an integral can be set in the same fashion by typing `V`. Vertical scaling of the integrals is changed with the scroll bar on the left of the window. The position of the base of the integrals can be changed with `Z`, which brings up a new scroll bar on the left of the screen. Typing `B` allows the slope and intercept of the integration to be set by dragging the left and right mouse buttons, respectively. When you are satisfied with the integration, type <RET>. `AF` turns the integral display off, while `AN` turns it on. `^I` toggles between integrals on and off.

Peak Picking

Hold the left mouse button down to display the cross-hairs. Set the horizontal line at the minimum level for peak picking. Press M before releasing the mouse button. `^B` toggles the peak table on and off. `DP` can be used to label a single peak. `PD` can be used to reposition a label. `PN` and `PF` turn peak label display on and off, respectively.

Notations

`NO` allows you to place notations anywhere on the screen. Click once to position the label, type the label into the text box, then repeat as necessary. <RET> exits the label routine. `LP` will display the acquisition parameters on the left of the screen.

Plotting

Check PRINTER SETUP under the FILE menu to set whether you will plot in landscape or portrait mode. `PL` will print what is on the screen.

All Done?

`XX` exits Nuts.

If you are finished with the PC workstation, click on the Windows 95 START button (at the bottom-left of the screen), select Shut Down..., then select "Close all programs and log on as another user."

Nuts Command Summary

<	decrease vertical scale
>	increase vertical scale
^A	toggle axis units
^B	toggle peak pick list on/off
^E	show last expansion
^F	show entire spectrum
^I	toggle integrals on/off
^L	toggle acquisition parameters on/off
^P	toggle peak labels on/off
^Y	vertical auto-scale
PAGE UP	increase vertical scale
PAGE DOWN	decrease vertical scale
AF	turn integrals off
AI	autointegrate
AN	turn integrals on
AO	all off—exits from all subroutines
AP	autophase (for complex spectra)
BC	DC offset for fid or spectrum
BF	baseline flatten
EM	exponential multiplication of fid
FB	fit baseline with polynomial
FT	Fourier transform
GA	read new file (Nuts format)
ID	enter integral display
B	slope/intercept correction
D	delete integral
V	set value for integral
Z	set baseline value
IM	import file
LB	line broadening
LP	list acquisition parameters
LZ	jump to last zoomed region
M	set minimum height (while holding mouse)
MF	make full vertical scale
MH	set minimum height
NO	notation
O	set reference (while holdingn mouse)
PF	turn peak labels off
PL	plot
PN	turn peak labels on
PS	phase same (applies previous ph0 & ph1)
QP	quick phase
RD	rotate data
SR	spectrum reverse
XX	exit Nuts
ZL	clears the peak list
ZO	enter zoom routine