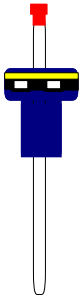
Folding instructions: www.pocketmod.com

3) Insert the sample



(a) Spinner into the depth measure then slide the tube down to the bottom (liquid level *c.a.* ≥ 3 fingers).
(b) Hold the tube above the spinner. Wipe the tube and spinner.
(c) Press the "lift on/off" (green = on)
(d) WAIT until you hear the air flow set the spinner on the air cushion.
(e) Press the "lift off" button (no light)

AV300 only:

4) Spin (optional)

(a) Press "spin on/off" (green = on)
(b) To check the spin rate:
orange plus spin rate/spin measure
(c) To deselect spin rate: stand-by

AV500 only:

4) atma

If it takes more than a minute, stop it (type: stop) and enter manual mode: atmm

5) Lock

(a) lockdisp
(b) rsh qnp (AV300)
rsh bbo (AV500)
(c) lock
Select your deuterated solvent
This sets the chemical shift scale

6) Shim

(a) Adjust "lock phase"
maximize the lock signal
(b) Adjust the shim currents
Z, Z^2, Z, Z^2, . . .
until no further changes
("fine", "onaxis" "Z1")
If the lock signal goes off the screen, reduce "lock gain" or "lock power."
To undo changes, press the upper-most lit button. To save press any other button.
*If not spinning (**AV500**):*
adjust: X, Y, XZ, YZ ("X" "Z0")
(c) Press "std by" when finished.

7) Parameter setup

(a) ased (showpp; ns 1, ds 0)
(b) rga
(c) zg (preliminary aquisition)
(d) tailor the parameters:
time domain (FID), aim: avoid clipping
x-axis: estimate the final acquisition time
(FID takes up ~ ½ the screen)
y-axis: if rga gave rg = 1, then reduce p1
frequency domain (spectrum)
proc *(this macro runs: ft, apk, abs)*
how is the shimming? more needed?
(d1 0 gs)
center the signals (o1p)
reduce sw
adjust td to get the desired aq
*(aq = td*dw = td/(2swh))*
adjust si = 2*td (zero filling)
set ns *(8 for a full phase cycle)*
set ds *(common value = 2)*
set d1 *(depending on T_1's)*
(t1ir1d, d7 0.1us phase, vary d7)
*(T1 = d7(longest to reach 0)*1.44)*
*e*xpt (experiment time)

8) Acquire a FID

(a) zg
(b) Options during FID acquisition:

tr saves without stopping
h HALTs and SAVEs
the FID is automatically saved after ns
go acquires more ns
added to the first FID
stop data will not be saved
kill data will not be saved

9) Processing

(a) ft (fourier transform)
ef *sensitivity-enhanced (lb > 0)*
gf *resolution-enhanced (lb < 0, gb > 0)*
right-click to alter the display properties
(b) apk (auto phase correction)
Manual phase correction: **.**ph

"0" = zero-order phase correction
"1" = first-order phase correction
right-mouse click to set the cursor
("set pivot point" left-click)
save and exit

(c) chemical shift calibration .cal

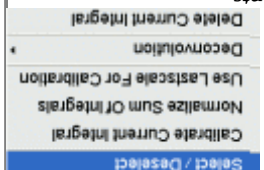
place the cursor at a known position
(e.g. $CDCl_3$ = 7.26 ppm)
click the left-mouse button to define it
(d) abs (automatic baseline correction)

Manual correction (no integration): .basl
save and exit
For more correction options, type: bas
(e) ppf (peak picking, full spectrum)
to toggle display units:
to change parameters: pp
or type values for mi, maxi, cy

Manual /interactive peak picking: .pp
define the range (green box)
draw a box around the peaks to pick
click on the "pick peaks icon"
save and exit

(f) integration
Automatic integration *and* baseline correction: **abs**

Manual integration (no baseline ops): .int
to delete all: "select all" with and delete with red "x" button
to define new integrals
right-click on an integrand to select:
save and exit
(g) plot (opens the plot editor)
"Data" expno's in use
green squares to select
"Edit" to change display
"Attributes"colors and fonts
"1D/2D Edit" interactive changes
File, Print to get a hardcopy (*i.e.* <ctrl>p).
File, Export to save as an image format
"Save" only saves the LAYOUT ONLY
NOT the picture on the screen
Please do not change the standard layout



10) Save your data

DATA MAY BE **DELETED at any time WITHOUT WARNING**
(a) Open my computer (nmr300 or nmr500)
(b) Click the "start" icon to get to the nmrlab4 network shortcut.
(c) Drag and drop files to nmrlab4 and preserve the hierarchy:
<*dir*>/data/<*user*>/nmr/<*name*>/expno

11) Remove your sample

(a) turn off: spin and lock (no lights)
(b) press "lift on/off" (green = on)
(c) gently remove your sample
(d) press "lift on/off" (no light)

12) Log off

13) On another computer

(a) Open the program Topspin.
(b) Navigate to your data via a the Browser.
(c) Drag your file into the display window.

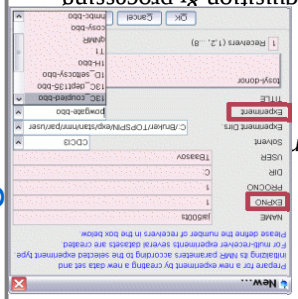
Bruker AV / Topspin 2.1

1) Login and open the program

(a) Sign the logbook
(b) Login to the computer.
user name
password
(c) Open Topspin

2) Create a new file

new
EXPNO
"*experiment number*"
one fid per expno



Experiment assigns standard acquisition & processing values (viewable in "eda" & "edp")