Bruker Avance DRX500 NMR Spectrometers  
(WTHR 367 and RPH G43)  
Basic Spectrometer Operation - Quick Reference Guide

Login and startup
Login to Linux with username and password
topspin (in Linux window) - start TopSpin program

Setup
edc - enter new dataset name and expno
rpar exp.bbo  (exp = h1, f19, c13, cosy, hmqc, etc.)
NOTE: always run a proton acquisition before running any other nucleus or experiment
ased , AcquPars tab - check / edit acquisition parameters

Change sample
lockdisp - open lock display window
bsmsdisp - open BSMS display (optional - the physical keypad may be used instead)
remove sample using BSMS display or keypad - turn off lock and shim, use lift key to eject
change sample, set sample depth, clean
insert sample - turn off eject, start spin on BSMS display/keypad
lock  (select solvent from popup menu)
shim Z1, Z2, Z3 using BSMS display/keypad
gradshim - open gradient shimming control panel (see Basic 1D Training Guide pp. 10 – 11)

Acquisition
atma - initialize current dataset and tune the probe - WAIT UNTIL ATMA COMPLETES!
NOTE: if you are running the same experiment on multiple samples with the same solvent, it is
not necessary to execute atma between each sample
rga - set receiver gain (do not use for C13)
zg - acquire FID (use halt to stop acquisition, if needed)

Processing and plotting
edp , ProcPars tab - check / edit processing parameters
ef - Fourier transform
Phase icon - phase spectrum with mouse
apk - automatic phasing
abs or abs13c - automatically flatten spectrum baseline
Calibrate icon - check / set chemical shift reference
Right-click on spectrum - define current displayed region of spectrum for plotting
cy - adjust y-scale of plot
setti , Title tab - open text editor to edit plot title
pps - view list of picked peaks on screen
mi - adjust peak picking threshold
Integral icon - enter integration subroutine
print - plot using either XWinPlot or internal plot routine
Finish-up and logout
change sample and insert standard CDCl₃ sample
re , data browser - read a proton dataset
standard - set up and lock on standard sample (touch up shims after locking completes)
close lock window - use return icon in icon-bar of window
exit - exit TopSpin
right-click on display background, select Logout and confirm - logout from Linux

Bruker DRX500-1 and -2 NMR Spectrometers
Parameter Sets w/BBFO Probes (05-01-2021)

Parameter Sets
h1.bbo
c13.bbo
c13dept.bbo
f19.bbo
p31.bbo
p31nd.bbo (no decoupling)
presat.bbo
c13hsqc.bbo
cosy.bbo
hmqc.bbo
hmbc.bbo
noesy.bbo
tocsy.bbo
al27.bbo
b11.bbo
h2.bbo
li7.bbo
na23.bbo
n15.bbo
n15hsqc.bbo
si29.bbo
si29nd.bbo
sn119.bbo
sn119nd.bbo
te125.bbo
te125nd.bbo

Parameter sets for other nuclei can be set up upon request.

Shim Files
shims.bbo