Bruker AV-III-800 (BRWN B124), AV-III-500-HD (DRUG B055) and AV-III-400-HD (WTHR 369) NMR Spectrometers
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 experiment number (expno)
rpar exp.probe (exp = h1, p31, c13, cosy, hmqc, etc; probe = cryo (500/800), bbo (400))
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
remove sample using BSMS display - turn off lock and shim, use lift key to eject
change the sample, set the sample depth, clean the tube
insert sample - turn off eject, start spin (if using) on BSMS display
lock (select solvent from popup menu)
topshim (perform automatic shimming) or manually shim Z1, Z2, Z3 using BSMS display

Acquisition
atma - initialize current dataset and tune the probe - WAIT UNTIL ATMA COMPLETES!
NOTE: if you are running the same experiment on multiple similar samples, it is not necessary to execute atma between each sample
rga - set receiver gain (do not use for C13 data acquisition)
zg - acquire FID (type 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
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 internal plot routine
plot0 - plot using XWinPlot (separate window)

Finish-up and logout
change sample and insert standard $CDCl_3$ sample
re , data browser - read a proton dataset
standard - set up and lock on standard sample
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 AV-III-800, AV-III-500-HD and AV-III-400-HD NMR Spectrometers Parameter Sets (06-15-2017)

AV-III-800

Parameter Sets
h1.cryo
presat.cryo
p31.cryo*
p31nd.cryo*
c13.cryo
c13dept.cryo
cosy.cryo
cosypr.cryo
tocsy.cryo
tocsypr.cryo
noesy.cryo
noesypr.cryo
noesypr1d.cryo
hmqc.cryo
hmbc.cryo
3d-hnca.cryo
3d-hnco.cryo
c13hsqc.cryo
n15.cryo
n15ineptrd.cryo
n15hsqc.cryo
n15hsqc3919.cryo
h2.cryo

*PINMRF staff assistance required

Shim Files
shims.cryo

AV-III-500-HD

Parameter Sets
h1.cryo
presat.cryo
f19.cryo
p31.cryo
p31nd.cryo
c13.cryo
c13dept.cryo
cosy.cryo
cosypr.cryo
tocsy.cryo
tocsypr.cryo
noesy.cryo
noesypr.cryo
hmqc.cryo
hmbc.cryo
c13hsqc.cryo
si29.cryo
si29nd.cryo
n15.cryo
n15hsqc.cryo
h2.cryo

Shim Files
shims.cryo

AV-III-400-HD

Parameter Sets
h1.bbo
presat.bbo
f19.bbo
p31.bbo
p31nd.bbo
c13.bbo
c13dept.bbo
cosy.bbo
cosypr.bbo
tocsy.bbo
tocsypr.bbo
noesy.bbo
noesypr.bbo
hmqc.bbo
hmbc.bbo
c13hsqc.bbo
si29.bbo
si29nd.bbo
n15.bbo
h2.bbo

Shim Files
shims.bbo