Bruker Avance 400 NMR Instructions for 1D Experiments

Dissolve solid or liquid into 600 uL deuterated solvent.
Double click on TOPSPIN 3.5 icon, if program not already open

Action	Description
“ej”	eject standard - replace with your sample
“ij”	inject sample
“new file” or new file icon	NAME: begin with your initials (example: JAT-aminothiazole-part1) EXPONO: 1, PROCNO: 1 (increment the EXPONO as you take additional spectra of the same molecule, but do not change PROCNO) Experiment: see experiment names below (PROTON, C13CPD…) Set the correct solvent Execute ‘getprosol’ must be selected - this one’s easy to forget! DIR: C:\data\CHM411 Create a descriptive title
“lock”, then select solvent from list.	auto lock procedure will lock and adjust gain/power based on solvent choice
“atma"	auto tune and match. Experiment PROTON tunes only ^{1}H, but many others tune both ^{1}H and ^{13}C. If moving to a ^{13}C-based experiment after running a ^{1}H experiment, alma must be re-executed.
“ro”	rotation - make sure this is ON when performing 1D NMR experiments.
“topshim”	auto shim.
"rga"	auto adjust receiver gain
adjust “ns” if needed	PROTON: ns = 1 x n (recommend 4) C13CPD: ns = 1 x n (recommend 64 for ~ 5 minute experiment) C13DEPT135p: ns = 4 x n (recommend 64 for ~ 5 minute experiment)
"zg"	begin acquisition
click Process tab, then Proc. Spectrum tab	processes data by applying exponential window function, fourier transform and phase correction; make sure phase correction is sufficient.
Click  if spectrum is raised off the bottom of screen	Do not do this for DEPT experiments - it should adjusted to the center of the screen so you can see positive and negative peaks.
if calibration needed, zoom in on region, then select Calib. Axis tab	select and calibrate to TMS or other known signal.
if needed, “pp” to pick peaks	make sure Auto-Pick peaks on full spectrum is selected, and value of mi is > 0. For DEPT experiments, “Pick peaks of sign” should read, “both”.
if needed, select Integrate tab	click and drag with left mouse button through each signal of interest. You can calibrate a signal to 1, 2, 3 or another known value by right-clicking and choosing calibrate. Save and return.
“plot”	enters plot window
open and apply layout	choose down arrow next to Layout and open appropriate layout within Turk Layouts
adjust axis, if needed	select spectrum by clicking on it. If x and y axis parameters do not appear, select “Axes, Grids, Curve…”, then adjust according to experiment. I generally use 10.5 ppm to -0.5 ppm for ^{1}H, and 210 ppm to 0 ppm for ^{13}C. If there are peaks further downfield or only upfield peaks, adjust your print width accordingly.
print	click on print icon

JAT 04-30-2017

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“ej”	eject standard - replace with your sample
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Command	Description
“re” *filename expno procno*	open file
“ns”	# scans
“expt”	experiment time
“mi”	adjusts threshold for peak picking
“i”	increment EXPNO
“ro"	sample rotation/ spin control

Experiment Files make sure Source = C: \Bruker\Topspin3.5pl5\exp\stan\nmr\par	
PROTON	^{1}H
C13CPD	^{13}C
C13DEPT135P	DEPT 135

JAT 04-30-2017