

Bruker Avance 300 NMR Instructions for 1D Experiments

Dissolve solid (20 - 40 mg) or liquid (20 - 40 μ L) into 600 μ L deuterated solvent for ^1H and up to 80 mg or μ L for ^{13}C .
Double click on TOPSPIN 1.3 icon

Action	Description
"new file" or new file icon	NAME: begin with initials EXPONO: 1, PROCNO: 1, DIR: /disk2 USER: CHM411 Experiment: see options in table on right
"lockdisp"	opens lock level display
"bsmsdisp"	opens bsms control panel
in BSMS window, select [Lock]	turn lock off
select [LIFT]	eject standard - replace with your sample
select [LIFT]	inject sample
if deuterium signal shows in the center of the lock display, select [Lock] - otherwise, "lock solvent"	lock on deuterium signal or begin autolock procedure using <i>solvent</i> parameters you chose when creating the file
wait for [SPIN] to turn green, then adjust lock power/gain as needed	see table to right
shim z & z ²	adjust to maximize signal strength z is sensitive and should be adjusted with step-size < 10, whereas z ² is less sensitive and can be adjusted with step-size = 10.
close BSMS window	
adjust "ns" if needed	if 20 mg for ^1H , then ns=16 (multiple of 4) if 80 mg for ^{13}C , then ns=16 (multiple of 16)
"rga"	set receiver gain
"zg"	begin acquisition
"ft" (proton) or "ef" (carbon)	process data
select interactive phasing icon	optimize 0 & 1 - save changes
if needed: select calibration icon	calibrate TMS or other known signal
if needed: "pp" to peak pick	peak pick entire spectrum
select interactive integration icon (^1H only)	select pick range icon, then drag with left mouse button through each signal
"plot"	enter plot editor
<file>, <open>	select: turk1H, turk13C or turkDEPT
for DEPT, add full ^{13}C spectra beneath DEPT spectra	select spectral region, then [data]. Choose ^{13}C experiment, then [append] and [apply]
adjust spectral height if needed	select spectral region, then 1D/2D edit
<file>, <print> or ctrl-P	print

Command	Description
"re" name expno procno	open file
"ns"	# scans
"expt"	experiment time
"mi" - can also be edited in "pp" window	adjusts threshold for peak picking

Adjustment	CDCl_3	DMSO
Lock Power	-25	-30
Lock Gain	120-125	150
Values are approximate		

Experiment Files	
protonC	^1H NMR: CDCl_3 , MeOD-d ₄
protonD	^1H NMR, DMSO-d ₆
carbonC	^{13}C NMR, CDCl_3
carbonD	^{13}C NMR, DMSO-d ₆
DEPT135	All solvents

