

How to Acquire a Proton Spectrum

rev 6/10/08 jgb

Eject sample in magnet and turn on the air flow	e <input type="text" value="↵Return"/> on the Gemini 400, push down the black button on the H-tower by the magnet
Insert your sample into the magnet and turn off the air flow	i <input type="text" value="↵Return"/> on the Gemini 400, slowly pull up the black button on the H-tower by the magnet
Select a set of standard parameters	<input type="text" value="Main Menu"/> <input type="text" value="Setup"/> <input type="text" value="H1,CDCl3"/> or <input type="text" value="Nucleus, Solvent"/> for another combination su <input type="text" value="↵Return"/>
Load a good set of shims	rts('best') su load='n' <input type="text" value="↵Return"/>
Open the Lock & Shim window	<input type="text" value="Acqi"/>
Find and optimize the Deuterium lock signal	<input type="text" value="Lock"/> <i>-Turn the lock off</i> <i>-Increase the lock gain all the way</i> <i>-Increase the lock power until the signal is evident</i> <i>-Adjust Z0 until the signal is on-resonance</i> <i>-Turn the lock back on</i> <i>-Lower Lock power to less than 30</i> <i>-Lower Lock gain so intensity of lock signal is >20 and <80</i> <i>-Adjust the Lock phase for the highest intensity lock signal</i>
Go to the Shim Window	<input type="text" value="Shim"/>
Shim the magnet	<i>-Adjust Z1C for the highest intensity lock signal</i>

	<p>-Adjust Z2C for the highest intensity lock signal</p> <p>-Readjust Z1C and Z2C until the best combination is found</p> <p>-Adjust Z1, Z2, Z3, and Z4 for the highest intensity lock signal</p> <p>-Iterate through Z1-Z4 until the highest lock signal intensity is found</p>
Set the number of transients to 1 and acquire a test spectrum	nt=1 ga ↵
Display the spectrum	f aph vsadj full ↵
Find the narrowest peak in the spectrum (typically the residual solvent signal) and put a cursor on each side of it	Expand
Place a cursor near the top of the peak	nl ↵
Measure the line width at half-height	dres ↵
Shim more if the line width is greater than 1 Hz or if the peak is asymmetric	Shim
Acquire a final spectrum with signal averaging if the shimming is acceptable	nt=16 ga ↵
Associate text with the spectrum before saving it	text('your text') ↵
Save the spectrum	svf('your filename') ↵
Phase the spectrum	aph ↵
Reference the spectrum: put a cursor on the peak to be referenced (e.g. chloroform peak)	nl rl(7.26p) ↵
Display integration of the spectrum peaks, scale the peaks and integral, and clear old zero points	Part Integral cz f full vsadj isadj ↵
Integrate individual peaks of your choice	Resets -Click left mouse button once on each side of every peak you want to integrate isadj ↵
Normalize the integrals to a particular peak	-Place cursor on known integral region (e.g. a peak that corresponds to 1 Proton)

	Set Int 1.00 <input type="text"/>
Select the starting point and total width of the spectrum to be plotted (e.g. -0.5ppm to 10.5 ppm)	wp=11p sp=-.5p <input type="text"/>
Set the threshold for peak picking	Th <i>-Move the yellow threshold line up or down with the mouse to select only those peaks above the threshold</i>
Plot the spectrum and integral graphics	pl <input type="text"/>
Plot the scale	pSCALE <input type="text"/>
Plot the integral values	pir <input type="text"/>
Plot the peak frequencies (above the threshold)	ppf <input type="text"/>
Plot the text (units out, units up)	pltext(150,150) <input type="text"/>
Plot all the parameters	pap <input type="text"/>
Start plotting	page <input type="text"/>