NMR User Guide for Avance NEO with IconNMR in Topspin 4

- (1) To submit a sample on the Bruker NMR Autosampler, first prepare your sample in ~0.6 mL deuterated solvent in a 5 mm NMR tube. Then gauge the tube properly such that the sample is centered about the RF coil (as circled in red in the picture below) in the NMR probe. Do not move the bottom white stopper.
- (2) Next, put the NMR tube in the Autosampler, e.g. position 4 (as circled in blue in the picture below).





(3) Next, click "**Change User**" (circled in red below) in the IconNMR interface and then log in your user account.



(4) In the IconNMR interface, double click the position # where your sample is located, e.g. 4. Then enter your sample name (e.g. Test), select an experiment # (e.g. 10), choose a solvent (e.g. D2O), and then select an experiment to run (e.g. PROTON).

Expe	erimer	nt Table	00	¥	2					
Hold ▶ 1 ▶ 2 ▶ 3		Гуре Ц Ц	Status Available Available Available	Disk	Name	No.	Solvent	Experiment Pri	Analysis Type	Analysis Settings
- 4		ter 1	Available							
	ŀ	4	Available	/opt/nmrdata/user	✓ Test					
▶ 5	l]	Available		Test	• 10	D2O	de - N PROTON -	No Analysis	
▶ 6	L]	Available					NUMBER OF		
▶ 7	L	l	Available							
▶ 8	L	1	Available							
₽ 9	L		Available							
▶ 10			Available							
D 11	ı L		Available							
▶ 12	2		Available	Hander Hand			1111111	111111111		

(5) Next, click the = sign (see red box below) to pop up the parameter menu where you can edit some of the most important parameters in the experiment.



(6) To edit more parameters in the experiment, click "**Parameters**", "**Edit all Acquisition Parameters**" (circled in blue below) in IconNMR, then it will switch to the Topspin interface where you can edit all the acquisition parameters. When done, click "**Return to IconNMR**" (circled in green below) to switch back to the IconNMR interface.

lconNMR: /	Automatic	on Sep03-20	021-1055-nmr		
<u>Eile R</u> un	Holder N	<u>/iew</u> Find	Parameters Optio	ns <u>T</u> ools	Help
🐯 Sta	rt		Edit <u>all</u> Acquisition I Edit Processing Par Pertinent Acquisitio	rameters n Parameter	
Experime	nt Table		User Specific Comm	ands	-
Holder ▶ 1	Туре	Status Available	Disk		Name
▶ 2	Ш	Available			
⊳ 3	U	Available			
⊽ 4	1 1	Available			
	er	Available	/opt/nmrdata/use	er 🗸	Test

SPECTRUM PR	OCPARS ACOUR	ARS THE PULSEPROG PEAK
бл ѕ 🖌 🗄	St 1,2, Return t	to IconNMR
Experiment Width	Experiment	
Nucleus Receiver	PULPROG	zg30
Durations	AQ_mod	DQD
Power	TD	65536
Program Probe	DS	2
Lists	NS	16
Wobble	TD0	1
Automation Miscellaneous	🔿 Width	
User	SW [ppm]	19.9851
Routing	SWH [Hz]	10000.000

(7) Next, click the Title icon (circled in red below) to pop up a window where you can enter your email address to receive the NMR data when the experiment is finished.



(8) To add another experiment for the current sample, make sure you have the first experiment highlighted, click "**Add**" in IconNMR as shown below and another entry line will pop up where you can set up another experiment.



(9) Finally, highlight the Holder # (e.g. 4) and then click "**Submit**" to submit all experiments for that sample.

(10) When all experiments are finished, your sample will be returned back to the Autosampler if there is another queue after your run. However, if there is no queue after your run, your sample will stay in the magnet. To retrieve your sample, press the green button (circled in green below) to eject your NMR tube. Next, press the blue button with the white arrow to the left of the green button to advance the autosampler. It's best to advance it twice (push, wait a bit, push again).

Please also note that your NMR tube should not be higher than the red bar (circled in red below), otherwise, your sample will not be run.

(11) To log out your account, click "Change User" in IconNMR and then click "Lock IconNMR".

Holder	Type	Status				
▶ 1	L .	Available	Disk	Name	No.	Solvent Fy
▶ 2	Ū	Available			110,	Solvent Ex
▶ 3	ũ	Available				
~ 4	er 1	Available				
	Her	Available	/opt/nmrdata/user	+ Test		
▶ 5	U	Available			• 10	D2O dt - NF
▶ 6	Ū	Available				
▶ 7	U	Available				
▶ 8	L	Available				
₽ 9	U	Available				
▶ 10	U	Available				
D 11	U	Available				
▶ 12	U	Available				
▶ 13	U	Available				
▶ 14	U	Available				
▶ 15	U	Available				
D 16	L	Available				
D 17		Available				
<u>S</u> ubmi	t (Cancel	Edit Delete	Add 1 Copy 1	<u>+</u>	

