## Acquiring Spectra using ICON-NMR The University of Southern Mississippi

1. Open Top Spin 2.1 by double-clicking on the TOPSPIN 2.1 icon.



2. To start ICON-NMR, type 'iconnmr' in the command line (outlined in red in the picture below) and press **Return** or **Enter**.



3. Select Automation (in red) from the list provided.



- 4. Verify that the User ID selected matches your login name.
- 5. Click OK.

🍓 ICON-NMR: Id	entify User	
🗉 Help on logg	ing in	
User ID	User's Full Name	
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final	final haung	
holder	holder	
jojo Johnson	jojo Johnson	
ledford masterson nmr phillips polymer schanz scigen wallace	ledford masterson NMR User NMR SuperUser phillips polymer schanz scigen wallace	
User ID <b>John</b> s	son	·
ОК	Cancel	

6. To set up Sample 1 double-click Holder 1.

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7. An input line will appear below Holder 1.

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- 8. For Sample 1, enter the file **Name** to save data under, the number (**No.**) of the experiment, **Solvent** used and **Experiment** to run.
- 9. Click **Submit** (in red).

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- 10. To run additional experiments on Sample 1, click **Add** (in red above). A new input line will appear below Holder 1.
- 11. Repeat steps 8-10 until all experiments have been entered.
- 12. To run additional samples, repeat steps 6-11 using the next Holder number.
- 13. After all samples and experiments have been entered, select the green gear shaped icon (in red).



14. A new window will pop up. In this window, select Start.

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The  $H_2O/D_2O$  standard will be ejected and your first NMR sample inserted into the probe. The technician will move the  $H_2O/D_2O$  standard to be reinserted once all samples are run. A new window will appear giving the status of the current run.

👋 ICON-NMR: auto Online Controls 🛛 🗖 🔀								
Automation In Progress								
Current Experiment	Info							
Holder No:	1							
Name:	2ethyl1indanone							
No.	30							
Time Remaining:								
Current Expt :	PROTON							
1H experiment 16 so	ans							
View								
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Stop	Search							
Stop Automation								

The status of the run can be followed in the automation window.

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Once the acquisition has begun, information on residual time and scans can be found in the TOPSPIN window, below the command line (in red).



Once all samples are complete, your last sample will eject and the H<sub>2</sub>O/D<sub>2</sub>O standard will be reinserted into the probe. The technician will remove all samples from the carousel.

15. To begin shutting down ICON-NMR, select **Stop Automation** in the ICON-NMR: auto Online Controls window. Select **Yes** in the window that asks, "Really stop the run?"

🎂 ICON-NMR: auto Online Controls 📃 🗖 🔀								
Automation In Progress								
Current Experiment Info								
Holder No:	1							
Name:	2ethyl1indanone							
No.	30							
Time Remaining:								
Current Expt :	PROTON							
1H experiment 16 sc	ans							
View								
Lock								
FID	Spectrum							
Controls								
Halt	Autoplot							
Stop	Search							
Stop Automation								

16. In the ICON: Automation window, select File > Close All. Select No in the window that asks, "Save set up before closing?" Select OK in the window that warns, "You do not have permission to change the configuration of ICON-NMR."

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Print (List Setup) Print <u>H</u> istory File						
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17. In the ICON-NMR: spect window, select **File > Exit**.



18. In the Bruker TOPSPIN 2.1 window, select File > Exit.

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Open [Ctrl O]
Reopen
Close [Ctrl W]
Close All
Save [Ctrl S]
Print [Ctrl P]
Export
Send To
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Delete
1 MentholH 10 1 C:\Bruker\TOPSPIN Johnson
2 Carbon 1 1 C:\Bruker\TOPSPIN Johnson
3 MentholC 20 1 C:\Bruker\TOPSPIN Johnson
4 MentholC 40 1 C:\Bruker\TOPSPIN Johnson
5 MentholC 10 1 C:\Bruker\TOPSPIN Johnson
6 2ethyl1indanone 10 1 C:\Bruker\TOPSPIN Johnson
Exit [exit]

- 19. Select **OK** in the window that warns, "Close Top Spin. This will terminate all possible active commands. Exit anyway?"
- 20. From the Start menu, select Log Off to end your session.