User's Guide to NMR, 2024 Without Autosampler: Draft 2/1/2022. Help: Dr. Jasperse, Hagen 407J, 477-2230

- 1. Prepare sample in lab; add sample to sample-holder; adjust sample depth using golden depth finder
- 2. Eject/Insert (Sample Exchange):
 - a. Hit "eject" button (below black field) to eject existing sample. (If not visible, click "start" button to make it so)
 - b. Manually lift out sample-in-sample-holder combination from the probe (place it in a box)
 - c. Place your sample-in-sample-holder into the probe
 - d. Hit "insert" button on the computer. (Wait ≥ 5 seconds before proceeding with step 3a).



- 3. <u>Spot Assignment</u>: (Each sample needs to be assigned a sample spot number)
 - a. Right-click on the lowest-numbered gray spot number in the zones map. (A pulldown will appear)
 - b. Select "Sample in Magnet" (<u>3rd line from the bottom</u> of the pulldown);
 - c. Enter your spot number into the upper field. (Remember your spot number)
 - d. Hit <u>OK</u>.



⊖ Leave	current sam	nple in the	magnet			1	~
○ Rem	ve current sa	ample fror	n the mag	gnet		1	
Repla	ce current sa	ample in ti	he magne	t with new s	ample	11	_

- 4. NMR-Experiment Submission:
 - a. Click "New Study" button in lower left. (A yellow experiment file-name will appear).
 - b. The default experiment is "Proton-8"; for something different select from panel on upper left.
 - c. Left-mouse single-click on your sample spot. (A white circle will appear around the sample spot)
 - d. Enter student name(s) into Sample Name field, which is underneath the black field
 - e. Submit: click the green "Submit" button on the lower left side. (your sample spot should turn color)
 - f. Hit "Cancel" to leave submit-sample mode.
 - a. Don't forget to do this. If you do, it will cause problems for both you and the ensuing user.
 - b. The yellow experiment file-name will disappear; unfortunately the zones map will too.
 - g. Re-open "zones" map: Click on little circle icon (2) to the upper left of the big gray/black panel, and the zones map with all the sample spot numbers should re-open.
 - Note: An experiment should take about 7 minutes.
 - There should be an automatic one-page printout upon completion.

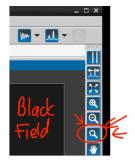


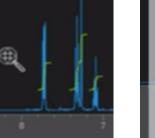
- 5. <u>Printing an extra copy</u> of spectrum (in case you have a partner)
- Must be in zones-map display. If not, click on little circle icon () upper left of the spectra-display panel.
- a. Right click on sample number, and a pulldown will appear
- b. Click "Show Study"
- c. <u>Double click</u> on green "PROTON_01" file that will appear in the lower left-hand area. (below your name)
 a. Your spectrum should now appear in the display field, where the zones-map appeared before
- d. Click "Process" button underneath the spectrum display field. ("Start" was highlighted previously)
- e. Click blue-text-on-white-background "Print" button on lower right to print another copy.



6. <u>Horizontal Expansions</u>

- a. Steps 5a-d above describe how to get your spectrum loaded into the display field.
- b. With spectrum displayed on screen, use a panel of display icons on the far upper right
- c. Click on the magnifying glass icon (6th icon down, \square)
- d. Move your cursor to the left end of the zone you want to expand, then hold down left mouse button and slide it to the other end of the zone you want to expand, then release the button.
 - a. To return to the full display, you can either click on the 3^{rd} icon (E) or the 5^{th} icon (E).
- e. Click blue-text-on-white-background "Print" button on lower right to print a copy. (Twice for 2 copies)











7. Exiting so that NMR is Ready for the Next user

- a. Click "Start" button underneath the spectrum display field. ("Process" was highlighted previously)
- b. Re-open "zones" map: Click on little circle icon ((a)) to the upper left of the big gray/black panel, and the zones map with all the sample spot numbers should re-open.



