

Bruker Prodigy User Guide
500 MHz
March 2017

General Considerations

Be aware of the stray magnetic field. Keep all ferromagnetic items outside the five-gauss perimeter (delineated by the yellow chain).

Always use tubes that are not cracked at the top, not single-use tubes, and preferably are rated for 500 MHz instruments to avoid damaging the probe. Do not use J Young tubes, Shigemitsu tubes, or other non-standard NMR tubes.

Never close any of the windows, even if you think you may have opened the window.

If a sample breaks or the instrument stops functioning, stop immediately, contact staff, and place the “Do not use” sign on the keyboard.

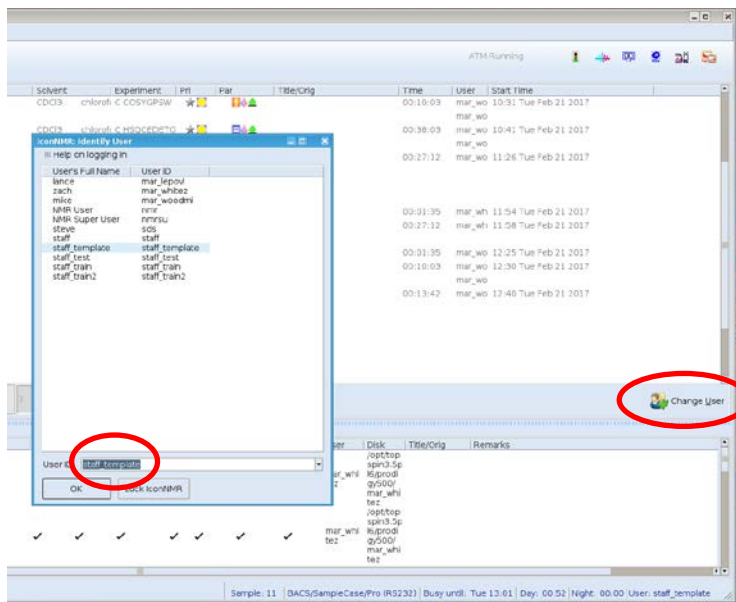
The time limit during the day (8 am – 10 pm) is 2 hours. A full set of 2D data takes approximately 1-2 hours. Please be considerate of other users when submitting samples. The night queue is from 10 pm until 8 am. The time limit for the night queue is 8 hours.

Liquid nitrogen fills are at 8 am on Monday and Wednesday mornings. Please plan accordingly.

Bruker Prodigy data cannot be processed on the Agilent workstations.

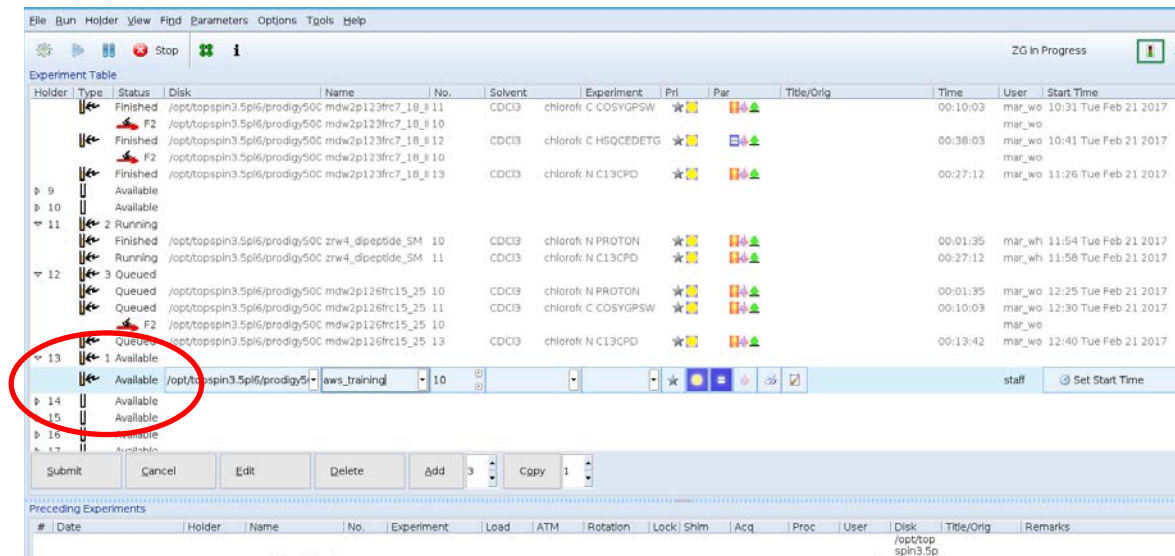
Sample Submission

Log in by clicking your username in the list, followed by “OK.” (You may have to click the “Change User” button if the last person forgot to do so.)

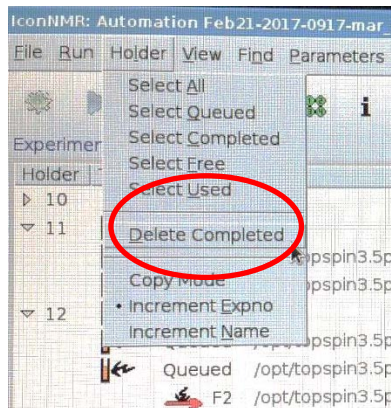


A window will appear prompting you for your password. Enter your password.

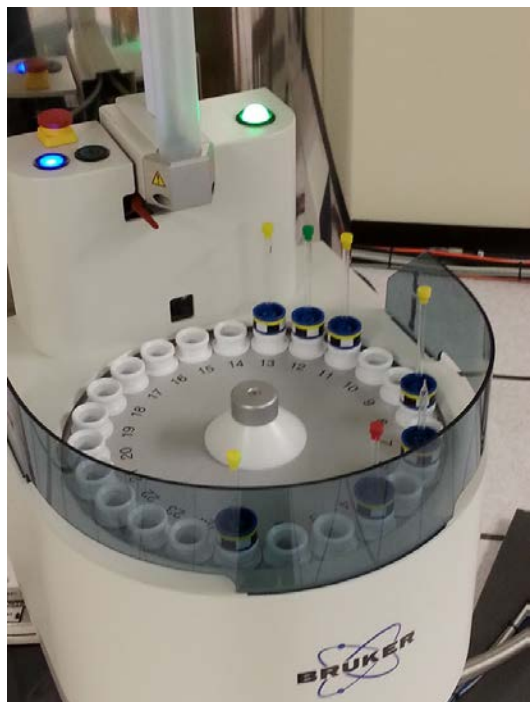
Choose a position that is "Available." Double click the number (in this example, # 13). A new line will appear.



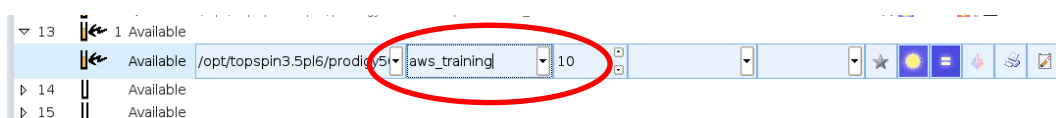
If no positions are available, go to "Holder" in the menu bar, and choose "Delete Completed," then choose an available position.



Carefully wipe your tube, insert it into the spinner, and depth-gauge the tube. Place the tube in the appropriate position in the carousel.



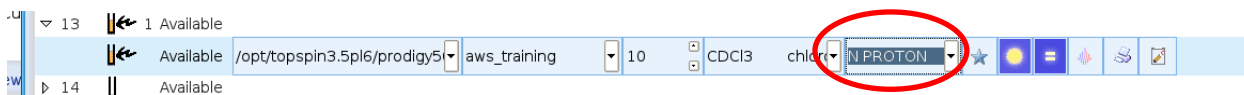
Enter your sample name in the “Name” field. The experiment number (10 in this case) will be filled in automatically. You have the option of changing the number.



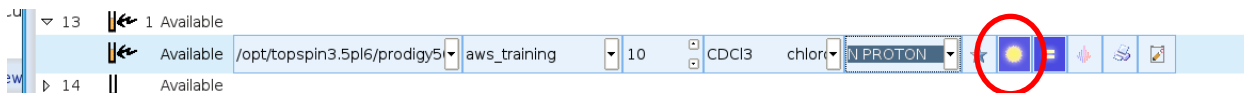
In the “Solvent” field, choose your deuterated solvent from the drop-down menu.



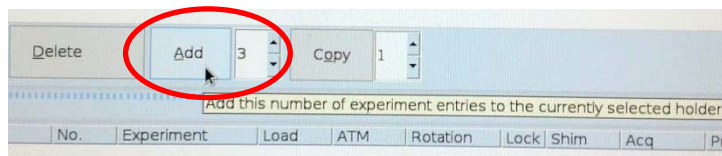
In the “Experiment” field, choose your experiment.



Use the “sun/moon” button to choose whether your sample runs on the day queue or the night queue.

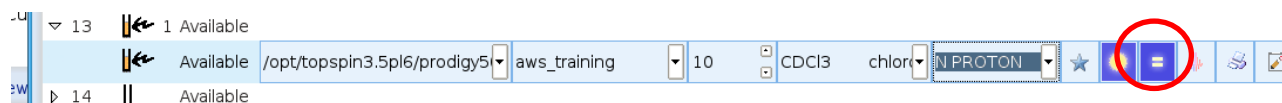


To add additional experiments (for example, to add a COSY, HSQC, and Carbon), enter the number of experiments to be added (3 in this example), then click “Add.”

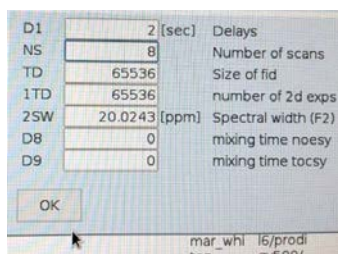


Desired Experiment	Select (default parameters can be changed for these experiments)
PROTON	1H experiment
CARBON	13C experiment with decoupling, 1024 scans, 235 ppm
COSY	Gradient selected COSY
HSQC	1H-13C multiplicity edited HSQC with gradient selection BF1 <= 600 MHz
PRESAT	CMC Single

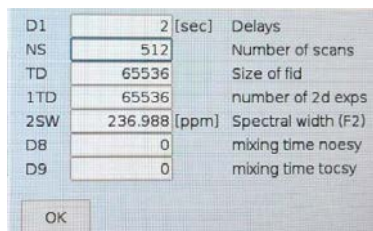
To edit the acquisition parameters for an experiment, click the blue icon with the yellow “=” sign on the row.



- For a proton spectrum on a small molecule (not a polymer), D1 should be set to 2 seconds. The number of scans will depend on the concentration of the sample. Set NS (number of scans) to a minimum of 8.



- For a carbon spectrum on a small molecule, D1 should be set to 2 seconds. Again, the number of scans will depend on the concentration. For a sample that contains 10 mg or more of a small molecule, 256 (15 minutes to acquire) or 512 (30 minutes to acquire) may be sufficient.



- For a COSY spectrum, D1 should be 2 seconds. The number of scans (NS) will depend on the concentration. For samples containing at least 10 mg of compound, 1 scan is probably sufficient. The minimum number of increments (1TD) is 256. For better resolution, increase 1TD to 512.

D1	2	[sec]	Delays
NS	1		Number of scans
TD	2048		Size of fid
1TD	256		number of 2d exps
2SW	13.0028	[ppm]	Spectral width (F2)
D8	0		mixing time noesy
D9	0		mixing time tocsy

OK

- For an HSQC, D1 should be 2 seconds. The minimum NS is 4. The minimum 1TD is 256.

D1	2	[sec]	Delays
NS	4		Number of scans
TD	2048		Size of fid
1TD	256		number of 2d exps
2SW	15.9769	[ppm]	Spectral width (F2)
D8	0		mixing time noesy
D9	0		mixing time tocsy

OK

- For a NOESY, D1 should be 2 seconds. The minimum NS is 4. The minimum 1TD is 256. D8 should be changed to 0.8.

D1	2	[sec]	Delays
NS	4		Number of scans
TD	2048		Size of fid
1TD	256		number of 2d exps
2SW	15.9769	[ppm]	Spectral width (F2)
D8	0		mixing time noesy
D9	0		mixing time tocsy

OK

0.8

Be sure the first line (the one with the carousel position number) is highlighted.

Click the "Submit" button.

▶ 16 Available
▶ 17 Available


Submit Cancel Edit Delete Add 3 Copy 1

Preceding Experiments

When you are finished submitting samples, click “Change User.”



Please come back when your sample is scheduled to be completed and take it out of the carousel so that others may use it.

If your sample is positioned below the pneumatic tube, press the blue  button to advance the carousel.



To download your data from the Welch server using Filezilla, go to:

/mnt/prodigy

