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

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.

To log out your account, click “Change User” in IconNMR and then click “Lock IconNMR”.