

NEO300 General Instruction Sheet

When you set up your automated runs you will first need to log in to iLab and start a short session on the Bruker neo300. This will turn on the computer display so that you can enter your information. This session only needs to be long enough to cover the amount of time needed to set up your information in IconNMR.

During the daytime please limit your submissions to experiment(s) which will take no longer than ca. 30 minutes. This is 6 ^1H acquisitions, or two $^1\text{H} + ^{13}\text{C}$ acquisitions, using the standard parameters. If you want to run longer experiments please set these up during the evenings or weekends.

If there are locations free in the carousel you may use those for your sample(s). If there are entries in the IconNMR software which show the status "Completed" you may remove the associated samples from the carousel and place them in the correctly numbered positions in the white plastic sample tube rack labeled "1." You may also delete these entries from IconNMR and then replace them with your own.

You may use the blue button on the carousel unit to rotate the carousel to allow easy changing of the samples.

Please keep unused spinners in their dedicated case.

NOTE: sample tubes may be **NO LONGER THAN 9 inches**.

Please clean your samples and spinners before putting them in the carousel. Keep any unused spinners in the case. Position 24 in the carousel is reserved for the autotest sample with the yellow spinner, which stays there.

The first step is to pick a sample holder and use the "Add" button and the number increment adjustment to add the number of experiments you want to run on this sample.

The NMR data directory is: /opt/nmrdata - please do not change this.

The "Name" field (dataset name) must contain the user's Purdue ID and the date in the following format:

jharwood-05012023-extrainfo

additional text can be appended as shown by the "-extrainfo" text above. The first - between ID and date **MUST** be present.

You may change the parameters ns (number of scans), d1 (relaxation delay) and td (digital resolution). You may toggle hardcopy printing on and off as desired.

In the "Title/Orig" field the user's account number (digits only, no letters or periods) and their Purdue email address must be entered in the associated blanks.

After you have completed the entry for your first sample you can use the "Copy" button and its number increment adjustment to duplicate this entry for however many sequential holder numbers you select.

The standard setup will generate processed data with peak picking and integration as well as a PDF-format printout included in the processed data directory.

Ultimately we expect to set up the automation so that it will email each user a notification when their samples are finished and also send the data as a zip file. However, you may also log in to the neo300 host and retrieve your data using the following information:

IP address: 10.166.20.6

Full name: neo300.pinmrf.purdue.edu

Shared login & password: localnmr WTnmr#00

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