**Quick guide for Icon NMR automation mode (400 MHz) (version 1.2)**

When you approach the magnet, always make sure you leave behind electronic or magnetic devices and small loose ferromagnetic objects. People with medical implants like pacemakers are generally not allowed into the lab and must stay well outside indicated lines on the floor. Violation of these rules can also cause severe damage to the instrument.

* Change user name (talk to administrator if you don’t have a user name yet)
* Select a vacant position in the autosampler. If all positions are taken, remove one which is finished and delete that entry in the program (and attach the correct label on the sample and place sample in correct position of the sample rack on the table)
* Select a name for your experiment, experiment number (if more than one experiment is run for the same sample), solvent, parameter file, parameters (number of scans, temperature, etc), title and priority (night/day). Priority is only to be used for unstable compounds or when approved by administrator. Long runs (>2 hours) should be run at night.
* Wipe off the tube to remove greasy fingerprints. Place your sample in a blue spinner using the fixed depth gauge (squared, 2.0 cm), and position it in the correct place in the autosampler. If you are running high temperature (50 – 100 oC) use the gray spinner. High temperature experiments must be approved by administrator. All samples must have a corresponding label that should be placed in the sample rack on the table.
* Click “submit”. Samples will be run in the order submitted to the queue.

The parameter list will be changed continuously. If you don’t know what parameter files to use, ask administrator or other experienced users. If you want other experiments included in the list, or need to make specific modifications to the experiment setup, please contact administrator. Generally, all experiments are run at 25 oC, but higher temperature is possible (users need special privilege). When running high-temperature experiments, always end with an experiment at 25 oC (set to 297 K because of calibration) so that temperature is correctly set for the next user (and instrument is not subjected to high temperature longer than necessary). The program only reads the temperature setting from the first experiment for each sample! Low temperature is not possible in automation and must be arranged with administrator.

If nobody is waiting in line, you may process and print out your results with the 400 MHz workstation. Alternatively you may use the workstation “pecan” or download the data to your own computer (recommended).

For more elaborate description on how to use Icon-NMR, see manuals available at the NMR-lab or online at <http://www.bruker-biospin.com/documentation_nmr.html> (requires log in).