

# KINETICS EXPERIMENTS ON BRUKER AVIIHD 500

There are many different options for running kinetics experiments using IconNMR, the front end to TopSpin.

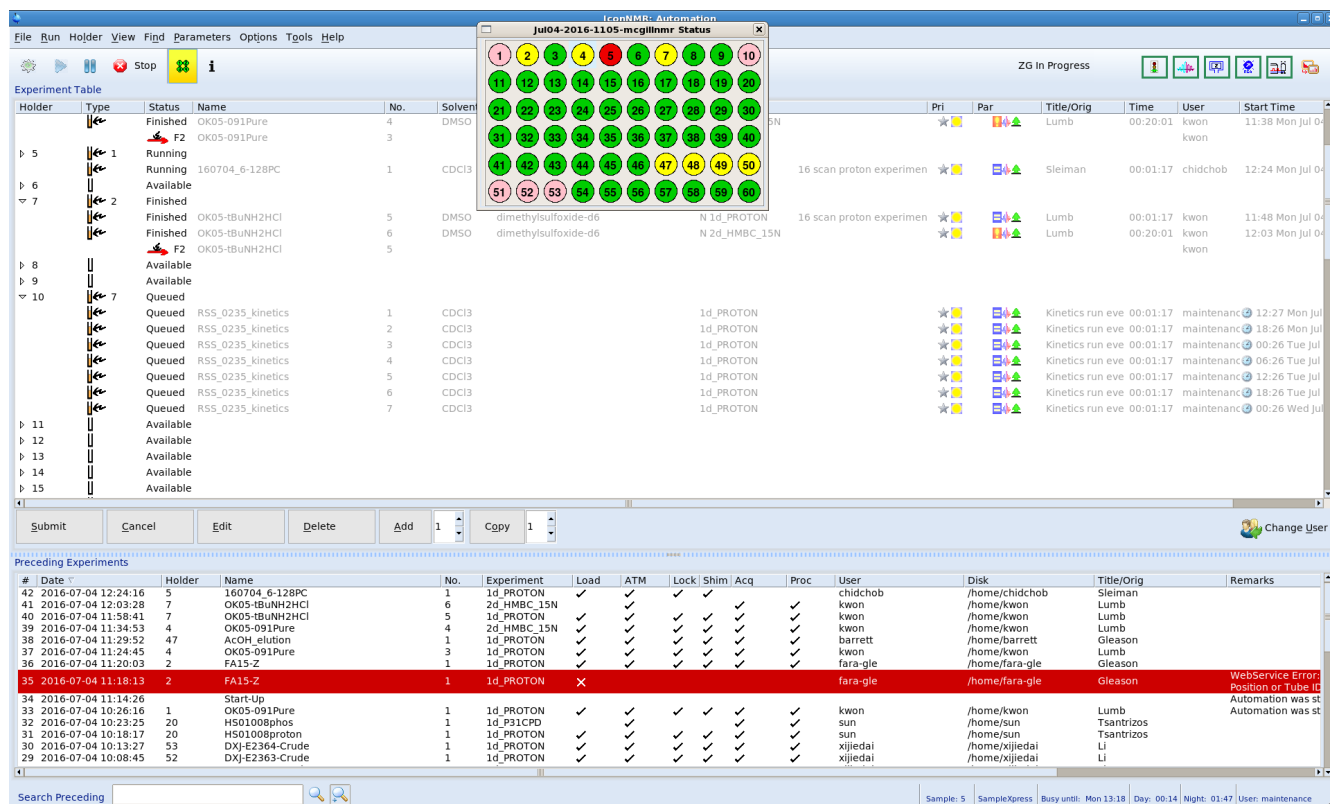


Figure 1: IconNMR, the automation front end to TopSpin.

## General notes

1. During the night (after 7 PM), please do not run experiments more frequently than every 3:10 (three hours and ten minutes), so as to allow long carbon experiments to run between the kinetics experiments.
2. The spectrometer will do its best to run the experiments at the requested times, but there will always be a slight difference between the requested start time and the actual experiment run time. To find out exactly when an experiment was run, use the command `date` in TopSpin after running the experiment and loading it in TopSpin. Or, in Mnova, use View / Tables / Parameters.
3. If you must keep your sample not at room temperature in between NMR experiments, then you can still line up experiments in the queue (see options 1 and 2 below). You must place another sample in the sample changer to hold your position until the time comes to run the sample.

## Option 1: Specify exact start time

After entering information for an experiment, you can click on the Set Start Time button and

enter an exact time when you would like the experiment to run.

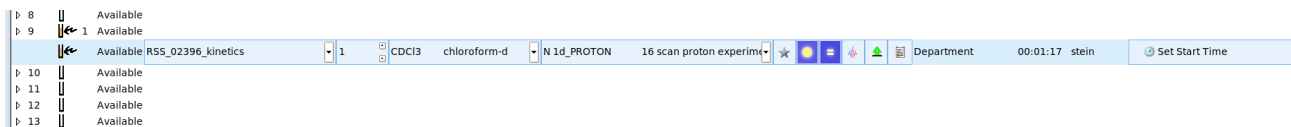


Figure 2: Submitting an experiment to IconNMR

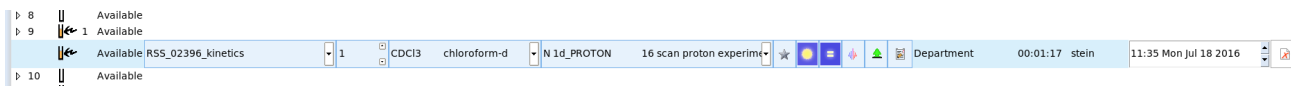


Figure 3: When submitting an experiment to IconNMR, clicking on the Set Start Time button on the far right enables you to select an exact time to run an experiment at.

You can run multiple experiments on the same sample at defined times using this method, and you can set up different experiments to run this way.

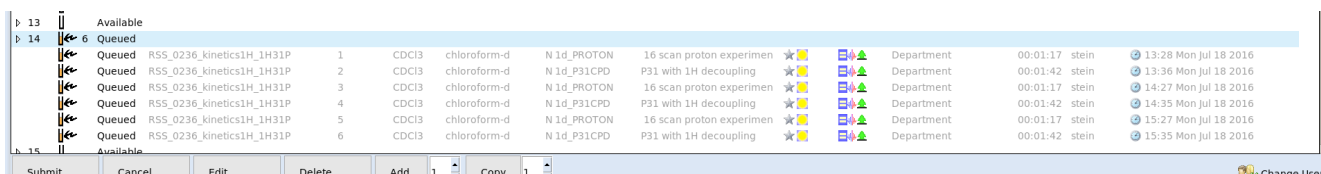


Figure 4: Proton and phosphorus experiments scheduled to run every hour

## Option 2: Use Tools / Run an Experiment Periodically to set up periodic experiments

This method works particularly well if you want to run a lot of experiments. Use the Tools menu and choose Run an experiment periodically to set up periodic experiments.

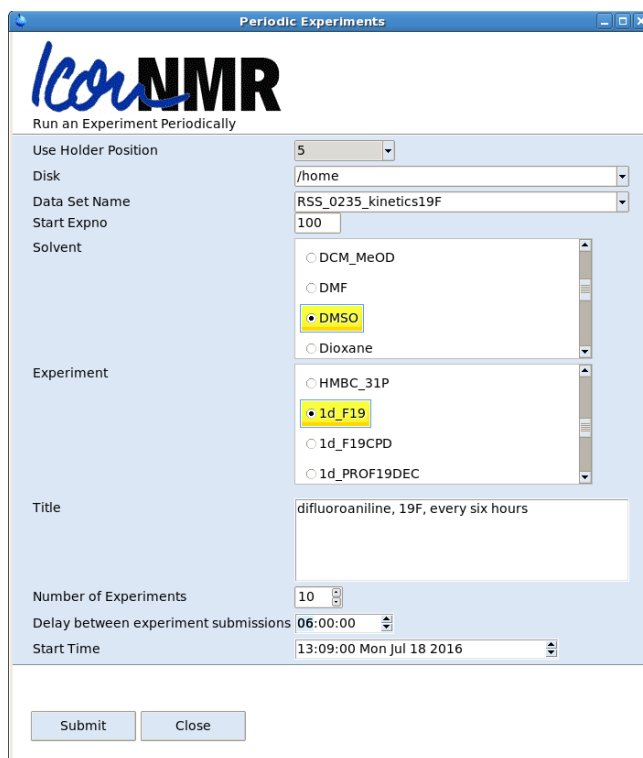


Figure 5: Setting up to run an experiment periodically. You can use Tools / Run an experiment periodically for different experiments for the same sample, but be sure to change either Start Expno or Data Set Name to avoid datasets being overwritten.

You can use the same menu entry to set up multiple experiments for the same sample (e.g. proton and fluorine). However, if you are submitting two different experiments for the same sample, change Data Set Name or change the expno so that there is no overlap between the two experiments. For example, if you run proton experiments with Start Expno = 1 and Number of Experiments = 10, then any other experiments you run on that sample must have Start Expno greater than 10, or a different Data Set Name. The reason for this is that every piece of data that TopSpin creates requires a distinct combination of Data Set Name and Expno.

Status	Expno	Solvent	Experiment	Title	Start Time
Finished	1	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	13:10 Mon Jul 18 2016
Queued	2	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	13:19 Mon Jul 18 2016
Queued	3	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	13:29 Mon Jul 18 2016
Queued	4	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	13:39 Mon Jul 18 2016
Queued	5	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	13:49 Mon Jul 18 2016
Queued	6	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	13:59 Mon Jul 18 2016
Queued	7	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	14:09 Mon Jul 18 2016
Queued	8	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	14:19 Mon Jul 18 2016
Queued	9	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	14:29 Mon Jul 18 2016
Queued	10	DMSO	1d_PROTON	difluoroaniline, 1H, every 00:01:17	14:39 Mon Jul 18 2016
Running	100	DMSO	1d_F19	difluoroaniline, 19F, ever 00:00:32	13:10 Mon Jul 18 2016
Queued	101	DMSO	1d_F19	difluoroaniline, 19F, ever 00:00:32	13:20 Mon Jul 18 2016
Queued	102	DMSO	1d_F19	difluoroaniline, 19F, ever 00:00:32	13:30 Mon Jul 18 2016
Queued	103	DMSO	1d_F19	difluoroaniline, 19F, ever 00:00:32	13:40 Mon Jul 18 2016
Queued	104	DMSO	1d_F19	difluoroaniline, 19F, ever 00:00:32	13:50 Mon Jul 18 2016
Queued	105	DMSO	1d_F19	difluoroaniline, 19F, ever 00:00:32	14:00 Mon Jul 18 2016

Figure 6: Proton (expno 1-10) and fluorine experiments (expno 1-10) queued to run every ten minutes.