

Running Multiple Experiments on the Same Sample Automatically (multizg, spooler/queue, iconnmr)



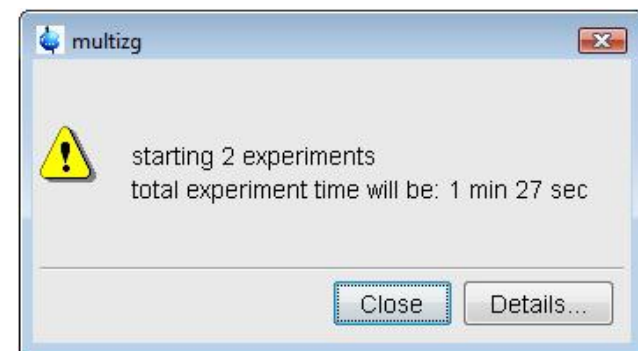
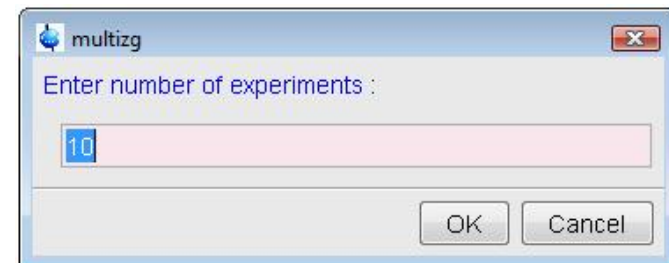
Multiple Experiment Setup

- If you have one sample that requires full characterization (e.g. ^1H , ^{13}C , COSY, HMBC etc.) and you do not want to wait until the previous experiment finishes to start the next one. There are ways to setup you experiments and have them run automatically.
- For systems without an auto sampler, this can only be done on one sample at a time.
- There are various way in which this can be achieved, here touches upon three common methods:
 - Using the *multizg* command
 - Setting up a queue of experiments
 - Through iconNMR (only available for UTL300 with an autosampler)



Multizg

- Multizg runs experiments that have been setup sequentially within the same experiment folder automatically.
- **Setup**
 1. Create a new experiment folder, insert sample and do the preacquisition processes as usual (e.g. lock, tune, shim, adjust receiver gain)
 2. Make new experiment files for each type of experiment that you want to acquire. Keep the same folder but change EXPNO.
 3. Go back to the first experiment of the list and execute the *multizg* command. A popup window will ask “How many experiment do you want to perform” so enter the number of experiments that you created.
- **Advantages**
 - Only one command needed
- **Disadvantages**
 - Once the multizg is running it is difficult to stop the entire process
 - Additional experiments cannot be appended to the list

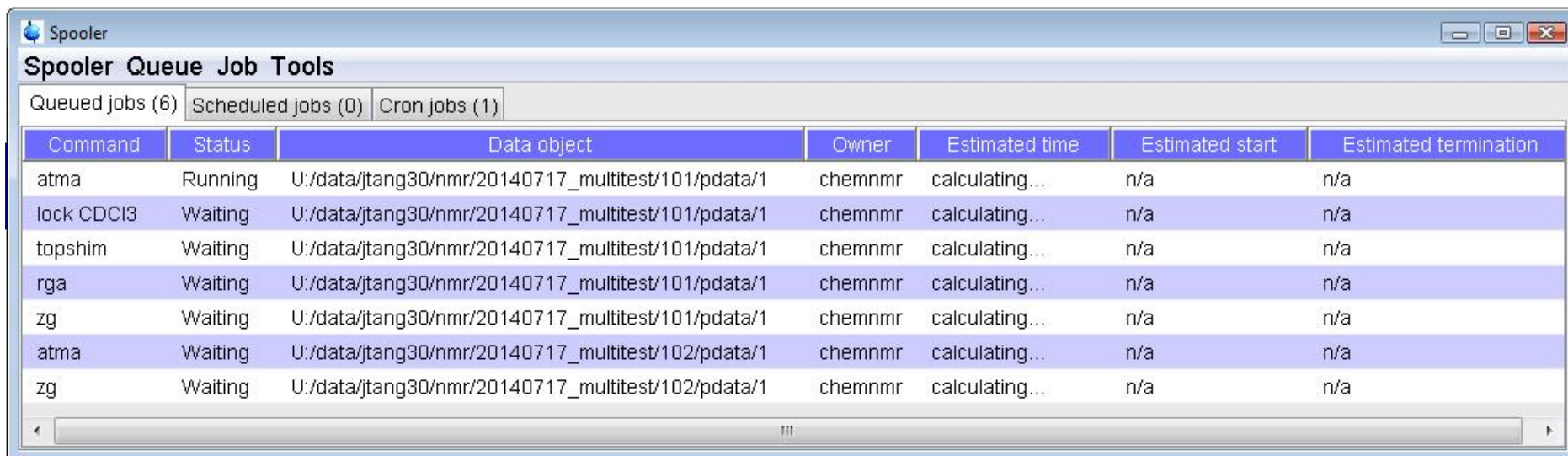


Spooler / Queue

- A better alternative is to use the *spooler* command and setup a study queue.
- **Setup**
 1. Create a new experiment folder, insert sample and do the preacquisition processes as usual (e.g. lock, tune, shim, adjust receiver gain)
 2. Enter the command *spooler* in the command line which will bring up the spooler window. This lists all the commands that are in queue.
 3. To add a command to the queue list use the command '**qu <command>**' (e.g. **qu zg**). You can input any type of Topspin command, acquisition and processing.
 4. If multiple experiments are desired, read in the next experiment number then queue the commands for that experiment.
 5. Alternatively, for multiple EXPNOs use the command '**qumulti**'. This will bring up a New Job window with all experiments listed in the current data set. Enter the command to be executed and check off all EXPNOs for it to be executed on.



Spooler Window



The screenshot shows a window titled "Spooler" with a sub-header "Spooler Queue Job Tools". Below the sub-header are three tabs: "Queued jobs (6)", "Scheduled jobs (0)", and "Cron jobs (1)". The "Queued jobs (6)" tab is active, displaying a table with the following data:

Command	Status	Data object	Owner	Estimated time	Estimated start	Estimated termination
atma	Running	U:/data/jtang30/nmr/20140717_multitest/101/pdata/1	chemnmr	calculating...	n/a	n/a
lock CDCI3	Waiting	U:/data/jtang30/nmr/20140717_multitest/101/pdata/1	chemnmr	calculating...	n/a	n/a
topshim	Waiting	U:/data/jtang30/nmr/20140717_multitest/101/pdata/1	chemnmr	calculating...	n/a	n/a
rga	Waiting	U:/data/jtang30/nmr/20140717_multitest/101/pdata/1	chemnmr	calculating...	n/a	n/a
zg	Waiting	U:/data/jtang30/nmr/20140717_multitest/101/pdata/1	chemnmr	calculating...	n/a	n/a
atma	Waiting	U:/data/jtang30/nmr/20140717_multitest/102/pdata/1	chemnmr	calculating...	n/a	n/a
zg	Waiting	U:/data/jtang30/nmr/20140717_multitest/102/pdata/1	chemnmr	calculating...	n/a	n/a

- When using the lock command, ensure you specify which solvent to lock on. If not, you will be prompted to select the solvent and the queue will not continue until then.
- When doing multiple nuclei on one channel ensure that you retune the probe before the next experiment is acquired as seen above.
- To delete a command, right click on command line and select 'Delete' in options menu.



Spooler / Queue

- **Advantages over *multizg***
 - Displays all experiments to be run in a easy to use GUI
 - Able to stop acquisitions easily in the event of improper parameter setup
 - Typing '**stop**' in the command line will auto-suspend all spooler commands
 - Delete any or all items in the spooler by right-clicking and select delete
 - Able to queue any Topspin command (i.e. **atma**, **rga**, **ef**, **apk**, etc.)
 - Displays exact end time for each experiment
 - Able to manipulate experimental parameters for acquisitions already in the spooler (i.e. number of scans, number of 2D/3D increments, etc.) and end time will be automatically recalculated
 - Not necessary to run experiments that are in sequential EXPNOs or even under the same experiment name

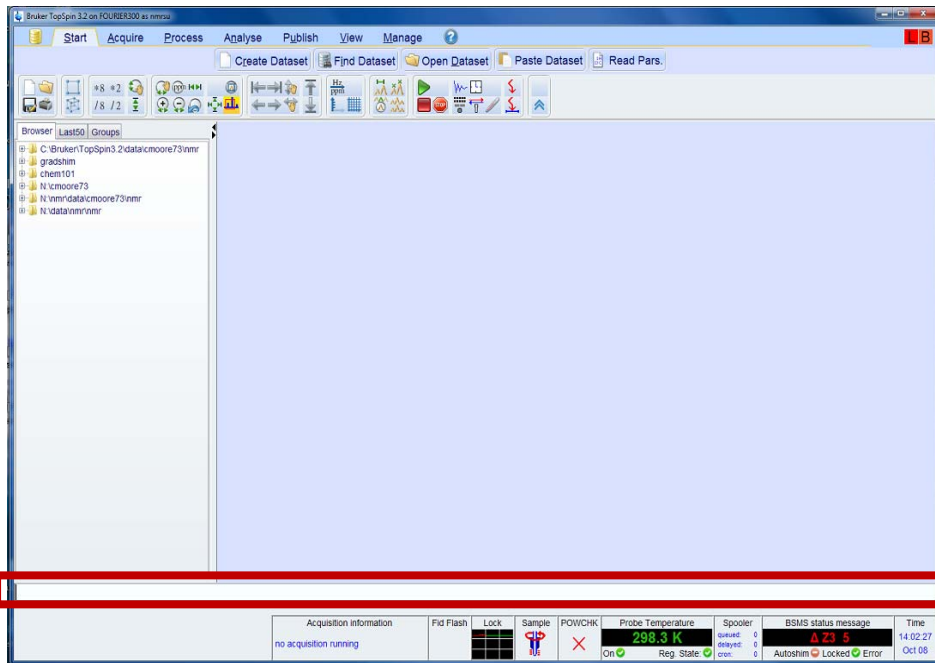


iconNMR

- IconNMR should only be used on the UTL300 spectrometer equipped with an autosampler.

- **Steps:**

Open Topspin, if it is not already open



Type *iconnmr* on the command line

Choose **Automation**

Pick userID and provide password with prompt



File Run Holder View Find Parameters Options Tools Help

Start [Icons]

Experiment Table

Ho...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	1	[Icons]	N:\	20131008-sample1	10	CDC13	chlo	N PROTON.f	[Icons]	test		nmr	[Set Start Time]
2	[Icons]	[Icons]											
3	[Icons]	[Icons]											
4	[Icons]	[Icons]											

Populate 6 fields:

- Disk: N:\ (auto populates)
- File Name
- Experiment number (auto populates)
- Solvent (from drop down)
- Experiment (from drop down): N PROTON.f or N PROTON
- Title (if needed)

[Submit] [Cancel] [Edit] [Delete] [Add] 1 [Copy] 1

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig	Remarks

Highlight experiment to copy and click **copy** button and change number to the number of samples you have to run. Then edit sample name and/or text

[Submit] [Cancel] [Edit] [Delete] [Add] 1 [Copy] 1

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig	Remarks

Highlight experiments to run and click **submit** button

HoL...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	1		N:\	20131008	10	CDCB3	chlorof N PROTON.f			test	00:00:51	nmr	14:09 Tue Oct 08 201
2													

Status light will be yellow after submitting

HoL...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	1		N:\	20131008	10	CDCB3	chlorof N PROTON.f			test	00:00:51	nmr	14:09 Tue Oct 08 201
2													

Once all samples are submitted click the green **start** icon

SampleXpress/Pro WebService

First sample: 1

First sample in the magnet (locked and shimmed)?

Start Cancel

A new window will pop-up, click **start** again

2	1		N:\	20131008-test	20	CDCB3	chlorof N PROTON.f			test	00:00:51	nmr	14:21 Tue Oct 08 201
3	1		N:\	20131008-test	30	CDCB3	chlorof N PROTON.f			test	00:00:51	nmr	14:23 Tue Oct 08 201

Status light will stay yellow until sample is progress, at which time it turns green



The screenshot displays the IconNMR software interface. At the top, a menu bar includes File, Run, Holder, View, Find, Parameters, Options, Tools, and Help. Below the menu is a toolbar with icons for Stop, information, and other functions. The main area features an "Experiment Table" with columns for Holder No., Type, Status, Disk, Name, No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, and Start Time. The table lists three experiments (1, 2, 3) for holder 20131008-test, all using CDCB solvent and N PROTON.f experiments. A pop-up window titled "IconNMR: auto Online Controls" is open, showing "Automation In Progress" and "Current Experiment Info" for holder 2, name 20131008-test, no. 20, with 1H exp. 16scans remaining. The window includes "View" options (Lock, FID, Spectrum) and "Controls" (Halt, Autoplot, Stop, Search, Stop Automation). A blue box highlights the "Stop Automation" button, with arrows pointing to it from a text box on the right that says "current function highlighted." The bottom status bar shows a search function, a search bar, and system information: SampleXpress/Pro WebService, Busy until: Tue 14:25, Day Experiments: 00:01, Night Experiments: 00:00, User: nmr.

Holder No.	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
20131008-test	1	●●●	N:\	20131008-test	10	CDCB	chlo N PROTON.f			test		nmr	
20131008-test	2	●●●	N:\	20131008-test	20	CDCB	chlorof N PROTON.f			test	00:00:51	nmr	14:21 Tue Oct 08 201
20131008-test	3	●●●	N:\	20131008-test	30	CDCB	chlorof N PROTON.f			test	00:00:51	nmr	14:23 Tue Oct 08 201

Automation In Progress

Current Experiment Info

Holder No: 2
Name: 20131008-test
No: 20
Time Remaining:
Current Expt: N PROTON.f 1H exp. 16scans

View

Lock
FID Spectrum

Controls

Halt Autoplot
Stop Search
Stop Automation

Search
Preceding

SampleXpress/Pro WebService | Busy until: Tue 14:25 | Day Experiments: 00:01 | Night Experiments: 00:00 | User: nmr

Also new pop-up window allows you to stop the automation run

Lower portion of the screen summarizes experiment and provides any errors in the remarks.

