Running Multiple Experiments on the Same Sample Automatically

(multizg, spooler/queue, iconnmr)

Multiple Experiment Setup

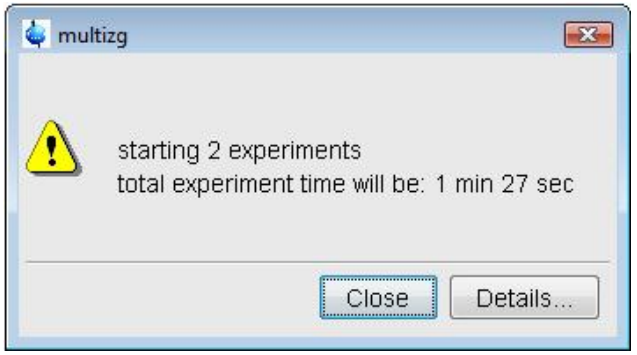
- If you have one sample that requires full characterization (e.g. ^{1}H, ^{13}C, COSY, HMBC etc.) and you do not want to wait until the previous experiment finishes to start the next one. There are ways to setup you experiments and have them run automatically.

- 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.

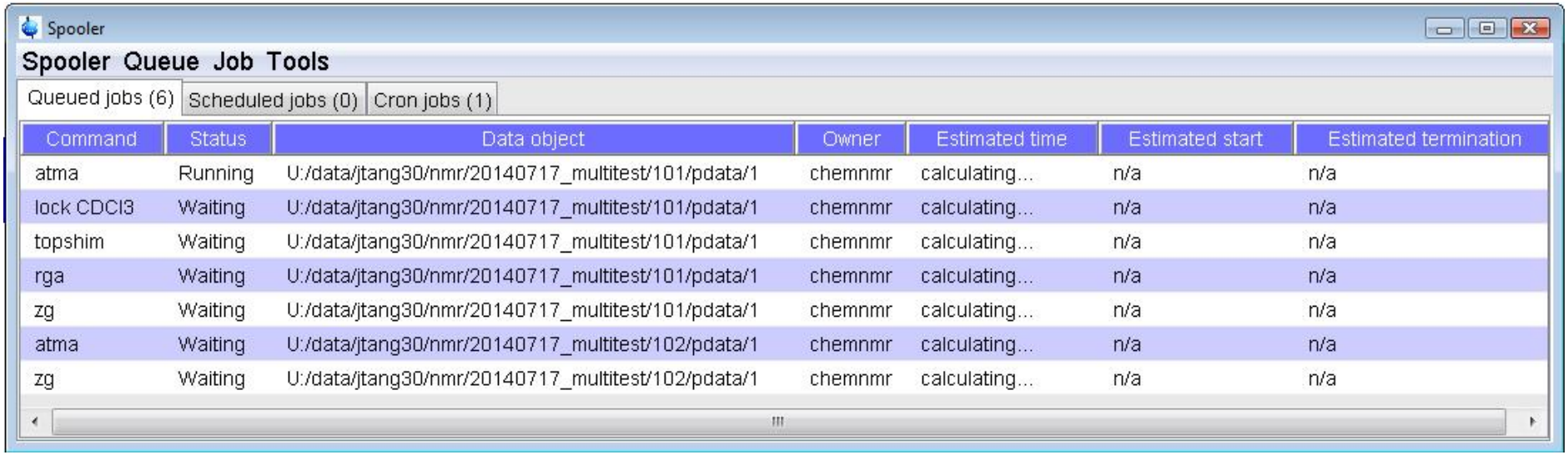


- **Advantages**
  - Only one command needed
- **Disadvantages**
  - Once the multizg is running it is difficult to stop the entire process
  - Additional experiments cannot be appended to the list

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



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 CDCl3	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.

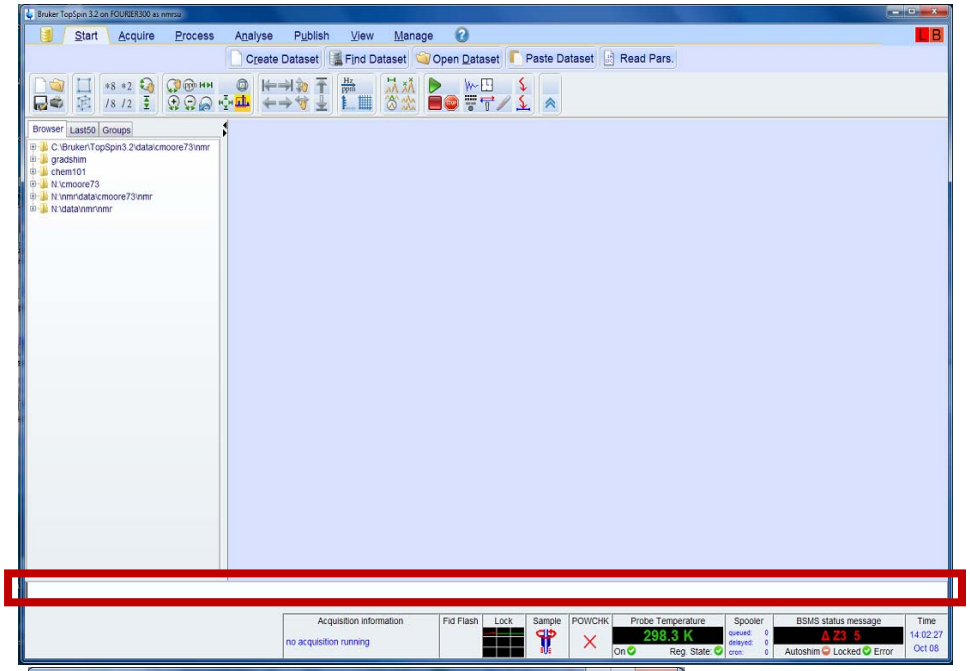
Spooler / Queue

- **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:**

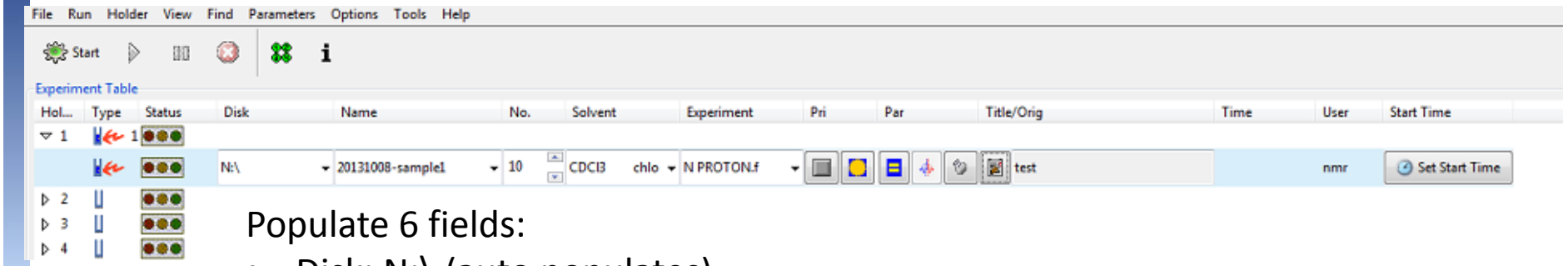
Open Topspin, if it is not already open



Type ***iconnmr*** on the command line

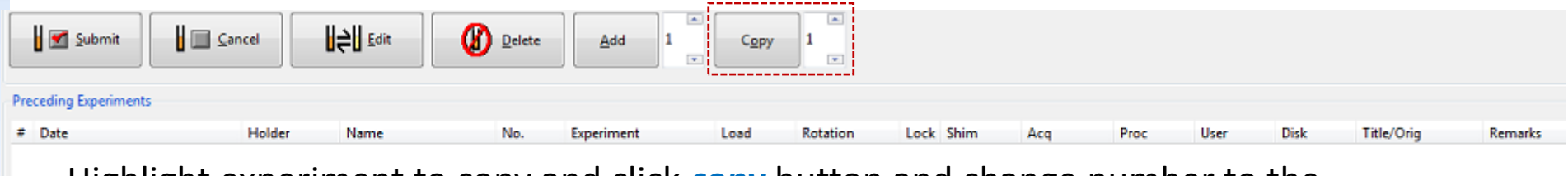
Choose **Automation**

Pick userID and provide password with prompt

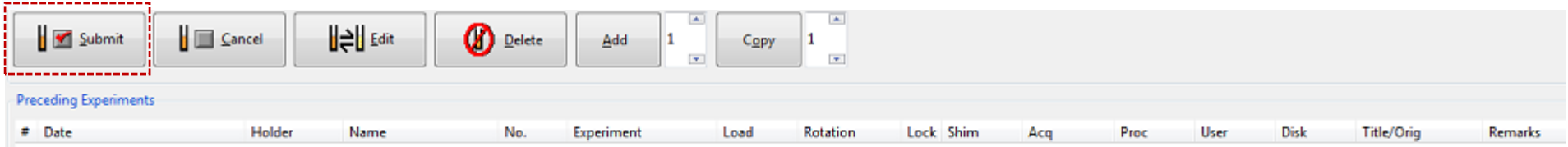


Populate 6 fields:

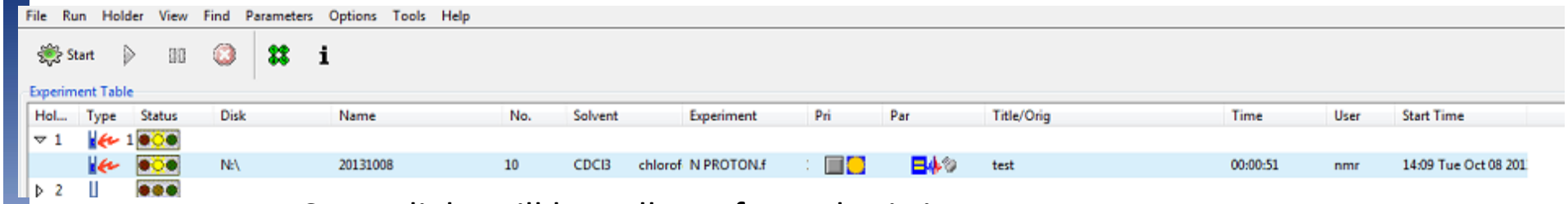
- Disk: N:\ (auto populates)
- File Name
- Experiment number (auto populates)
- Solvent (from drop down)
- Experiment (from drop down): N PROTON.f or N PROTON
- Title (if needed)



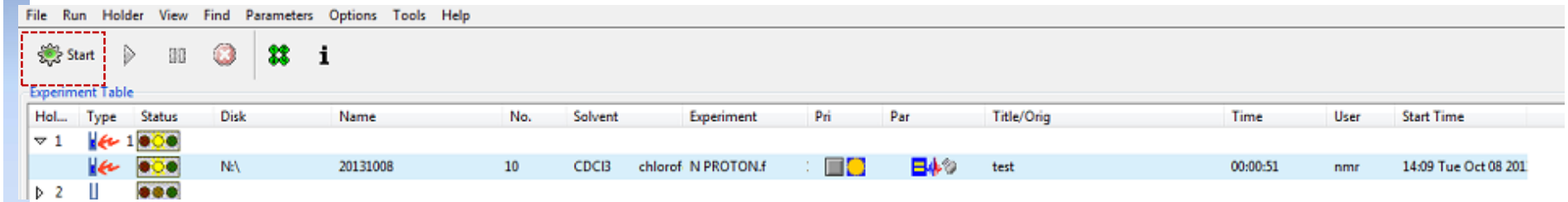
Highlight experiment to copy and click ***copy*** button and change number to the number of samples you have to run. Then edit sample name and/or text



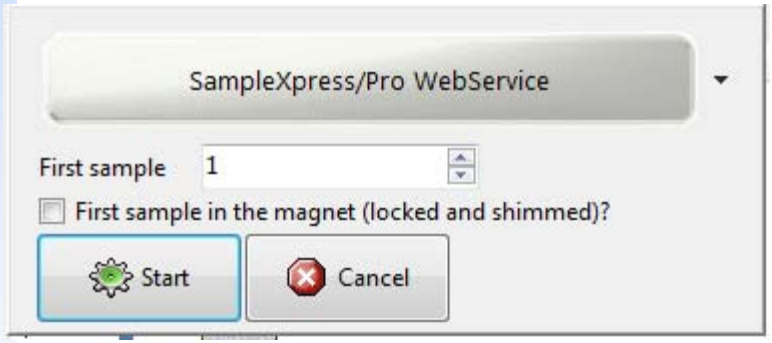
Highlight experiments to run and click ***submit*** button



Status light will be yellow after submitting

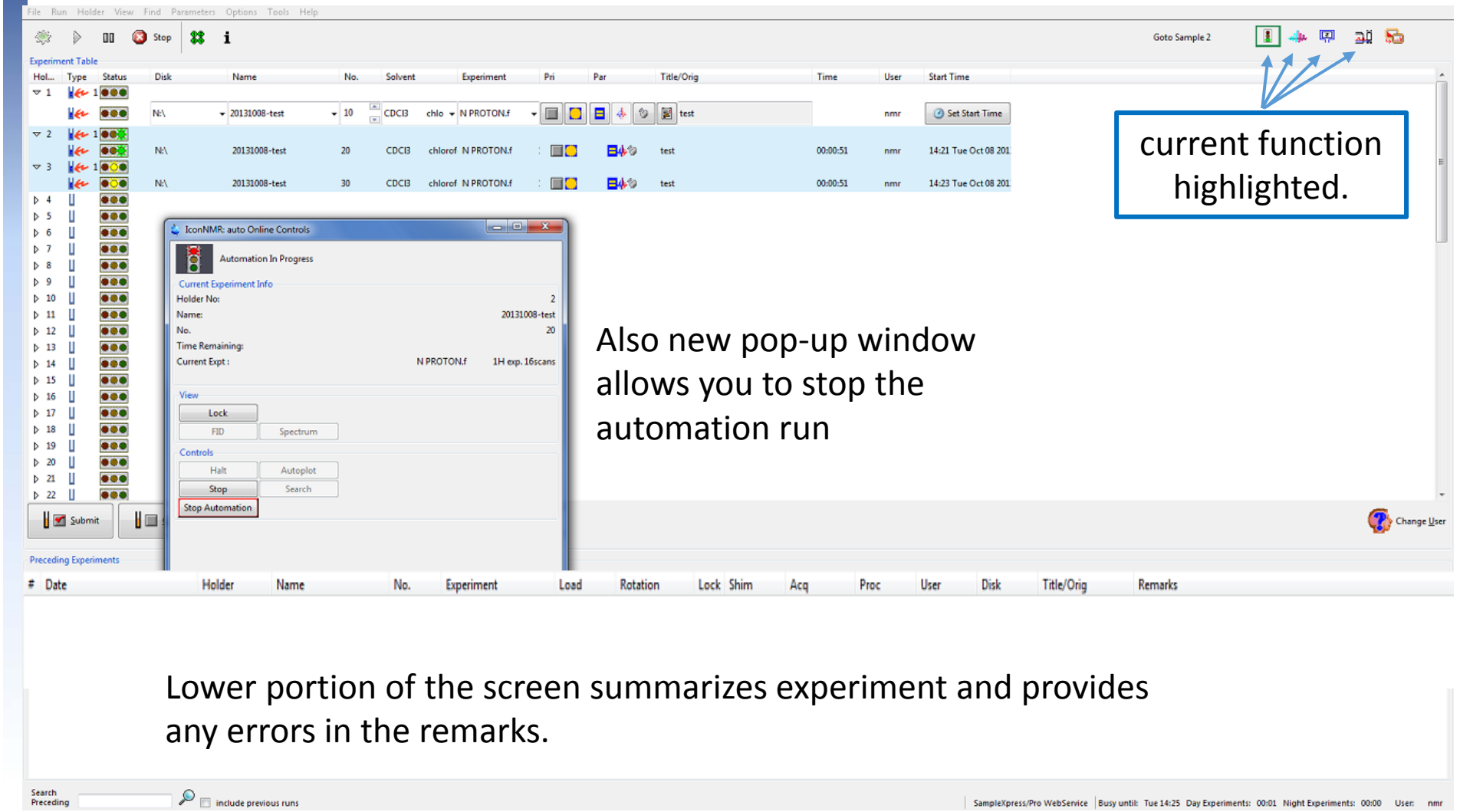


Once all samples are submitted click the green ***start*** icon



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

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


current function highlighted.
IconNMR: auto Online Controls
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
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.