Delta V5 operation

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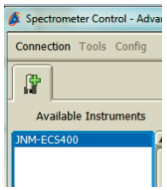
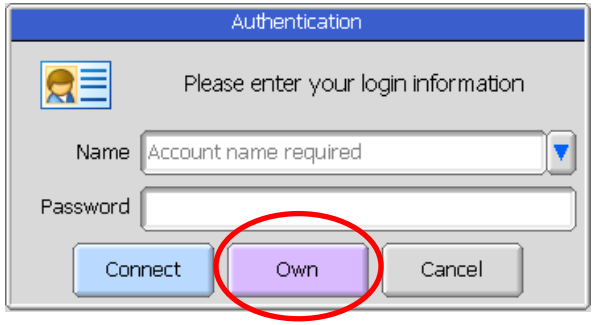
Progress through Synergy

Connect to spectrometer

1. Start Delta V5 (double click).
2. Open Spectrometer Control (click).
3. Select spectrometer on Available Instruments.



4. Click Connect and login with delta account (click Own) .

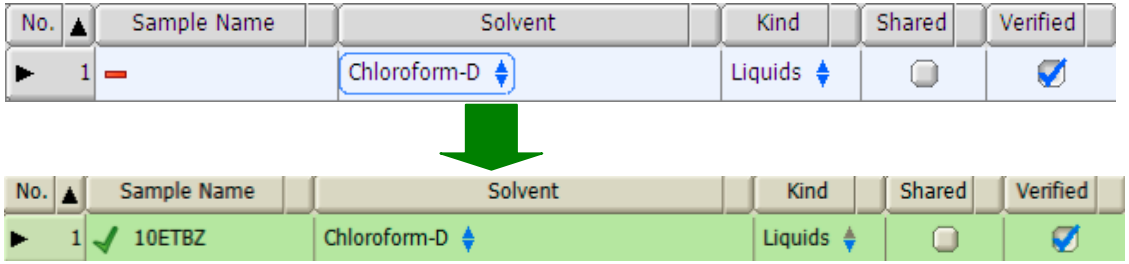


Name	Password	remarks
delta	delta	For installation account

Sample preparation

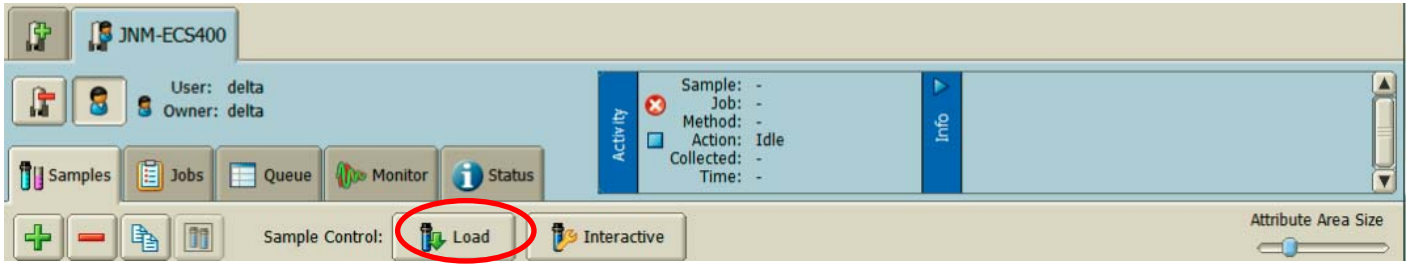
1. Set sample tube on SCM .
2. On Samples tab 

, you must defined your sample information.
3. On Samples tab, click  . You can see new sample definition space on sample list.
4. Input sample name.
5. Select solvent.
6. Click Verified.
7. Click sample number. Clicked sample box becomes green color.

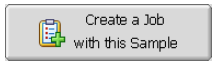


8. Click 

for sample loading.

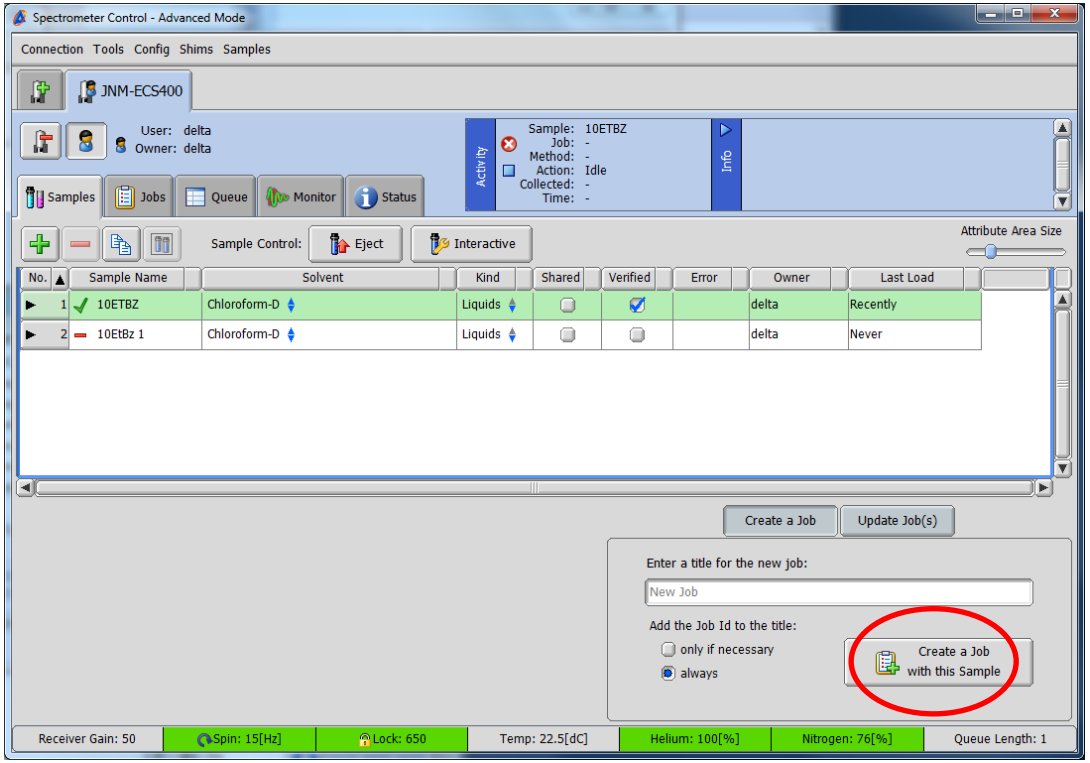


Set up experiment (automation)

1. Click 

on Samples tab or key in the job name which you want to define your job. You can see the next tab 

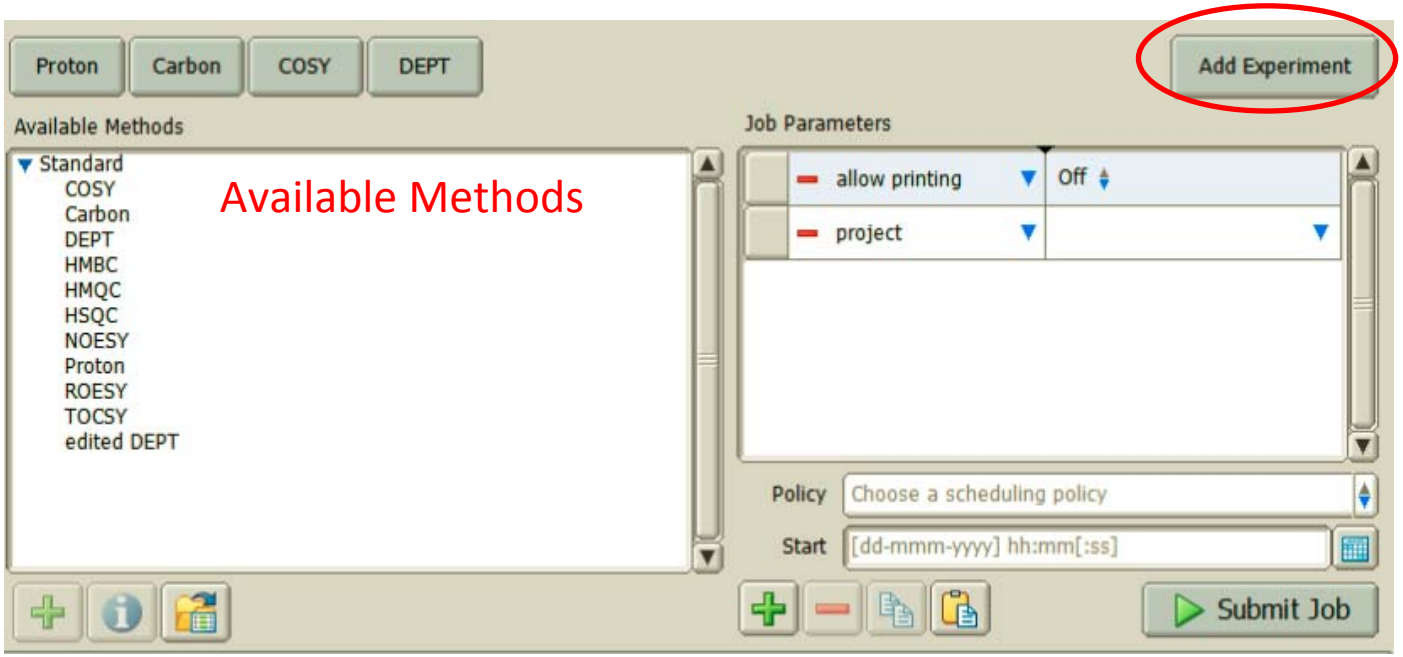
(Jobs tab).



Set up experiment (automation)

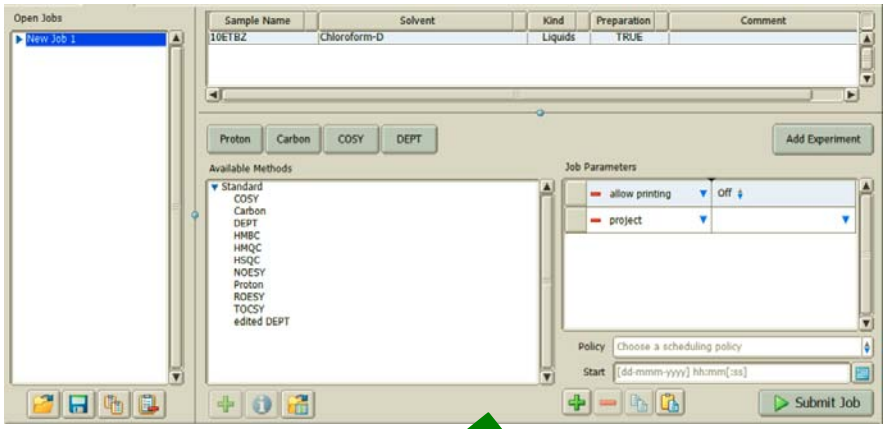
2. We can choose some experiments which user want to do on Job Parameters box.

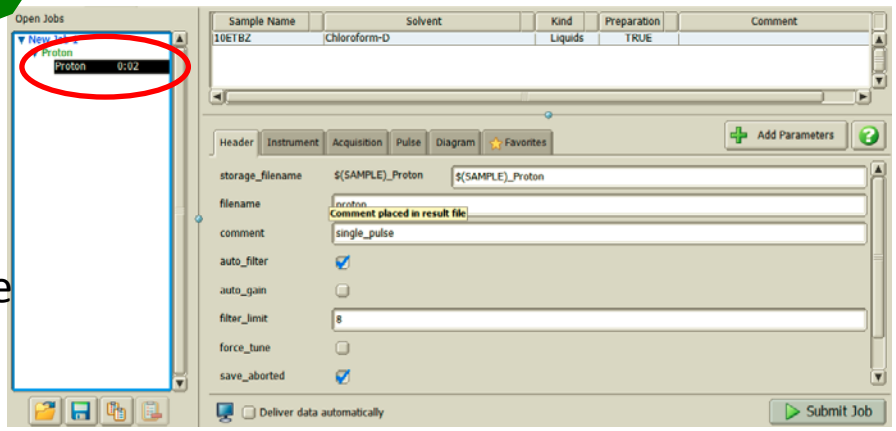
3. If user want to do another experiment which is not save in available methods, click Add Experiment for another experiments.



Set up experiment (automation)

4. If you want to change the more detail parameters, select experiment name on Open Jobs list.



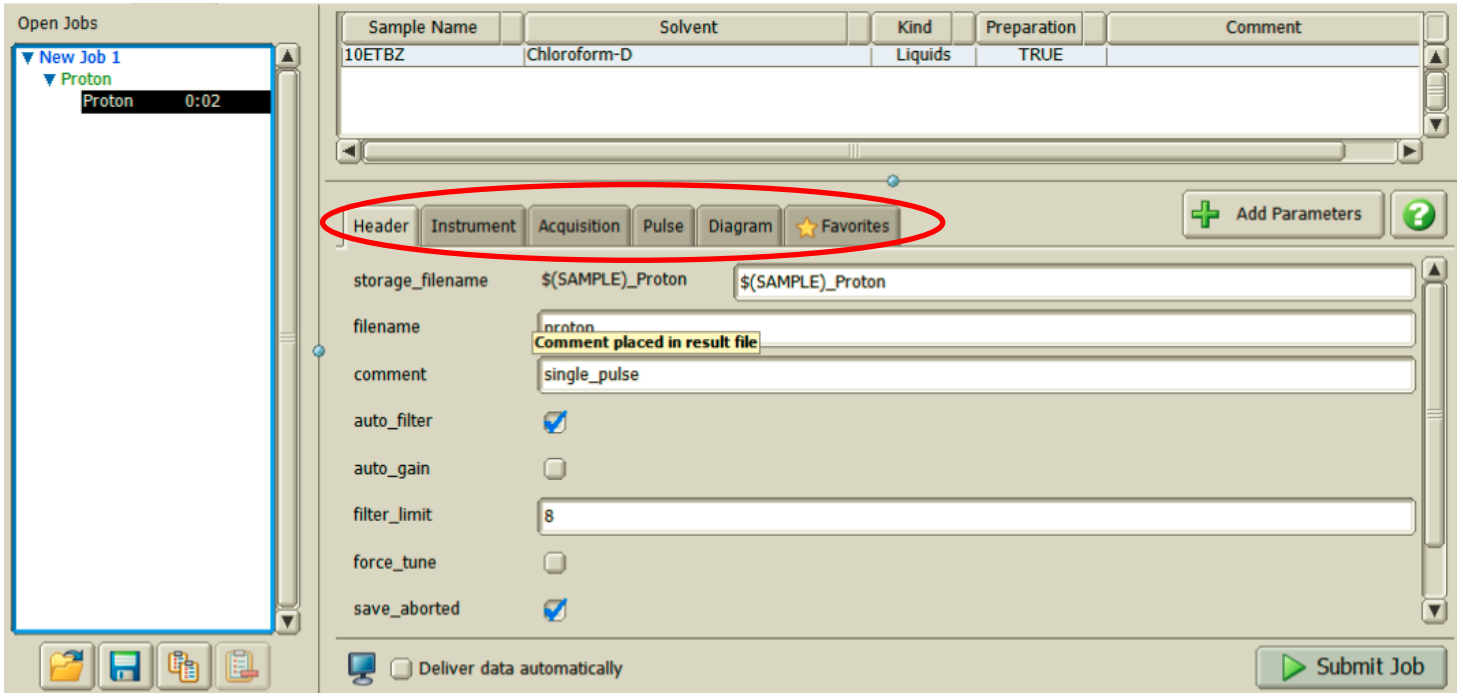


- Job Name
  - Method Name
    - Experiment Name

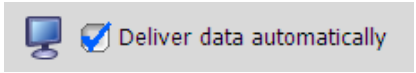
Progress through Synergy

Set up experiment (automation)

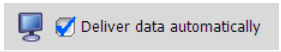
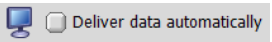
5. We can change some experiments parameters on Job Parameters box.

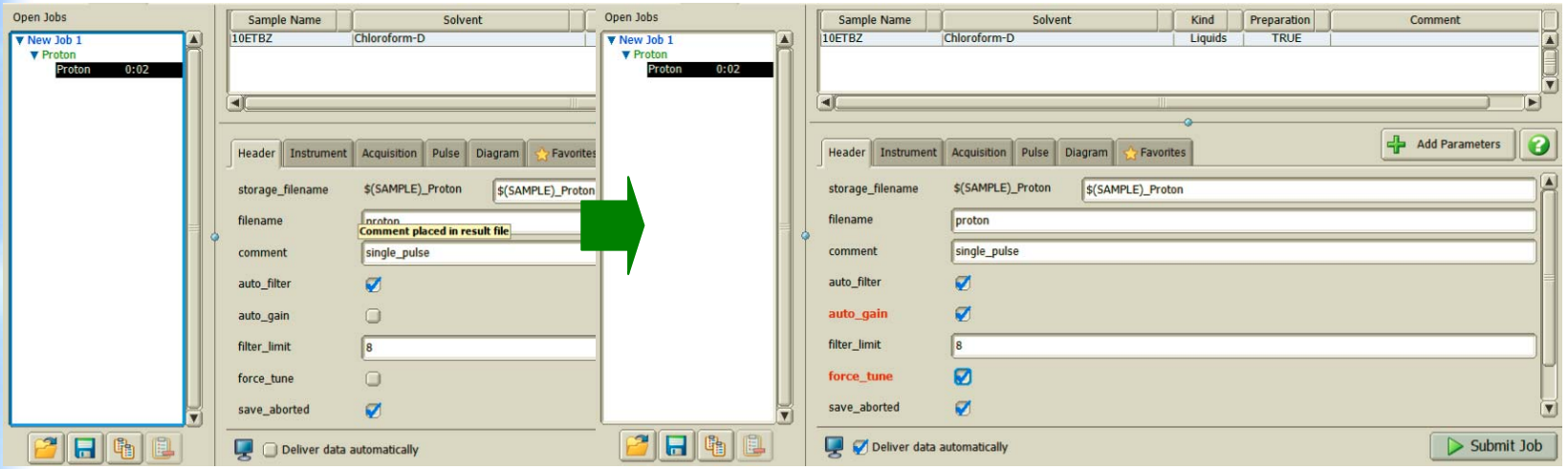


Set up experiment (automation)

6. If you first time do this sample, click “Force tune” and “Auto_gain”.
7. If you tick “Deliver data automatically “ 

, you can see the results on your display.
8. The parameters became red word when changed.

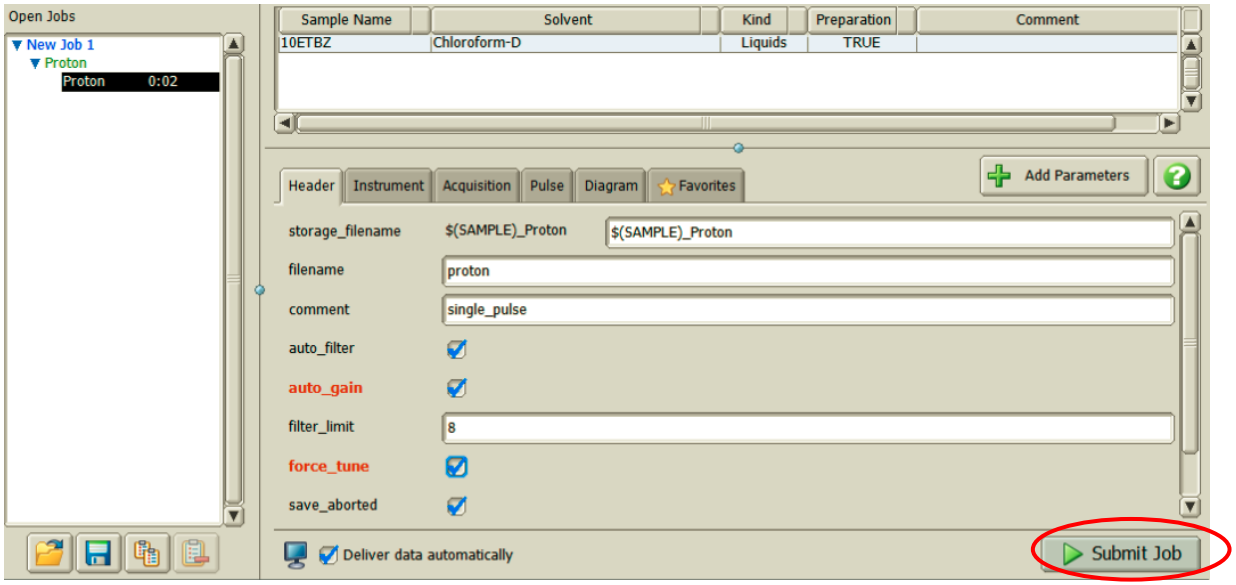
Deliver data automatically	results	Data is saved to …
	You can see results on your display.	Data Servers (spectrometer) and your workstation
	You can’t see results on your display.	Data Servers (spectrometer) only



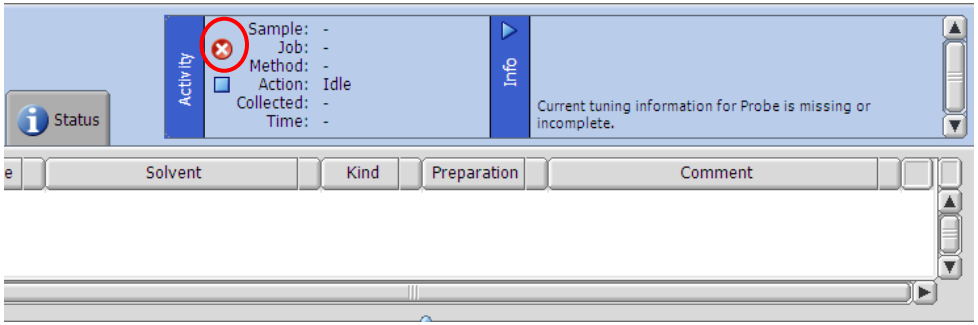
Submit experiment (automation)

9. Click 

. The experiments are started.



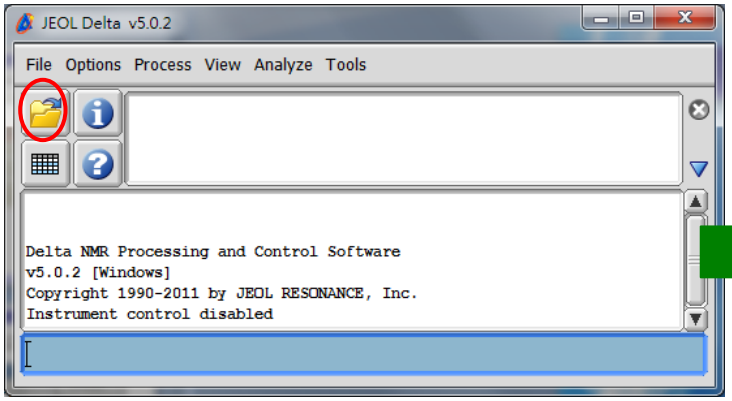
10. If you want to stop experiment, Click  .

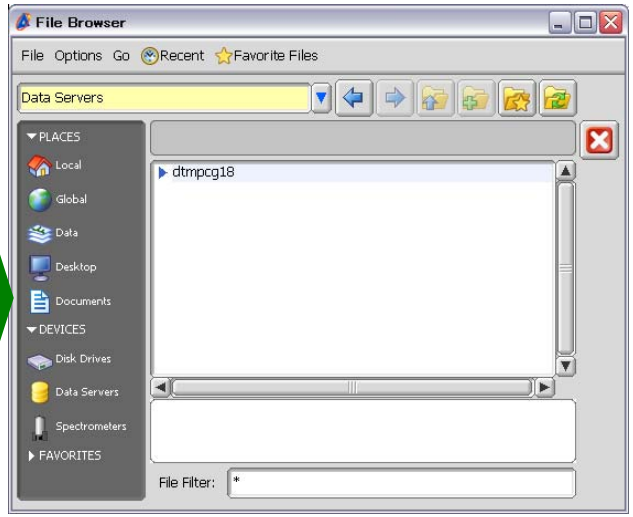


Open data (1)

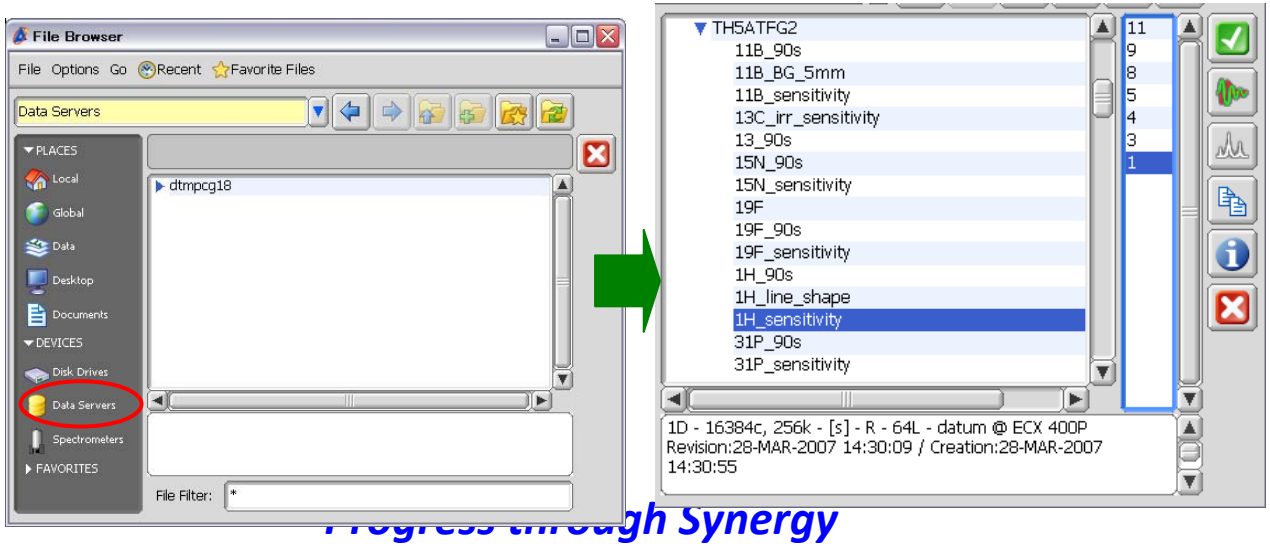
Case A: You have already connected to spectrometer.

1. Click  on Delta Console window.



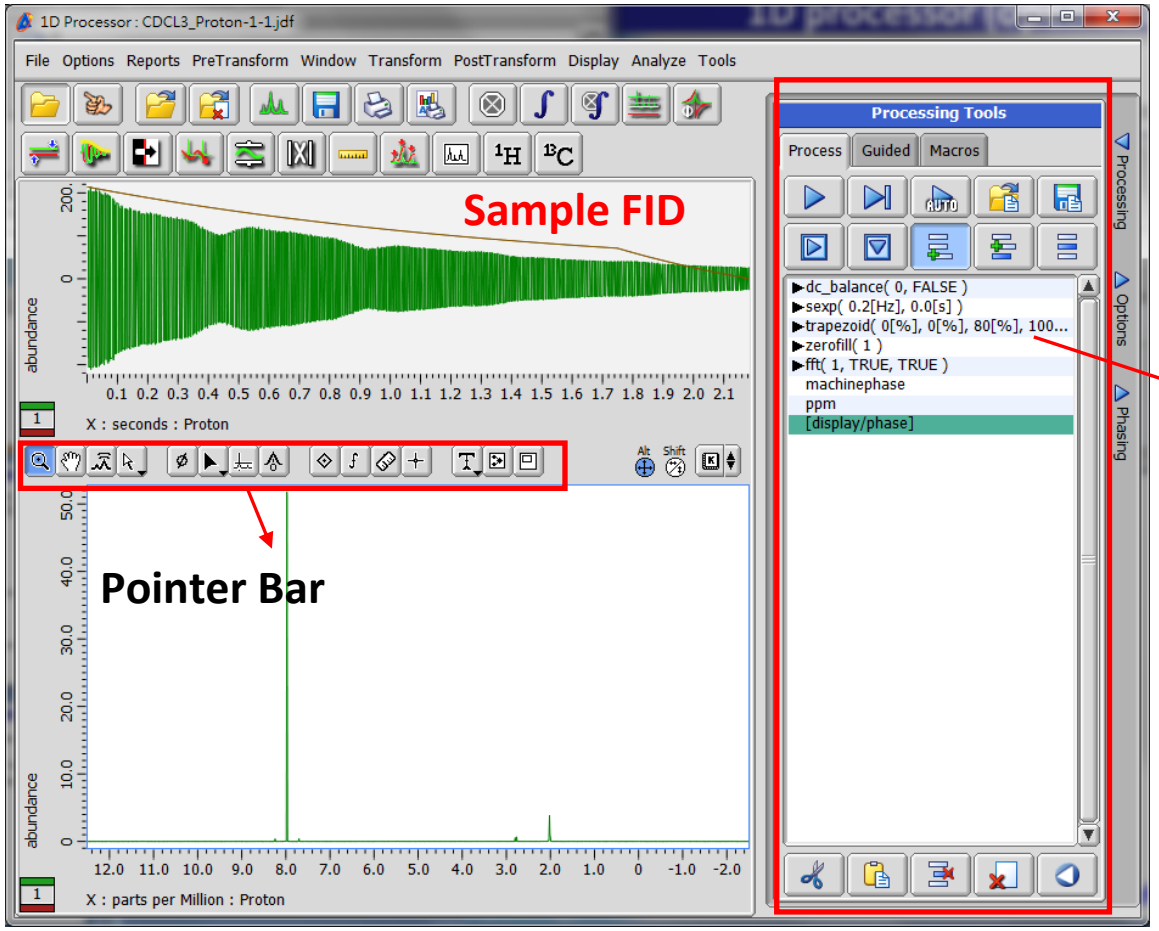


2. Click  for downloading from spectrometer. You can select and download data.



1D processor (open data file)

1. When you open 1D NMR data, you can see 1D processor window.



Processing

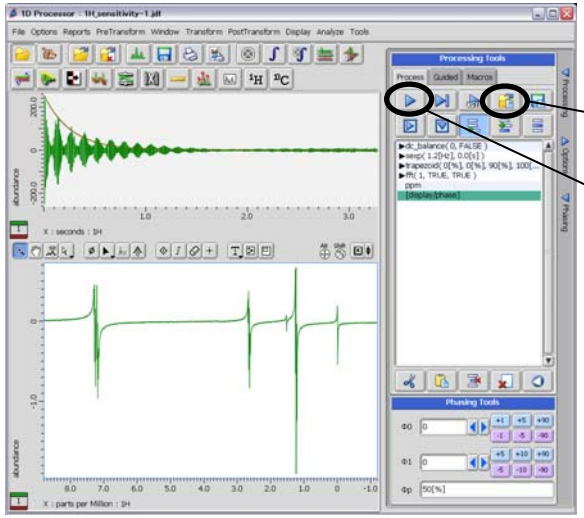
1D processor (Pointer Bar)

1. When you open 1D NMR data, you can see “Pointer Bar” .

: Zoom (Zoom view of data)
: Pan View (Pan view of data or slide view)
: Amplitude gain (apply amplitude gain)
: Select (To select data of geometry)
: Phase correct (To adjust the phase of spectra)
: Copy position (Copy position to paste buffer)
: Peak threshold (Adjust the peak threshold)
: Reference (To set a chemical shift reference axis marker)
: Peak (Peak picking tool)
: Integral (Integral tool)
: Measure (To measure distance between peaks)
: Cursor (make the horizontal and vertical line)
: Annotation (edit annotation in the geometry)
: Molecule (To display a structural formula and molecular formula in the geometry)
: PiP (Picture in Picture)

1D processor (open process list)

1. When you open 1D NMR data, you can see 1D processor window.

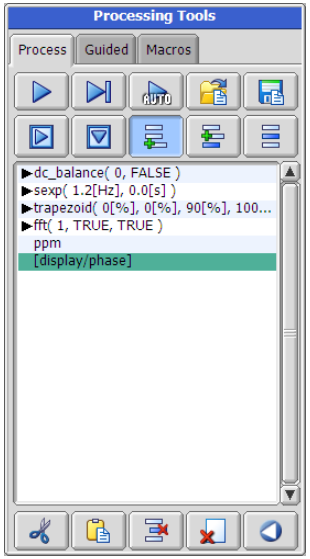


2. If you want to open process_list, click  .
3. When you apply process_list, click  .

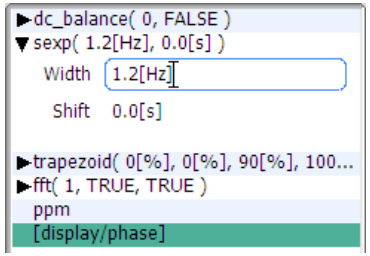
*  : for 1H process_list,  : for 13C process_list

1D processor (edit process list)

1. When you want to edit process, you can edit on Processing tool.



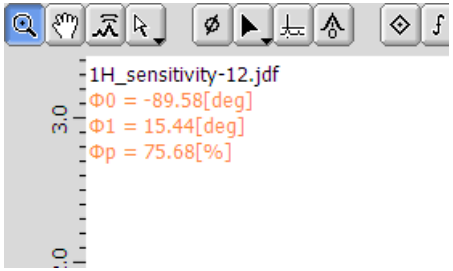
2. If you click ▶, you can see detail parameters for processing command.



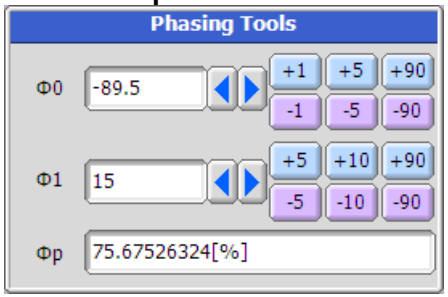
3. When you apply process, click  .
4. If you click  , you can undo your process list.

1D processor (phase correction 1)

1. When you click  (auto phase), the phase of spectrum is adjusted.
2. You can see phase correction values on the left upper in spectrum.



3. Those values are inputted in Phasing Tool.



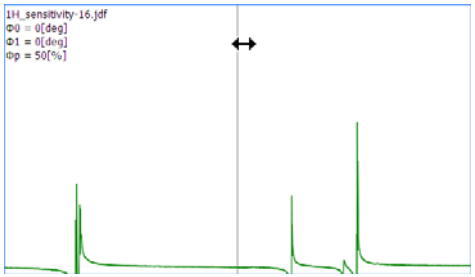
4. If you want to adjust those, you can manipulate with Phasing Tool.
5. When you finish to adjust, click  .

(If you can't see Phasing Tool, please click 

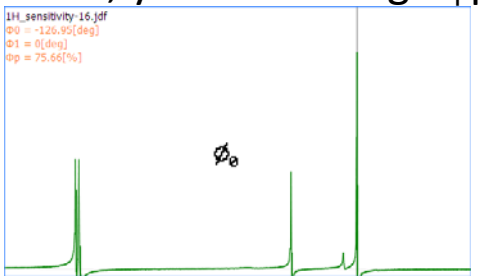
on the left.)

1D processor (phase correction 2)

1. Click  at “Pointer Bar”. (Pointer bar is  on processor window.)
2. You can see the vertical line on you spectrum.



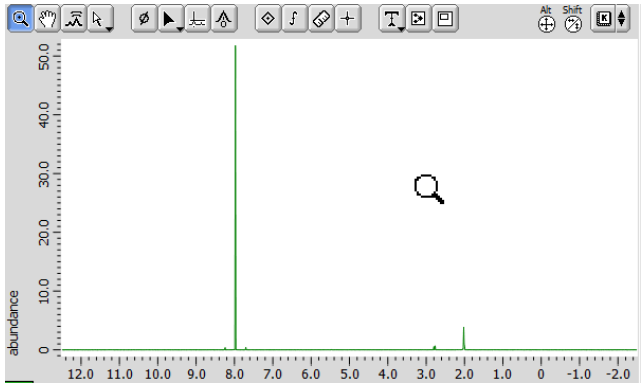
3. When your mouse cursor moves to that line, mouse cursor is changed to ⇔.
4. In that situation, you can change ϕp with dragging.



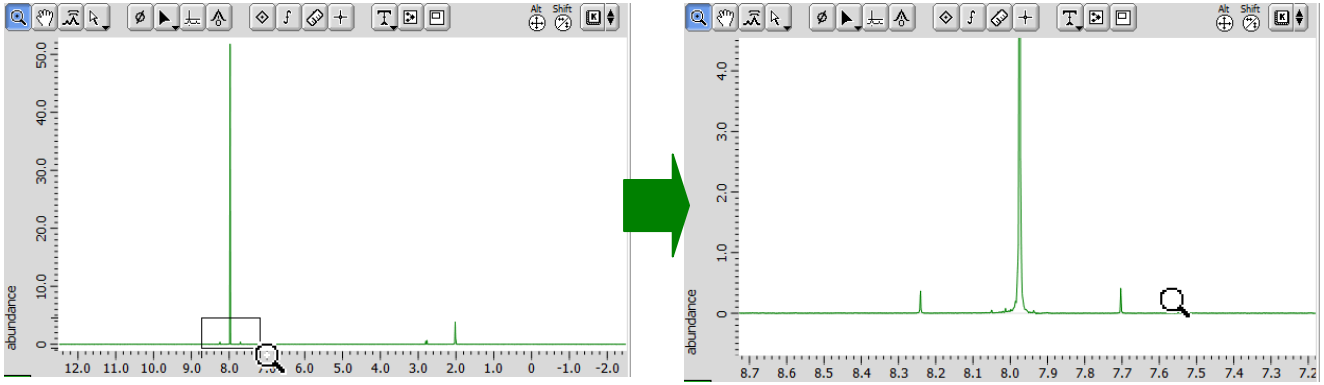
5. If you want to adjust ϕ0 and ϕ1, you can manipulate with Phasing Tool.

1D processor (Zoom process)

1. Click  at “Pointer Bar”. (Pointer bar is  on processor window.)
2. You can see your mouse cursor became magnifer.

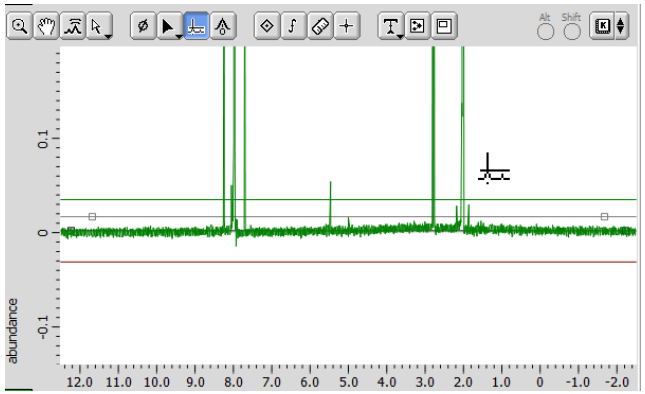


3. When you drag any region or the border, the process window zoom will be changed.

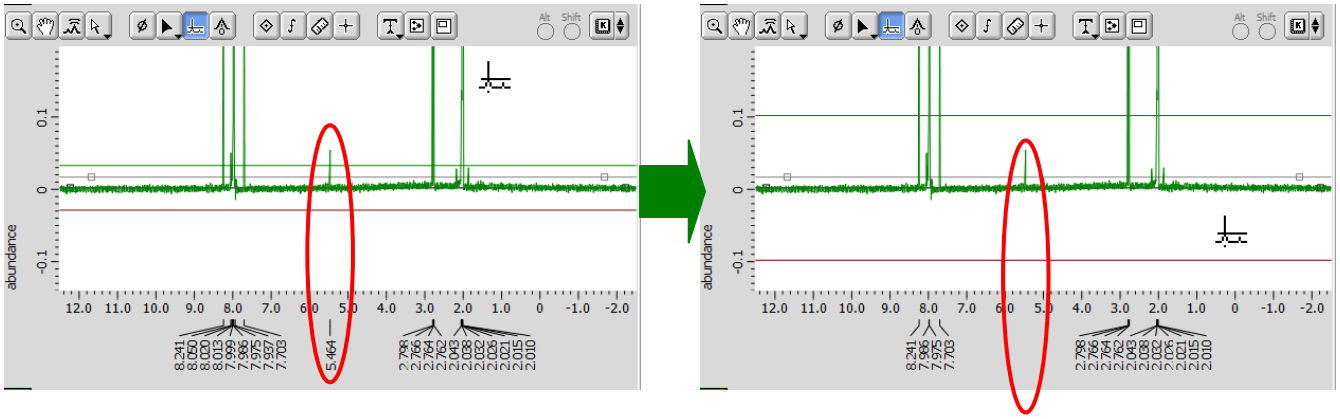


1D processor (Peak threshold)

1. Click  at “Pointer Bar”. (Pointer bar is  on processor window.)
2. You can see your mouse cursor became peak threshold.

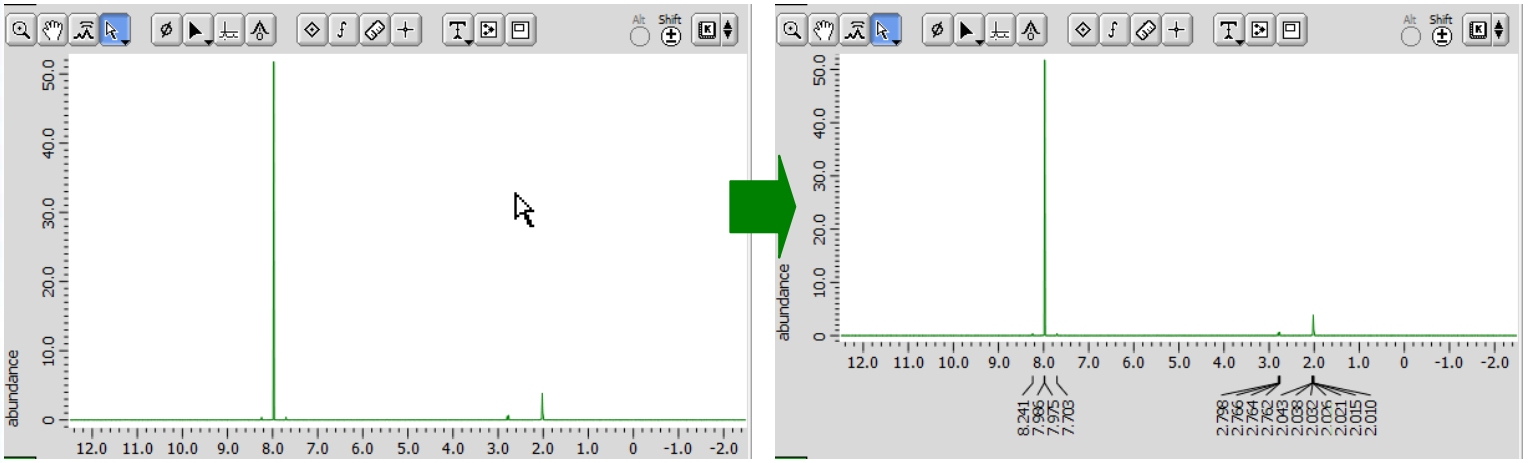


3. You could drag the green line or red line, this process influence peak picking and integral.



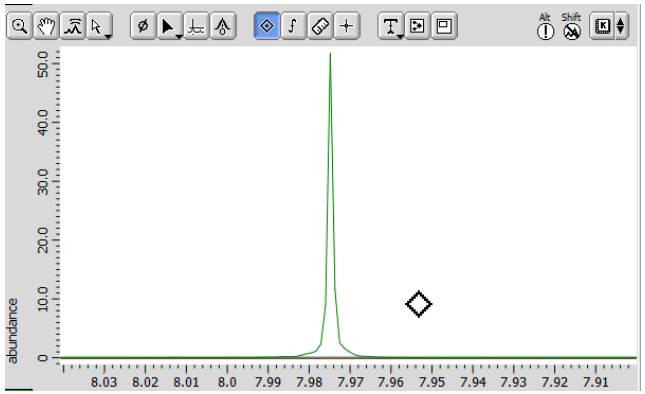
1D processor (Peak picking 1)

1. When user decide their peak threshold, click  for auto peak picking

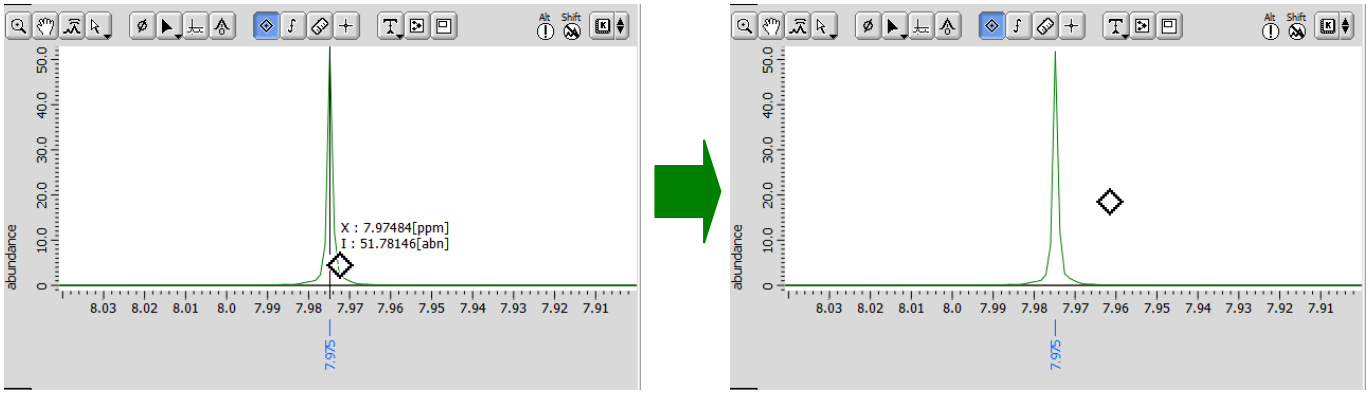


1D processor (Peak picking 2)

1. Click  at “Pointer Bar”. (Pointer bar is  on processor window.)
2. You can see your mouse cursor became peak picking.

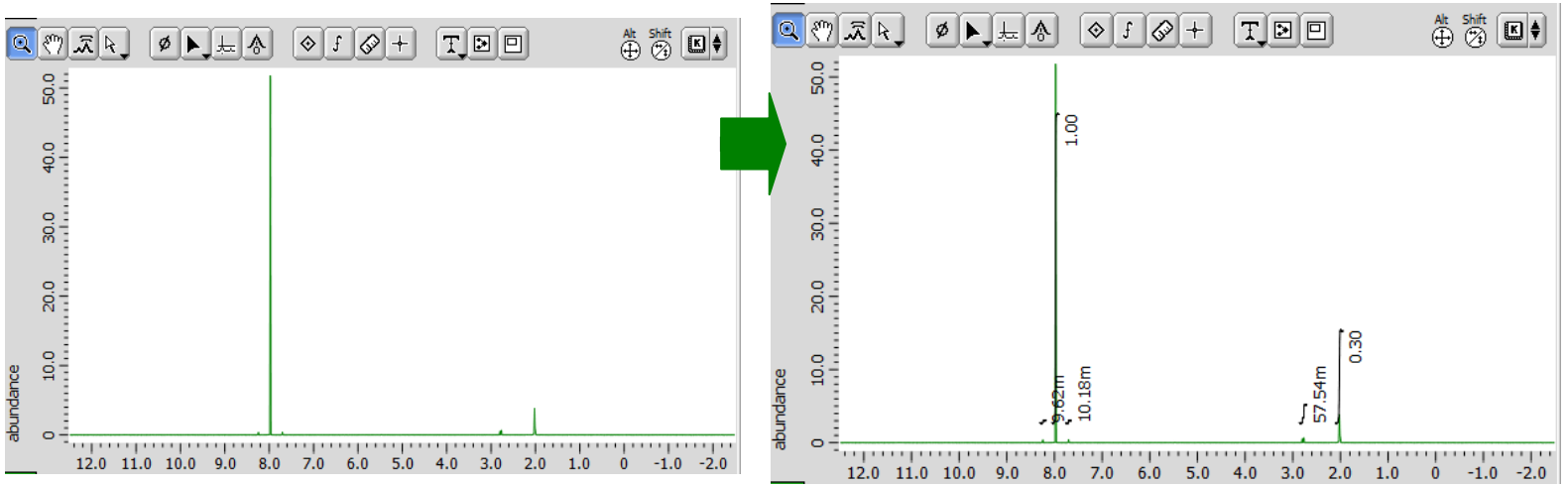


3. Which peak you want to pick, move the mouse cursor to peak and click left mouse button.



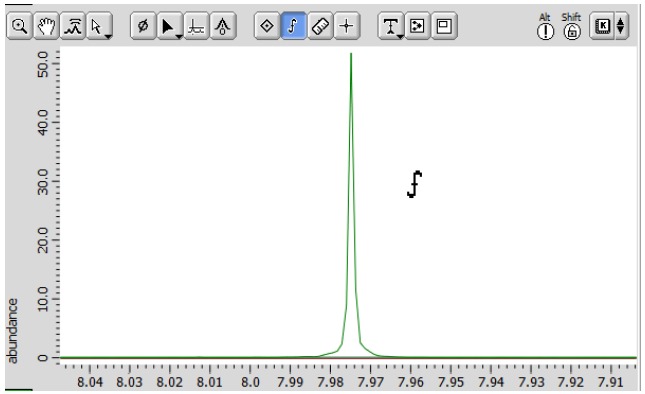
1D processor (Peak integral 1)

1. When user decide their peak threshold, click  for auto peak integral.

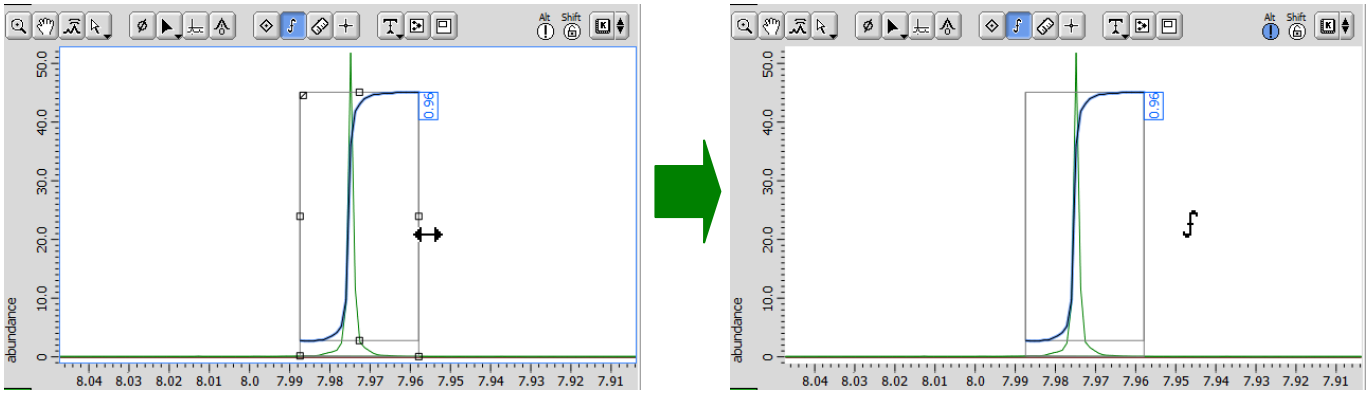


1D processor (Peak integral 2)

1. Click  at “Pointer Bar”. (Pointer bar is  on processor window.)
2. You can see your mouse cursor became peak picking.

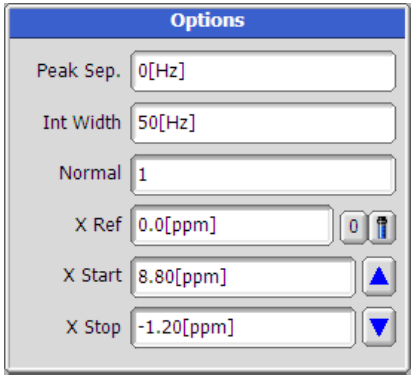


3. Which peak you want to integral, move the mouse cursor to peak and drag the region by left mouse button.



1D processor (options)

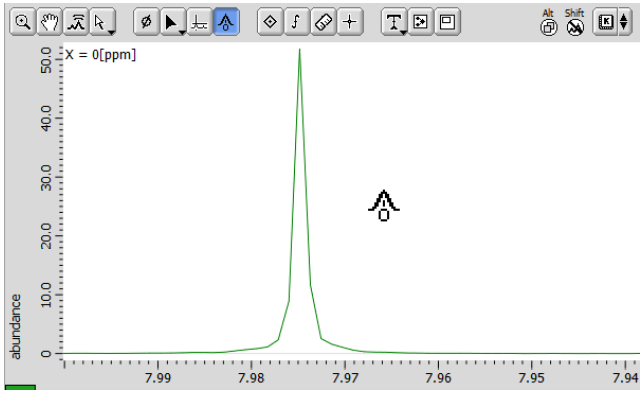
If you can't see "Options" panel, please click △ Options on the left.



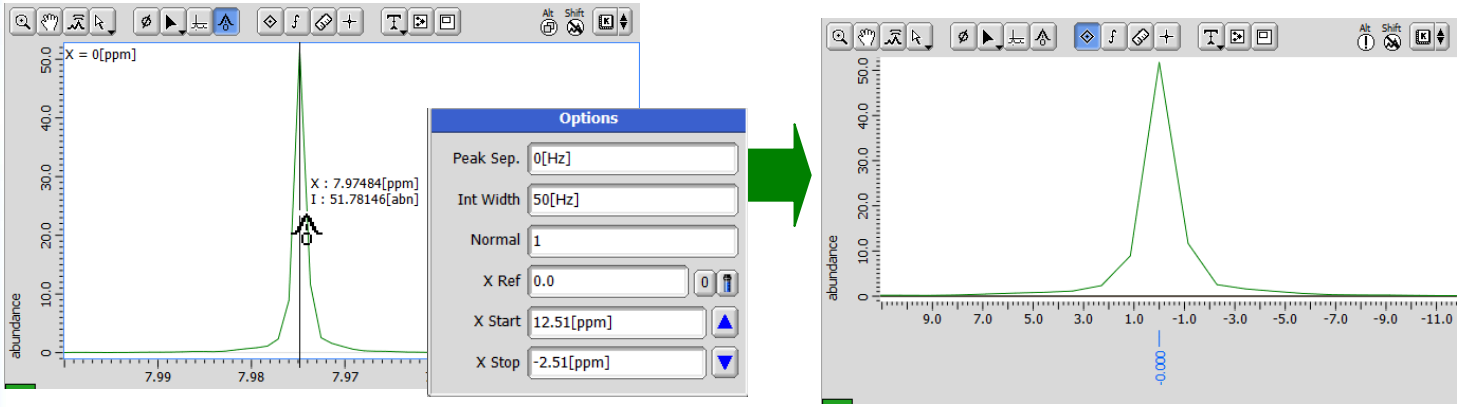
Peak Sep. : The minimum value between peak and peak for peak picking.
Int Width : The range of integral.
Nomal : Normalize value for integral.
X Ref : the value for calibrating chemical shift.
X start : the right edge of the spectrum.
X Stop : the left edge of the spectrum.

1D processor (Peak reference)

1. Click  at “Pointer Bar”. (Pointer bar is  on processor window.)
2. You can see your mouse cursor became reference.

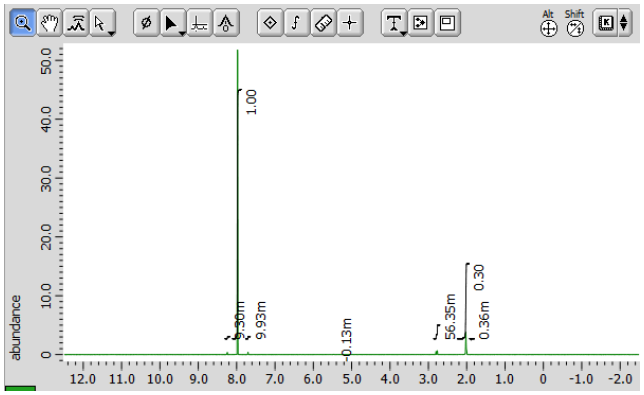


3. Which peak you want to decide reference peak, set the value in X ref on option bar and move the mouse cursor to peak and click by left mouse button.

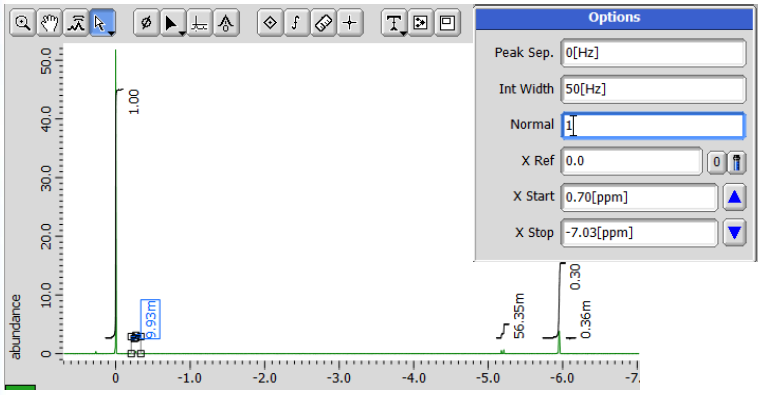


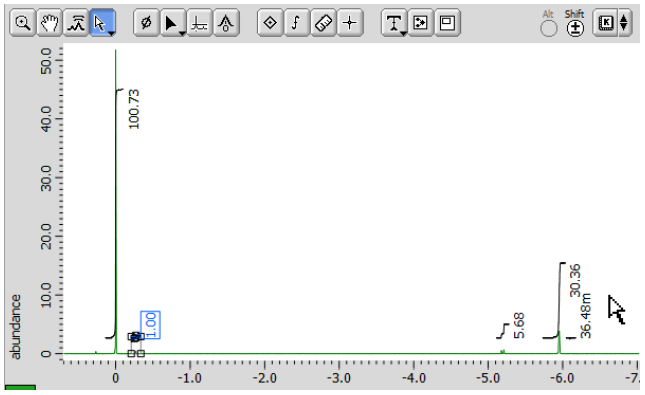
1D processor (Peak integral normalized)

1. After auto integral, user could see the result about integral.



2. Click  at “Pointer Bar”. (Pointer bar is  on processor window.) , select the integral and key in the value which user want to normalized on option bar

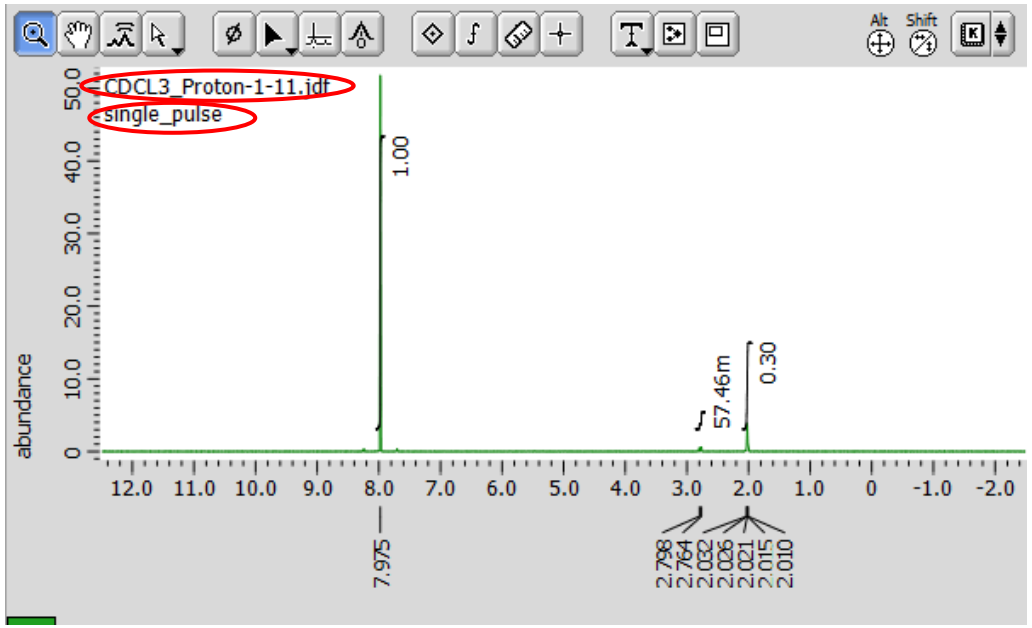




Progress through Synergy

1D processor (prepare print)

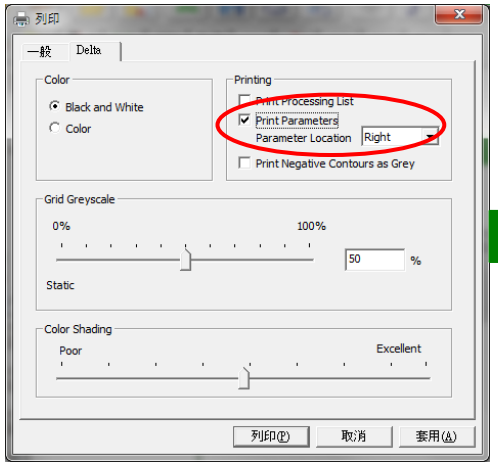
1. After data process, click alt+f for data file name and alt+shift+c for method.

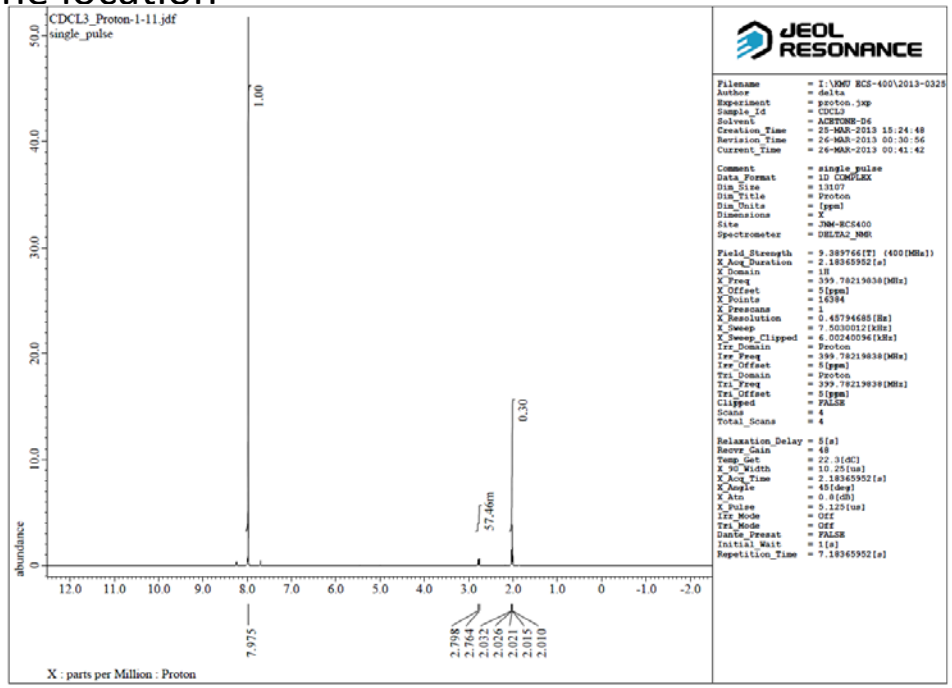


1D processor (prepare print)

1. Click  For pint data file.

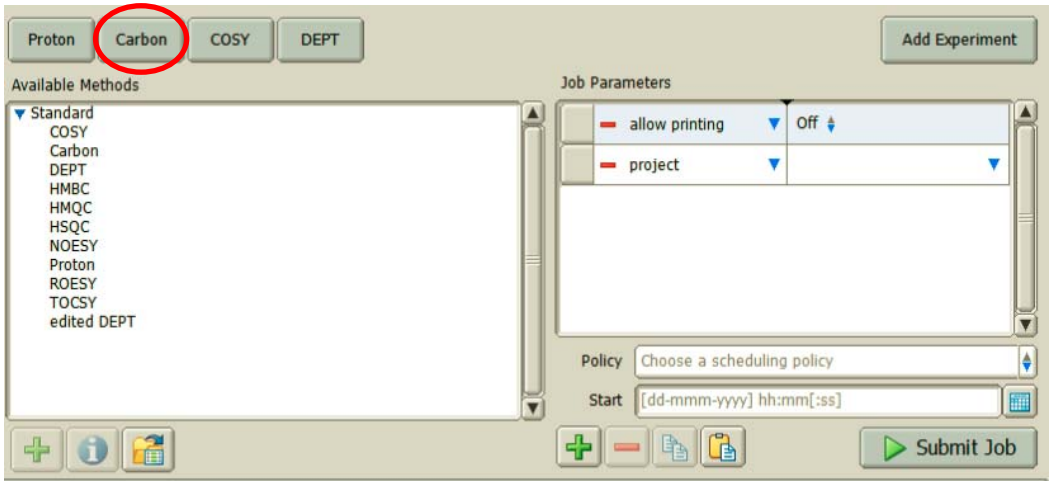
2. If user want to print shim parameters, click delta and tick the print parameters and choose the location

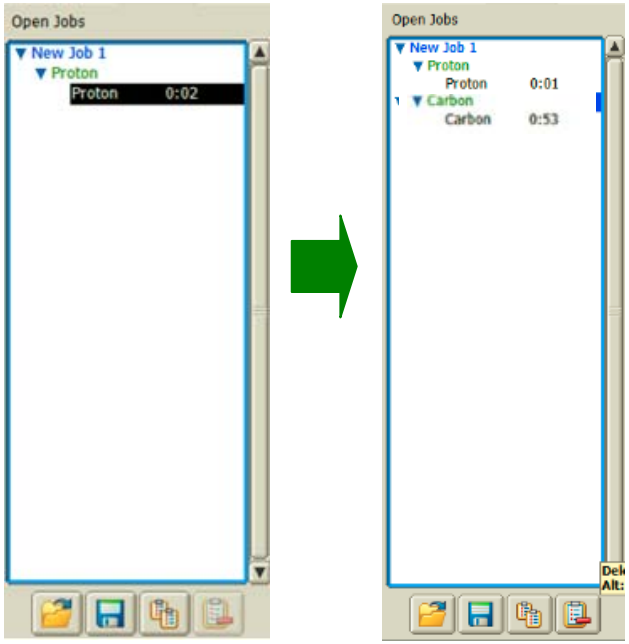




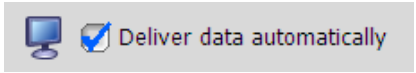
Set up experiment (^{13}C automation)

1. We can click the carbon experiment icon on Job tab.

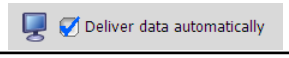
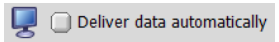


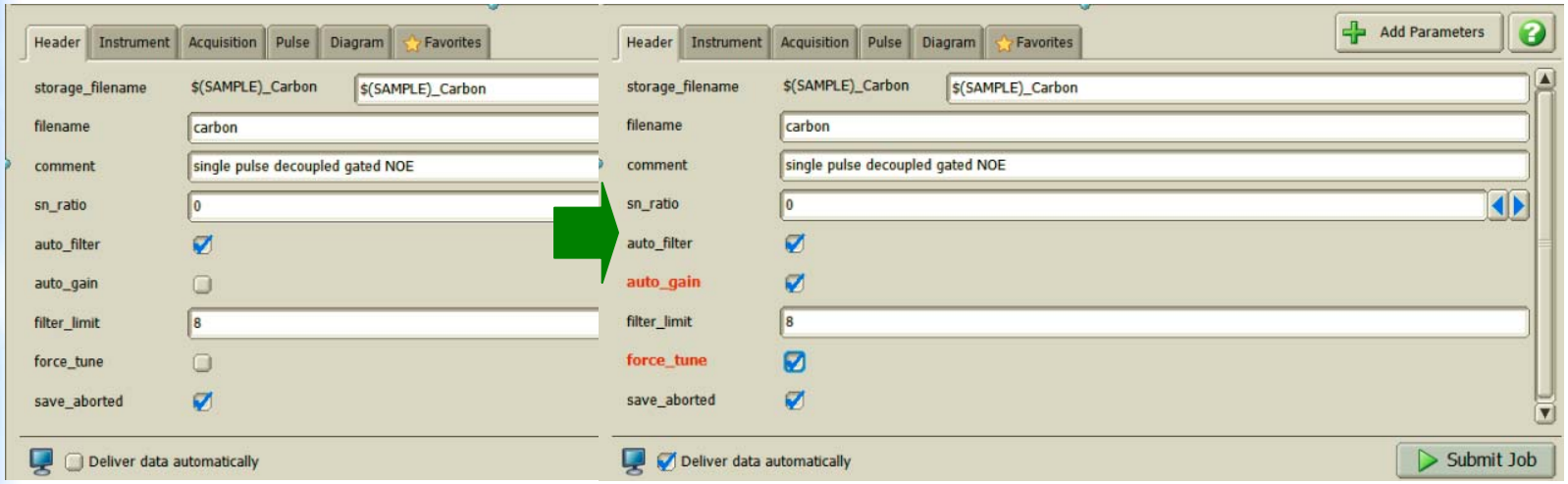


Set up experiment (^{13}C automation)

1. If you first time do this sample, click “Force tune” and “Auto_gain”.
2. If you tick “Deliver data automatically “ 

, you can see the results on your display.
3. The parameters became red word when changed.

Deliver data automatically	results	Data is saved to …
	You can see results on your display.	Data Servers (spectrometer) and your workstation
	You can’t see results on your display.	Data Servers (spectrometer) only

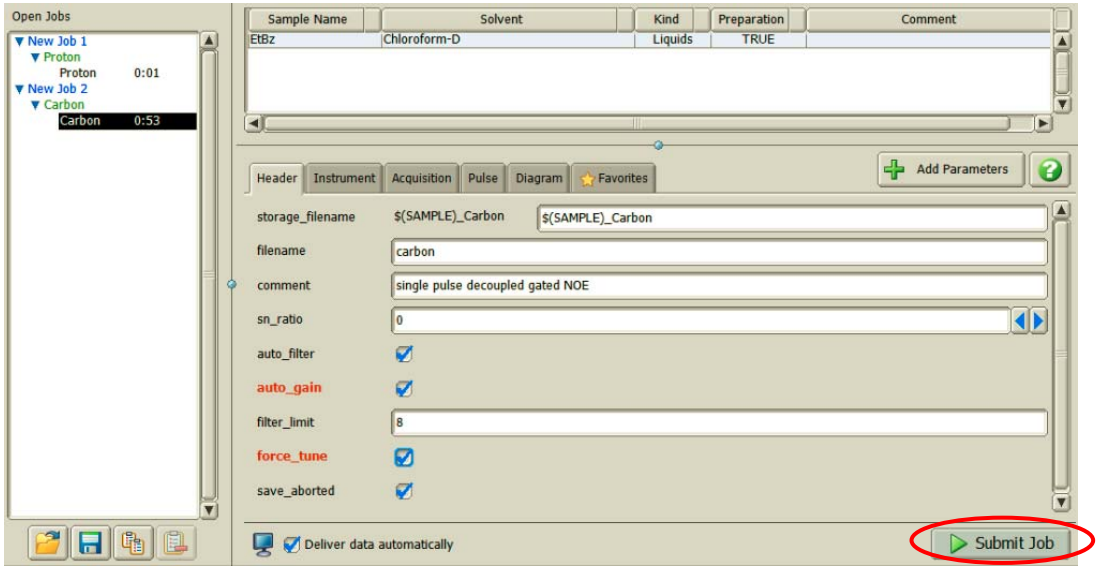


Progress through Synergy

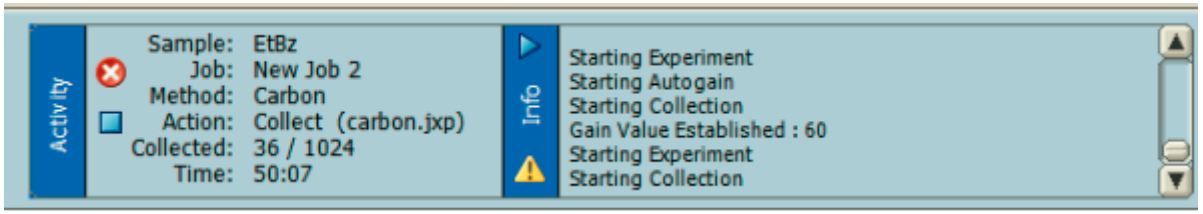
Set up experiment (^{13}C automation)

1. Click 

The experiments are started.



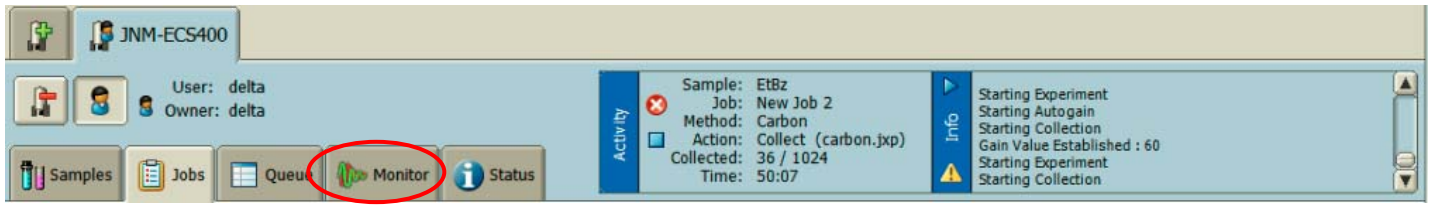
2. Wait to collect data.

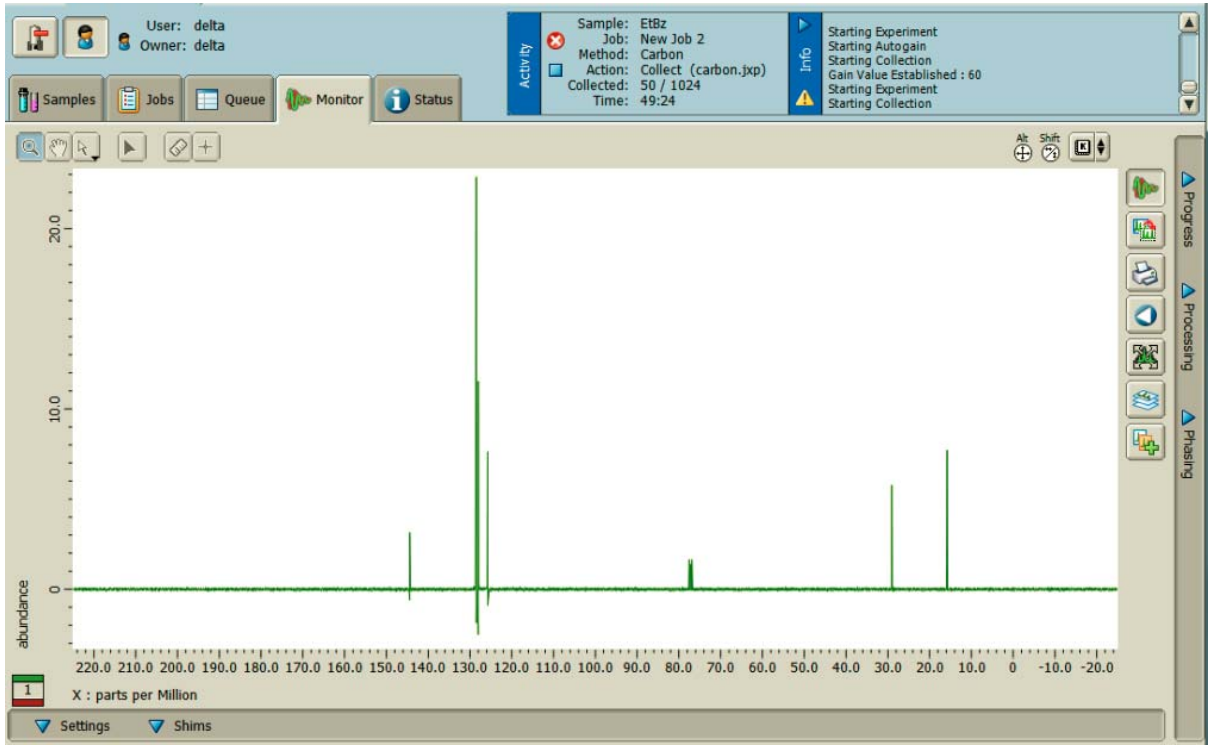


Set up experiment (^{13}C automation)

1. Click 

, and observed the real time spectrometer.

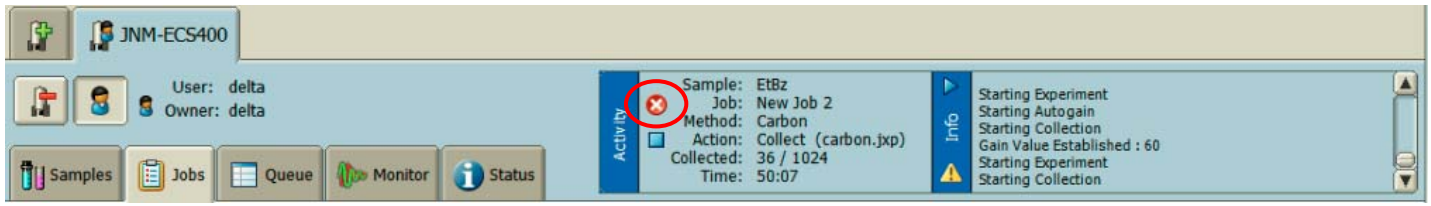




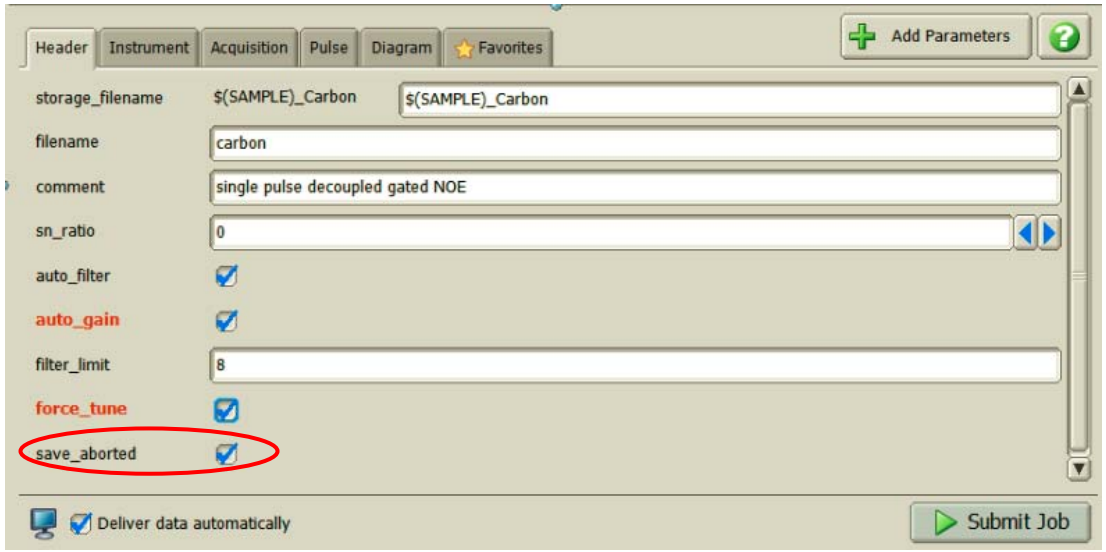
Progress through Synergy

Set up experiment (^{13}C automation)

1. If you want to stop experiment, Click  .



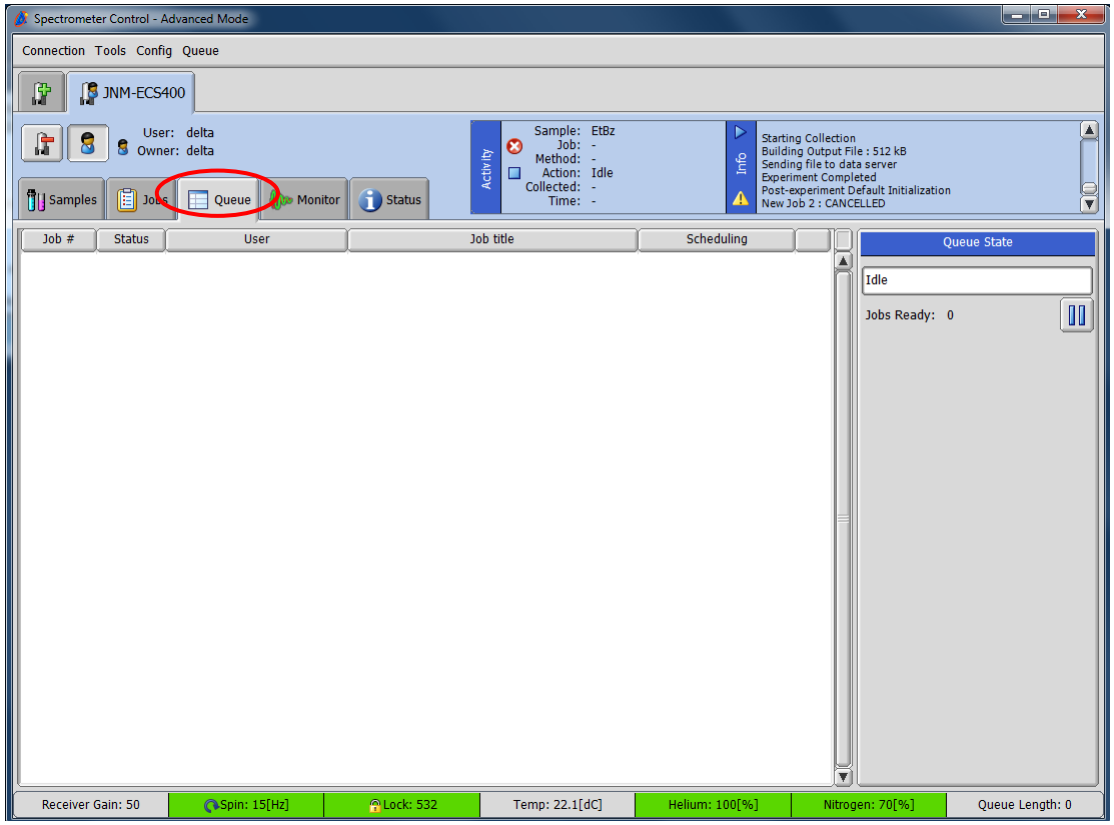
2. If tick save_aborted (default parameters), stop experiment, the data file will be saved in console



Finish experiment

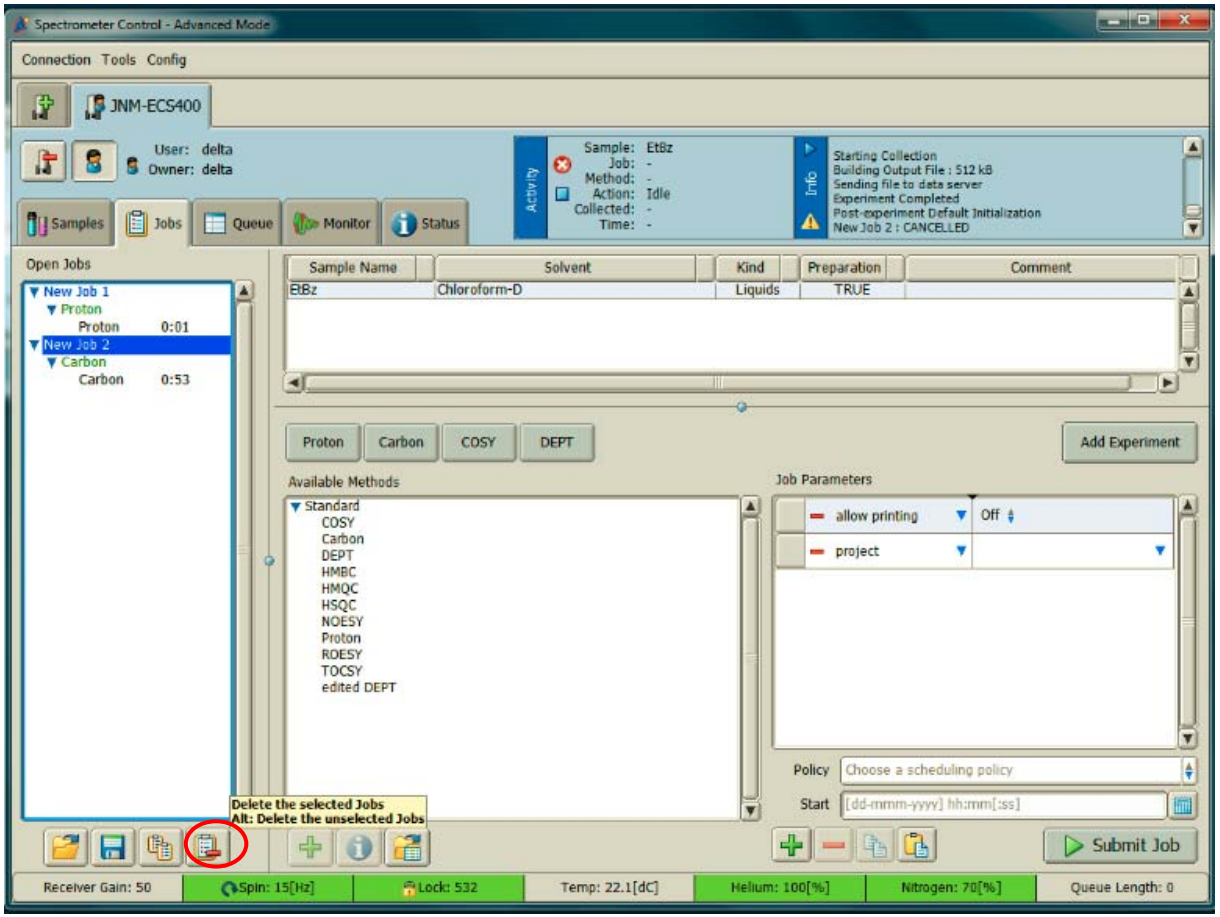
1. When finish your experiment, click 

and check the Quene tab which is empty.



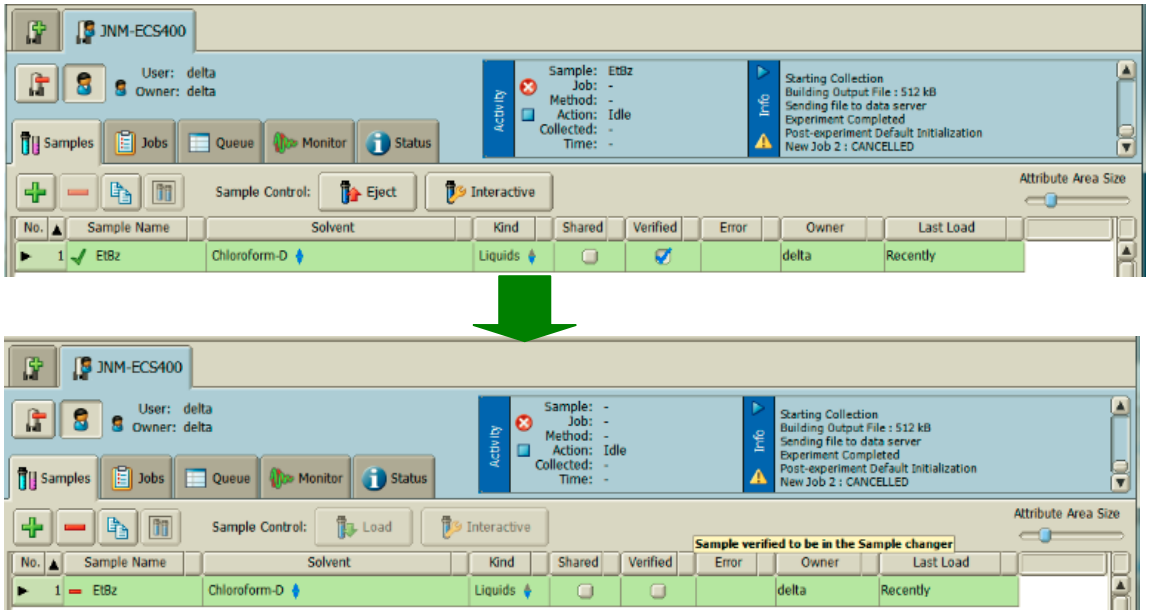
Finish experiment

1. Click  and check the Job tab which is empty.
2. If not empty, click the Job and click  to delete Job.

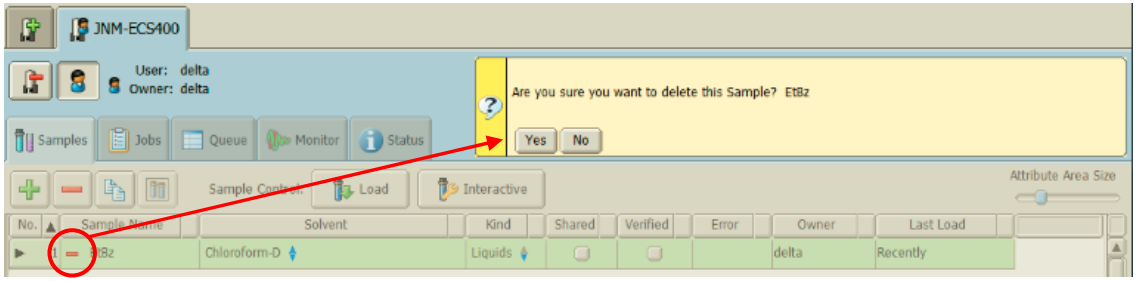


Finish experiment

1. Click  and click verified.
2. Sample will eject



3. Click  to delete sample for next user to use software.



Progress through Synergy

Finish experiment

1. Check all your file will be save and click  to close delta software.