Delta software

Hints and tips

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What kind of hints?

- System architecture
- Delta updates
- Automation setup
- Other
- PFG offset
- Gradient shimming

System architecture

Some highlights of JEOL NMR history

1956
JNM-1

(32MHz commercial spectrometer)

1972
JNM-FX60

(Fourier Transformed NMR)

2002
JNM-ECA series

(Modular NMR with full automation)

2014
JNM-ECZ series

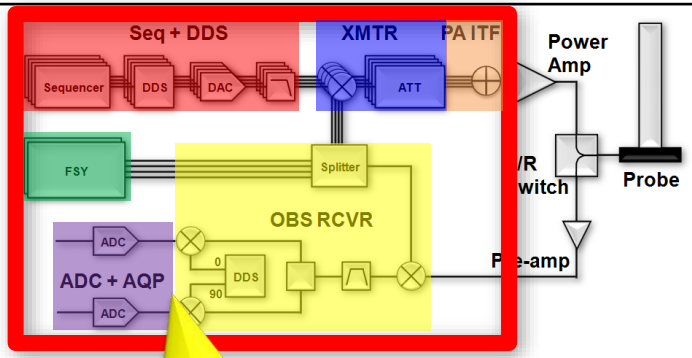
(Transceiver system)

2021
JNM-ECZL series

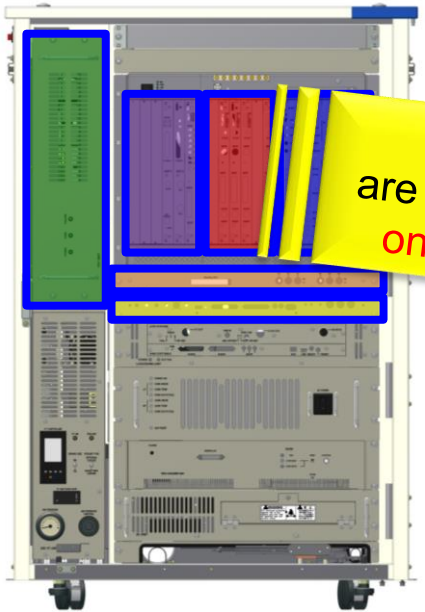
(Multi-frequency transceivers)

ECS vs ECZL

Block diagram of ECS→



ECS



Unit groups are integrated into only one board

ECZL

NMR spectrometer

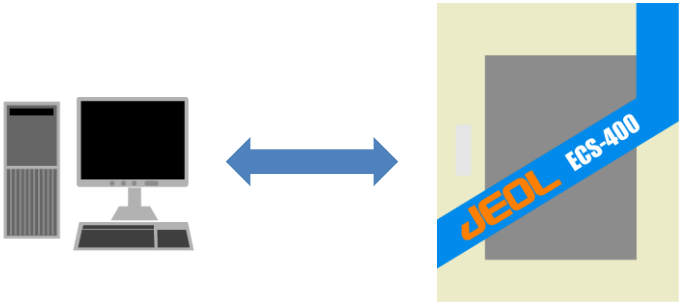
Console	ECS
Event time resolution	20 nsec
Minimum event duration	380 nsec
Frequency step	0.01
Switching time	100 nsec
Max. spectrum bandwidth	2 MHz
Sequence memory	512 Mbyte

More reliable
Faster service

* RF: Radio Frequency, Transceiver: transmitter and receiver

Solutions for Innovation JEOL

Delta 4 (ECS) vs Delta 5+ (ECZL / ECZ / ECS (II))



ECS

automation

Sample No.1

PROTON 1D

CARBON 1D

Sample No.2

PROTON 1D

CARBON 1D

Queue

The host PC sends queue elements one by one and waits for feedback

The **connection** between the host PC and the spectrometer is **required during automation**

Data is saved in host PC

ECZ Luminous

Job group

Sample No.1 PROTON 1D

Sample No.2 CARBON 1D

Automation / Queue

One job group is sent to the spectrometer when submitted

The connection is not required during automation

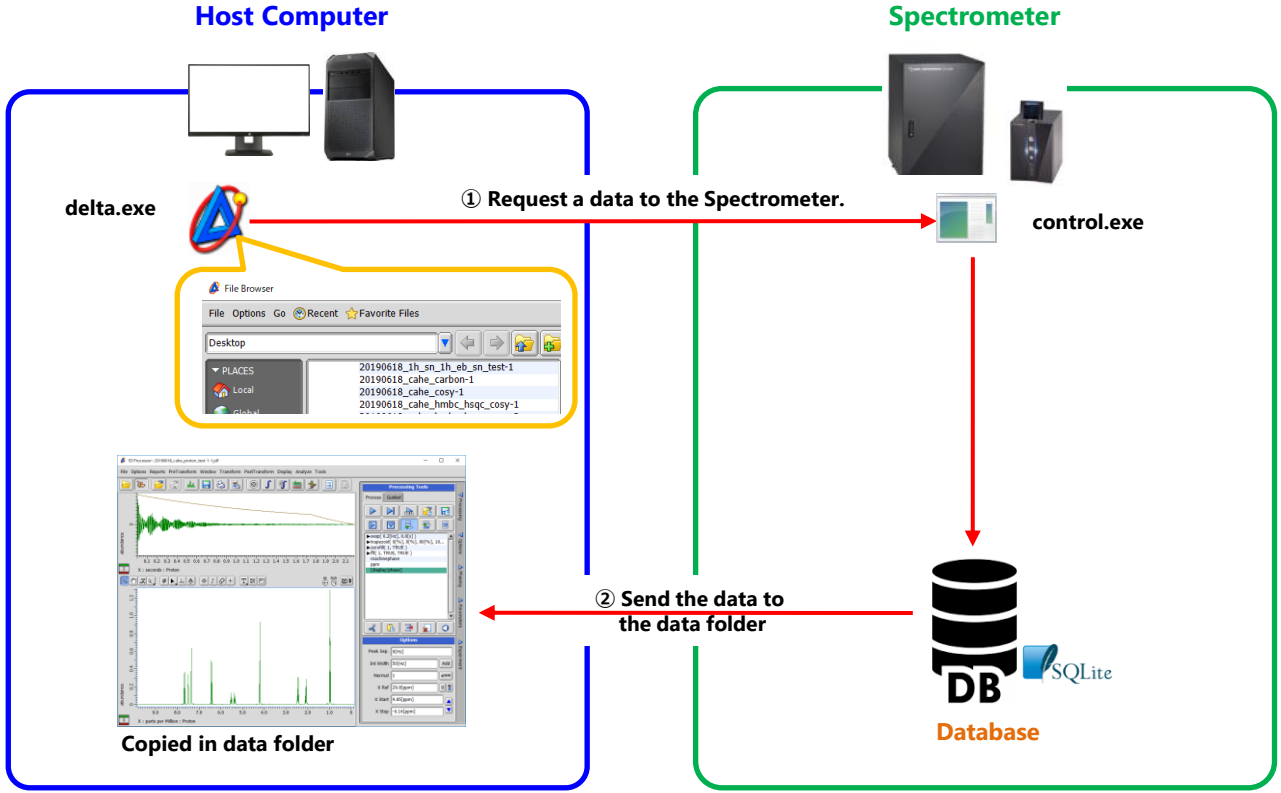
Data is saved in spectrometer

Solutions for Innovation JEOL

Delta Database System

- Workstation (Host computer)
  - Delta: Data processing and Interface to Control
  - RMT: Automatic copy of data from console database
  - Default IP: 172.20.1.201
  - Windows 7, 8,10 or 11

- Console
  - Control: Console and database operation
  - RMT(Instrument): Database and console maintenance
  - Default IP: 172.20.1.210
  - Windows 7 Embedded (ECZ) or Windows 10 IoT Enterprise 2016 LTSB (ECZL and some ECZ)



Solutions for Innovation JEOL

Software configuration

- Workstation
  - RMT: *C:\Program Files (x86)\JEOL\Remote Maintenance Tool* (install folder)
    - ***MaintenanceService.ini*** **(config)**
  - Delta: *C:\Program Files (x86)\JEOL\Delta 5.3.3.app* (install folder)
    - ***C:\Program Files (x86)\Common Files\JEOL\Delta 5.3*** **(manuals, license, permanent GMP mode) [All users]**
    - ***C:\Users\<Windows user>\AppData\Local\JEOL\Delta 5.3*** **(local configuration) [Windows user]**
    - ***C:\Users\<Windows user>\Documents\JEOL*** **(local files,e.g., experiments, scripts, etc.) [Windows user]**
    - *C:\Users\<Windows user>\AppData\Local\VirtualStore\Program Files (x86)\JEOL\Delta 5.3.3.app* (it should be empty, but trying to do a restricted operation may lead to files being stored here)
- Console
  - Control: C:\Program Files (x86)\JEOL\Control 5.3.3.app (install folder)
    - C:\Program Files (x86)\Common Files\JEOL\Control 5.3 (local folder, backed up by RMT (Instrument). Contains both spectrometer configuration, spectrometer user configuration, and local files uploaded to console)*
      - C:\Program Files (x86)\Common Files\JEOL\Control 5.3\users (spectrometer user specific files)
      - C:\Program Files (x86)\Common Files\JEOL\Control 5.3\web_server (SQL database)
  - RMT(Instrument): *C:\Program Files\JEOL\Remote Maintenance Tool*
    - ***MaintenanceService.ini*** **(config)**
    - ***files\configurations*** **(Control backup files)**

In bold: configuration to backup

*** Control local folder can be backed up via RMT and the backup downloaded with RMT(Instrument) (options to backup config/logs/data)**

Users? Which users?

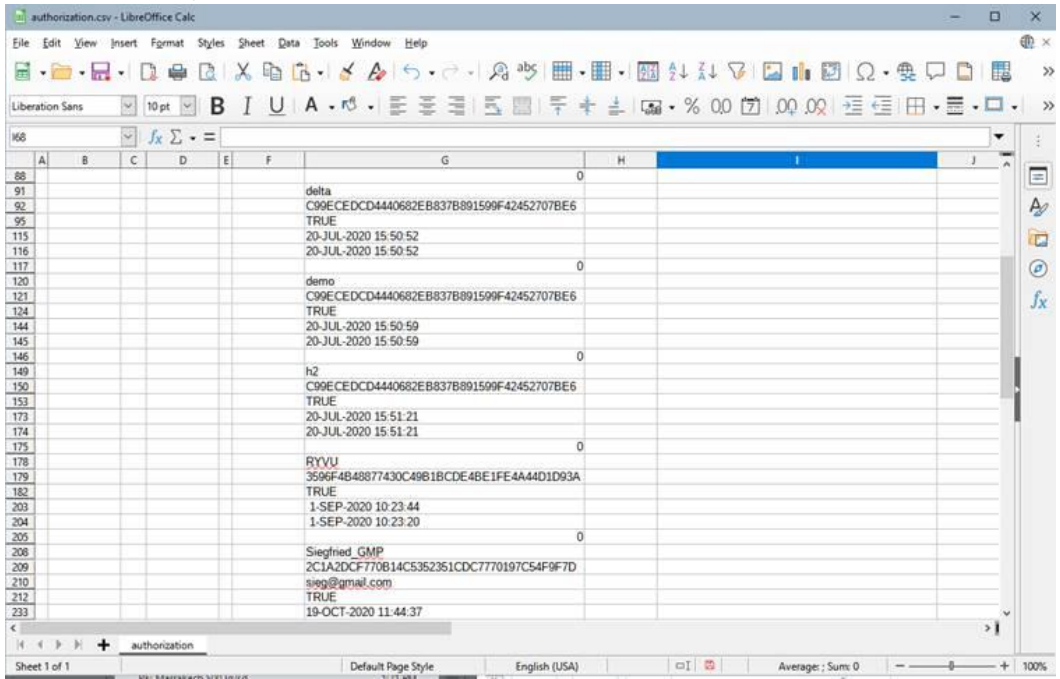
- **Workstation Windows user account**: Linked to Delta preferences, including GMP mode, Spectrometer operation mode and can be used to customize automation. **Windows user account is linked to processing actions.**
- **Spectrometer user account**: How users log into the spectrometer control in Delta. Managed within Delta. **Spectrometer user account is linked to acquisition actions.**

- Console Windows user account: Typically this is only Administrator, only used for internal file manipulation, such as customization including Smart mode buttons

- RMT Spectrometer user account: These are linked to spectrometer user accounts. console has access to Administrator menu (restarting control, solvent control). Datum in addition has access to Service menu (updating software).
- RMT Workstation user account: console and Windows user accounts. console has access to Administrator menu (backup management, printer config). Datum in addition has access to Service menu (updating software, change password for RMT Workstation user account).

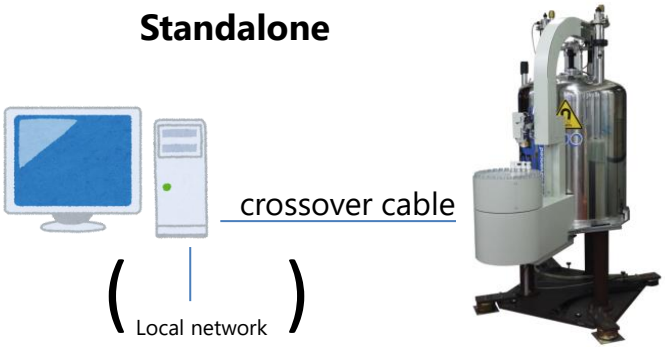
List of users with emails

If you do remote desktop into the console and locate:
C:\Program Files (x86)\Common Files\JEOL\Control 5.3\configuration
There is a file called authorization.jts
This contains the list of all users. It is perhaps in a not very convenient format to extract emails as it also contains other user data. But you can make a copy, change extension to csv, open it with LibreOffice or similar ensuring you also use spaces as delimiters, then you will have in a column all names with emails, hash code, dates, brackets and empty spaces. If you do an autofilter on that column to remove empty spaces and brackets you will get something like (note that I don't have emails assigned other than for Siegfried_GMP user, which you can see has an email just after the hash code):

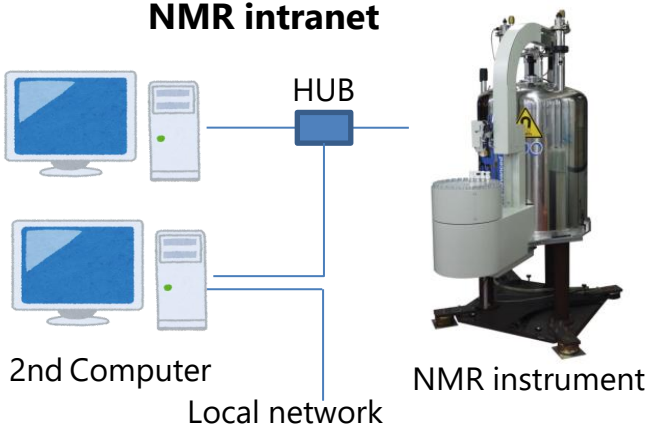


Network configurations

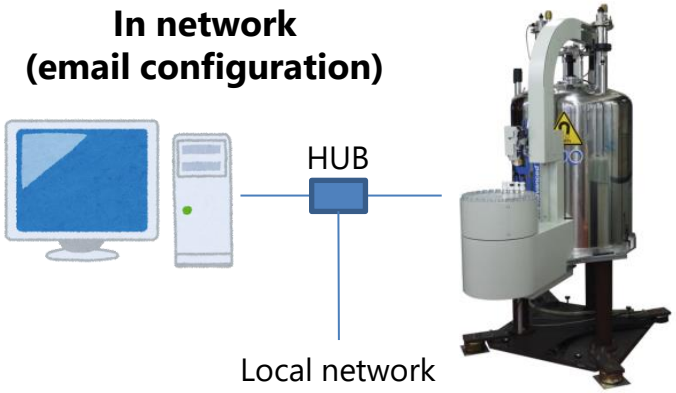
Standalone



NMR intranet

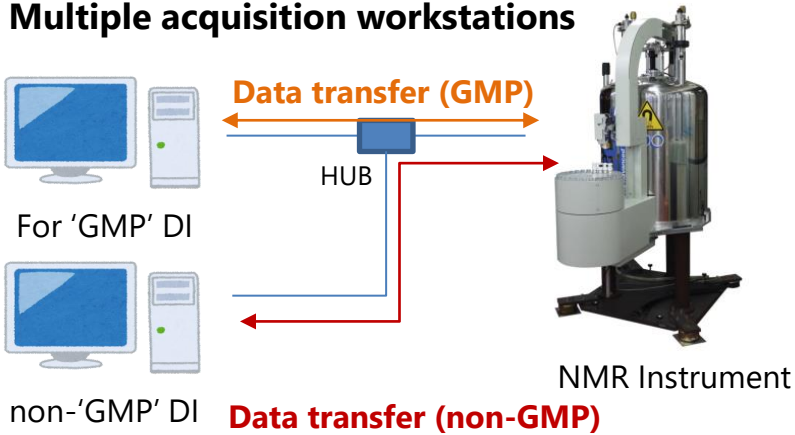


In network (email configuration)



The email functionality requires the acquisition computer to have access to an SMTP server and does not support authentication.

Multiple acquisition workstations



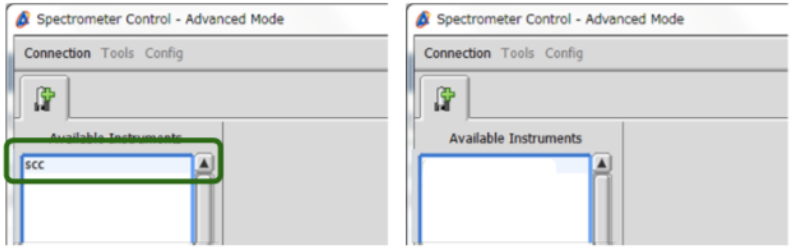
Solutions for Innovation JEOL

Network requirements

- The following networking ports and services are required for normal spectrometer operation between the **workstation** and **acquisition computer** and should be considered when configuring either hardware or software firewalls:
  - TCP: 6241, 6242, 6243, 6244
  - UDP: 6241, 6242, 6243, 6244
- All normal spectrometer operations are routed through the aforementioned TCP/UDP ports and these ports must be considered if installing the system behind a firewall or software firewall.
- Microsoft Remote Desktop (RDP) Client may be used between the **workstation** and **acquisition computer** for spectrometer maintenance; thus the following ports should be open in that network TCP: 3389 UDP: 3389
- The ports used for data backup are 80, 1080, 139, 445. The Remote Maintenance Tool service from the **workstation** can do the data backup from the **acquisition computer** onto a Windows / SAMBA shared drive.
- The **workstation** and **acquisition computer** as installed are only minimally configured for network security. If the user's network environment is not secure, **JEOL** recommends that a separate firewall be installed to secure the NMR spectrometer and workstation(s) requiring access to the NMR spectrometer.
- The use of a switch between the workstation and the NMR instrument may slow down system operation.
  - Test: Load Edited HSQC twice in Advanced mode and check how long it takes before the methods are loaded and its estimated time is calculated. Check this connecting directly the spectrometer to the workstation and via a router. If it is substantially slower via a router, the router is not fast enough to handle the data transfer.
  - E.g. 10s when directly connected and 35s when connected via a router.

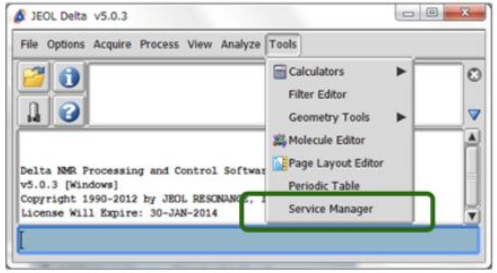
When the spectrometer is blocked

After Delta is restarted, if the spectrometer is not displayed, it may be blocked.



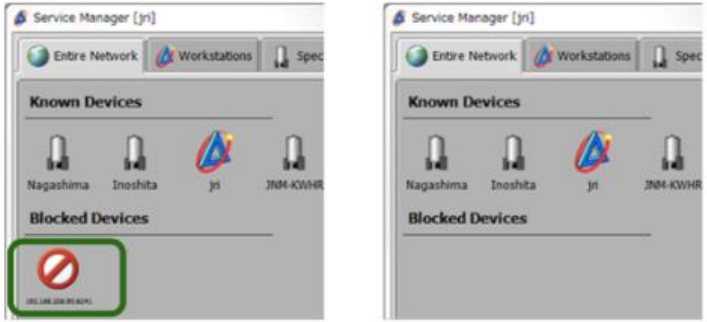
Spectrometer list display **No display**

From the Delta console pull-down menu, select **Tools** – **Service Manager**.



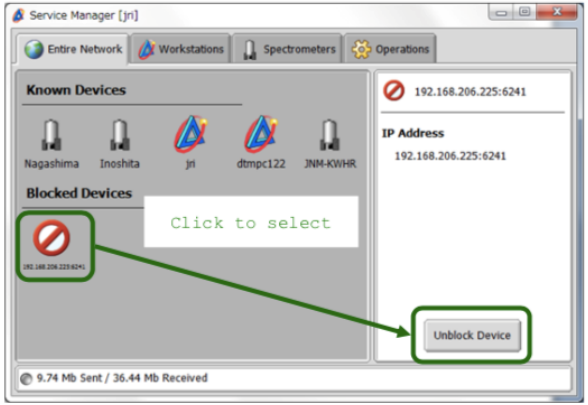
Check the section "Blocked Devices".

The IP addresses of the blocked devices are shown.



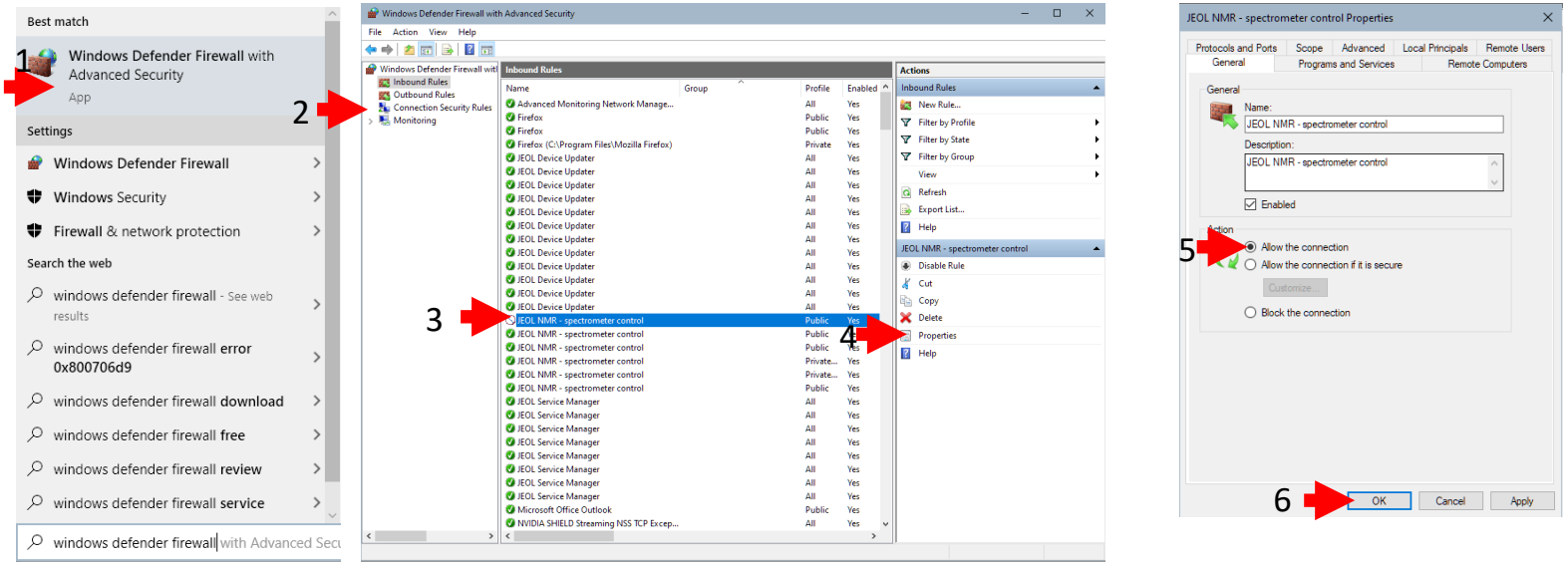
Block display **No display**

Select the spectrometer from the "Blocked Devices", and click the **Unblock Device** button.



After a few seconds, the spectrometers that can be connected will be displayed in the spectrometer list

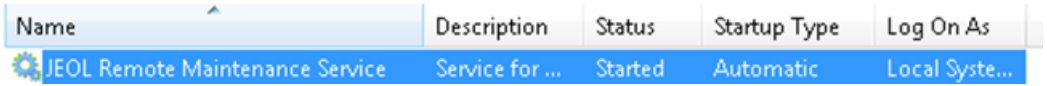
When the spectrometer is repeatedly blocked or is invisible



1. Open Firewall Advanced security
2. Inbound rules
3. Find blocked rules
4. Open properties
5. Select “Allow the connection” in the Action
6. Click Apply and OK button.

When RMT for workstation is not working

Log into Windows as datum, click on the Windows menu, type services and press enter.
Look for JEOL Remote Maintenance Service. It should have Status as Started, and Startup Type as automatic:



If not, Start it either from here or from the services tab in task manager, and right click, properties and change Startup type to automatic.

If for some reason the user is disabled from modifying this, it may be possible to edit the registry:
Locate the JEOL Remote Maintenance Service under HKLM:

And ensure that Start reg_dword is set to 2

Delta updates

Delta 6 why?

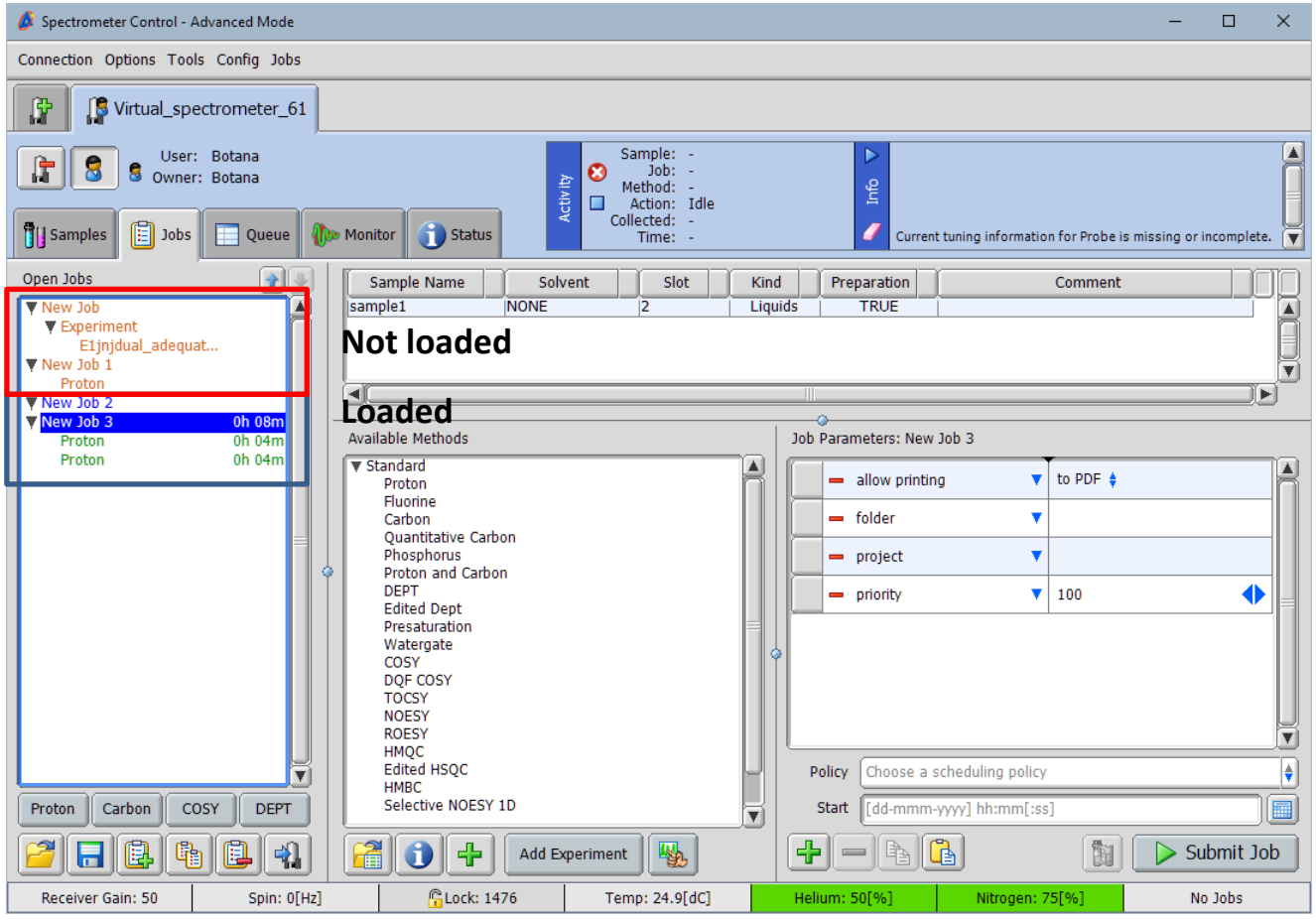
- 64 bits (Delta only, Control is still 32 bits)
- New automation capabilities
- New shape viewer
- New search tool
- Resolved bug: temperature not reset in walkup
- Resolved bug: sample location gets corrupted
  - Note that delete job related files deletes Smart mode method buttons (stored in console under C:\Program Files\Common Files\JEOL\Control 6.x\users\<username>.jobs)

- Delta 6.2 brings personas, monikers, announcement editor

Shortcuts:	Ctrl-Sh-Alt-A	- Advanced Mode
	Ctrl-Sh-Alt-S	- Smart Mode
	Ctrl-Sh-Alt-W	- Walkup Mode

- Delta 6.3 brings solvent editing from Delta, easy datafile signing

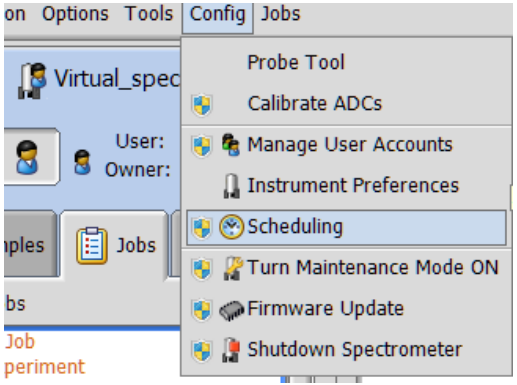
Advanced mode job loading



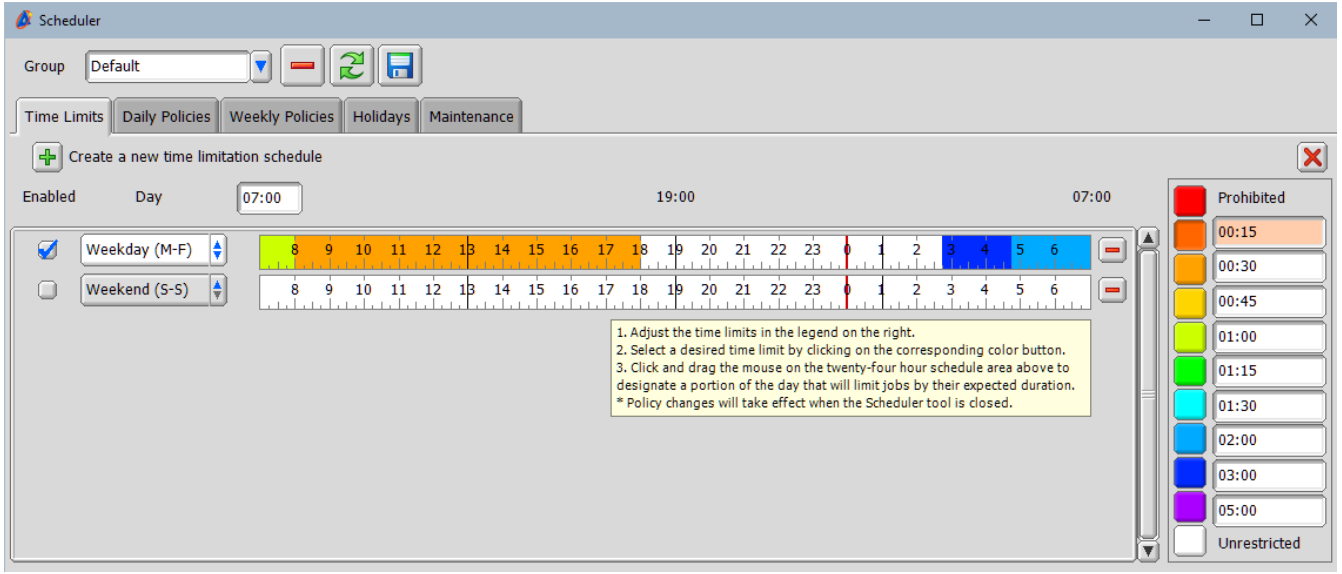
- Now jobs are not all loaded at once, only loaded when selected

If you want to run measurements that take time at night, you can put off measurements that take a long time for other measurements by setting a priority for the job to be measured. This function is available in Advanced mode and Walkup mode.
Enabling **Queue Control — Job Priority Allowed** from the Spectrometer Control window system settings allows you to select the "priority" parameter from the job parameter created herein. Setting the priority measures jobs with the smallest job number before jobs with larger numbers regardless of when the job was registered for measurement. Put simply, if there are jobs with "priority" 10 and 20, the job with the priority of 10 will be measured before the job with the priority of 20, even if the job with the priority of 20 was registered first. You can assign numbers from 0 to 100. Jobs that do not have a "priority" parameter are handled as jobs with the lowest priority (priority = 100).
You can determine the highest priority value that can be set by user (smallest value that can be specified for that user) from the account control screen on the Spectrometer Control window. Additionally, you can also overwrite numbers for the index that indicates the priority with characters using the pencil button on the same screen. (E.g., priority=10 → priority="high")

Scheduling



- When time limits are enabled, jobs with a duration exceeding the maximum allowed time limits of that time of the day are postponed
- Combined use of time limits and policies can lead to huge system slowdown



Cryogen filling intervals

5.4 Coolant Filling Date Setting and Log Function

It has become possible to pre-register the coolant charging date on Delta.
Alert display of the spectrometer control connection window and the log function for recording results have also become available.

5.4.1 Setting the filling intervals

1. Connect to the spectrometer and log on as a console user.
2. Select **Config — Instrument Preferences** in the Spectrometer Control window.
3. Select the Magnet Probe tab.
4. Select Cryogen Fill Tracking ☑ and enter the number of days in "Fill Cycle: Helium" and "Fill Cycle: Nitrogen".

- Fill Cycle: Helium: 0 to 365 (days) can be entered.
- Fill Cycle: Nitrogen: 0 to 18 (days) can be entered.

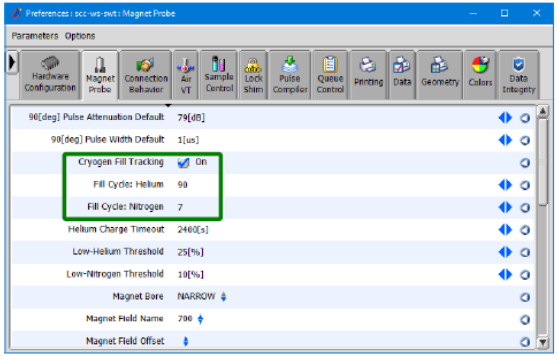


Figure12 Magnet Probe tab panel

The number of days that the coolant is remaining differs depending on the specifications of the SCM.

5. Close the Preference window.

Cryogen filling log

5.4.2a Starting filling of Nitrogen and Helium

1. Connect to the spectrometer and log on as a console user.
2. Select the **Status** tab.
3. Click the **Fill** button for Liq. Helium.

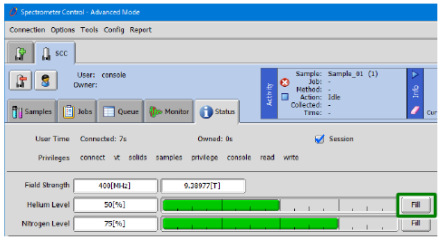


Figure5.13 Fill button for Liq. He

The Charging Helium window is displayed.

4. Enter current He level in the Start Level text box.

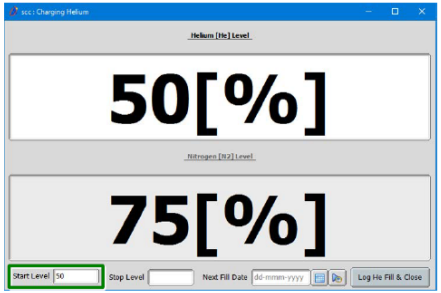


Figure5.14 Charging Helium window

5. Start filling of Liq. He.

5.4.2b Stopping filling of Liq. He and creating a filling log

1. After completion of filling, enter the coolant level when the filling is completed in the Stop level text box.

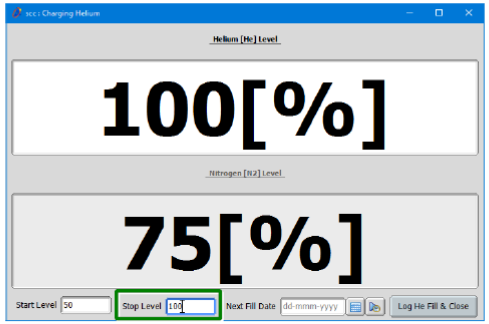


Figure5.15 Charging Helium window

2. Click the button.
The next filling date is automatically calculated and displayed by referring to the value of "Fill Cycle: Helium" set in the Preferences window.

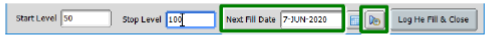


Figure5.16 Automatic calculation of the Next Fill Date

The date can be also entered manually using the button.

3. Click the **Log He Fill & Close** button.

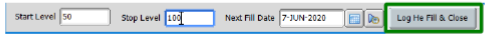


Figure5.17 Fill button for Liq. He

The filling log is created and the Preference window closes.

5.4.2e Fill log

You can check the log of coolant filling start level and filling completion level.

After creating the filling log, it can be checked the next time the spectrometer is connected.

1. Select the Status tab.
2. In the Log Files pane, select **cryogen_fill.log**.

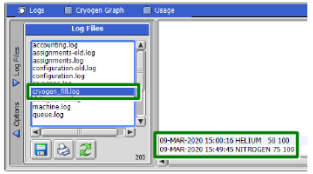


Figure5.23 cryogen_fill.log

5.4.2f The next filling date displayed in the Available Instruments information window

After setting the filling date, the scheduled filling date is displayed in the coolant level information from the next connection of the spectrometer.

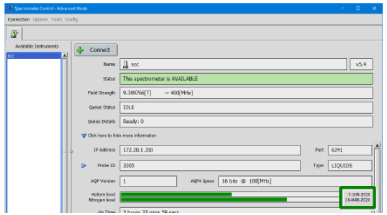


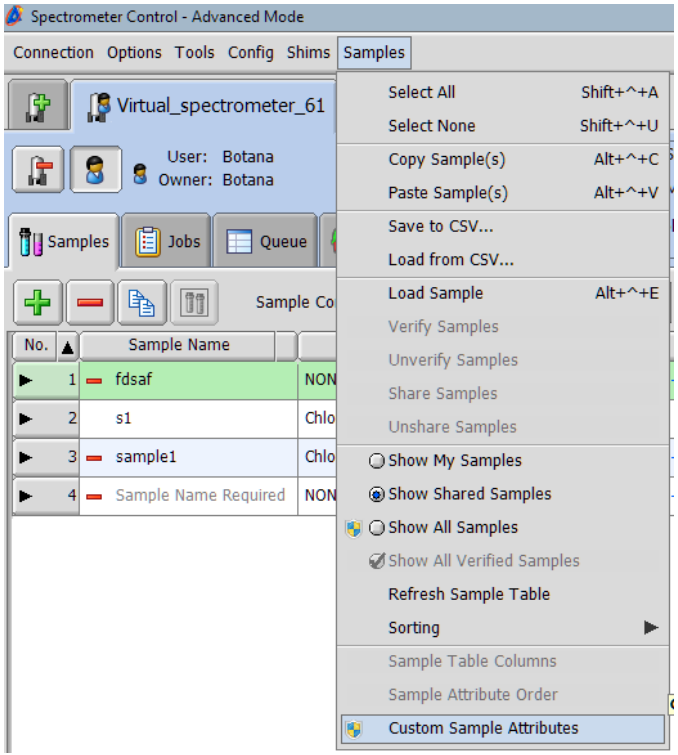
Figure5.24 Displaying the next filling date

When the next filling date is passed, the date will be shown in red to indicate alert status.

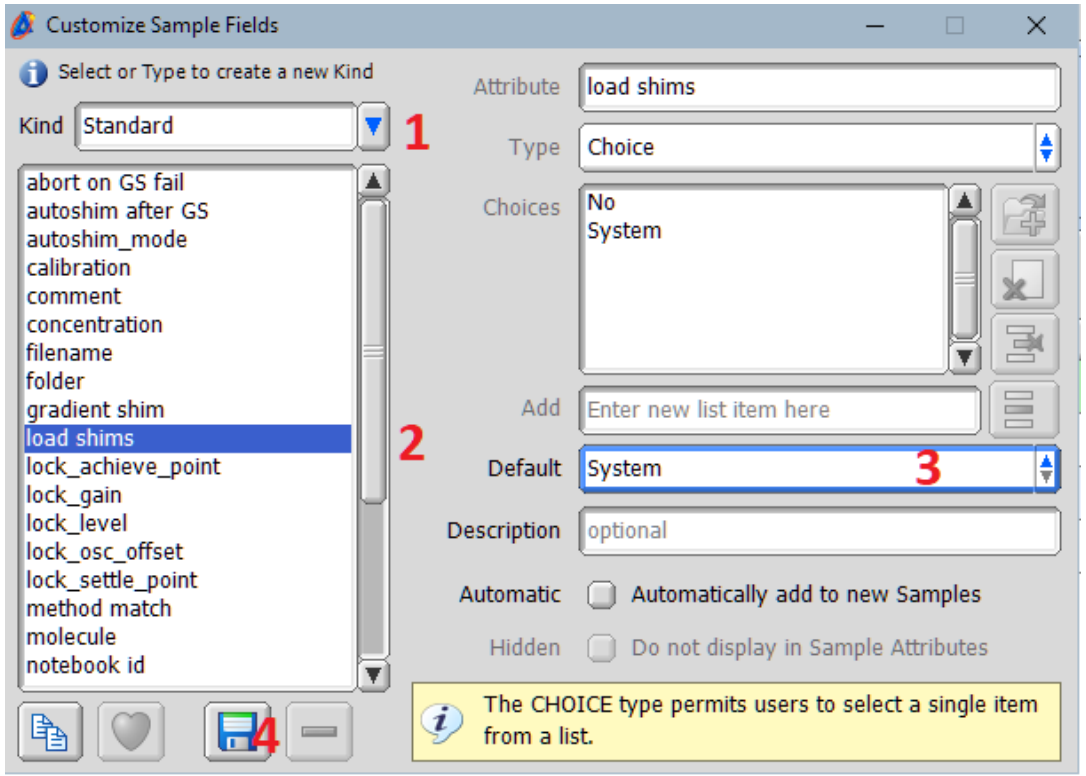
Figure5.25 Alert indication

New way to change sample attributes

- Log in as console



- Find attribute, change it, save it



Loading default shims (classic way)

-Specific sample. Click on the > to expand sample definition. Click on + to add a field, choose Load Shims and set it to system. Now this sample will load default shims before shimming.

-Load default shims for any sample before shimming:

1. Login with console user to spectrometer.
2. Open Preferences.
3. Open Edit.
4. Input the following sentence in Title. (Copy & paste is better.)
   sample_fields.standard."load shims"(default)
5. When you hit "enter" key, we can see "No" in Value box (If you can't see, please check spell and hit enter key again.)
6. Please change to "System" and hit "enter".
7. Click close button.
8. Open Edit again.
9. Input the following sentence in Title. (Copy & paste is better.)
   sample_fields.standard."load shims"(automatic)
10. Change to "TRUE" from "NULL".
11. Close edit preferences.
12. Close every Delta windows and restart spectrometer.
13. After initializing, please please create a new sample definition.
14. If you can see "Loaded System Shims for Current Probe" in Info box, you succeeded to modify.

Changing default sample settings (classic way)

To perform auto shim after gradient shim, change user to console and open Instrument preferences from Spectrometer control>Instrument preferences

- **Choose parameters>edit from preferences window drop down menu.**
- **Enter exactly, sample_fields.standard.”autoshim after gs”(default) in the title box**
- **Enter exactly Z1 Z2 in the value box or AUTOSHIM OFF**

Turn spinning off:

- **Enter exactly, sample_fields.liquids.spin_state(default) in the title box**
- **Enter exactly SPIN OFF in the value box instead of SPIN ON**

Setting a default temperature:

- **Enter exactly, sample_fields.liquids.temp_state(default) in the title box**
- **Enter exactly TEMP ON in the value box instead of TEMP OFF**
- **Choose temperature with sample_fields.liquids.temp_set(default)**
- **Choose delay with sample_fields.standard.temp_delay(default)**

sample_fields.standard.temp_delay(automatic) set to TRUE

Increasing RT shim limits

1. Login with console user to spectrometer.
2. Open menu Config> Instrument Preferences.
3. Open menu Parameters> Edit.
4. Input the following sentence in Title depending on system:
   shim.*[dm/lg/mx]*.shim*_[shim]*(*[UPPER/LOWER]*)

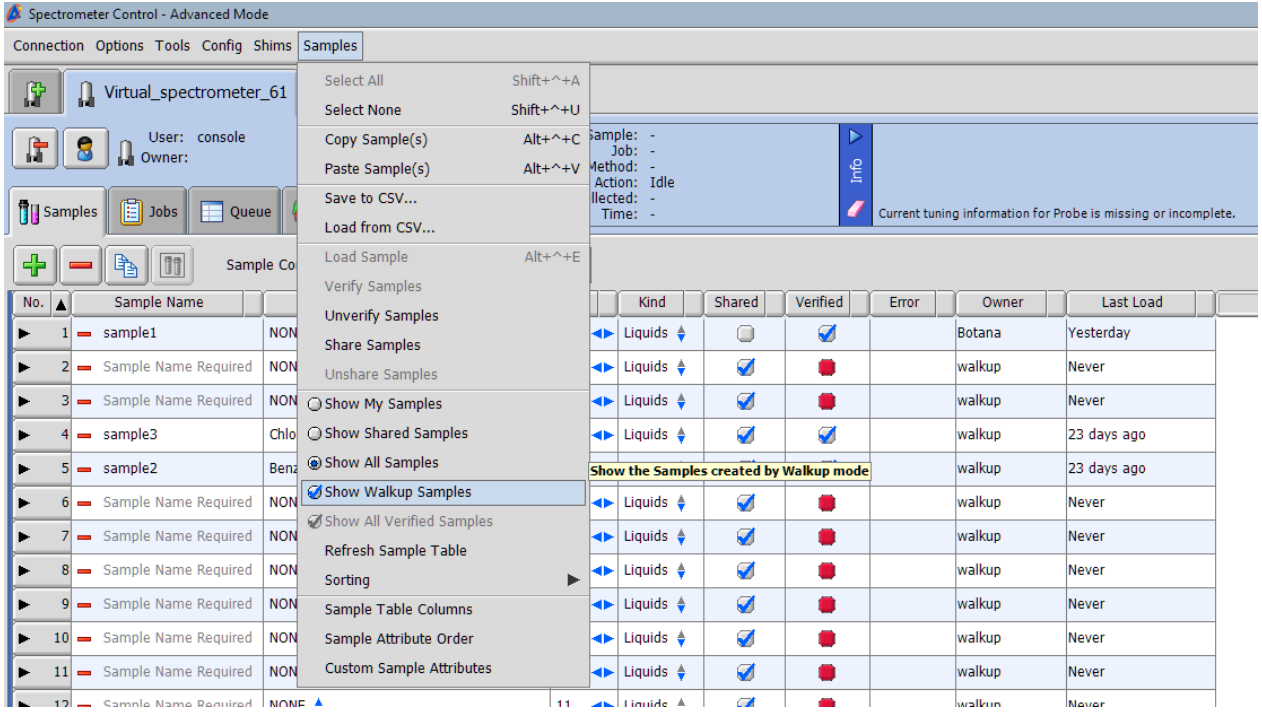
e.g.:
   shim.dm.shim_z1(UPPER)

5. Please change to new desired limit and hit "enter".

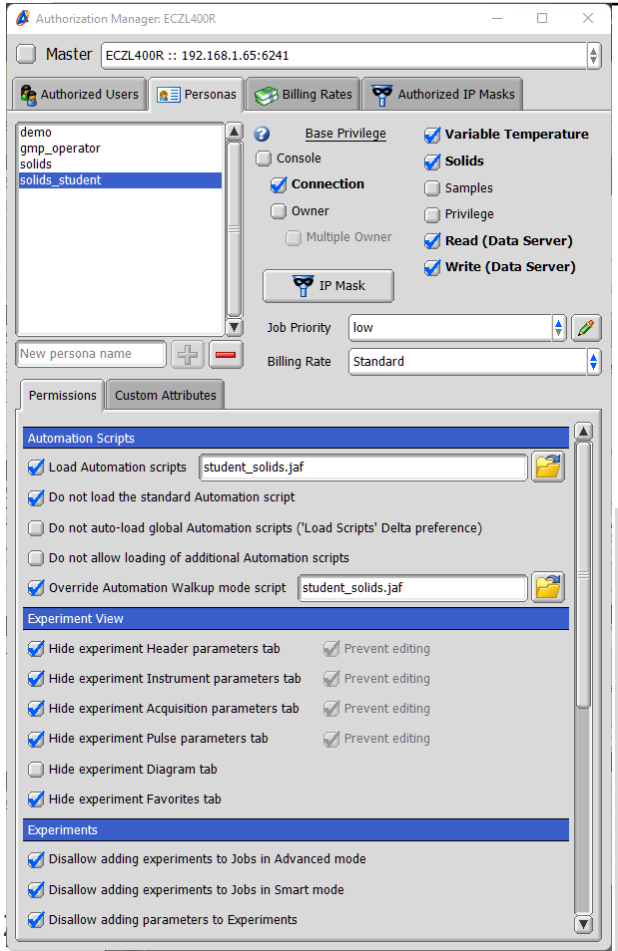
Note: dm is for 400, lg is for 500+, mx is for legacy systems. If the current value is null, probably the wrong type of shim is selected or there is a typo.

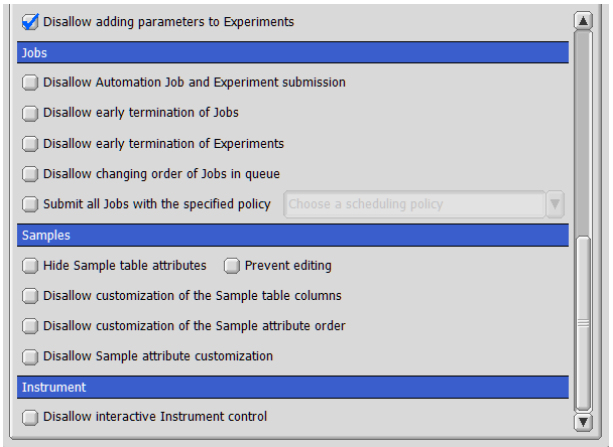
Walkup mode

- Changing sample default parameters does not change the parameters of samples currently defined, e.g., Walkup samples.
- Log in as console, Show walkup samples, select all samples, delete them

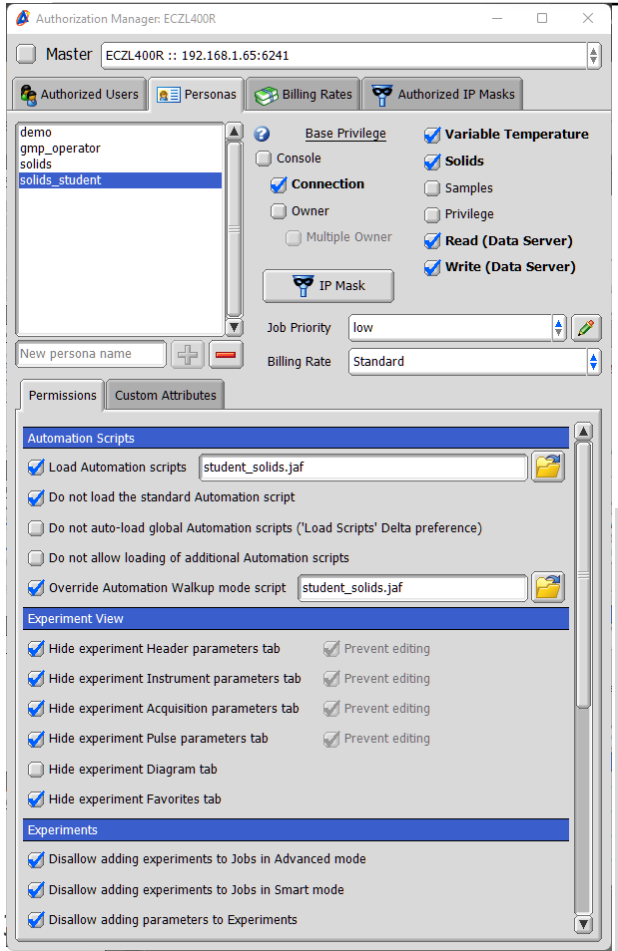


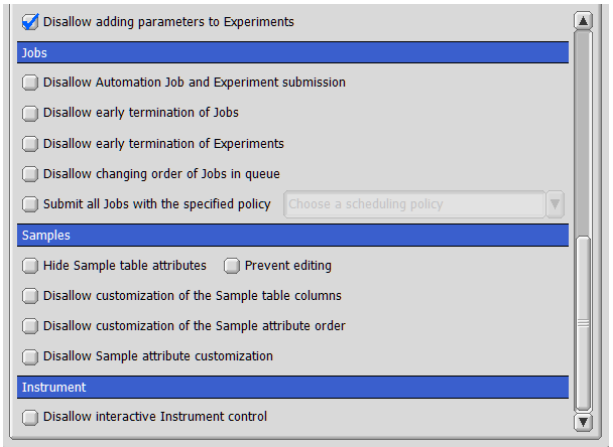
Persona manager

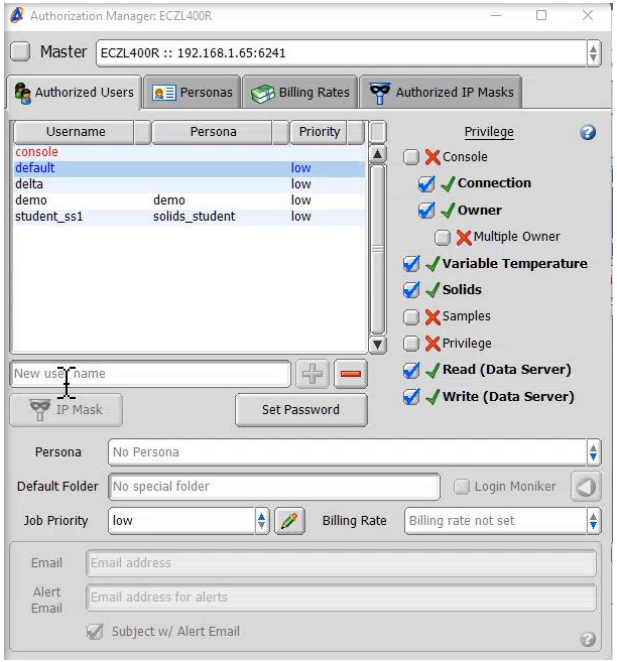




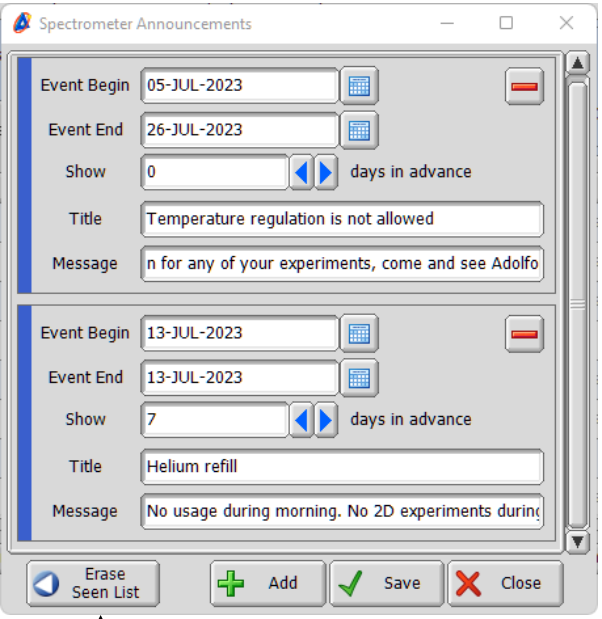
Persona manager







Announcement editor

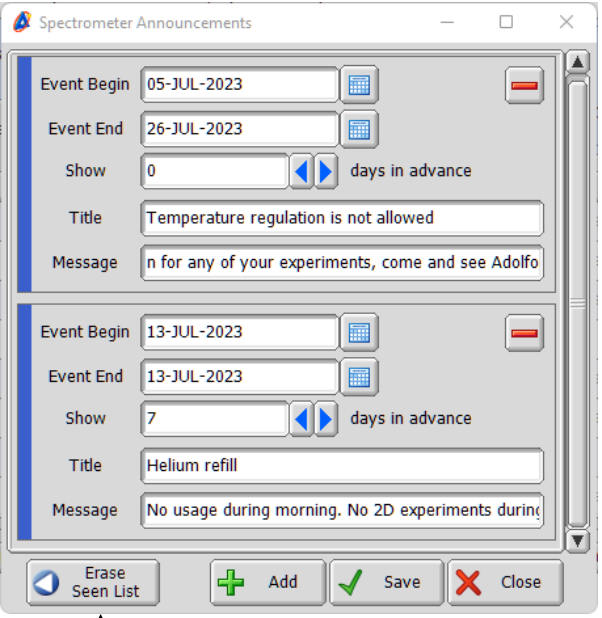


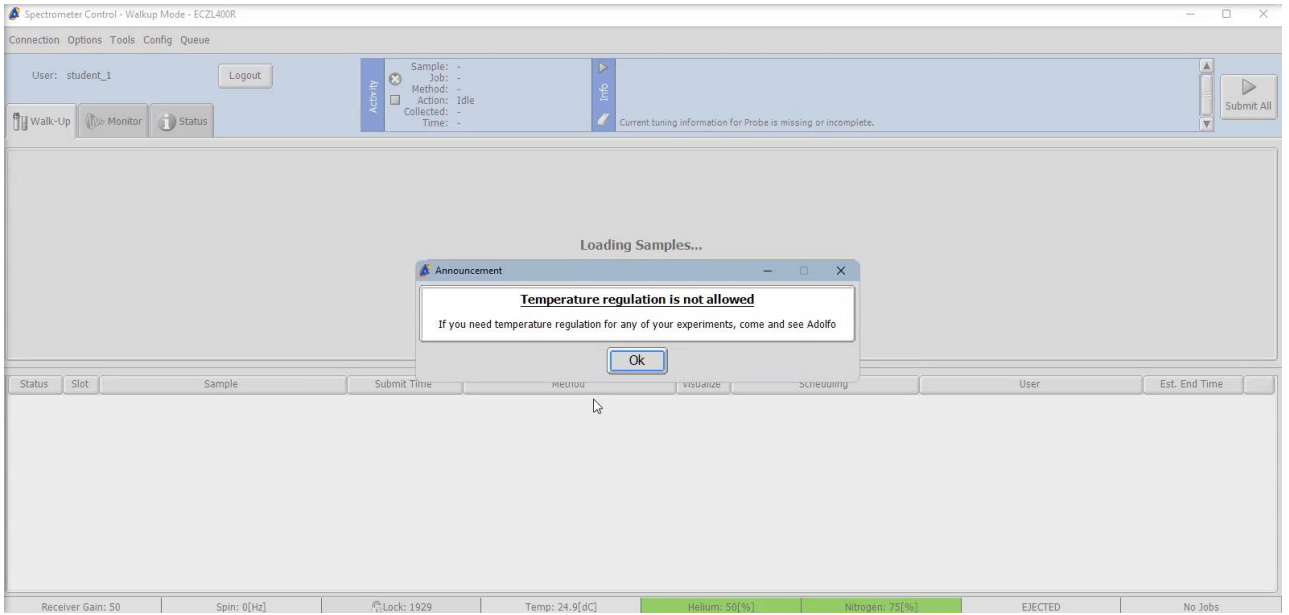
Announcements show up only on first login once the announcement is active.

Push this button to show again.

Solutions for Innovation JEOL

Announcement editor





Announcements show up only on first login once the announcement is active.

Push this button to show again.

Solutions for Innovation JEOL

Automation setup

Automation setup

Flexible configuration of defaults and privileges for different users, including:

Variable temperature, Solids mode, Data folder, Email address, **user operators**, multiple backup structure as per user, project, date, etc.

Automation setup

Flexible configuration of defaults and privileges for different users, including:

Variable temperature, Solids mode, Data folder, Email address, user operators, …

Usage reports, logs, statistics and billing:

JEOL Instrument:	Virtual_spectrometer			
Usage Log Report:	1-AUG-2022 - 18-AUG-2022			
User	Cost Center	Active(min)	Rate/Hr	Active Charge
Botana	<blank>	63	0.00	0.00
console	<blank>	0	0.00	0.00
Delta	<blank>	200	0.00	0.00
demo	<blank>	35	10.00	5.83
tesT	<blank>	2	0.00	0.00
		300		**5.83**

Automation setup

Flexible configuration of defaults and privileges for different users, including:

Variable temperature, Solids mode, Data folder, Email address, user operators, …

Usage reports, logs, statistics and billing:

Detailed output:

* Breakdown of folder 'demo'

Operation Began	Operation End	Duration	Duration/day	Username	Job Name	Experiment Began	Experiment End	Experiment Duration	Experiment Duration/day	Experime	Project Na	Folder	Filename	Job Result
14-12-22 23:14	14-12-22 23:14	0 days 00:(	0.00037037	demo	Proton	14-12-22 23:14	14-12-22 23:14	0 days 00:00:18	0.000208333	proton.jxp		demo	test1_1H	FINISHED
15-12-22 10:19	15-12-22 10:19	0 days 00:(	0.000208333	demo	Proton	15-12-22 10:19	15-12-22 10:19	0 days 00:00:08	9.25926E-05	proton.jxp		demo	sample1_1H	FINISHED
21-01-23 21:46	21-01-23 21:46	0 days 00:(	0.000300926	demo	Proton	21-01-23 21:46	21-01-23 21:46	0 days 00:00:18	0.000208333	proton.jxp		demo	aa1_1H	FINISHED

* Breakdown of folder 'organometallic/PhD_1'

Operation Began	Operation End	Duration	Duration/day	Username	Job Name	Experiment Began	Experiment End	Experiment Duration	Experiment Duration/day	Experime	Project Na	Folder	Filename	Job Result
29-06-23 9:38	29-06-23 9:38	0 days 00:(	0.000243056	test	1H	29-06-23 9:38	29-06-23 9:38	0 days 00:00:10	0.000115741	proton.jxp		organome	sampl3_PROTON	FINISHED

* Breakdown of folder 'organometallic/PhD_2'

Operation Began	Operation End	Duration	Duration/day	Username	Job Name	Experiment Began	Experiment End	Experiment Duration	Experiment Duration/day	Experime	Project Na	Folder	Filename	Job Result
16-12-22 19:21	16-12-22 19:22	0 days 00:(	0.000196759	test2	1H	16-12-22 19:21	16-12-22 19:22	0 days 00:00:10	0.000115741	proton.jxp		organome	fds_PROTON	FINISHED

Automation setup

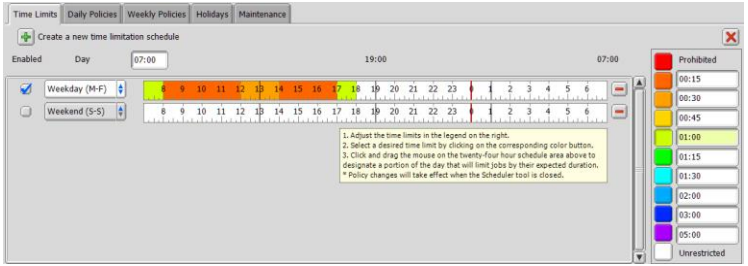
Flexible configuration of defaults and privileges for different users, including:

Variable temperature, Solids mode, Data folder, Email address, user operators, …

Usage reports, logs, statistics and billing:

JEOL Instrument:	Virtual_spectrometer			
Usage Log Report:	1-AUG-2022 - 18-AUG-2022			
User	Cost Center	Active(min)	Rate/Hr	Active Charge
Botana	<blank>	63	0.00	0.00
console	<blank>	0	0.00	0.00
Delta	<blank>	200	0.00	0.00
demo	<blank>	35	10.00	5.83
tesT	<blank>	2	0.00	0.00
		300		**5.83**

Custom time limitations:



Automation setup

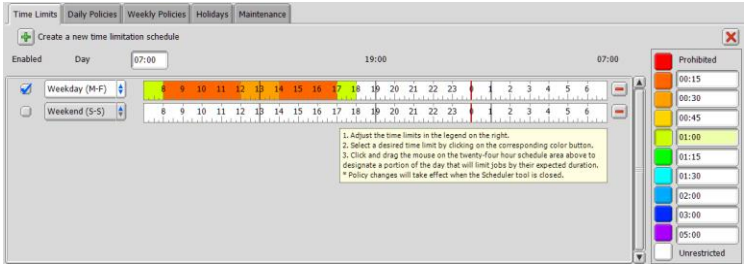
Flexible configuration of defaults and privileges for different users, including:

Variable temperature, Solids mode, Data folder, Email address, user operators, …

Usage reports, logs, statistics and billing:

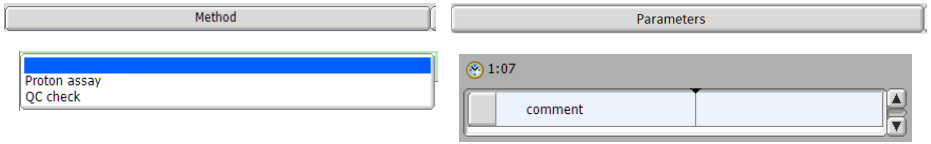
JEOL Instrument:	Virtual_spectrometer			
Usage Log Report:	1-AUG-2022 - 18-AUG-2022			
User	Cost Center	Active(min)	Rate/Hr	Active Charge
Botana	<blank>	63	0.00	0.00
console	<blank>	0	0.00	0.00
Delta	<blank>	200	0.00	0.00
demo	<blank>	35	10.00	5.83
tesT	<blank>	2	0.00	0.00
		300		5.83

Custom time limitations:

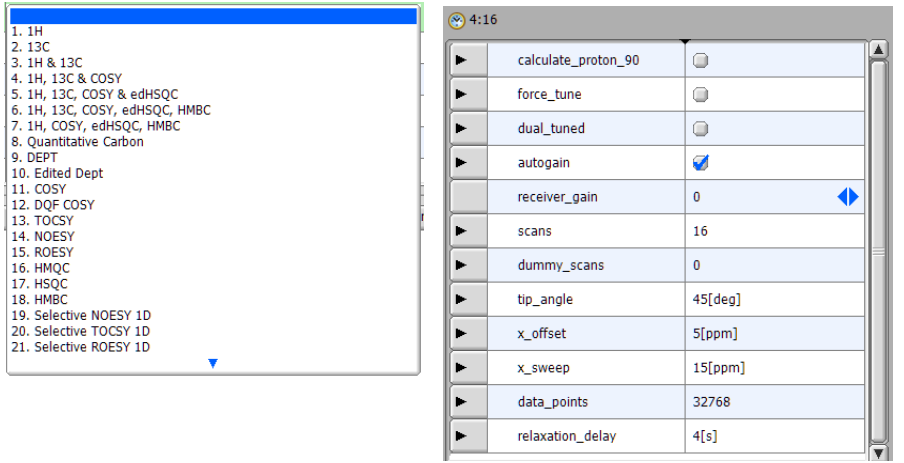


Fully customizable methods for each user

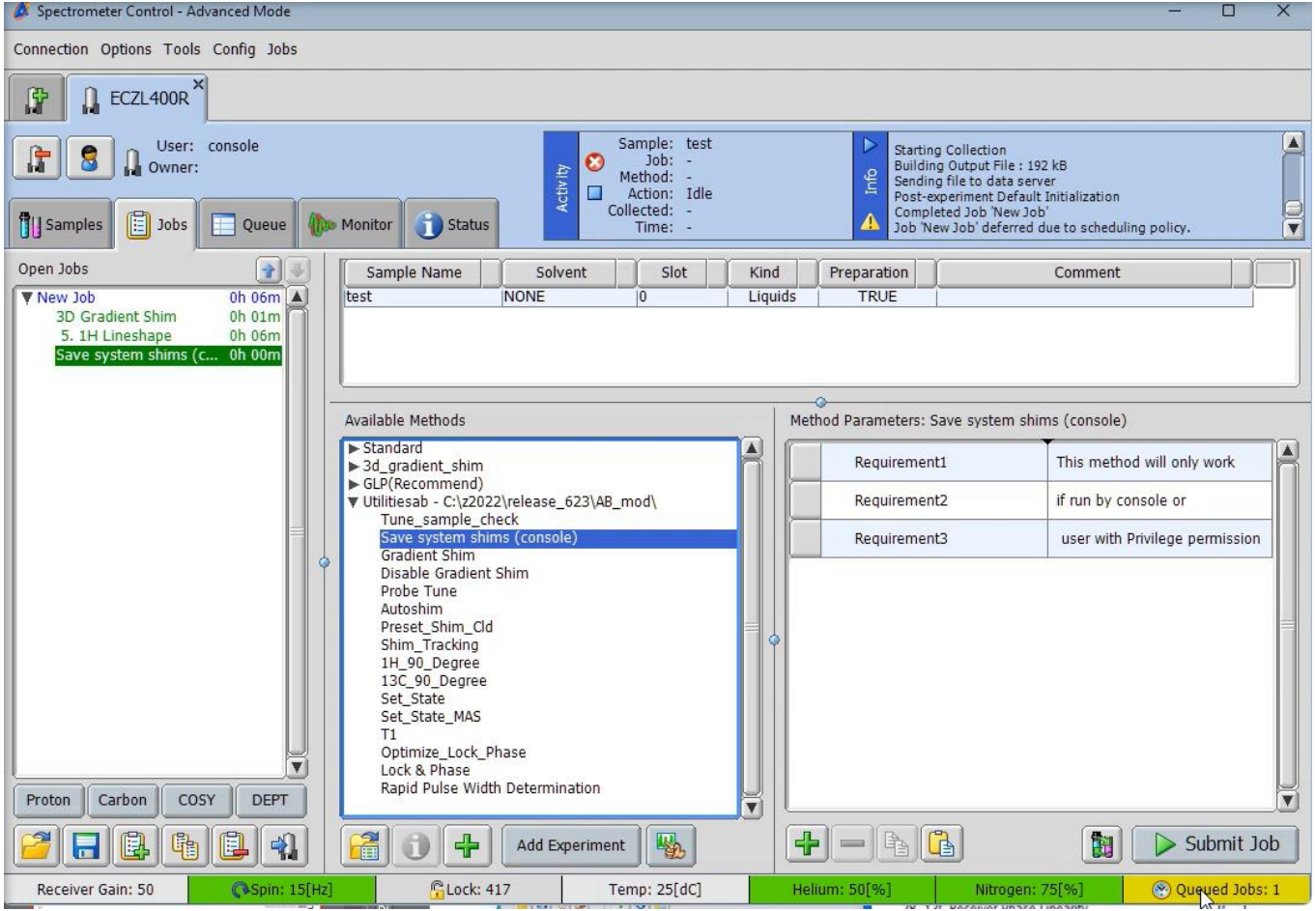
User 1



User 2



Recurrent jobs



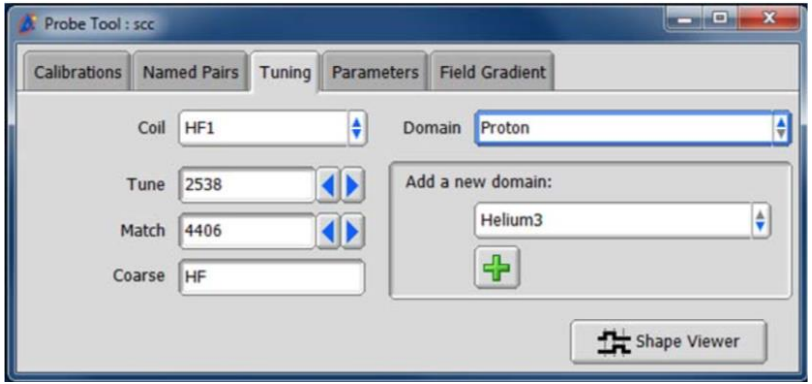
Solutions for Innovation JEOL

Other

Update the probe file.

The LFT & LFM for 31P, found by manual tuning now need to be entered in the probe file for pretune to use them.

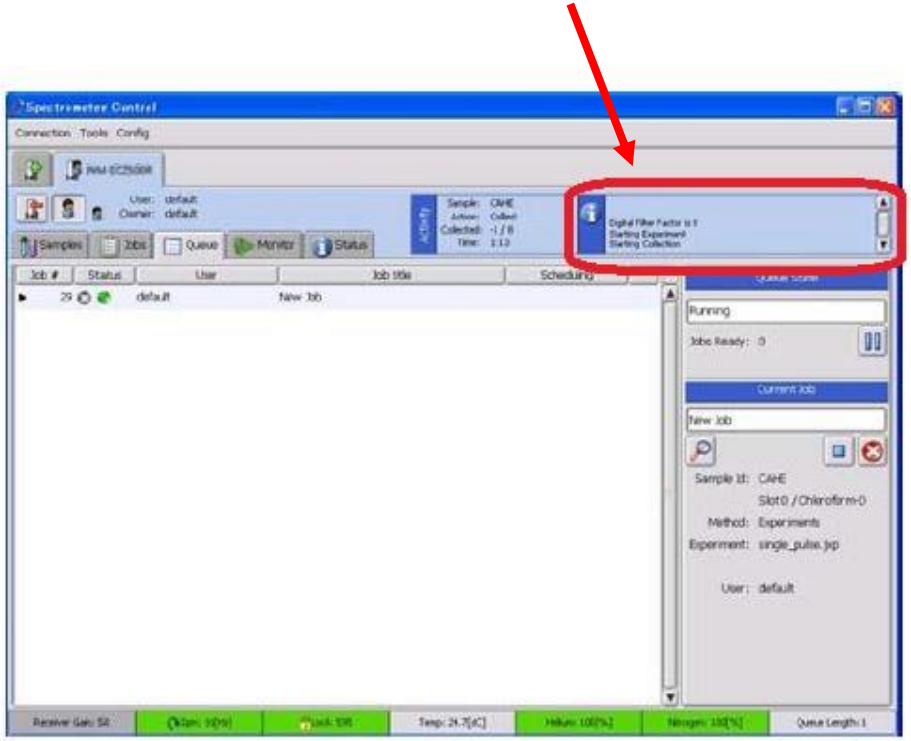
- Change user and connect as console mode, to allow probe tool editing.
- Choose the 'Configuration' drop down menu, then 'Probe Tool'.
- When the probe tool opens, select the 'Tuning' tab.



- Choose Coil = LF, Domain = Phosphorous 31.
- Edit the Tune & Match with the new values found by manual tuning **+ an offset of 50**.
- Close the Probe Tool window.
- Reconnect the autotune drive cables, turn on the AT unit, note the probe dial values and attempt the pretune again.

Delta Software, Alarm Status

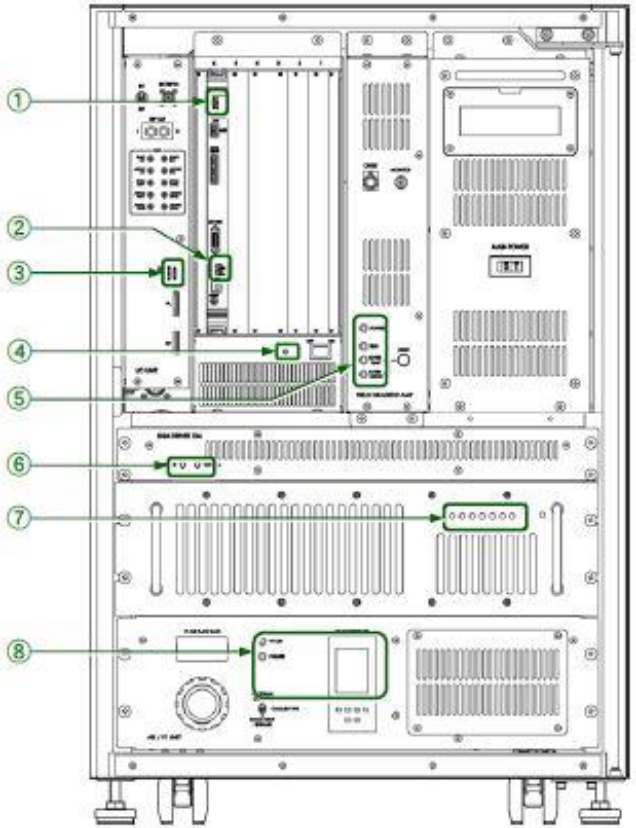
During normal operation, spectrometer alarms will appear in the information panel, spectrometer control window.



Solutions for Innovation JEOL

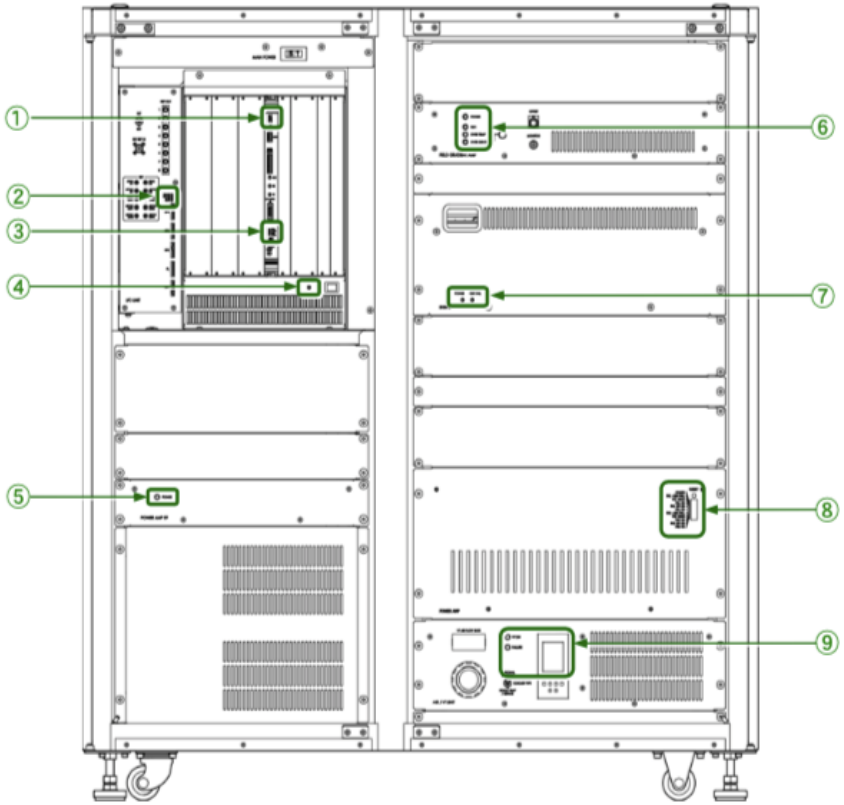
- Alarm Status, checking Hardware. ECZ400S

1. Shim Controller Display No.1
2. Shim Controller Display No. 2
3. Input / Output Unit
4. PCI Rack Display
5. Field Gradient Amplifier Display
6. Shim Driver Display
7. Power Amplifier Display
8. Air VT Unit Display



ECZ-R hardware locations

1. Shim controller display 1
2. I/O Unit display
3. Shim Controller display 2
4. PCI Rack display
5. Power Amplifier Interface display
6. Field Gradient Amplifier display
7. Shim Driver display
8. Power Amplifier display
9. Air/VT display



- Shim Controller display 1.
  - Only lamp 4 should flash.

- I/O Unit display.
  - Power lamp and REF CLK lamp should be lit.

- Shim Controller display 2
  - B-BUS and RUN lamp should be lit.
  - Check FAIL lamp.

- PCI Rack display
  - Lamp lights and buzzer sounds if a fan fails.

- P-Amplifier Interface display
  - Power lamp should be lit

- Field Gradient Amplifier display
  - Power lamp should be lit.
  - Run light on during operation
  - Over-Temp lit if internal temperature is too high.
  - Over-Drive lit if excessive FG power is used

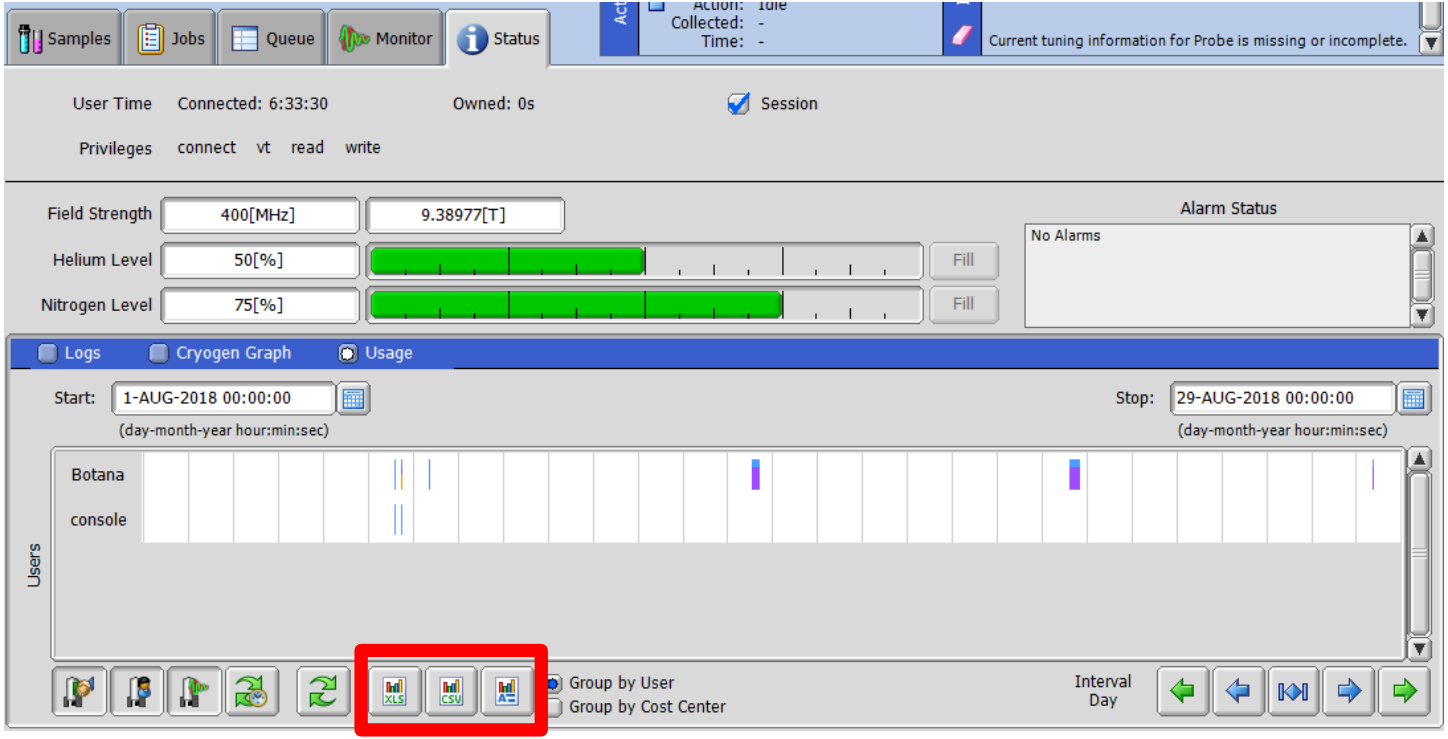
- Shim Driver display
  - Power lamp should be lit.
  - Out Fail on if shim coil is disconnected.

- Power Amplifier display
  - AC & HF/LF Enable lams should be lit.
  - Note which alarm is lit and press reset button.

- Air/VT display
- VT lamp on during operation. Failure lamp lit if air flow is low.
  400 deg C indicated thermocouple

Usage

- Available from Delta 5.3



Usage

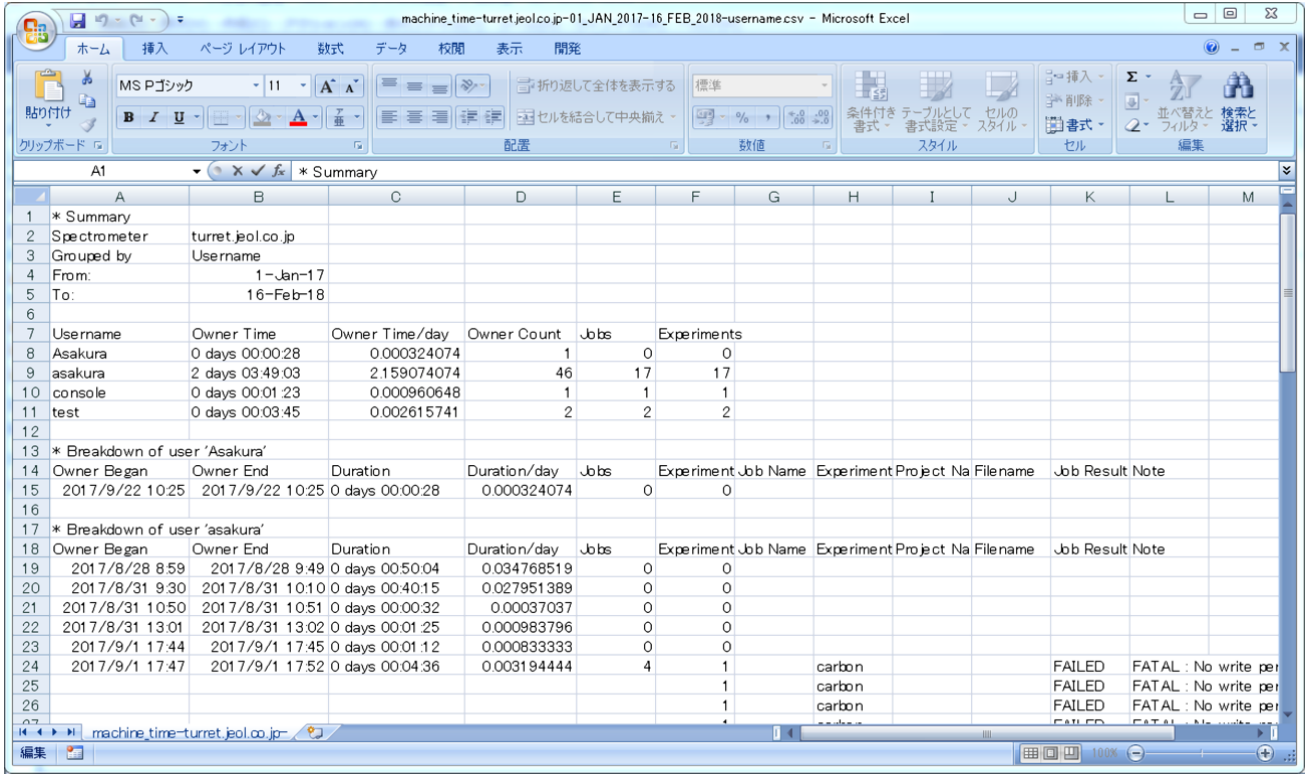
- Exported to .xls file:
- Rate/hr controlled in “Manage User accounts”

	A	B	C	D	E	F	G	H	I
1	JEOL Instrument:	ecz400s							
2	Usage Log Report:	1-AUG-2018 - 4-AUG-2018							
3									
4	User	Cost Center	Connected*	Owned*	Active*	Rate/Hr	Connected Charge	Owned Charge	Active Charge
5	console	<blank>	3	0	0	0.00	0.00	0.00	0.00
6	datum	<blank>	1	1	0	0.00	0.00	0.00	0.00
7	delta	<blank>	1238	1165	405	0.00	0.00	0.00	0.00
8			**1242**	**1166**	**405**		**0.00**	**0.00**	**0.00**
9									
10			* Numbers are rounded up to nearest minute						
11									

Solutions for Innovation JEOL

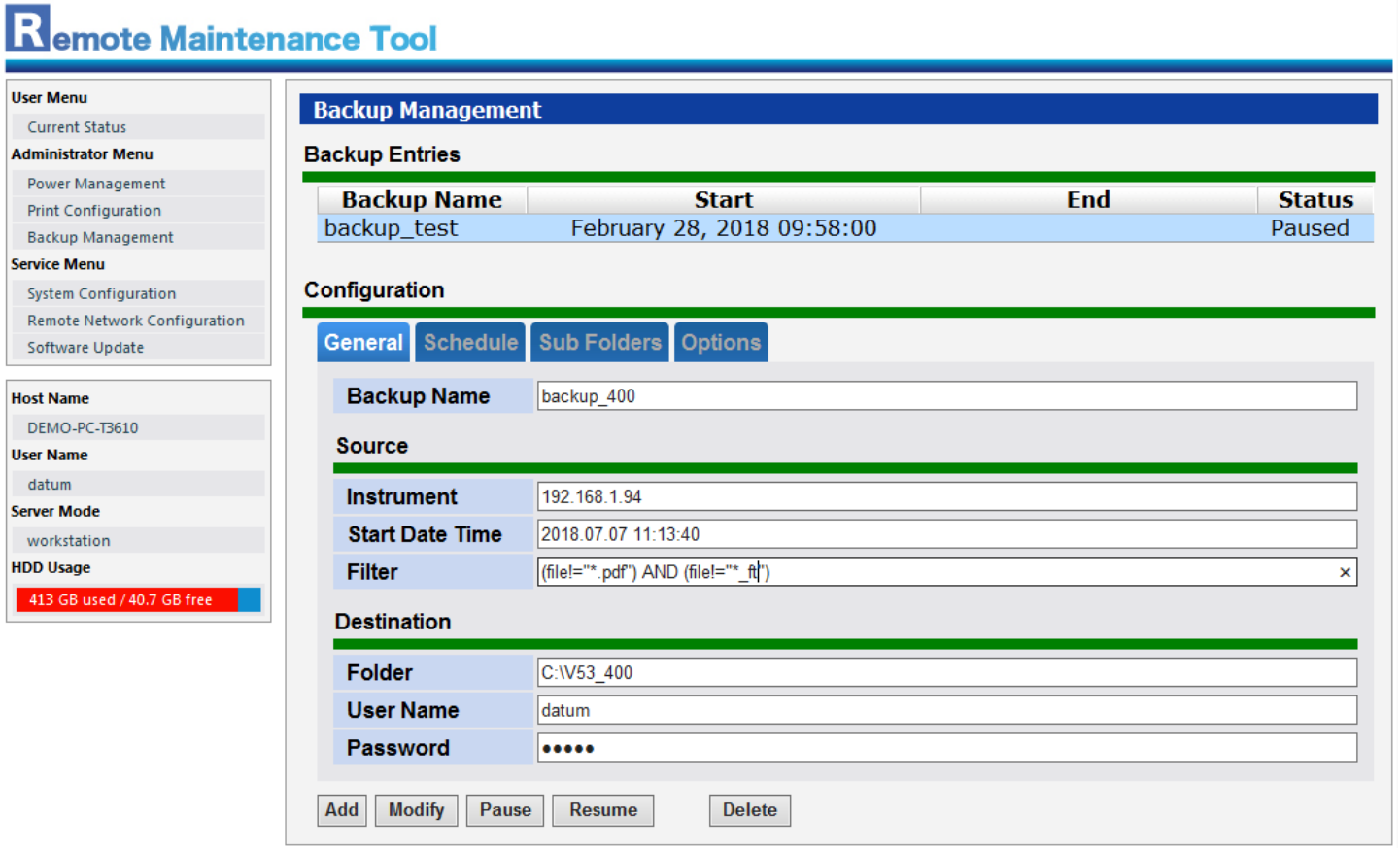
Machine Time calculator

Use MTC 2.1 and get full details of time employed for each experiment



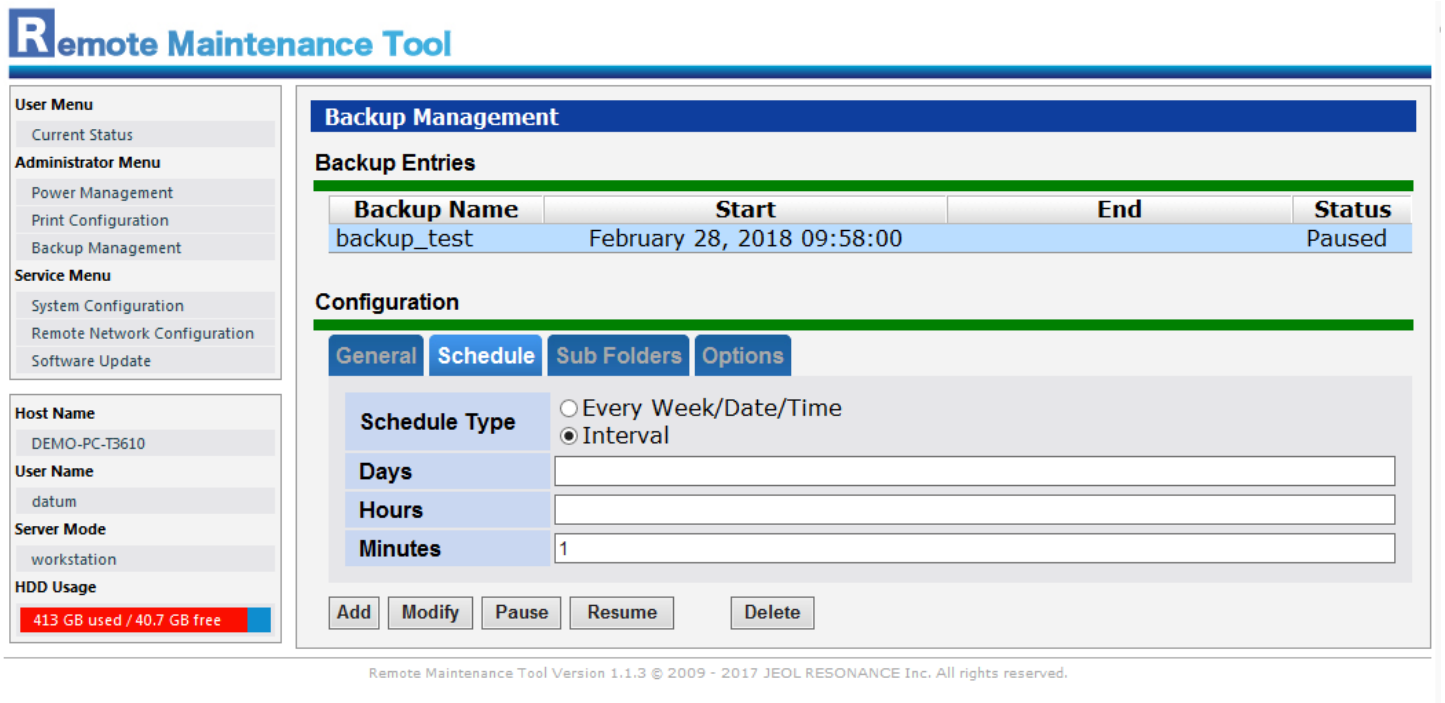
	A	B	C	D	E	F	G	H	I	J	K	L	M
1	* Summary												
2	Spectrometer	turret.jeol.co.jp											
3	Grouped by	Username											
4	From:	1-Jan-17											
5	To:	16-Feb-18											
6													
7	Username	Owner Time	Owner Time/day	Owner Count	Jobs	Experiments							
8	Asakura	0 days 00:00:28	0.000324074	1	0	0							
9	asakura	2 days 03:49:03	2.159074074	46	17	17							
10	console	0 days 00:01:23	0.000960648	1	1	1							
11	test	0 days 00:03:45	0.002615741	2	2	2							
12													
13	* Breakdown of user 'Asakura'												
14	Owner Began	Owner End	Duration	Duration/day	Jobs	Experiment	Job Name	Experiment	Project Na	Filename	Job Result	Note	
15	2017/9/22 10:25	2017/9/22 10:25	0 days 00:00:28	0.000324074	0	0							
16													
17	* Breakdown of user 'asakura'												
18	Owner Began	Owner End	Duration	Duration/day	Jobs	Experiment	Job Name	Experiment	Project Na	Filename	Job Result	Note	
19	2017/8/28 8:59	2017/8/28 9:49	0 days 00:50:04	0.034768519	0	0							
20	2017/8/31 9:30	2017/8/31 10:10	0 days 00:40:15	0.027951389	0	0							
21	2017/8/31 10:50	2017/8/31 10:51	0 days 00:00:32	0.00037037	0	0							
22	2017/8/31 13:01	2017/8/31 13:02	0 days 00:01:25	0.000983796	0	0							
23	2017/9/1 17:44	2017/9/1 17:45	0 days 00:01:12	0.000833333	0	0							
24	2017/9/1 17:47	2017/9/1 17:52	0 days 00:04:36	0.003194444	4	1		carbon			FAILED	FATAL : No write per	
25						1		carbon			FAILED	FATAL : No write per	
26						1		carbon			FAILED	FATAL : No write per	

RMT workstation: Backup

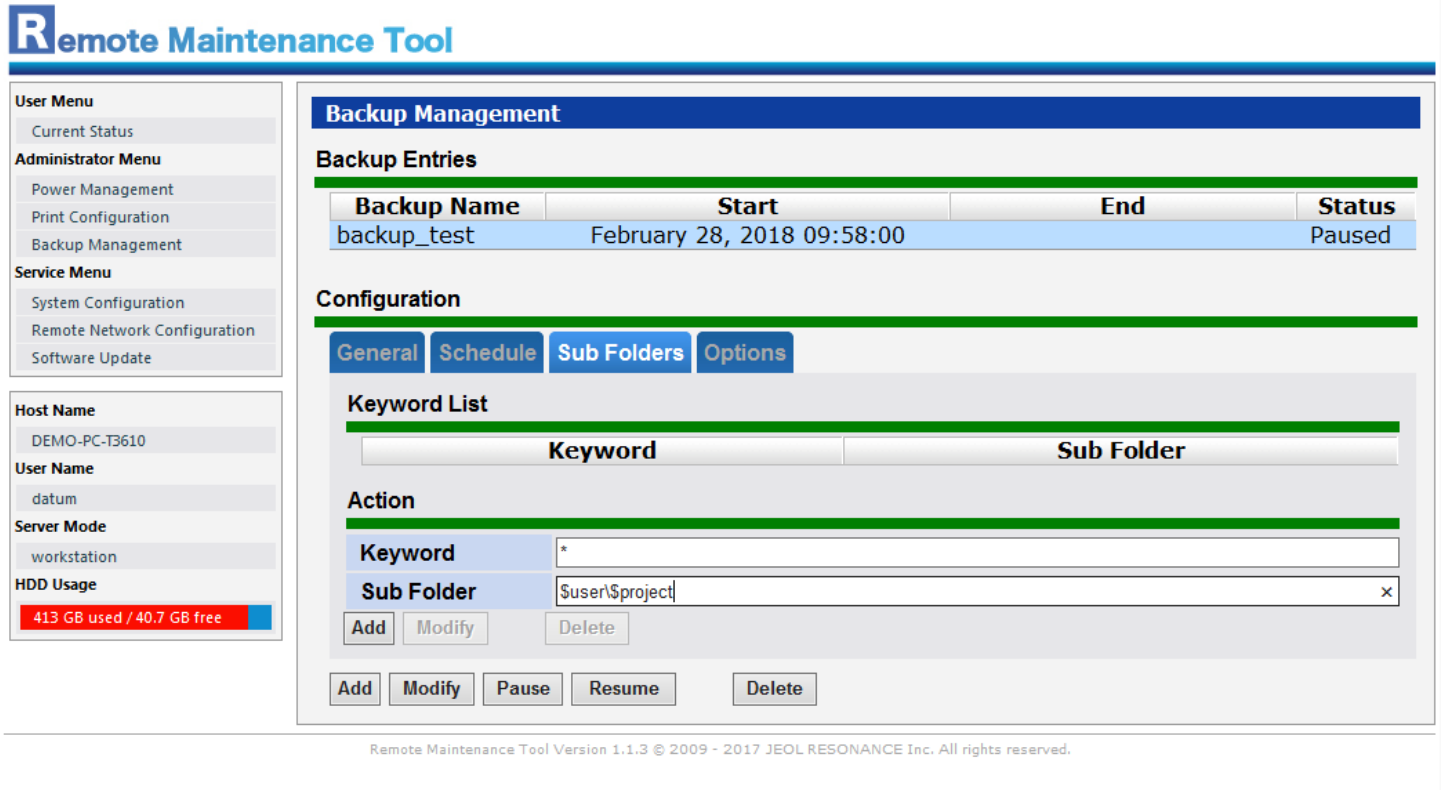


Remote Maintenance Tool Version 1.1.3 © 2009 - 2017 JEOL RESONANCE Inc. All rights reserved.

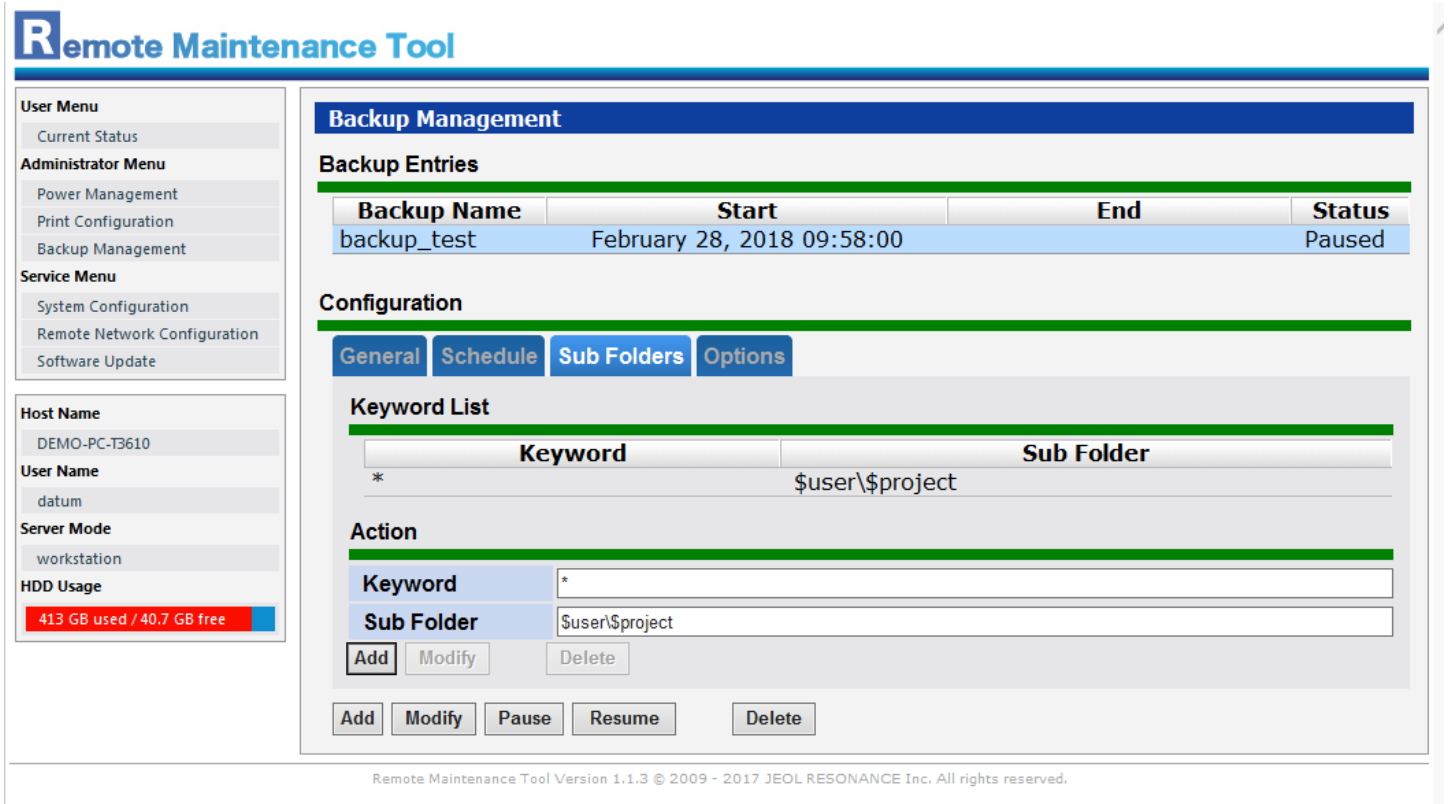
RMT workstation: Backup



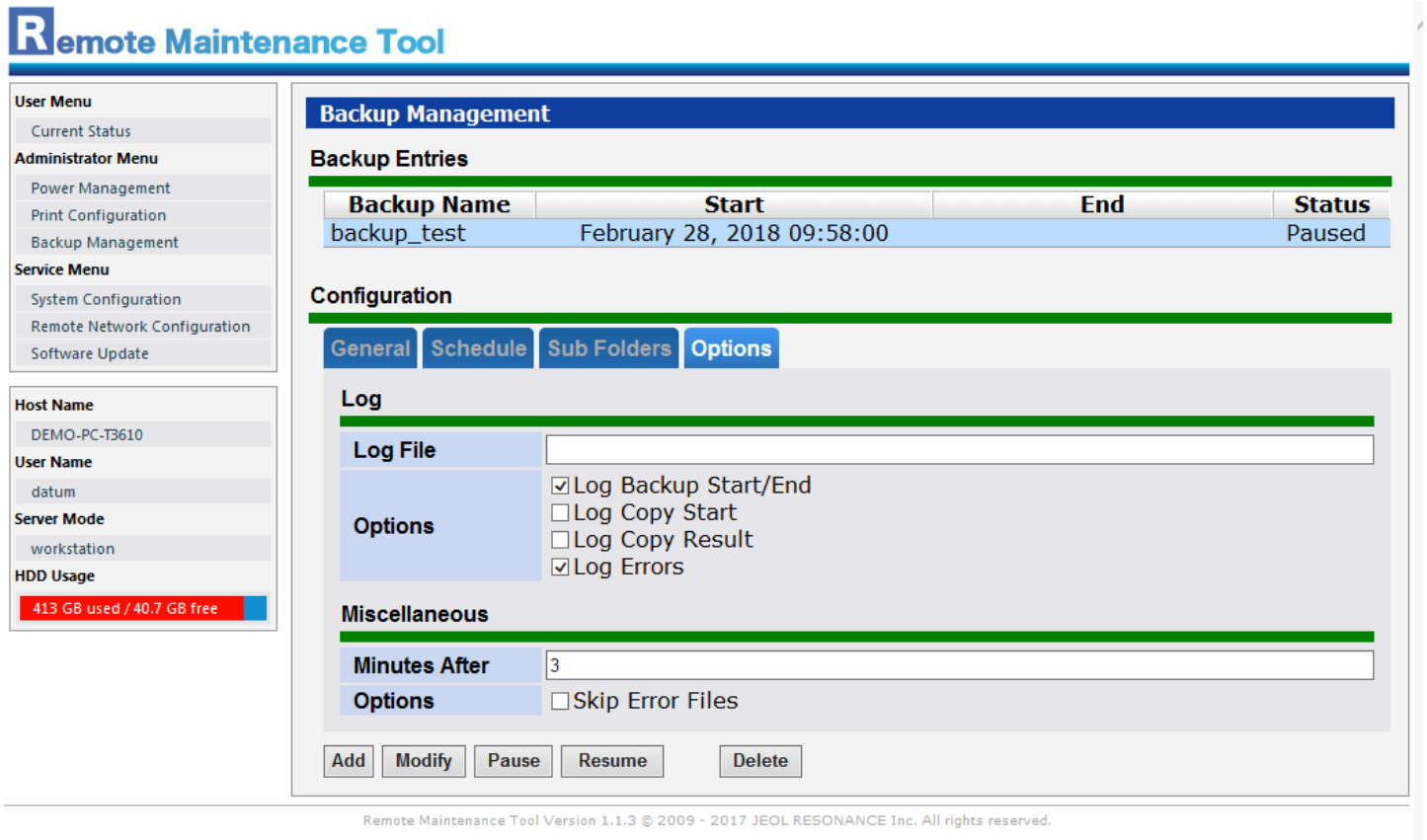
RMT workstation: Backup



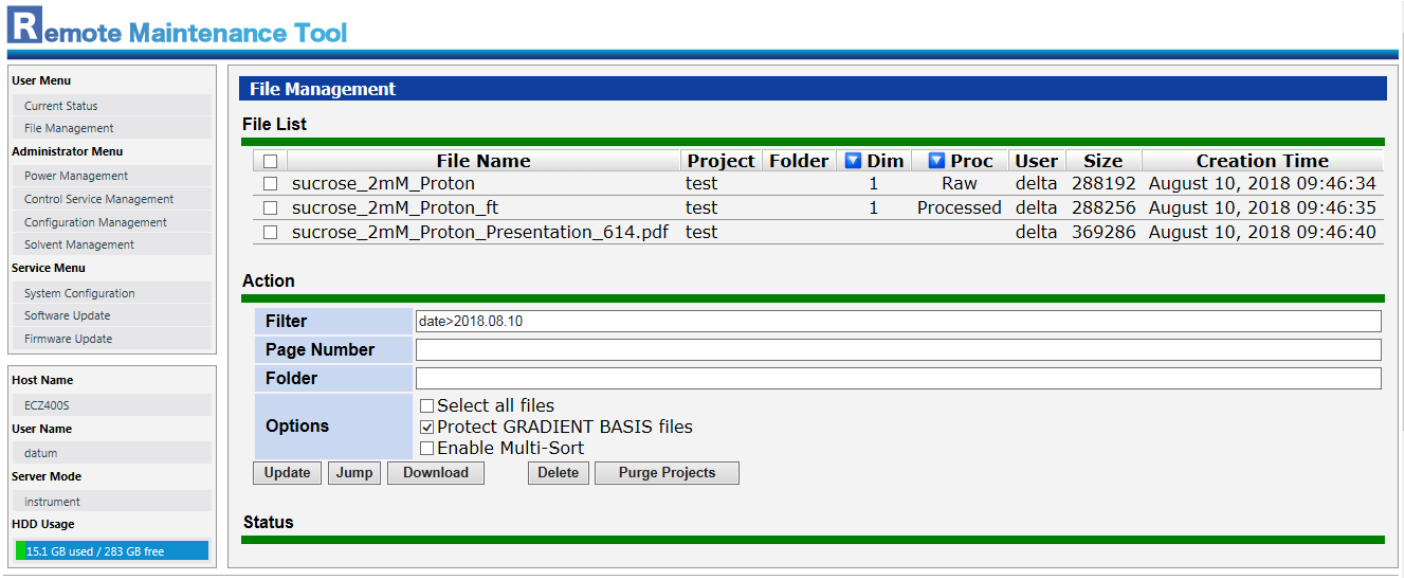
RMT workstation: Backup



RMT workstation: Backup



RMT console: File management



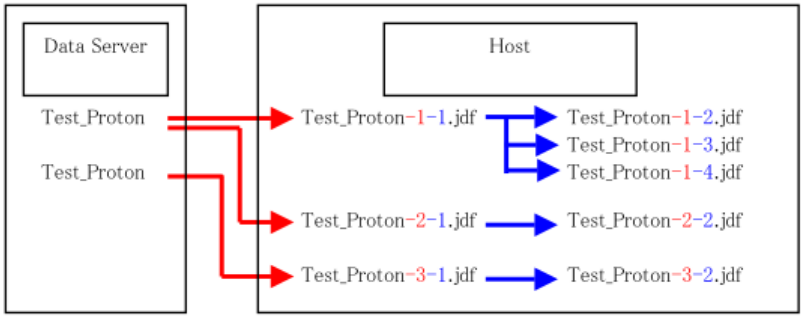
Delta V5 filenames

File name nomenclature

A8. (data filename) – X – Y . jdf

X: group number

Y: version number



Spectrometer

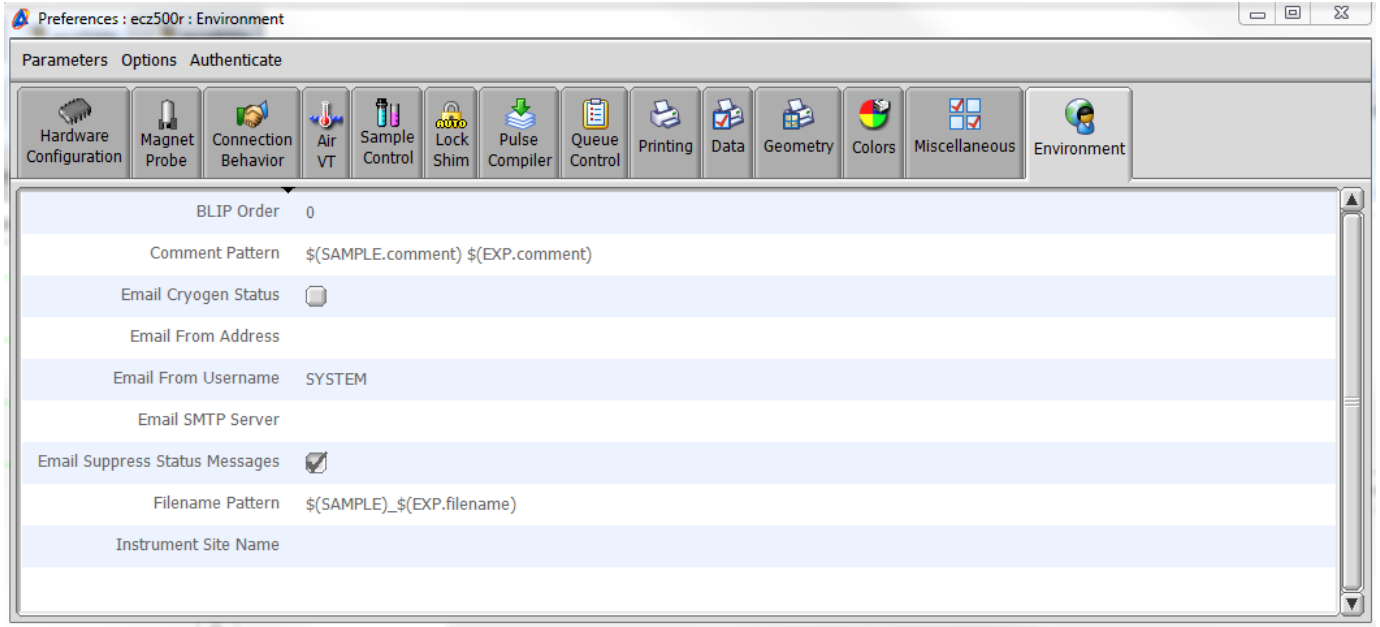
Workstation

Red arrows: downloaded data

Blue arrows: processed data on workstation

Solutions for Innovation JEOL

Changing the default filename



The default filename for data can be changed in the filename pattern in the instrument preferences

The folder in which data is saved can be customized through the Remote maintenance tool, so data can be automatically be stored in folders/subfolders depending on user, project, date, etc.

Changing the filename for an experiment

If the default filename is not suitable for a specific experiment, this can be changed

1. Specify the filename for the data you want to save in the storage_filename of the Experiment Tool panel.

   If not specified, the filename is set by the default rule.

   The name shown on the right side of storage_filename is the default filename.

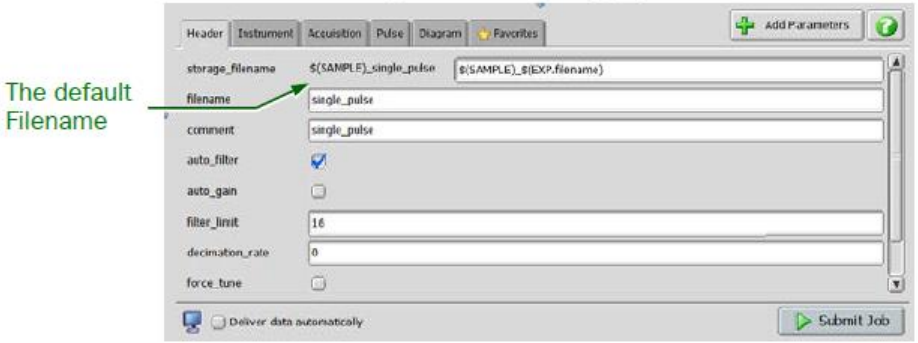


Fig. 6.1 Input box for a filename

Words that can be used in filenames (1)

These reserved words can be used not only in a storage filename but also in a various sentences of automation-templates.

Reserved Words	Contents after Expansion
$(DATA_SERVER)	Hostname of a dataserver.
$(DATE)	Generates a character string with format as "$(DAY_NUM)-$(MONTH3)-$(YEAR)".
$(DAY)	Day of the week.
$(DAY_NUM)	Date of the month.
$(ERROR)	Name of the error handler to be output when an error occurred during an automatic measurement. However, the automatic measurement must be designed to be output an error handler. If no name is specified, "NONE" is applied.
$(EVENT)	Name of event handler currently running. If no name is specified, "NONE" is applied.
$(EXP.FILENAME)	Filename as an Experiment attribute. Specifies at filename of Header tab of Experiment Tool panel.
$(FILENAME)	Subsitute the content filename variable determined in the inner most among variable scopes. The order of variable scopes is, from outside to inside, Job, Sample, Method and Experiment.
$(INSTRUMENT)	IP address of the spectrometer.
$(JOB)	Name of Job.
$(JOB_ID)	ID number of Job.

Words that can be used in filenames (2)

Reserved Words	Contents after Expansion
$(JOB.FILENAME)	Filename as Job attribute. Specify filename of Job parameter.
$(JOB.*ATTRIBUTE*)	Substitute Job attribute specified by *ATTRIBUTE*. If there are attribute with same name, it will be overwritten. By using asterisk, all the attributes can be listed, but this can be used only the statement that will accept multiple lines.
$(METHOD)	Name of method.
$(METHOD.FILENAME)	Filename as Method parameter. Specify by filename at method parameter.
$(METHOD.*ATTRIBUTE*)	Substitute attribute of Method specified by *ATTRIBUTE*. If there are attributes having more inner scope, this will be over-written. By using asterisk, all the attributes can be listed, but this can be used only the statement that will accept multiple lines.
$(MONTH)	English names of months, January, February and so on.
$(MONTH3)	Three letters abbreviations like, Jan and so on.
$(MONTH_NUM)	Number description of month like1, 2, and so on.
$(NOW)	Substitute date including current time with Control Panel¥System Preference. If not found, $(DATE)−$(TIME)−$(TIMEZONE) is used.
$(SAMPLE)	Sample name. Same as $(sample.sample_id).
$(SAMPLE_KEY)	ID of sample.
$(SAMPLE.FILENAME)	Filename as samler attribute. Specify by filename of Sample parameter.
$(SAMPLE.*ATTRIBUTE*)	Substitutes attribute of sample specified by *ATTRIBUTE*. If there are attributes having more inner scope, this will be over-written. By using asterisk, all the attributes can be listed, but this can be used only the statement that will accept multip le lines.
$(SITE)	Spectrometer name set at “Instrument site Name” in Sect. 1.1.14, ““Environment” Tab”.
$(TIME)	Current time in the manner of *HH:DD:MM*.
$(TIMEZONE)	Time Zone.
$(USER)	Name of user.
$(*VARIABLE−NAME*), $(VAR.*VARIABLE−NAME*)	Substitute any variable specified by *VARIABLE—NAME* (this also can be used for Method parameter). If *VARIABLE—NAME* itself is one of reserved words, $(*VAR.VARIABLE—NAME*) is used.
$(YEAR), $(YEAR_NUM)	anno Domini. (A.D.)

File information in Delta browser

The File Browser window opens.

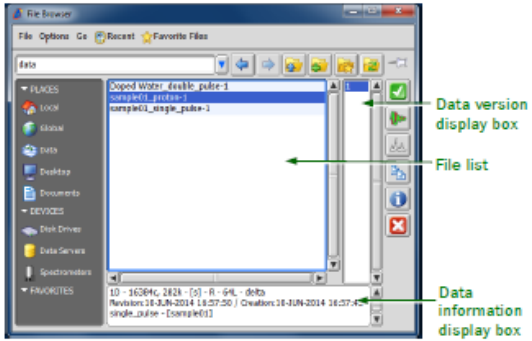
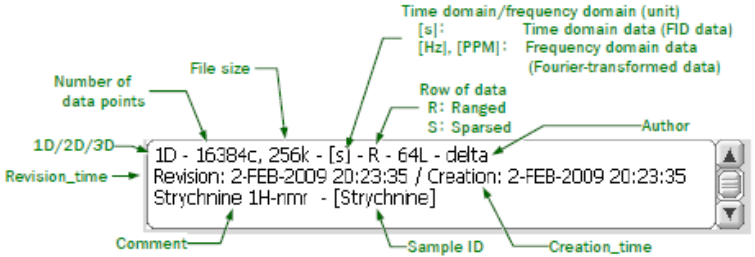


Fig. 6.4 File Browser window

2. Select the desired file in the file list, and click the ✓ button.

The most recent version of the data is displayed in the 1D Processor window or nD Processor window.

The following information on the most recent version of the data is displayed in the data information display box.



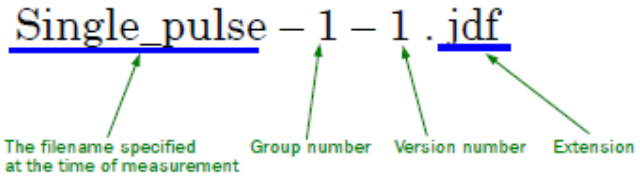
If you display earlier data, select the version number, referring to information in the data information display box, and click the ✓ button.

Note: detailed data parameter information and reports can be obtained from the information button

Numbers after filename

■ Version number

In the Delta program, when loading a data from the data server, the group number for avoiding a duplication of a file name and a version number are appended to each data filename.
Also, before data are processed, a new file is automatically created under the same file name with a version number higher than that of the original data. The original data are not processed, preventing corruption of the original FID data.
If you save data under the existing file name, the data are given a version number higher by one. Copied data are sometimes deleted after they are processed. Therefore, some of the version numbers in the file list are usually omitted.



In the File Browser window, the parts till the group number are displayed as a filename.

After the filename, two numbers are added to avoid data being overwritten
The first one is the raw data number
The second one is the processing version

Filename restrictions

Illegal Filename Characters	/\:"*?<>|

Username restrictions

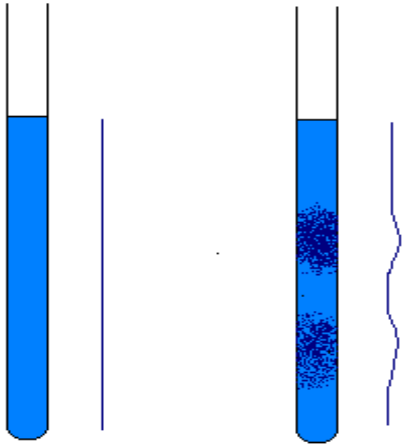
The following are reserved words for automation, their use would cause trouble

abort association	after attach	alert automation	all	and	as	assert
boolean	by					
call const	category constrain	coil context	collect continue	complete	conceal	console
data div	date divisible	day do	decrease domain	delay	depends	dialog
else experiment	email expired	end expose	enum	error	evaluate	exit
false	fatal	file	finish	for	from	
group						
help	hour					
if integer	in interim	include invoke	increase is	info	inform	inout
job						
limit	list	log				
machine	message	method	minute	mod	modulo	multiple
namespace	no	not	null	number		
of	offset	on	or	out		
parameter probe	percival process	precision processed	prepare project	presentation promote	print purpose	printer
raise	raw	ref	remark	repeat	retry	
sample status	save step	scout subject	second	service	set	shims
template true	terminate tune	text	then	time	to	translate
unit	until	user				
var	version	visualize				
warning	when	while	with			
xor						
yes						

Shimming

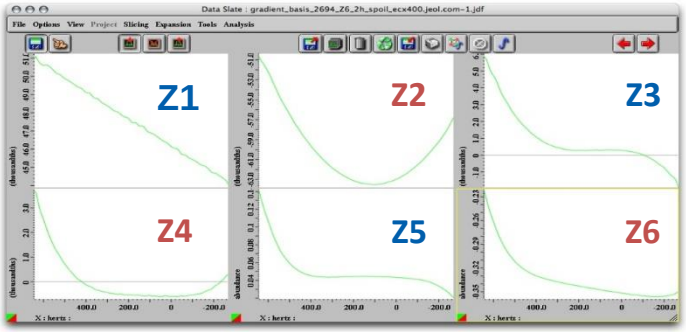
Sample homogeneity

Homogeneous sample Inhomogeneous sample



If your compound is not homogeneously dissolved, it causes high order distortion which is impossible to adjust by shimming

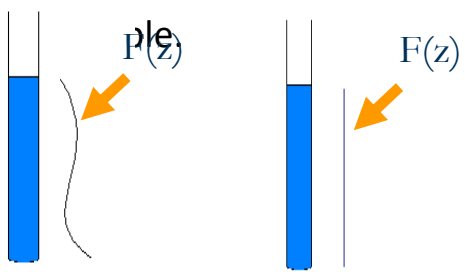
Just shake your sample
But do not allow bubbles to stay around the detection area



Solutions for Innovation JEOL

Shimming

An NMR instrument has a series of shims at room temperature to create small correcting magnetic fields.
Shimming is a process to find a combination of these RT shim to compensate for the in-homogeneous magnetic field caused by ple.

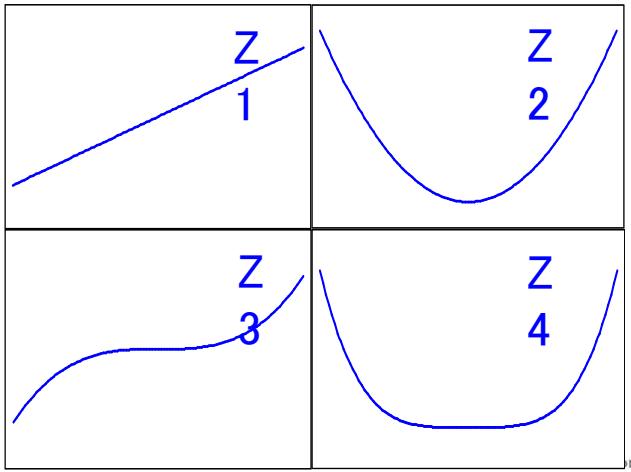


$$F(z)=az+bz^2+cz^3+dz^4$$

Z1 shim=-a, Z2 shim=-b

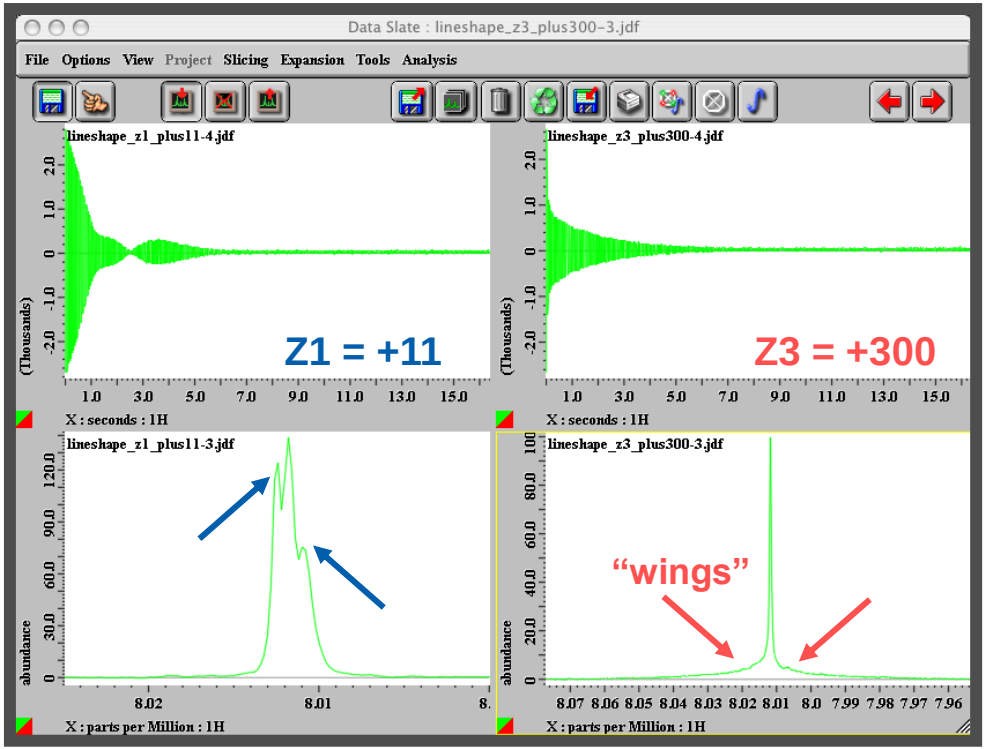
Z3 shim=-c, Z4 shim=-d

$$F(z)=az+bz^2+cz^3+dz^4$$
$$-aZ-bZ_2-cZ_3-dZ_4=0$$



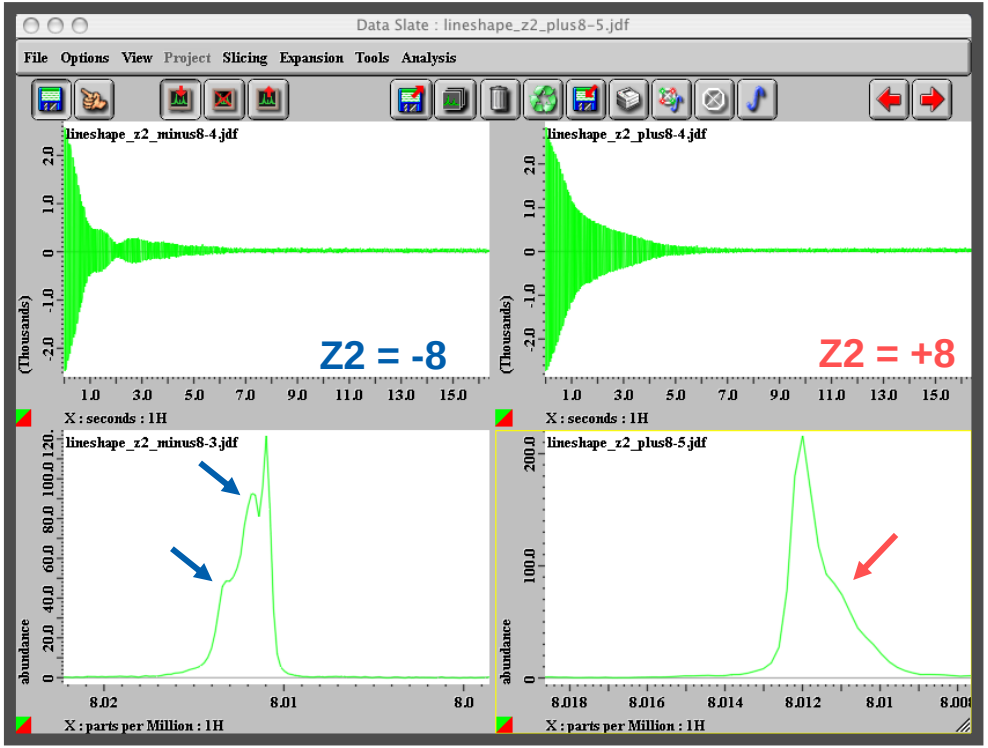
ns for Innovation JEOL

Z1, Z3 shims



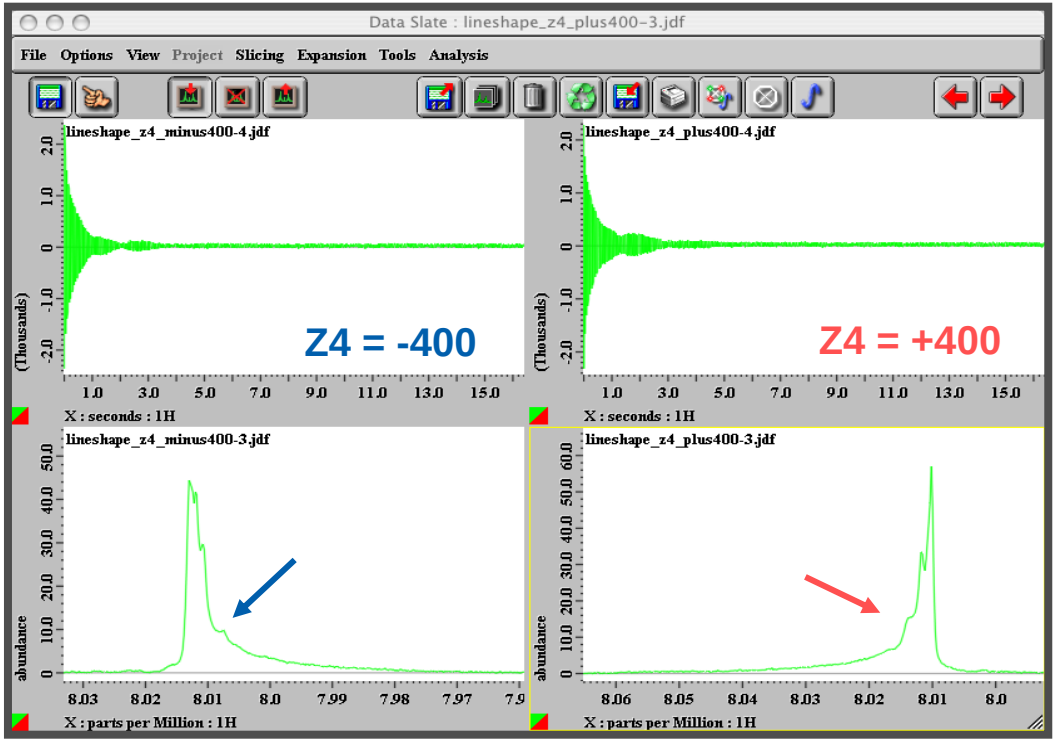
Solutions for Innovation JEOL

Z2 shim



Solutions for Innovation JEOL

Z4 shim



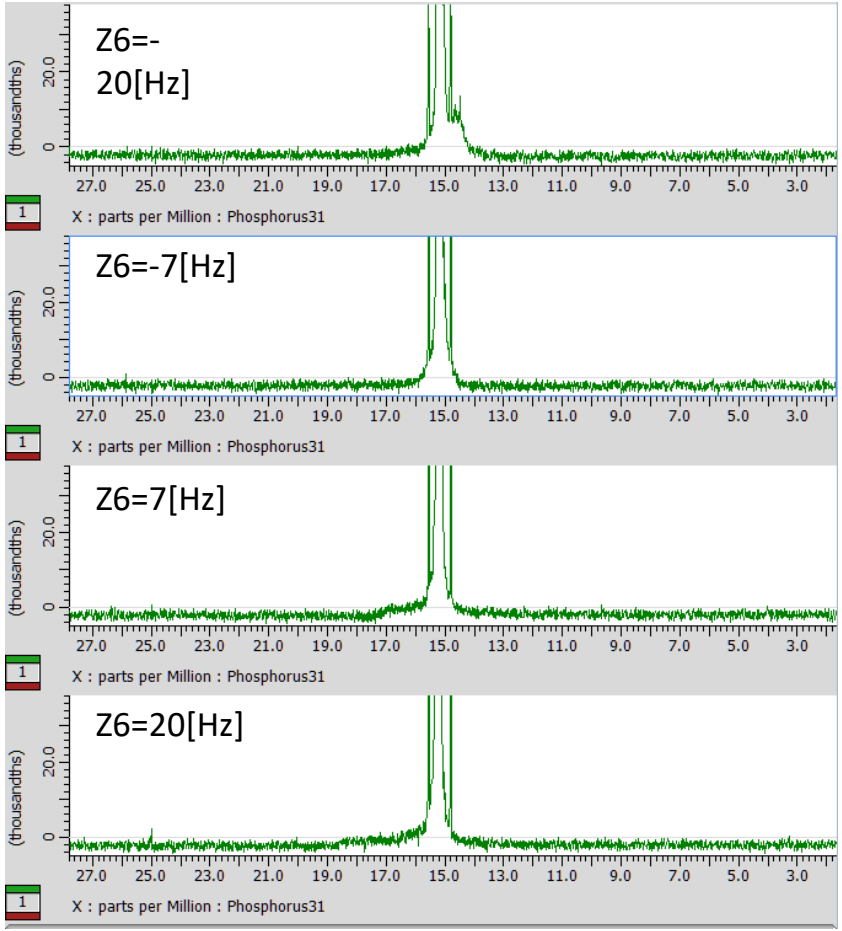
Solutions for Innovation JEOL

Effects of shims

- Lower-order shims (Z1, Z2) have larger effects on line-shape
- Odd shims (Z1, Z3) produce symmetric effects
- Even shims (Z2, Z4) produce asymmetric effects; direction depends on position relative to the optimum value
- Errors in X and Y produce sidebands at the spinning frequency
- Errors in XY and X2 – Y2 produce sidebands at twice the spinning frequency

Solutions for Innovation JEOL

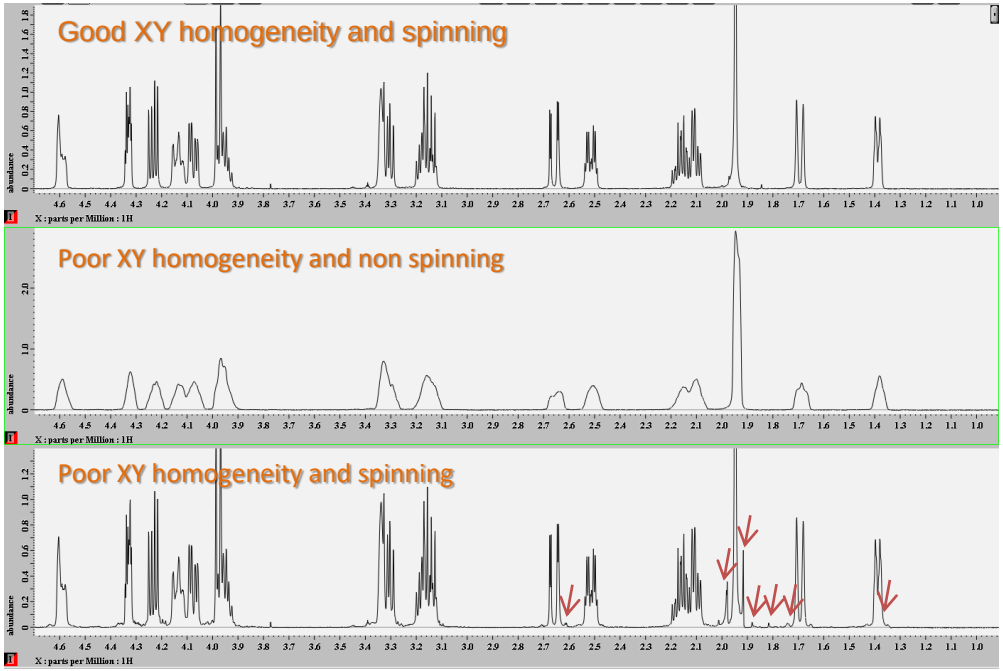
Z6 is quite insensitive to sample nature



Spinning

Sample spinning for what?

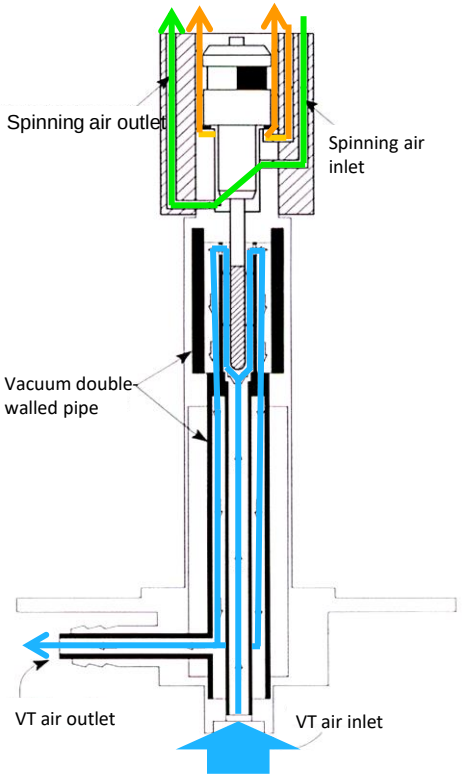
Sample spinning is to cancel magnetic field in-homogeneities along XY and improve resolution.



Solutions for Innovation JEOL

Probe air flow

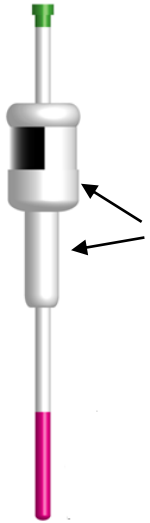
- Based on a counter-flow design
- VT exhausts through the bottom of the probe
- VT air is kept separate from the spinning air



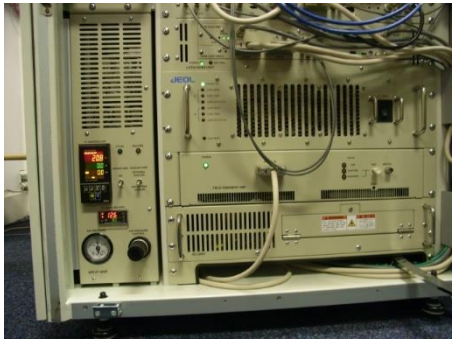
Solutions for Innovation JEOL

For stable sample spinning

- Fit a sample rotor and holder firmly
- Keep sample holders and rotors clean
- Check air pressure
- Check the probe



O-ring inside
Pull each other and rotate to fit

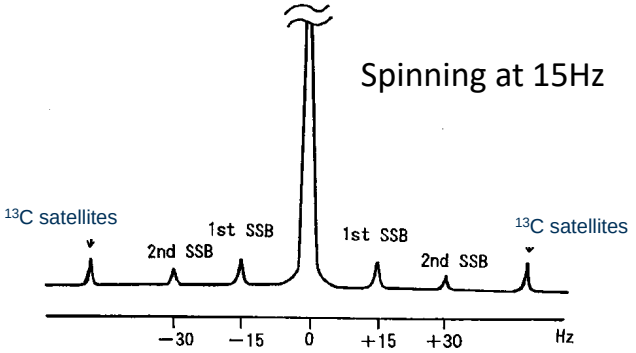


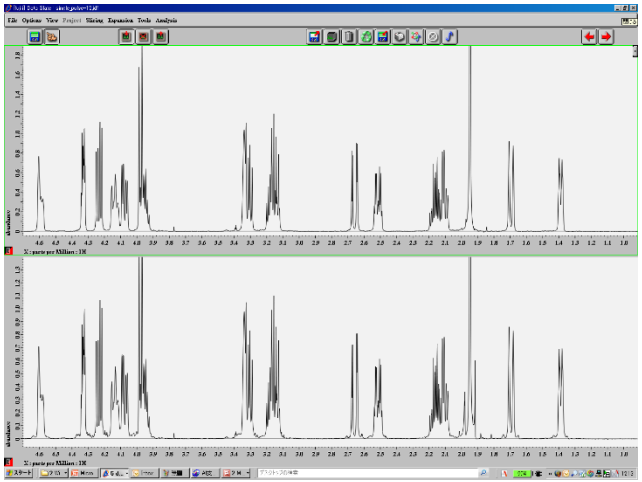
Solutions for Innovation JEOL

Spinning sidebands

Spinning sidebands are caused by poor magnetic field homogeneity along x or y

- 1st SSB appear at the spinning speed beside the main signal, adjust X,Y,XZ and YZ.
- 2nd SSB appear at twice spinning speed, adjust X2 or Y2 or other 2nd order shims





Other sideband sources

- Instable spinning causes phase distorted sidebands
- Floor vibration causes
- Strong ^{13}C signal may have decoupling sidebands

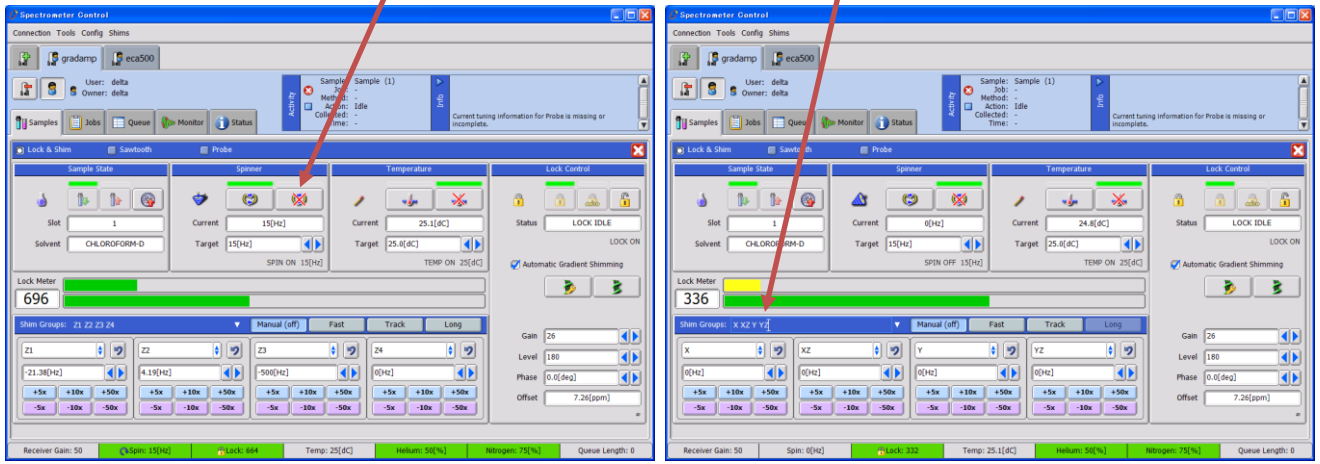
Solutions for Innovation JEOL

No spin shim

Delta version 5 series

Stop sample spinning first!

Change shim group



Adjust the non spin shim values
so that lock intensity becomes larger

Solutions for Innovation JEOL

How to setup 1D gradient shimming

Gradient shim calibrations (shim mapping)

- It is important that all the following gradient shim calibrations are done during installation

System Type	Nucleus	Comments
Homospoil	2H	By far the most used method; for deuterated solvents that have only one deuterium resonance (e.g. DMSO-D6, chloroform-D, acetone-D6)
Homospoil_selective	2H	Very important to calibrated, needed for solvents that have more than one deuterium resonance, e.g. Methanol-D4
Homospoil_selective	1H	Needed for non-deuterated solvents (No-D NMR)
Fast_homospoil_CC	2H	Needed for variable temperature (VT) measurements. Depending on solvent, can be needed for even modest temperatures.
Fast_homospoil_selective_CC	2H	As above; for solvents with more than one deuterium resonance

Fast types are faster because they assume shim behaviour. If the behaviour in a particular spectrometer deviates from the assumed behaviour, results are worse than the other types.

Gradient shim calibrations (shim mapping)

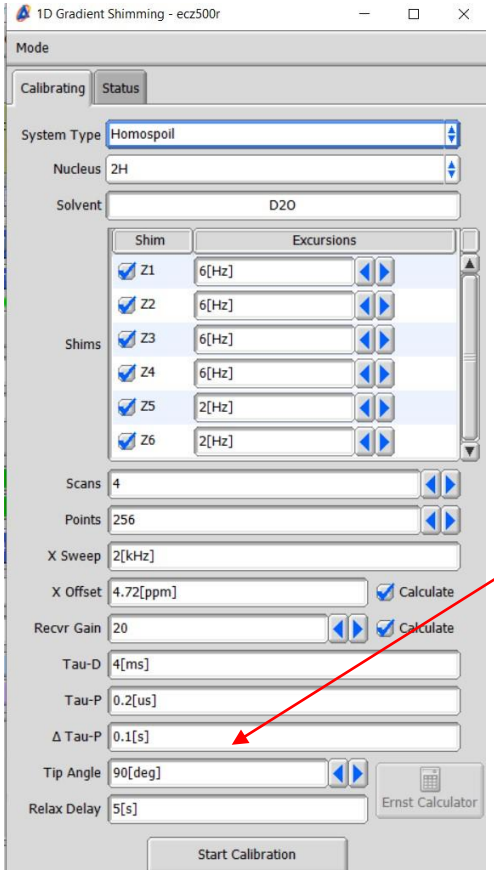
Samples

× 1H lineshape sample is not ideal (long T_1 relaxation, needs long relaxation delay, time consuming)
× 1H sensitivity sample is not ideal (low SNR for 2H, more scans needed, time consuming)
✓ Doped 1% H2O in 99% D2O is an excellent choice
✓ ASTM (40% p-dioxane) is also a good choice, and can be used for 1H calibration

System Type	Nucleus	Sample	Scans* (1H sensitivity)	Relaxation delay (1H lineshape)
Homospoil	2H	Doped H2O; ASTM; 1H lineshape; 1H sensitivity	4 (8)	2 (5)
Homospoil_selective	2H	As above	4 (8)	2 (5)
Homospoil_selective	1H	ASTM	4 (8)	2 (5)
Fast_homospoil_CC	2H	Doped H2O; ASTM; 1H lineshape; 1H sensitivity	8 (16)	2 (5)
Fast_homospoil_selective_CC	2H	Doped H2O; ASTM; 1H lineshape; 1H sensitivity	8 (16)	2 (5)

*For ROYAL/HFX probes. Older or direct-style probes may need more scans

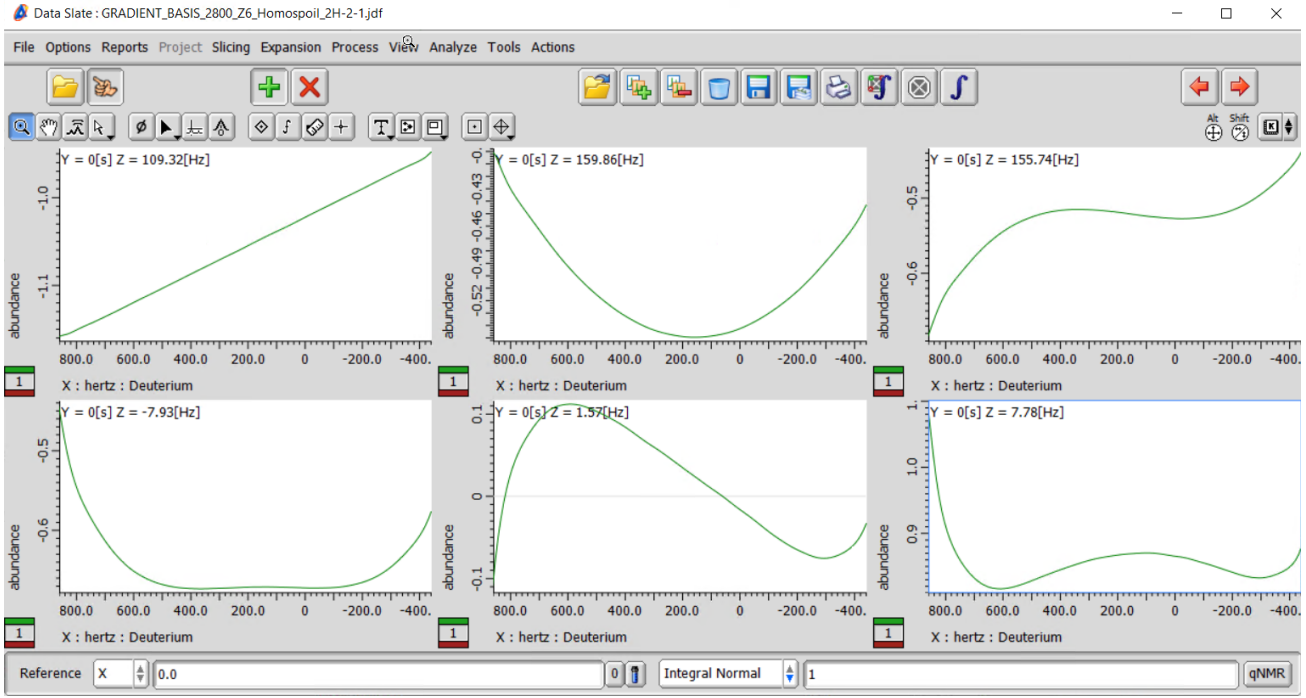
Gradient shim calibrations (shim mapping)



- Use a 90-degree tip angle for all calibrations
- Don’t bother with the Ernst calculator, no one uses it
- Leave the defaults as they are, including excursions (too large excursions will cause aliasing in the maps)
- For the 1H homospoil selective calibration, it can be useful to reduce Δ Tau-P from the default 20[ms] to e.g. 5[ms] to reduce issues with radiation damping

Gradient shim calibrations (shim mapping)

- After calibration, check the maps in a data slate
- “Trim” the edges so that Z1 (top left) is straight with no wiggles displayed either side
- The shim maps should show good symmetry
- A small asymmetry is acceptable but a large one could indicate a problem, e.g. probe vertical misalignment, issue with mapping



Setting up shimming parameters

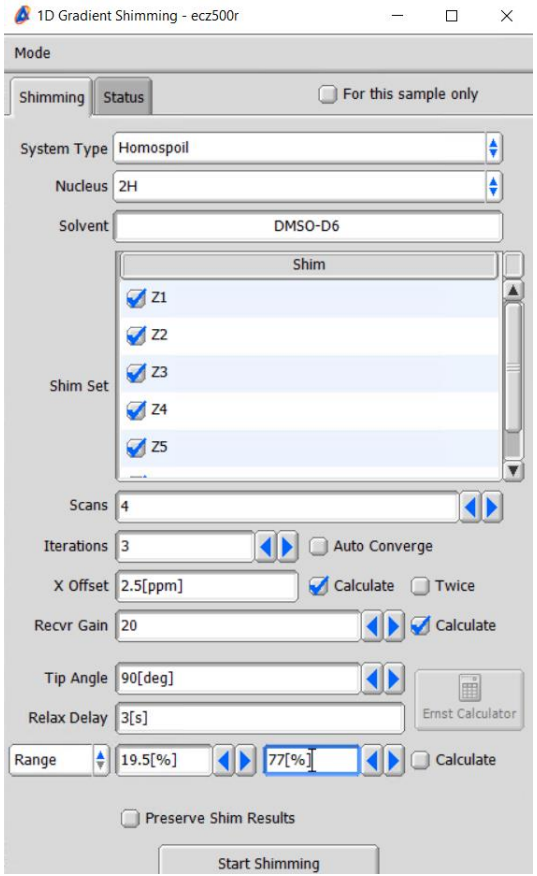
Setting parameters for gradient shimming

- Calibrating the shims (shim mapping) is only half the job

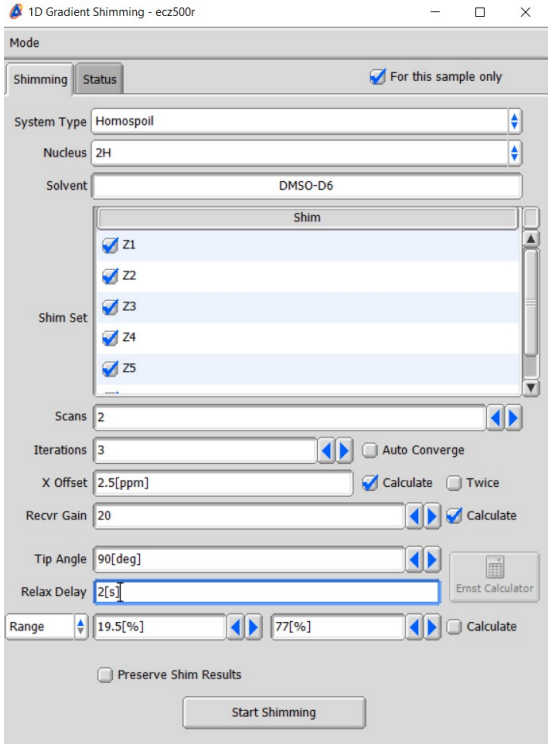
- Parameters for shimming different solvents need to be set for the different “System Types” (shim methods)

What does unchecking “For this sample only” do?

- Requires administrator (console) privileges
- Sets all default parameters, **including the “System Type” (shimming method)** , **<u>for the current solvent</u>**
- They apply ONLY to the current solvent/”System Type” combination
- **Checks and settings need to be made to ensure parameters are set for every solvent/method combination**



Sensible default parameters for different solvents

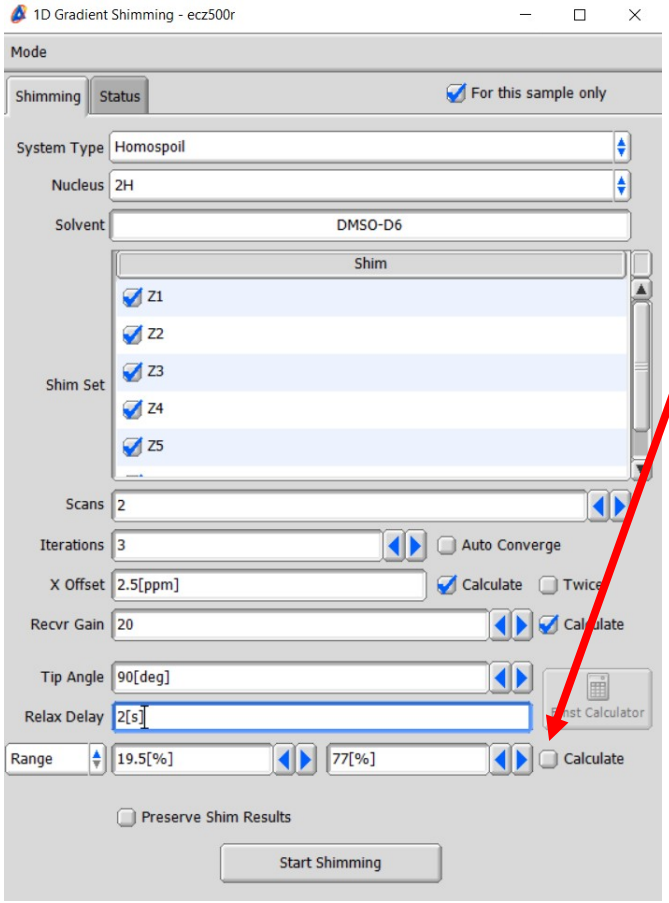


Solvent	Default shim method (System Type)	Scans* (CC methods)	Relaxation delay
Acetone	Homospoil	2 (4)	5
CDCl3	Homospoil	4 (8)	2
MeOD	Homospoil selective	2 (4)	2
DMSO-d6	Homospoil	2 (4)	2
D2O	Homospoil	2 (4)	2
Benzene-d6	Homospoil	2 (4)	2

*For ROYAL/HFX probes. Older or direct-style probes may need more scans

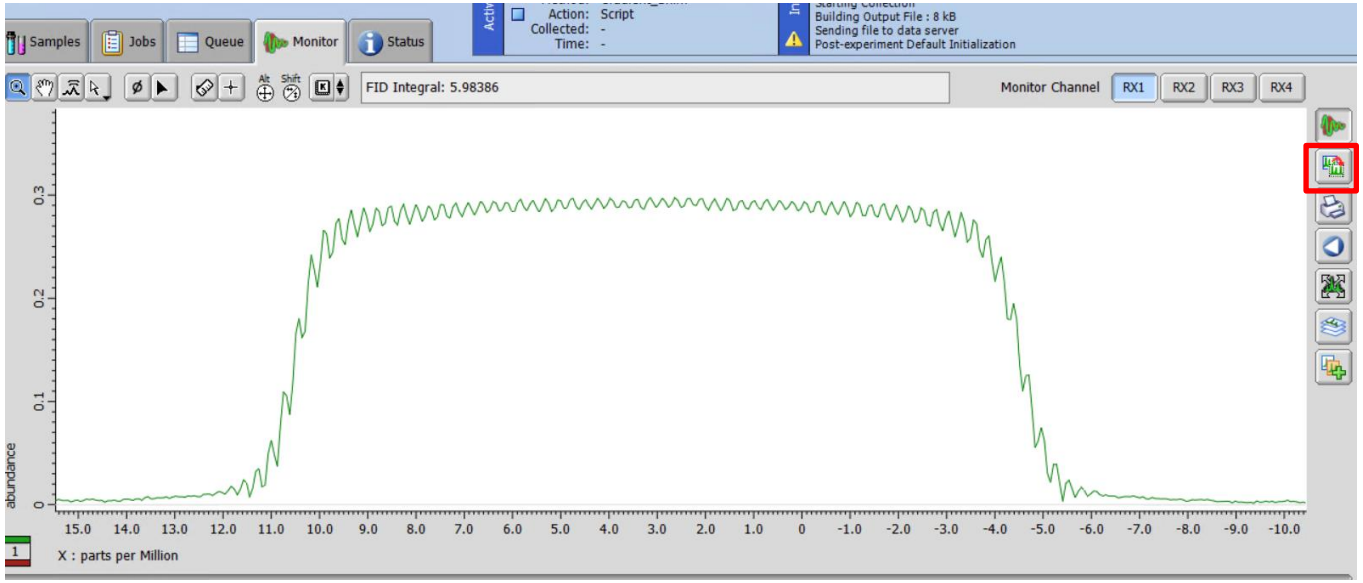
- Uncheck “Auto Converge”
- Set 3 iterations
- 90-degree tip angle for all methods
- Uncheck “Calculate” range and set manually (next steps)

Setting Range



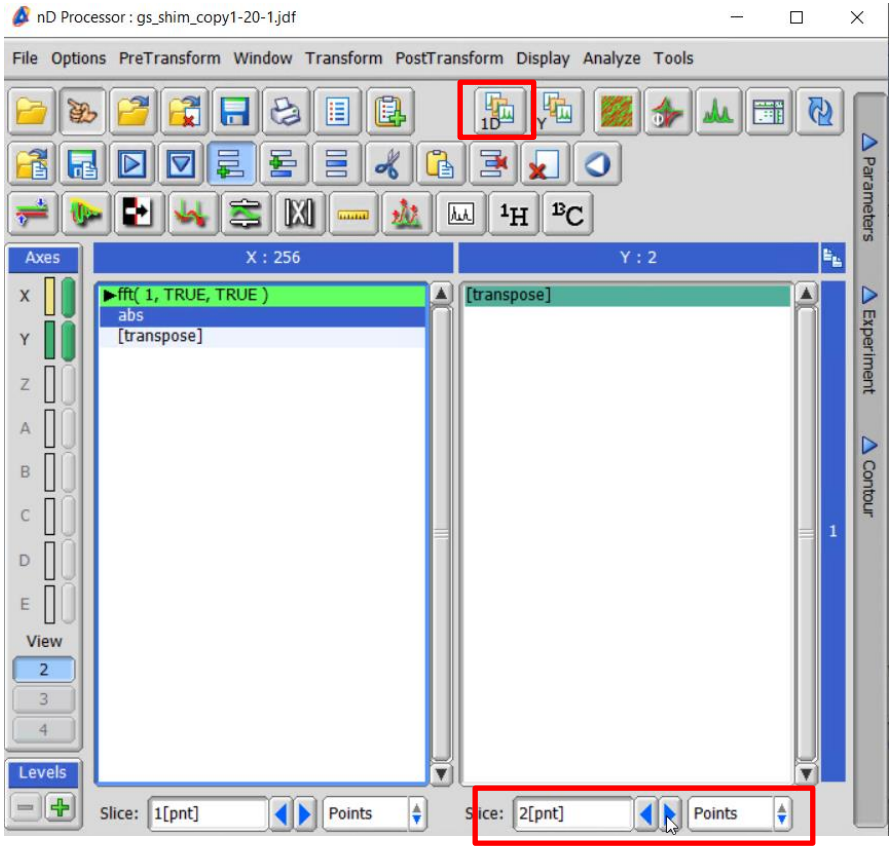
- "Calculate" option sets range too wide
- Better to determine range manually and set for all samples

Setting Range



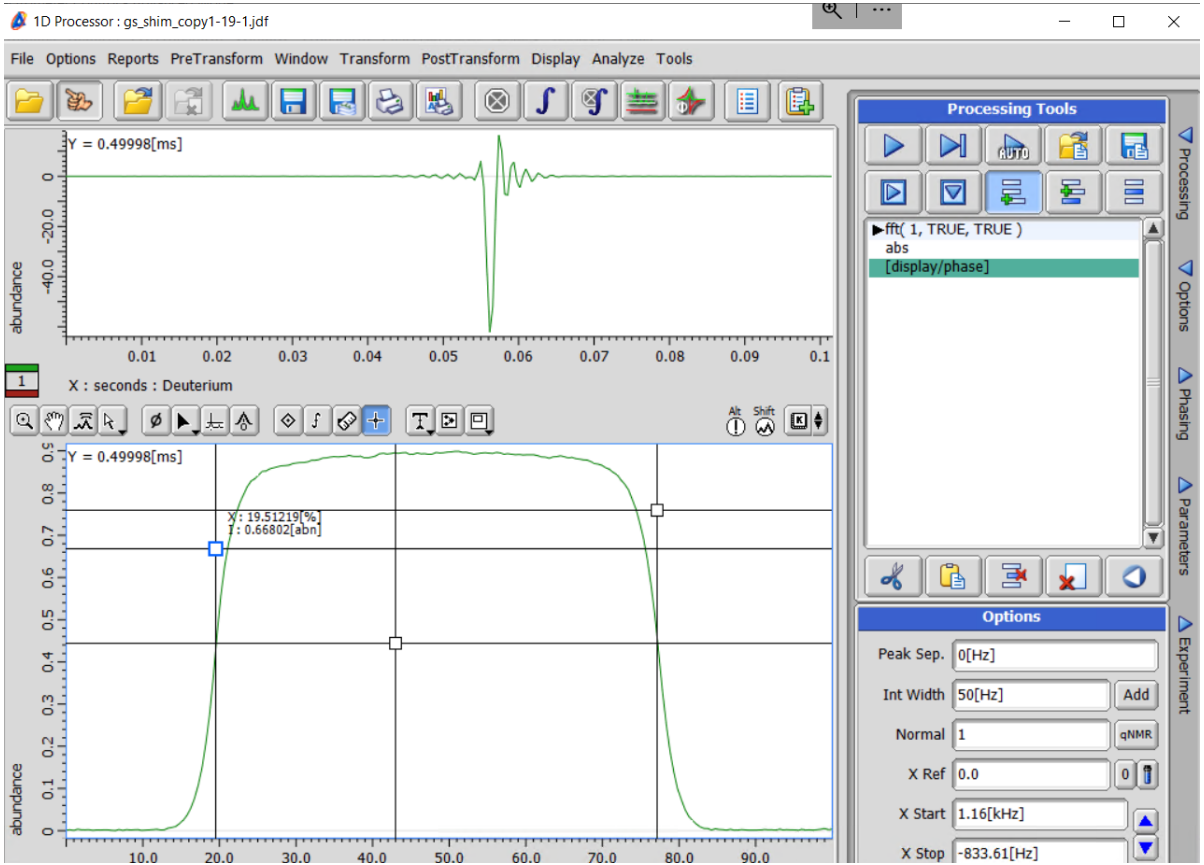
- A robust way to set range is to use ~50% amplitude points on second profile from gradient shimming
- Start gradient shimming with “calculate” option checked
- Go to “Monitor” window

Setting Range



- In nD Processor window, add FFT and Abs steps to X dimension
- Select 2[pnt] slice for Y dimension (i.e. second profile)
- Click 1D button

Setting Range



- Place cursor at top of profile and measure amplitude
- Place cursor at half that amplitude (i.e. 50% point)
- Place left and right cursors to intersect profile at 50% point
- Set X-axis units to %
- Read low and high range values
- IMPORTANT: range needs to be set for every method (“System Type”). E.g. setting range for “Homospoil” does not get automatically applied for “Homospoil selective”

Testing the gradient shimming

- After everything has been set up, it is essential to check that the shimming is working well

- A good test:

    - Remove and recreate sample definitions for standard test samples in the “Samples” tab. This will ensure that the default gradient shimming parameters will be used

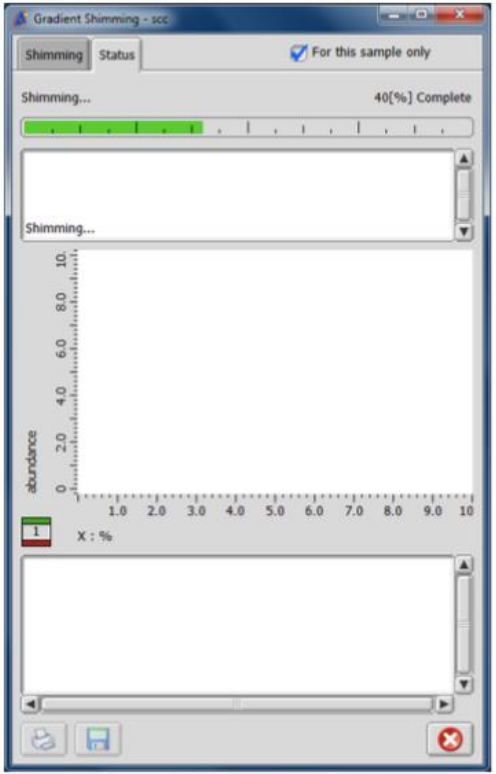
    - Run 1H lineshape, 1H sensitivity and 13C sensitivity GLP tests under automation – do the samples shim well and do the tests pass?

Troubleshooting

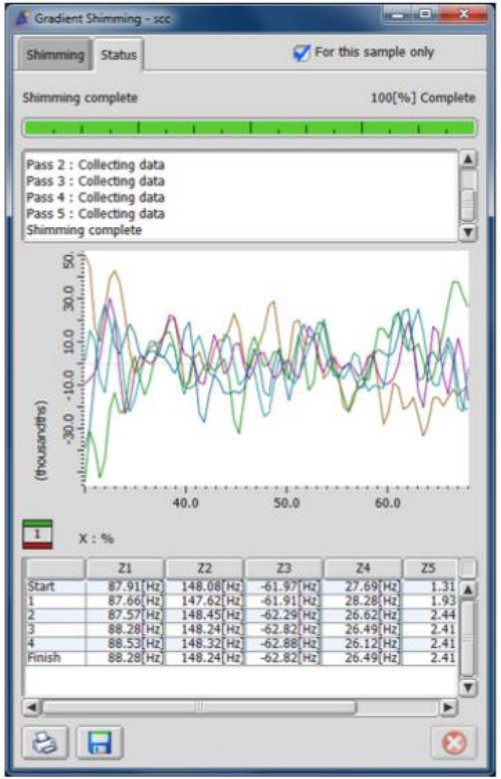
Occasionally, gradient shimming can fail to produce well adjusted line-shape.

Possible causes can include,

- Insufficient sample depth. Aim for a minimum 40mm sample depth. If this isn't possible for a particular sample, use the depth gauge to centre the sample against the centre of the RF coil.
- Dirty or scratched sample tube. Contaminated sample material.
- Temperature gradient. Insufficient wait time between VT on and starting gradient shimming. Remember, the temperature shown is that of the thermocouple NOT the sample. It takes time to catch up & settle(gradient shimming gives better results waiting 5 minutes than if just waiting 3 minutes, do not expect it to shim well without any temp_delay).
- Erratic spinning. Is the spinning speed stable? Try another rotor.
- Have the shim values been excessively adjusted. Try reloading the system shim file or a known good user shim file for the probe in use
- It can also help to check the gradient shimming is configured correctly and also the FG shim residual map.

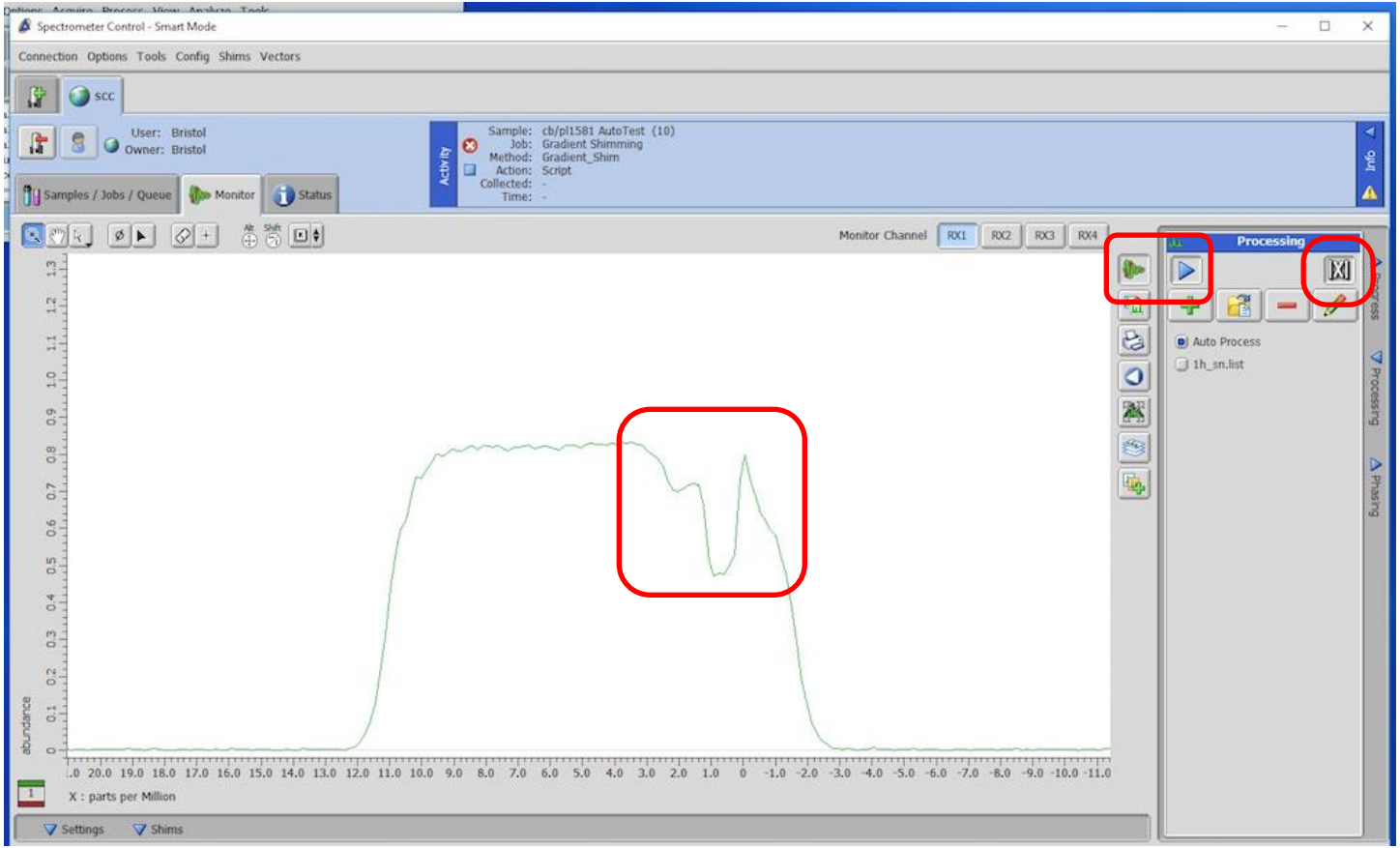


Click Start Shimming, the status tab is shown.

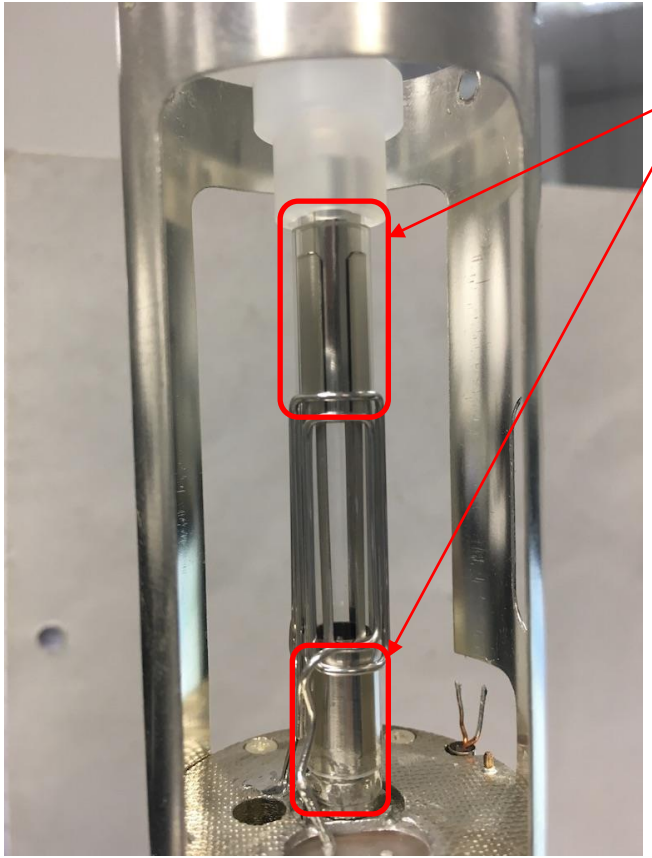


The residual plot should flatten out after each iteration.
Aim for less than +/- 0.1 abundance.

- The residual can bee seen in real time, from the monitor tab.
- Turn on FID, FT and ABS.
- Modern probes should have a square like profile, no notches as below.



The previous image indicates that either the sample tube is scratched/dirty, or that the detection coil area is dirty and needs cleaning. BUT…..

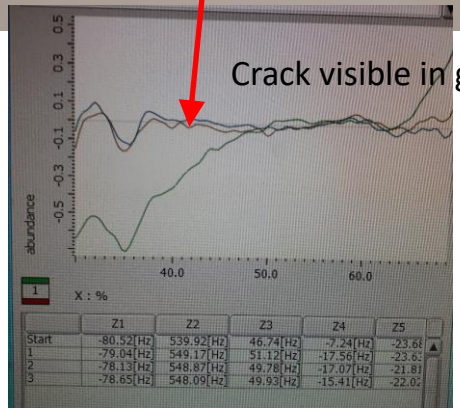


Modern sample coils have RF shielding above and below the detection coils.

They improve achievable line-shape by reducing end effects.

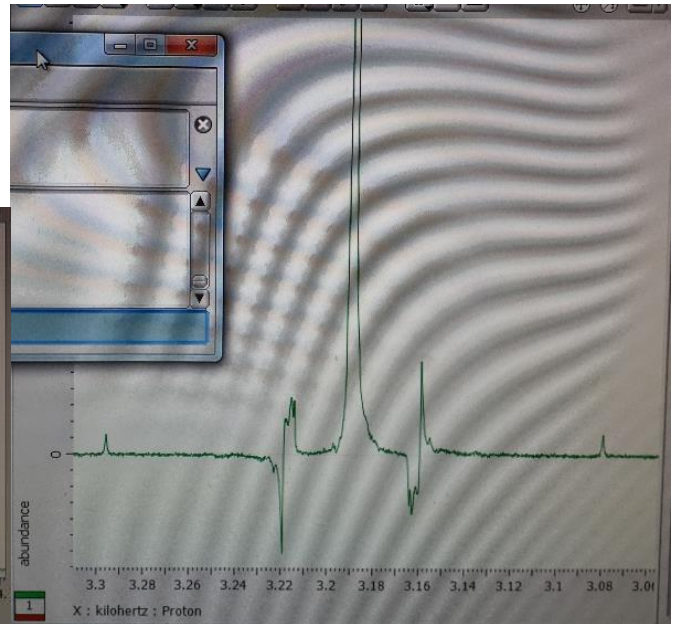
However, they make cleaning the detection coil area tricky.

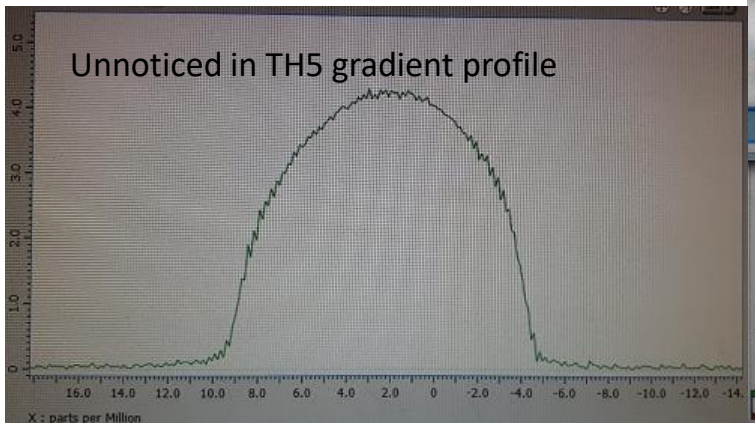
Vigorous cleaning with an aggressive solvent (e.g. Acetone) can lift the foil and prevent samples from spinning, as well as affecting the FG shimming performance.



Crack visible in gradient shimming fitting

Non-spin lineshape: cracked glass leading to bad coil fixing leading to vibrations





And finally…

When you update the system shims with an HFX probe, remember to do so for both single and dual mode as each mode uses a different system shimset in Delta 5. In Delta 6 this is not needed.

- At the end of the installation remember to do a backup of everything, including data. If the database becomes corrupted (which can happen with power cuts), it needs to be restored otherwise the gradient maps will be lost.

Gradient shimming files

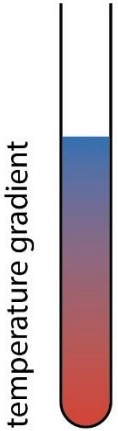
For a completely new and never used system, if you uncheck “For this sample only” and setup parameters, changes will be reflected for all samples except for those with different predefined parameters. Used systems may have other conditions and different solvents can have different parameters, and different specific samples can have different parameters.
A dive into the configuration of control in the console can clarify what is happening. Locate *C:\Program Files\Common Files\JEOL\Control 5.3\configuration*

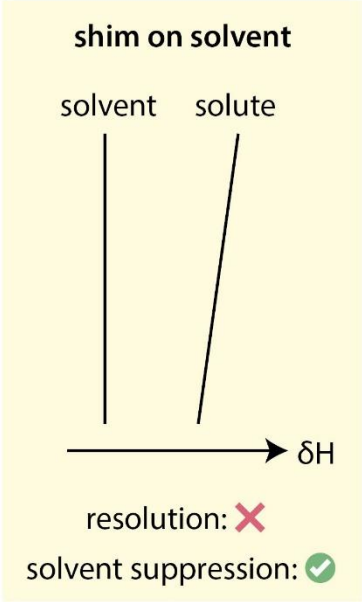
This folder contains several files related to the shimming:

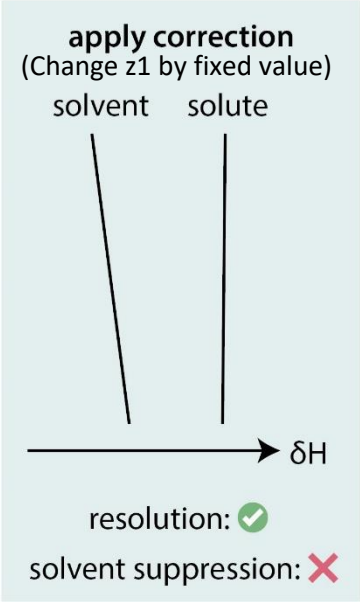
- *Solvent_reference.jnv*: It tells the system which type of shimming it should do for each solvent.
- *gradient_shim.jnv*: It tells which nucleus and shims to use in shimming
- *gradient_shim-homospoil-2h.jnv*: Contains the shimming settings for each solvent with this type of gradient shimming
- System shims are in probe file
- Shimmaps are in the database!

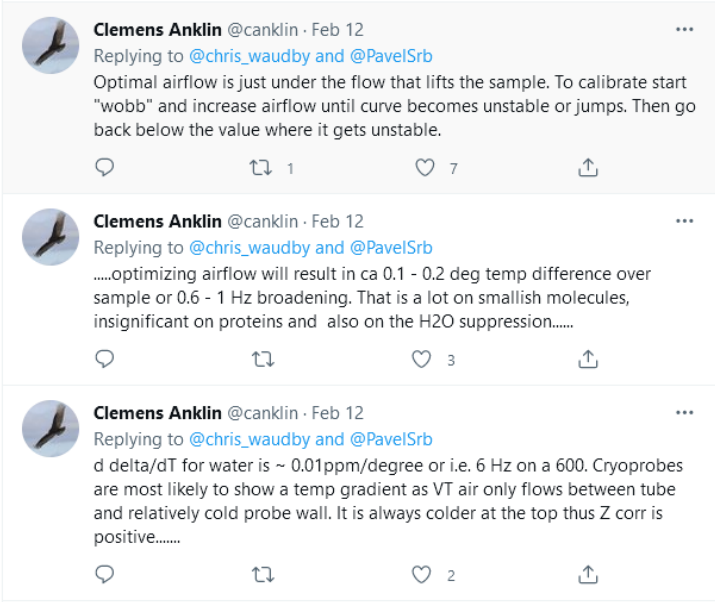
Temperature gradients

Temperature gradients are common









Clemens Anklin @canklin · Feb 12
Replying to @chris_waudby and @PavelSrb
Optimal airflow is just under the flow that lifts the sample. To calibrate start "wobb" and increase airflow until curve becomes unstable or jumps. Then go back below the value where it gets unstable.
1 7

Clemens Anklin @canklin · Feb 12
Replying to @chris_waudby and @PavelSrb
.....optimizing airflow will result in ca 0.1 - 0.2 deg temp difference over sample or 0.6 - 1 Hz broadening. That is a lot on smallish molecules, insignificant on proteins and also on the H2O suppression.....
3

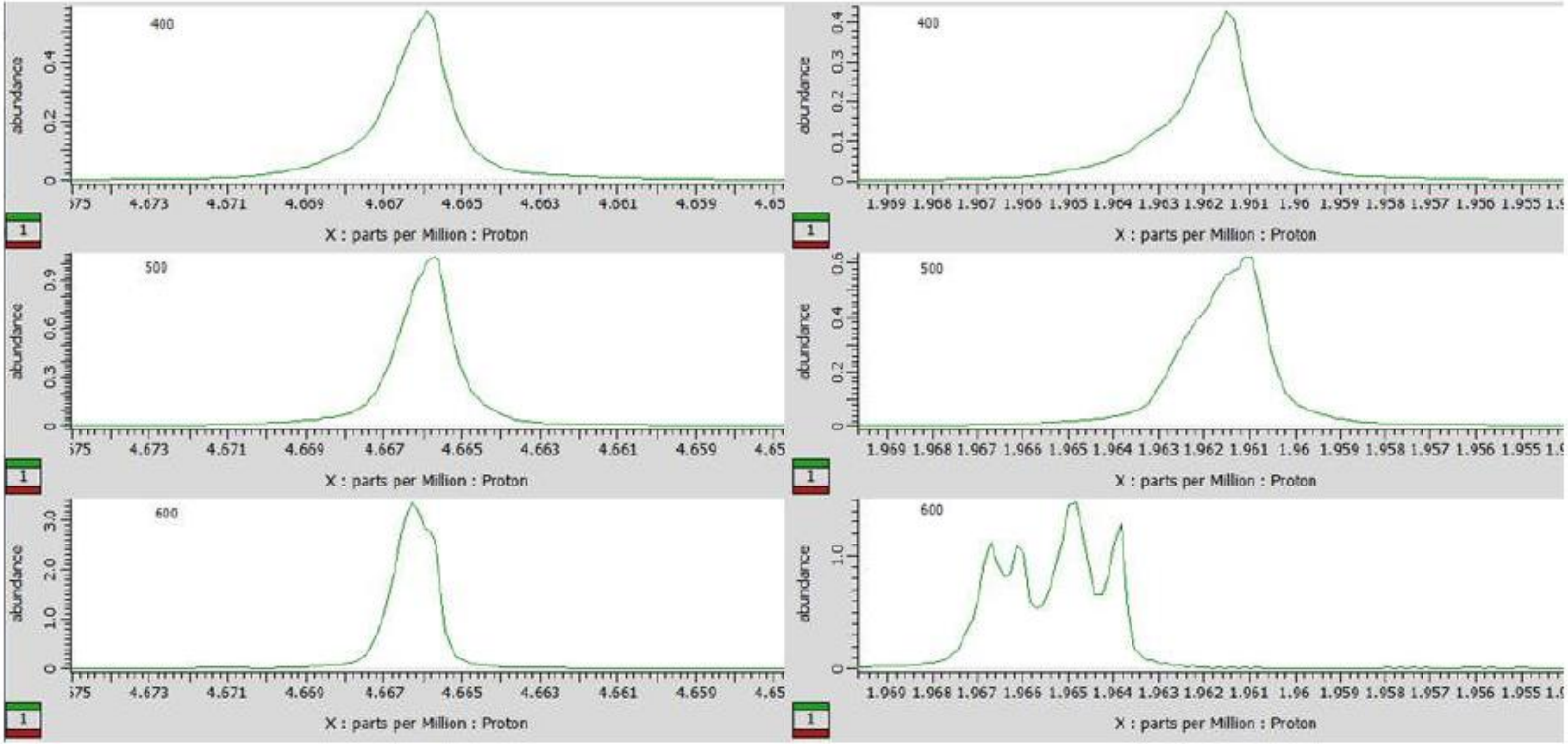
Clemens Anklin @canklin · Feb 12
Replying to @chris_waudby and @PavelSrb
d delta/dT for water is ~ 0.01ppm/degree or i.e. 6 Hz on a 600. Cryoprobes are most likely to show a temp gradient as VT air only flows between tube and relatively cold probe wall. It is always colder at the top thus Z corr is positive.....
2

https://twitter.com/chris_waudby/status/1492474822932275201

Solvent vs solute: 400 Demo HFX vs 500 Demo HFX vs 600 RO

	LW_D2O(Hz)	LW_ACN(Hz)
400	0.64	0.54
500	0.73	0.95
600	0.75	1.95

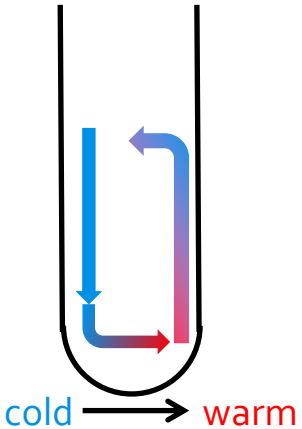
Varian temperature gradient standard
H2O vs CH3CN signals



Convection

- Hadley convection: Always present with temperature gradients
- Rayleigh–Bénard cells convection: Present once a critical Rayleigh number is reached (1700 for a Benard configuration, i.e., two parallel horizontal boundaries separated by a distance *d*).

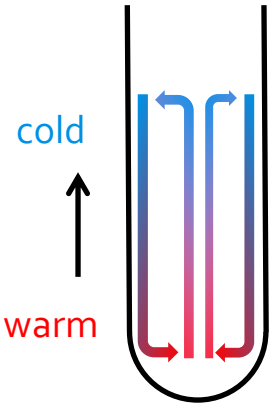
Hadley convection



$$\mathrm{Ra} = \frac{\rho\beta\Delta T l^3 g}{\eta\alpha}$$

g: gravity,
β: coefficient of thermal expansion
ΔT: temperature difference
l: length
η: viscosity
α:thermal diffusivity

Rayleigh–Bénard convection

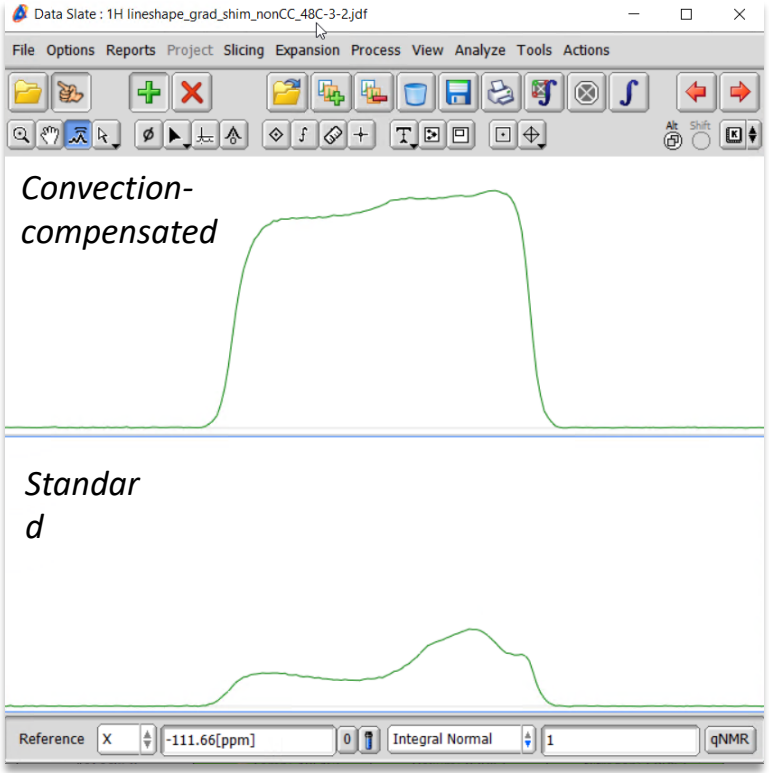


Convection-compensated gradient shimming

- At temperatures significantly away from room temperature, sample convection will occur

- This will cause the signal profiles collected by gradient shimming to be heavily attenuated and/or distorted

- Solution: use a pulse sequence that compensates for convection
  - Double spin echo refocuses additional phase shifts that accumulate due to convection

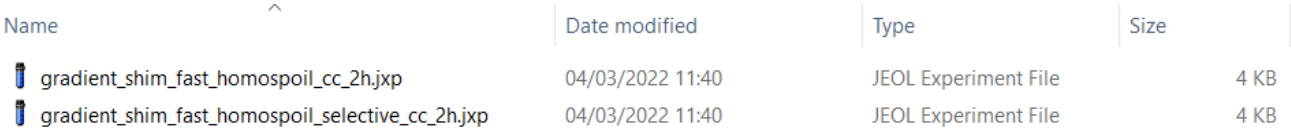


Acetone-d6 sample, 48° C

Convection-compensated gradient shimming

- Calibrate “Fast_homospoil_CC” and “Fast_homospoil_selective_CC” during installation

- Recommended use:
  - Working sequences have been renamed as “Fast” versions under service_experiments in AB_pack



Name	Date modified	Type	Size
gradient_shim_fast_homospoil_cc_2h.jxp	04/03/2022 11:40	JEOL Experiment File	4 KB
gradient_shim_fast_homospoil_selective_cc_2h.jxp	04/03/2022 11:40	JEOL Experiment File	4 KB

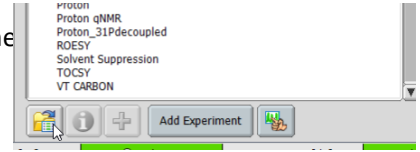
  - Log in as console and Upload to “Experiments folder on spectrometer and then calibrate these methods as described

3D gradient shimming

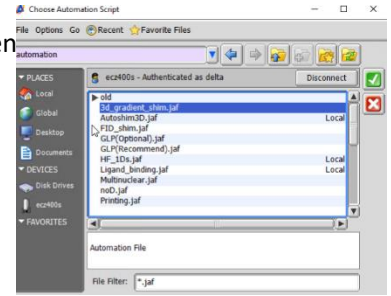
3D gradient shimming

Transverse shims need to be shimmed from time to time with a period ranging from every 3 days to every 3 months depending on magnet stability and nature of work.

1. Load the standard 1H lineshape sample if you have it
2. Use the gradient shimming tool to Z-gradient shim first
3. Create a job for this sample
4. Load the 3D_gradient_shim.jaf script by clicking on the button to the bottom-left of the “Available Methods” window as shown below



5. Navigate to the spectrometer using the window that opens and then select the 3D gradient shimming script as shown below



6. The 3D gradient shimming method should now be available

7. Load the method
8. Click the “Submit Job” button. The 3D shimming will take around hal an hour or so to complete.
9. After this check the lineshape. Save the system shims as console.

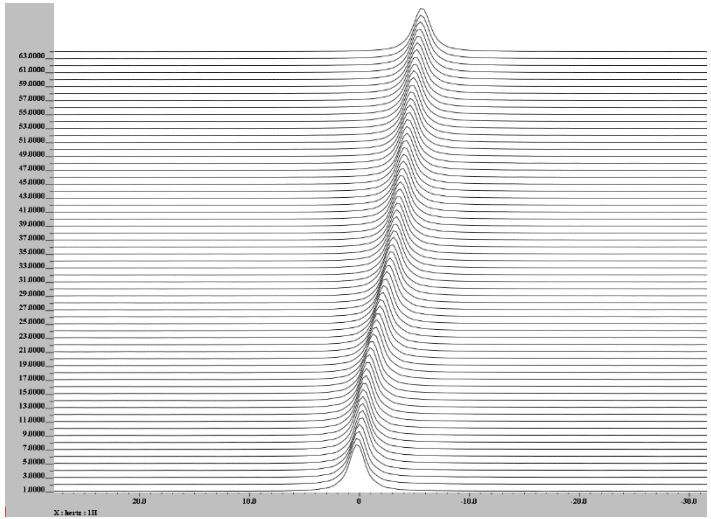
When to run it

- At installation
- Every week (if it works)

Lock

Lock

- Monitor ^{2}H signal from solvent to detect field drift
- If field changes, ^{2}H signal position also changes
- Adjust current in supplementary coil to compensate for drift
- Also used as signal in conventional shimming



Proton signal changes position without NMR lock

Solutions for Innovation JEOL

NMR LOCK failure for my sample, why?

- (Wrong solvent nominated)
- Insufficient solvent
- Sample is solid
- The magnet has drifted a lot
  (or you loaded very old shim file)
- Resolution is very bad for some reason
- Solvent is not deuterated

  e.g. CCl4

- Z0 is at its limit

Solutions for Innovation JEOL

Find lock signal with Sawtooth

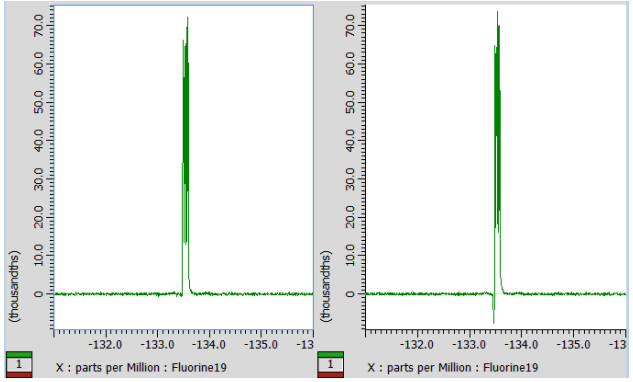
Delta version 5 series

1. Start SAWTH from interactive mode on Spectrometer control
2. Increase Lock Level
3. Increase Sawtooth Range
4. If you find it, click on the signal
5. If you find nothing, observe 1H without lock, then you should be able to estimate how far you missed the lock

Solutions for Innovation JEOL

Lock phase

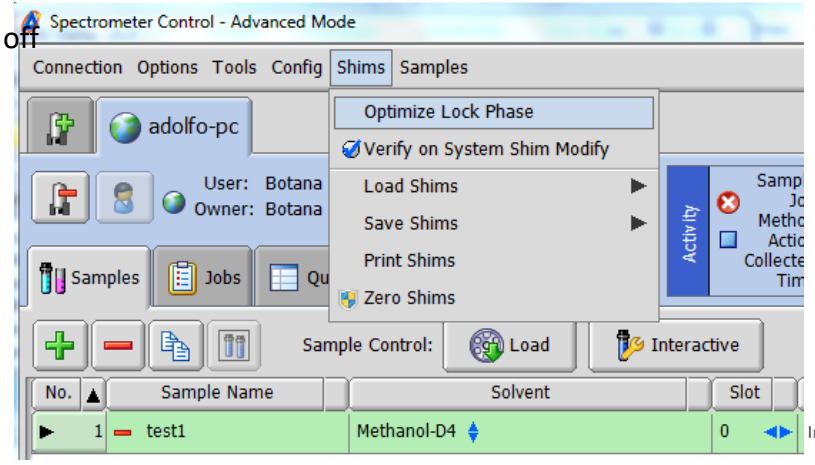
Selective 1D experiment



Lock phase correct

Lock phase off

Fig. 2.3 Lock signal observed in the sawtooth mode before and after adjusting the lock phase



Innovation JEOL

Calibration & Tests

Lineshape

- Use sample of chloroform in acetone-d_6
- Use standard 1D sequence
- Shim
- Process with no line-broadening
- If there are any problems:
  - ^2H gradient shim
  - check the probe for damage / dirt etc

Solutions for Innovation JEOL

Pulse Lengths

- Tune the probe
- Use a suitable pulse program
  - first run a test spectrum with a ‘small’ pulse to adjust receiver gain, offsets, phase etc.
  - set the plot region to the signals of interest

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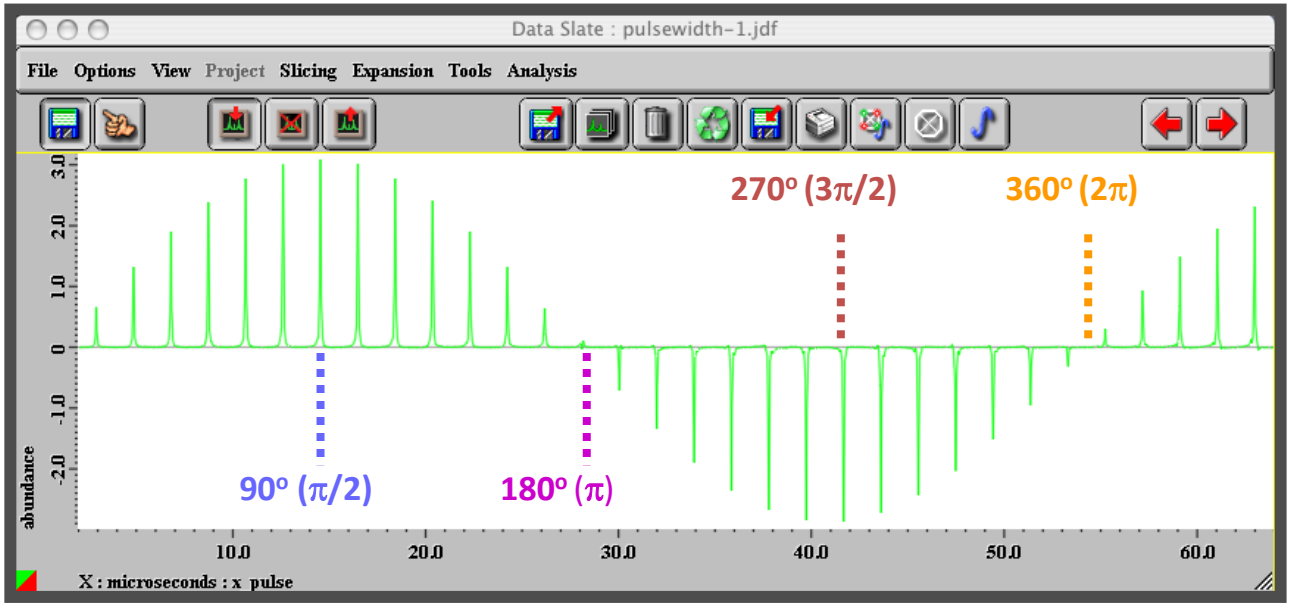
Find either 180 or 360



t_{pulse} →

Solutions for Innovation JEOL

Sensitivity

- The standard ^{1}H sample is 0.1% Ethylbenzene in $CDCl_3$
- Check probe tuning, pulse length, and shimming

Solutions for Innovation JEOL

Temperature calibration (methanol-d4?)

- Methanol

	with FTS			
No	Set Temp [deg C]	delta	real Temp [deg C]	delta T
1	0	1.7806	1.59	1.59
2	5	1.7377	6.46	1.46
3	10	1.6935	11.38	1.38
4	15	1.6485	16.30	1.30
5	20	1.6034	21.13	1.13
6	25	1.5580	25.90	0.90
7	30	1.5126	30.57	0.57
8	35	1.4678	35.08	0.08
9	40	1.4220	39.59	-0.41

~180K to 300K			between 178 and 330 K,					
http://staff.ustc.edu.cn/~liuyz/methods/NM			https://doi.org/10.1016/0022-2364(82)90147-0					
bruker	bruker T	bruker delta		T	delta	JEOL	T	delta
274.9833	1.833301	1.83330147	274.6607	1.510657	1.510657	274.9833	1.833301	1.833301
279.8487	6.698711	1.69871145	279.5307	6.380653	1.380653	279.8487	6.698711	1.698711
284.7596	11.60959	1.60958851	284.4539	11.30387	1.303866	284.7596	11.60959	1.609589
289.6705	16.52048	1.52048478	289.3853	16.23529	1.235293	289.6705	16.52048	1.520485
294.4901	21.34011	1.34011293	294.2335	21.08352	1.083519	294.4901	21.34011	1.340113
299.2555	26.10549	1.10549275	299.0359	25.88592	0.885915	299.2555	26.10549	1.105493
303.9112	30.76116	0.76115526	303.7367	30.58667	0.586671	303.9112	30.76116	0.761155
308.4171	35.26706	0.26705584	308.2952	35.14516	0.145164	308.4171	35.26706	0.267056
312.9195	39.76952	-0.23048113	312.8596	39.70956	-0.29044	312.9195	39.76952	-0.23048

- Ethylene Glycol

	without FTS			
No	Set Temp [deg C]	delta	real Temp [deg C]	delta T
1	20.0	1.693	22.18	2.18
2	22.5	1.672	24.30	1.80
3	25.0	1.651	26.44	1.44
4	27.5	1.630	28.57	1.07
5	30.0	1.608	30.76	0.76
6	32.5	1.586	32.97	0.47
7	35.0	1.564	35.12	0.12
8	37.5	1.542	37.38	-0.12
9	40.0	1.520	39.57	-0.43
10	42.5	1.498	41.84	-0.66
11	45.0	1.476	44.02	-0.98
12	47.5	1.453	46.33	-1.17
13	50.0	1.430	48.58	-1.42

~300K to 380K			between 273 and 416 K					
http://staff.ustc.edu.cn/~liuyz/methods/			https://doi.org/10.1016/0022-2364(82)90147-0					
bruker	bruker T	ruker delta		T	delta	JEOL	T	delta
295.3256	22.17557	2.175574	293.764	20.61402	0.61402	293.7884	20.63837	0.638375
297.4476	24.29758	1.797577	295.9213	22.77132	0.27132	295.9502	22.80017	0.300173
299.5866	26.43664	1.436636	298.096	24.94596	-0.05404	298.129	24.97899	-0.02101
301.7217	28.57168	1.071682	300.2665	27.11652	-0.38348	300.3034	27.15337	-0.34663
303.9129	30.76291	0.762913	302.4942	29.3442	-0.6558	302.5346	29.38461	-0.61539
306.1172	32.96719	0.467187	304.7351	31.58514	-0.91486	304.7787	31.62875	-0.87125
308.2703	35.12029	0.120292	306.9241	33.77406	-1.22594	306.9704	33.82043	-1.17957
310.5328	37.38276	-0.11724	309.2242	36.07416	-1.42584	309.273	36.12304	-1.37696
312.724	39.57399	-0.42601	311.4518	38.30184	-1.69816	311.5028	38.35278	-1.64722
314.9895	41.83947	-0.66053	313.755	40.605	-1.895	313.8077	40.65767	-1.84233
317.1747	44.02468	-0.97532	315.9766	42.82656	-2.17344	316.0305	42.88053	-2.11947
319.4823	46.33229	-1.16771	318.3226	45.17256	-2.32744	318.3775	45.2275	-2.2725
321.7277	48.5777	-1.4223	320.6053	47.45532	-2.54468	320.6608	47.5108	-2.4892

The chemical shift of water is temperature dependent (as well as pH dependent).
$\delta(H_2O) = 7.83 - T / 96.9$, where temperature is measured in Kelvins.
This equation is valid at pH 5.5. Dependence of $\delta(H_2O)$ on pH is about 0.02 ppm per pH unit.

Methanol-d4

- https://doi.org/10.1002/mrc.5216

$$T/\mathrm{K} = \sum_{i=0}^{4} a_i (\Delta\delta/\mathrm{ppm})^i. \quad (4)$$

Table 1 contains the polynomial coefficients of the fit function, and Figure 3a shows the graph of this function including the data points. In Figure 3b, the deviation of the individual data points from the fitted curve is depicted.

TABLE 1. Polynomial coefficients for the fit function in Equation 4

i	0	1	2	3	4
a_i	416.4745	−39.5133	−36.0620	11.4869	−2.4340

Temperature calibration

2-point calibration can be saved in VT controller

The shift value is calculated as **Δ shift value = (Actual Sample Temperature) – (Set Temperature)**. The +/- sign of the shift has to be used for the calibration.

Open the front door of the spectrometer and identify the OMRON E5ER temperature controller.

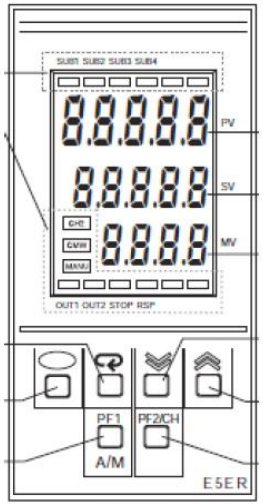


Figure 2

Gradient calibration

- As per manual with a Shigemi tube
- Using DOSY experiment

the known [2] diffusion coefficient at 25 °C for 1% H_2O/D_2O of 1.91×10^{-9} m^2 s^{-1}

Table 2
Experimental and literature values for diffusion coefficients of simple liquids.

		Experimental $D/10^{-9}$ m^2 s^{-1}	Literature $D/10^{-9}$ m^2 s^{-1}
a	4.28 m $MgCl_2$	0.472 ± 0.005	0.468 ± 0.008
b	Cyclooctane	0.55 ± 0.005	0.546 ± 0.006
c	Dimethylsulphoxide	0.73 ± 0.007	0.723 ± 0.008
d	3.21 m $MgCl_2$	0.779 ± 0.008	0.768 ± 0.008
e	Dioxane	1.09 ± 0.007	1.100 ± 0.01
f	2.02 m $MgCl_2$	1.203 ± 0.01	1.206 ± 0.01
g	0.995 m $MgCl_2$	1.728 ± 0.02	1.753 ± 0.02
h	0.372 m $MgCl_2$	2.036 ± 0.02	2.049 ± 0.02
i	Water	2.299 ± 0.005	2.303 ± 0.02
j	Methanol	2.42 ± 0.02	2.421 ± 0.03
k	Chloroform	2.43 ± 0.03	2.432 ± 0.03
l	Cyclopentane	3.1 ± 0.02	3.147 ± 0.03
m	Acetonitrile	4.37 ± 0.04	4.370 ± 0.04

https://doi.org/10.1016/j.jmr.2009.01.025

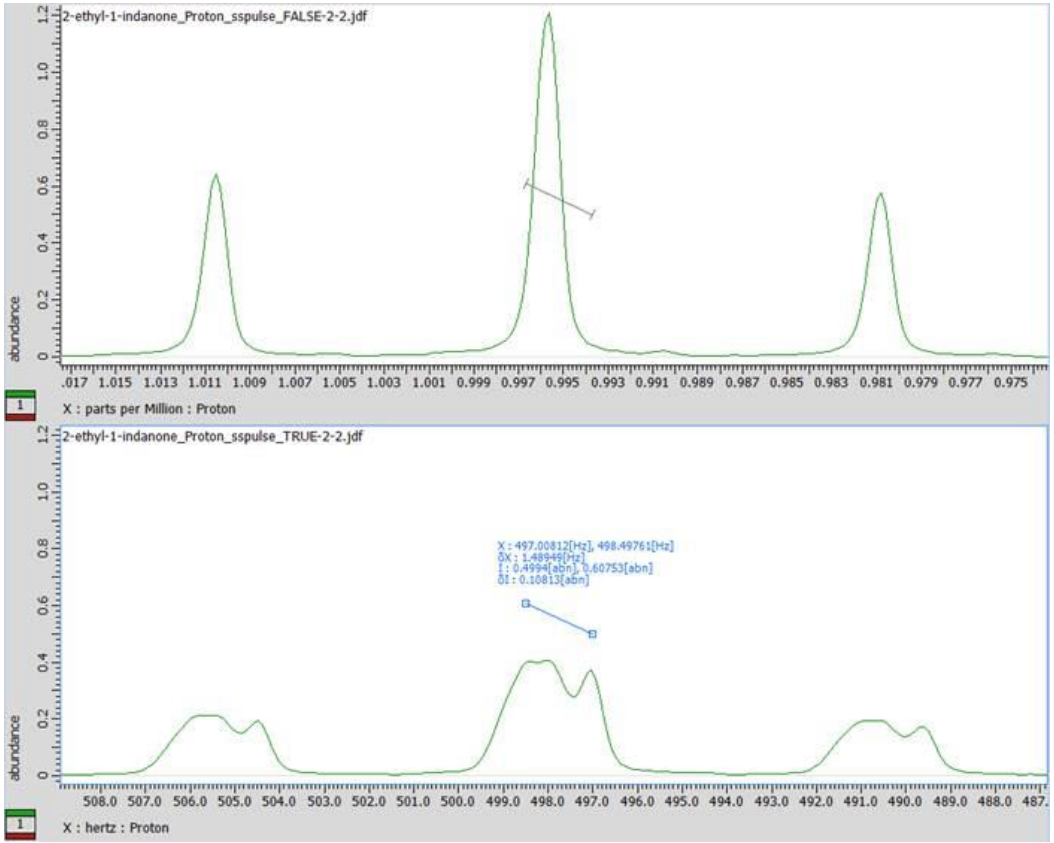
PFG amplifier offset

Gradient offset

- Check if experiments with gradients degrade linewidth (does a cosy with gradient set to zero degrade lock)?

PFG amplifier effect

Proton with an optional PFG pulse before the relaxation delay:



No PFG pulses
(ss_Proton_FALSE.jxp)

PFG pulse (even with gradient amplitude set to zero)
(ss_Proton_TRUE.jxp)

(measurement taken 3 months after adjusting PFG offset)

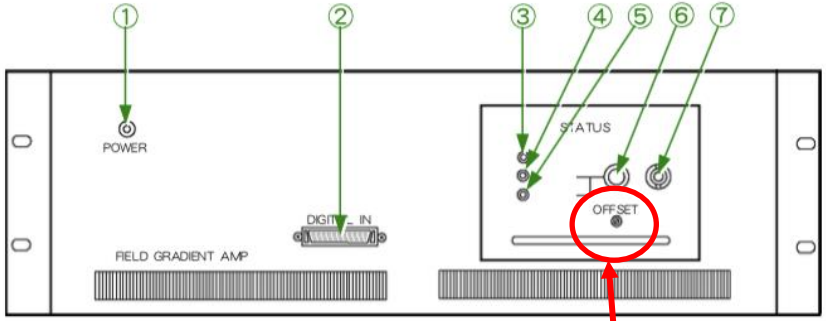
PFG amplifier offset correction

- If a pulse sequence uses gradients. The PFG amplifier will be on for the whole duration of the pulse sequence, introducing a residual current (offset).
- The PFG amplifier offset drift over time, with noticeable effects even one month after adjustment
- Ensure that the gradient offset is correctly set at any PM/installation. If not, any experiment with gradients will have poor performance.
- You can use the traditional check using cosy with gradients set to zero described in the ECZ service manual or the ss_proton.jxp experiment, which allows visualizing the extent of the issue.
- Use any sample of known and relatively narrow lineshapes, like 0.1% ethylbenzene where the triplet at 0.9 can be observed and compared the spectrum obtained with sspulse parameter enabled *(ss_Proton_TRUE.jxp)* against the spectrum obtained with sspulse disabled *(ss_Proton_FALSE.jxp)*. Intensities may be different, but the linewidth and shape should be the same (or less than 0.1Hz different). The gradient offset can then be corrected by running *ss_Proton_repeat.jxp* and trying to optimize the lineshape seen in the monitor while adjusting the offset.

  (The only difference between these pulse sequences are the repeat, relaxation_delay and sspulse parameters default values)

PFG offset is dependent on room temperature: ensure room temperature is stable

PFG offset pot



ECA/ECX FG Amp

DC Offset Adjustment

ECZ FG Amp

FG POWER SUPPLY OFFSET ADJUSTMENT

Measurement condition (Pulse sequence)	
Sample	3% $CHCl_3$ in Acetone-d6
Experiment	global/All Files/cosy_pfg.jxp
Process_lists	None
Template	None
Specification value	Adjustment items

1. Create a sample definition.
2. Click the Interactive button to open the "manual control panel".
3. LOAD the sample and perform SPIN and Auto_Lock.
4. Adjust the Lock_Gain value so that the Lock Signal will be approximately 2000.
   Remember the Lock Signal value.
5. Click the Add Experiment to open the specified Experiment and perform the following settings.

- Header tab: add repeat

  How to add repeat

  a. Click the Add Parameters icon and select repeat.
  b. Select the value check box Value.
  c. Click the Add icon Add.
  d. Click the Done icon Done and close the Add Parameter window.
- Acquisition tab: scans=1, x_prescans=0
- Pulse tab: grad_**1_amp=0%**

6. Click Submit Job and start the measurement.
7. Click the Samples tab, and click the Interactive icon.
8. Make sure that the Lock_Signal value does not differ significantly before and after the measurement.

If the shift in the Lock Signal is small, there is no need for adjustment.

If there is a large shift in the Lock Signal value.

9. Adjust with OFFSET at the front of the FG UNIT so that the Lock Signal value will be the same value as before the measurement.
10. Stop the measurement and check that the Lock Signal value does not change.
11. Perform the process again by repeating procedure 6 to 10.

Spectrometer Troubleshooting

Getting Information

- It will help if you can find as much detail as possible:
  - Software version
  - Error messages or other output
  - What made it happen
- View the history log

Solutions for Innovation JEOL

Experiment Problems

- Cannot get an experiment to work?
  - Check the parameters are set correctly (check pulse program, etc).
  - Insert a standard sample
  - Run a proton spectrum

Solutions for Innovation JEOL

Locking Problems

- If the system does not lock
- Possible causes:
  - Solid DMSO (melting point: 19°C)
  - Little or no ^{2}H in sample solvent
  - Poor shimming
  - Magnet quench

Solutions for Innovation JEOL

Shimming Problems

- Poor shimming may be due to a number of causes:
  - Poor sample preparation
  - Incorrect sample depth
  - Old system shimfile

Solutions for Innovation JEOL

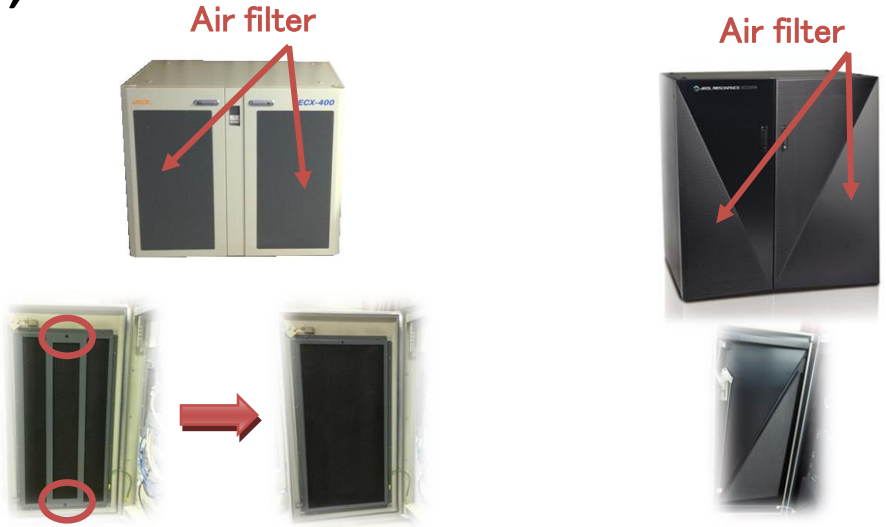
Console Problems

- It is a good idea to use preventative maintenance to avoid down-time
- Regulated room temperature is important (17 to 25°C) - have your AirCon regularly serviced!
- Problems arise due to overheating of the console electronics
- Regularly check airflow from rear vents (a rise in temperature may indicate fan failure)
- Replace any non-functioning or worn fans (squeaking noise / no airflow)

Solutions for Innovation JEOL

Cleaning the air filter

- Remove the front panel inside the door to free the filters, and then vacuum them



Powering Off

- Ideally if you know there will be a power cut you can shut the system down gracefully:
  - remove sample
  - shut down Instrument computer (RMT)
  - turn off the console

Solutions for Innovation JEOL

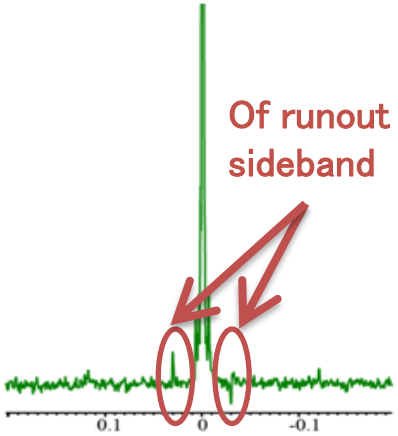
Powering On

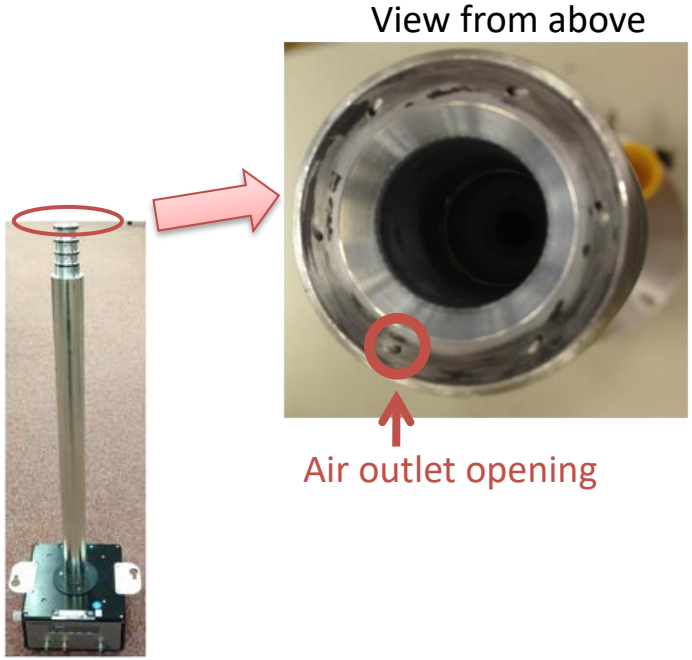
- To power on:
  - Turn everything on
  - Start Delta
  - Run proton experiment of a standard sample to check all is OK

Solutions for Innovation JEOL

Spinning problem

- Could be caused by dirt

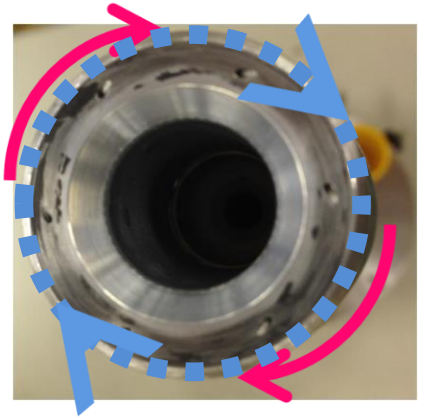




Solutions for Innovation JEOL

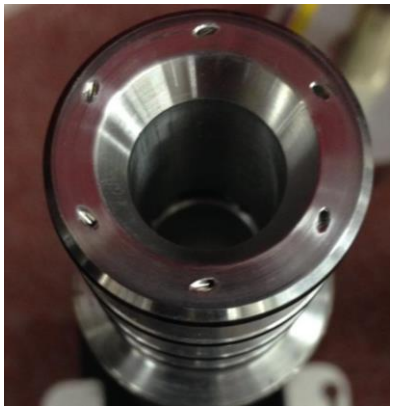
Cleaning of the probe head

- Wipe the probe head by applying ethanol in gauze. Wipe clockwise, without letting ethanol enter the air outlets.



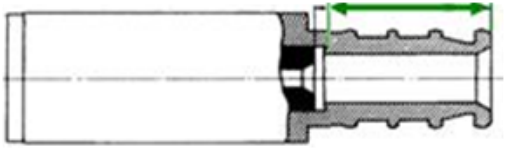
Air flow direction

Direction to wipe the probe head



Solutions for Innovation JEOL

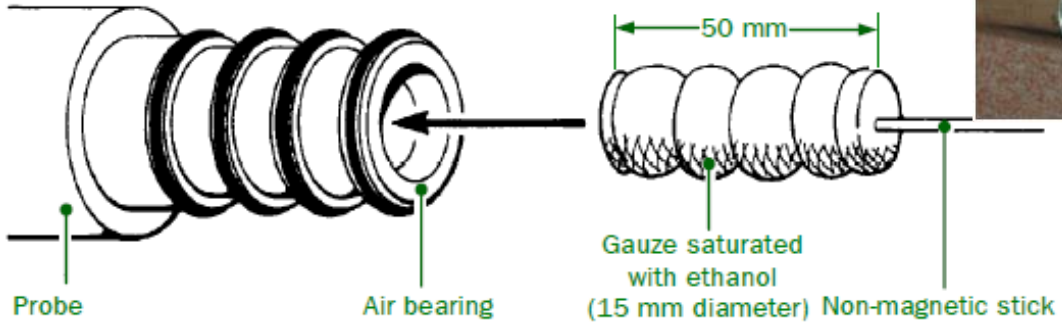
Cleaning the stator



The part to be cleaned

1. Prepare a non-magnetic material (for example, plastic, copper or aluminum) stick wrapped by gauze (Fig. 6.3, right).
2. Saturate the gauze with ethanol. Slowly wipe the inner wall of the stator with this cleaning stick to remove dirt and dust.
   - Ensure that no gauze material or lint remains inside.
   - Wring the gauze firmly so that ethanol does not drip inside the probe.

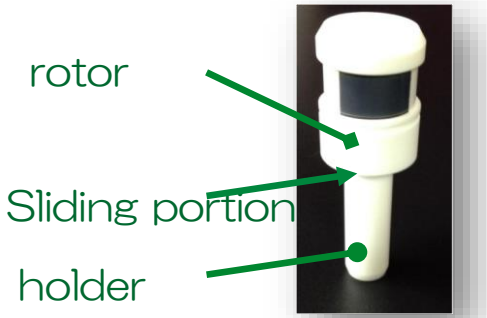
Wipe the air bearing by the same method, using fresh gauze.

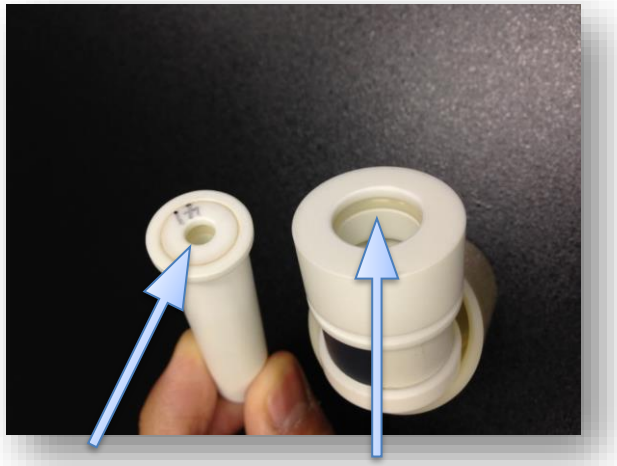


Solutions for Innovation JEOL

Cleaning spinner

- Clean the o-rings by applying ethanol in gauze.





- If spinner does not hold tube tightly, o-rings might need replacing

Solutions for Innovation JEOL

Trouble-shooting using the RMT

Remote Maintenance Tool

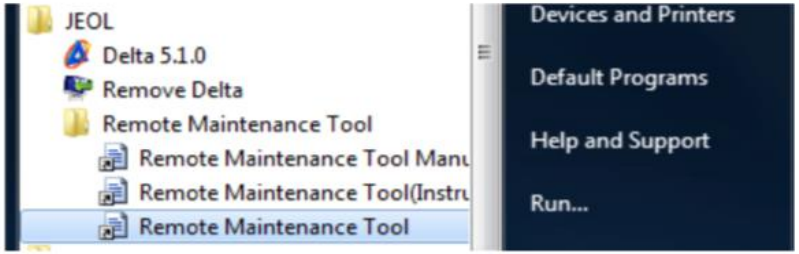
Starting the Remote Maintenance Tool

Start the Remote Maintenance Tool as follows.

1. Select All Programs — JEOL — Remote Maintenance Tool from the Start menu.
2. Select a mode to start.

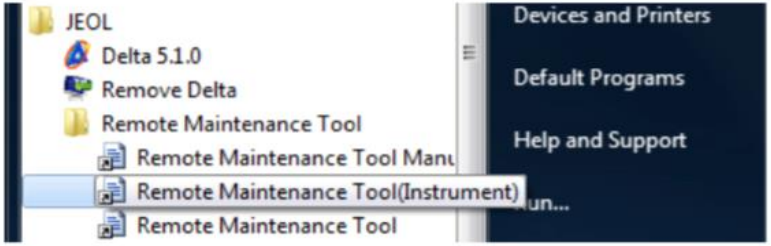
a. Starting with Workstation mode

Select "Remote Maintenance Tool".

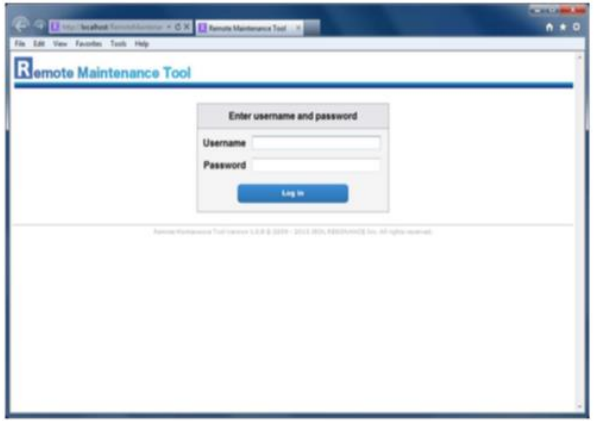


b. Starting with Instrument mode

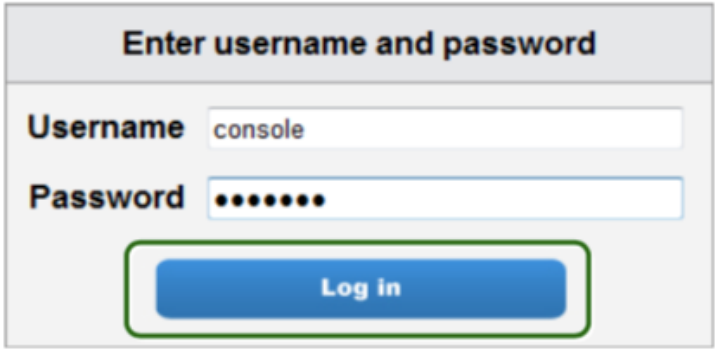
Select "Remote Maintenance Tool (Instrument)".



A login dialog box appears.

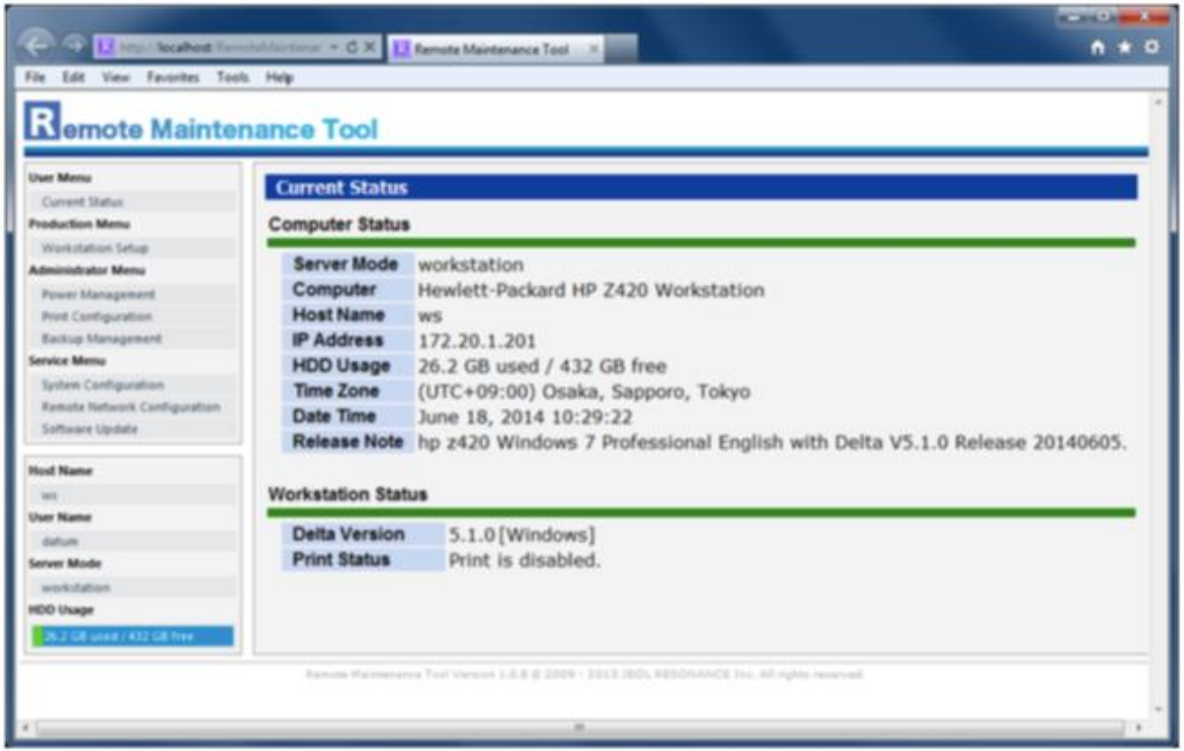


3. Enter the user name and the password.
   Username: console
   Password: console



4. Click **Log in**.

If the log in succeeds, the display changes as follows.



The figure is for the Workstation Mode.

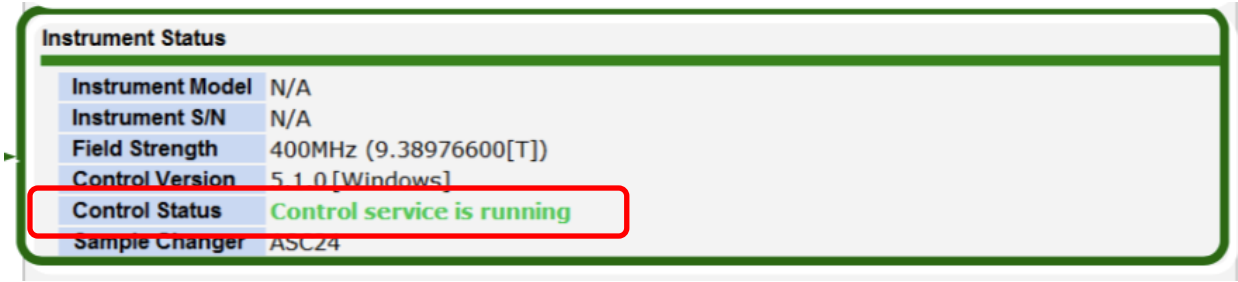
Instrument Mode

Current Status

In the Current Status pane, you can check the information about each item of the spectrometer.

1. Computer Status
2. Instrument Status
3. Instrument Configuration
4. Wiring Configuration

- Similar to a blocked spectrometer, if scc is not shown in the available spectrometers after a power cycle or a reboot. It's possible the control service has not started.
  - Log into the spectrometer via RMT.
  - Check Instrument Status, the control service should be running.



- If the control service is shown as not running it can be restarted.
- Select RESTART control service from the management window.

- If sample definitions and jobs cannot be deleted from the sample and job queue then log into the RMT and remove them via the Control Service Restart option.
  - Go to Control Service Management

  - Select 'Delete job related files'
  - Restart the control service. When reconnecting to the spectrometer, all samples and jobs will have been removed.
  - Untick again this option

Note this will cause Smart mode buttons to be reset. If want to keep them, make a copy of them before deleting job related files.
So remote desktop to the console once you are happy with the buttons, locate folder:
C:\Program Files\Common Files\JEOL\Control 5.3\users
And make a copy of it, for example in the desktop of the console.
After restarting spectrometer control with the delete jobs option enabled, copy this folder to the original location.

- Sometimes it may be necessary to use debugging mode, e.g. if a spectrometer alarm is stopping experiments but the alarm is vague.
- JEOL service may ask you to turn on enhanced debugging mode so detailed error logging records more detail of the error status.
  - Connect to the RMT and select control service management.
  - Stop the control service then expand the Debug Option.

- Change from Level(Simple) to Level (Detail)

- Either select all items or the relevant hardware, depending on advice from JEOL service.

- Once done, restart the control service.

- Once the alarm has occurred then the machine log should be downloaded and sent to JEOL service.

- Again, from the control service management window, expand the machine.log option.

- Select download machine.log file.
- This is a hyperlink and will allow you download the machine log to the workstation, by default to the downloads folder.

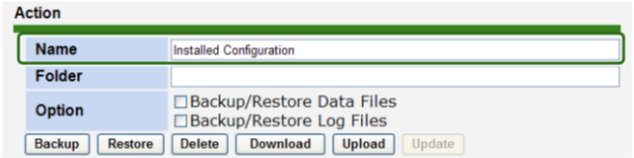
- The log file can then be emailed to JEOL service.
- If it's large, please use the JEOL ftp server,

- http://www.j-resonance.com/filex/

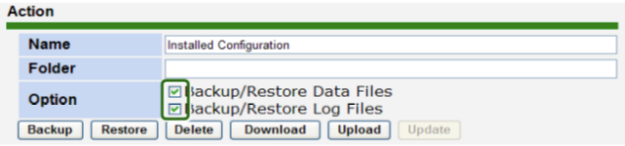
- Using configuration backups
  - JEOL service will make a configuration backup at the completion of the installation and before/after a major software update.
  - A backup can be made at any time. However, use the configuration restore carefully as some files may be lost and settings changed.

Backup of configuration

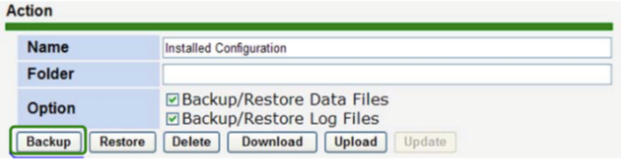
1. Enter the Backup name in the Name.



2. Specify the Options.

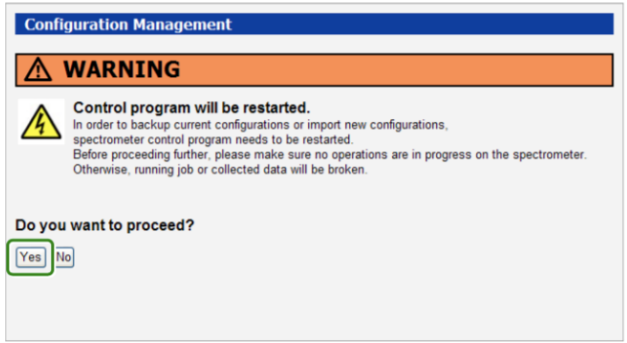


3. Click **Backup**.



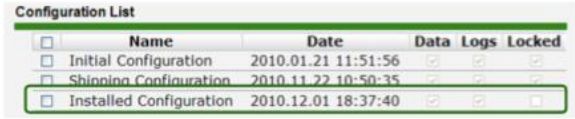
A warning dialog box appears because the Control program is restarted.

4. Click **Yes**.



The situation of the progress is displayed in the Status area.

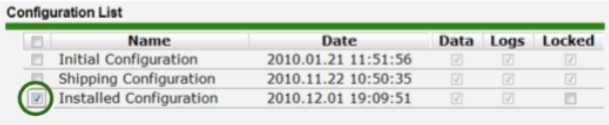
When the backup is completed, the backup information is added in the Configuration List.



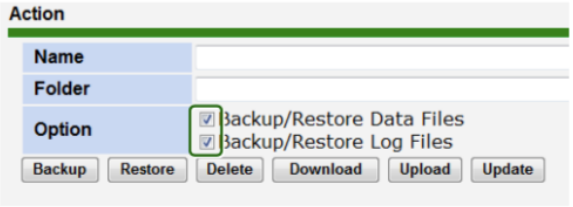
Restoring a configuration

This section explains the procedure to restore the Configuration and the environment original state.

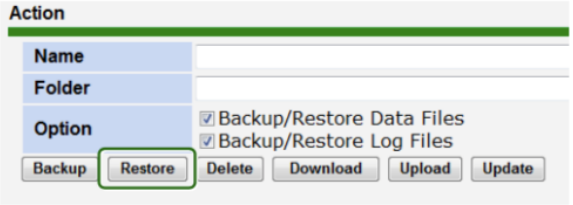
1. Select the configuration be restored from the Configuration List.



2. Specify the Option items.

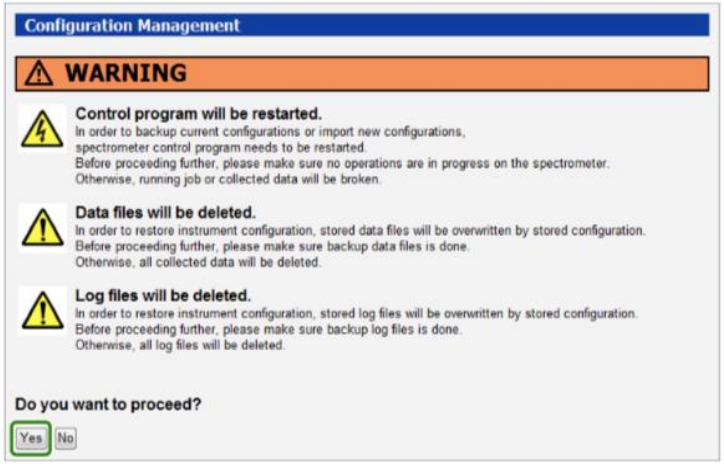


3. Click **Restore**.

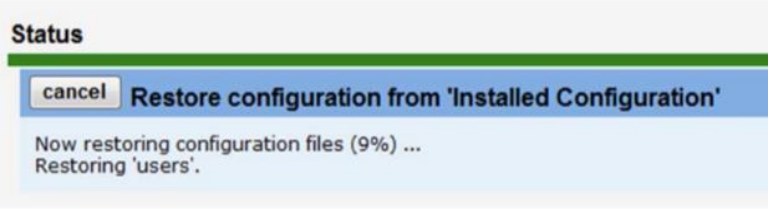


A warning dialog box appears because the Control program is restarted.

4. Click **Yes**.



The progress situation is displayed in the Status area.

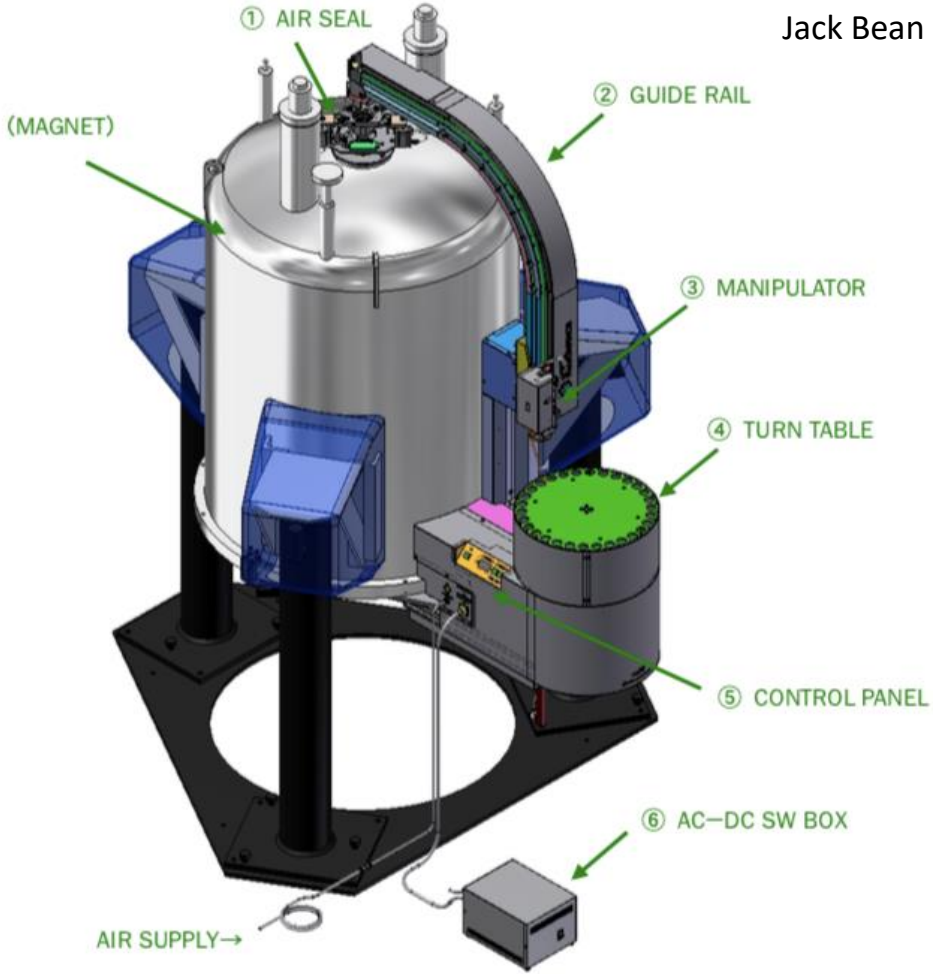


Clicking **cancel** stops the restoration.

When the restoration is complete, the following message is displayed.

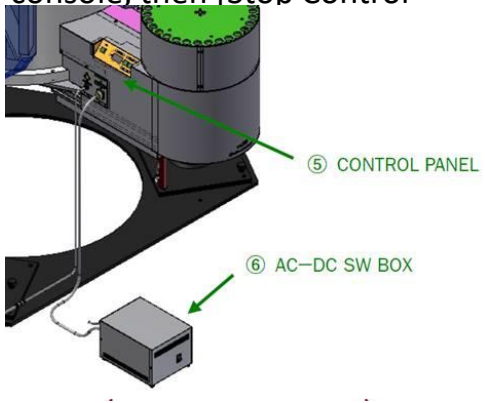
Auto Sample Changers

Jack Bean 30/64/100 position sample changer



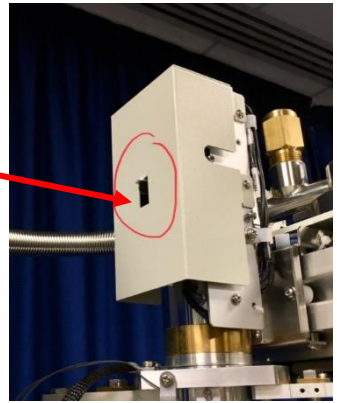
It’s possible for the ASC to become non responsive after a LOAD/EJECT error. If this happens, do the following.

- Login to RMT(Remote maintenance tool instrument) by console, then [Stop Control Service]
- Turn off the ASC AC-DC SW box
- Disconnect B-BUS cable from ASC connector panel
- Re-connect B-BUS cable to ASC
- Turn on the ASC AC-DC SW box
- Control Service Management, [Start Control Service]



If the ASC manipulator will not release a sample, this can be done manually.

- Place a hand under the manipulator to catch the sample.
- Operate the manual release lever on the side of the manipulator



ASC24 Sample Changer

Please turn OFF the control box of the autosampler.
Then turn it ON again, wait until display show 0 on the autosampler.
Then press S1 and S2 at same time and wait until there is an “.” next to the 0 (0.).
Then press S2, to get in position of slot 1.
Then check if it works.

A.1 Result from Miss operation

In the case of rebooting system, confirm no sample in the sample slot at the eject position.

Error message	Cause	Remedy
WARNING: Sample Changer Carousel does not detected. LED display: #50	No carousel or set it incorrectly	①Set carousel correctly. ②Confirm position of setting carousel correctly.
WARNING: Sample does not exist at the specified slot LED display: #54	No sample at position assigned by [Slot] number	Set sample at position assigned by [Slot] number.
WARNING: Sample is remained in the probe or spinner housing, or carousel. LED display: #56	The sample is remained in probe, spinner housing or carousel while [Load] enters.	Confirm the sample floating by ejecting from probe, spinner housing and carousel The eject air is readjusted if sample is not enough to float.
WARNING: Sample Changer Carousel is full. LED display: #58	At command of ejecting sample, do not eject sample because eject position of carousel is occupied with another sample.	Remove sample from eject position of Carousel.

A. 2 Result from System itself

Error message	Cause	Remedy
WARNING: Carousel rotation failed. LED display: #51	Sample or another object is caught between Carousel and the housing. Supply air decreases or stops.	①Confirm whether something between bottom of carousel and housing . ②Check air leakage or unfasten air tubes. ③Check input air (> 0.25MPa) ④Call SVC.
WARNING: Carousel position -1 indicator was never found LED display: #52	Position sensor fails at initialization or setting position.	①Sample caught somewhere. Remove it, load sample and calibration again. ②Call SVC
WARNING: Carousel position -1 indicator was not found where exported LED display: #53	Adjustment of initial Carousel position fails.	①Sample caught somewhere. Remove it, load sample and calibration again. ②Call SVC
WARNING：Sample is Not Floating. LED display: #55	Sample does not float enough due to less floating air. Sample is caught with gate pin of carousel.	①Adjust air for ejecting sample ②Release gate pin by hand to remove sample
WARNING：Specific sample number is more than 24 or the sample number is 0. LED display: #57	Wrong function of hardware. Normally this does not cause error due to input limit of software.	①Reboot spectrometer and ASC24 again. ②Call SVC

JEOL webinars (https://www.jeol.co.jp/en/news/seminar/webseminar/movie_index.html)

Webinar	Link
An Introduction to NMR: Practical Aspects	https://attendee.gotowebinar.com/register/6221243905175906829
Speeding up NMR: NUS and NOAH	https://attendee.gotowebinar.com/register/5215973618176042256
An Introduction to Pure Shift NMR	https://attendee.gotowebinar.com/register/7480233097627308048
Introduction to JEOL Delta: Processing of 1D NMR data	https://attendee.gotowebinar.com/register/3743196484819939856
An Introduction to Solid-State NMR	https://attendee.gotowebinar.com/register/1588889267810221067
Natural Products identification through JEOL systems	https://attendee.gotowebinar.com/register/987608140196536078
An Introduction to JEOL Delta pulse programming	https://attendee.gotowebinar.com/register/4684449906779482894
Main aspects and applications of FAST MAS Solid-State NMR	https://attendee.gotowebinar.com/register/3947946440960288782
Elucidating nano-crystalline structure by combining microED and solid-state NMR	https://attendee.gotowebinar.com/register/5151154110240940816
Delta processing part 2: quantitative NMR	https://attendee.gotowebinar.com/register/591245194184783115
Assignment strategies in NMR pt1: 1D NMR and coupling	https://attendee.gotowebinar.com/register/7874168324236508685
NMR application in battery research	https://attendee.gotowebinar.com/register/7305723011972237583
Gradient Shimming: Theory and Practice	https://attendee.gotowebinar.com/register/5291489178361927691
A Synergy between Cryo-EM and NMR	https://attendee.gotowebinar.com/register/7623552241737432588
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Ethyl Indanone: a user's perspective of the new JASON software	https://attendee.gotowebinar.com/register/3360923782708443918
Practical aspects of high-resolution 1H solid-state NMR at moderate MAS rate	https://attendee.gotowebinar.com/register/3873886639811883023
Your data in JASON: file formats and external access	https://attendee.gotowebinar.com/register/2441061364881739019
Selective Excitation of Overlapping Multiplets	https://attendee.gotowebinar.com/register/3213601326619561742
NMR Crystallography of Dynamically Disordered Solids	https://attendee.gotowebinar.com/register/3995403572903868683
Solid-State NMR Tutorial: Setting up CPMAS Probe	https://attendee.gotowebinar.com/register/477678849452440848
Quantitative 13C NMR	https://attendee.gotowebinar.com/register/2577550346473705743
A Practical Introduction to Diffusion-Ordered Spectroscopy	https://attendee.gotowebinar.com/register/4225933783914972175

JEOL webinars (https://www.jeol.co.jp/en/news/seminar/webseminar/movie_index.html)

Webinar	Link
Solving the Structures of Small Molecules Using Fluorine's Unique NMR Properties	https://connect.acspubs.org/CENWebinar_JEOL_10_22_19
Advances in Liquid Nitrogen Cold Probe Technology	https://connect.acspubs.org/CENWebinar_JEOL_11_19_19
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Proton, Fluorine and X: Practical Aspects and Real Life Applications	https://go.jeolusa.com/Webinar_031
AutoMAS Solid State NMR for Improved Sample Throughput	https://connect.acspubs.org/CENWebinar_JEOL_10_5_21
An Introduction to JASON NMR Processing Software using a number of worked examples	https://connect.acspubs.org/CENWebinar_JEOL_11_10_21
An Introduction of Delta NMR Data Processing Software ver.5	https://vimeo.com/755875413/1e71d583b0
Fluorinated Small Molecules at NMR -Simplifying Structure Elucidation of Fluorinated Small Molecules-	https://vimeo.com/755891713/a56376c521
Introduction to Quantitative NMR —Easy and Reliable Assay—	https://vimeo.com/755891839/c906767e0b
Introduction to solid-state MAS NMR	https://vimeo.com/755877206/48ed7afcb5
JASON a novel NMR tool	https://vimeo.com/755877511/17ebb853b4
To analyze the motion of molecule (ion) by NMR	https://vimeo.com/755879143/d15bc3a1c4
Tackling complex mixture by NMR	https://vimeo.com/755879270/6d88566cc4
SMILEQ Plugin in JASON Software for Automated Quantitative NMR System	https://vimeo.com/755880107/efb95e2646
NMR Techniques to Determine Local Structure and Ion Dynamics in Lithium Ion Batteries	https://www.bigmarker.com/azonetwork/NMR-Techniques-to-Determine-Local-Structure-and-Ion-Dynamics-in-Lithium-Ion-Batteries
Solid-state NMR to elucidate the atomic level structures: basic principles and applications	https://www.jeol.com/events_seminars/webinars/2023/20230213_01_movie.php
Introduction to solid-state NMR: half-integer quadrupolar nuclei	https://www.jeol.com/events_seminars/webinars/2023/20230707_01_movie.php
What makes solid-state NMR broadened and how to overcome it	https://vimeo.com/936545870/9a33a89f95

Thank you

Email: nmrapps@jeoluk.com

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- **http://nmrsupport.jeol.com/**
  - Free processing software Delta
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