Delta NMR Software Release Notes V6.1.0

JEOL RESONANCE Inc.
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CONTENTS

1 ABOUT THIS DOCUMENT

This document describes the functions of V6.1.0, the latest version of the application software program “Delta” for NMR (hereinafter referred to as “Delta”).

2 ABOUT Delta V6.1.0

- Delta V6.1.0 is software for data process and spectrometer control of JNM-ECZ/ECZL series spectrometers.
- To connect to a spectrometer running the spectrometer control software V6.1.0, you need Delta V6.1.0 installed on your control PC.
- Delta V5.1.x software or later is required for processing data acquired using JNM-ECZ/ECZL series spectrometers. Appropriate processing results cannot be obtained using software Delta V.5.0.x or earlier.
- Delta V6.1.0 can process data from JNM-ECA/ECX/ ECS/ECAII/ECXII/ECZ/ECZL series spectrometers.
- The workstation folder path for “automation”, “experiments”, “favorites”, “logs”, “process_lists”, “reports”, “source”, and “templates” folders is as follows:

  Delta V6.1: C:\Users\<User name>\Documents\JEOL\Delta 6.1

3 COPYRIGHT INFORMATION

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3-1-2 Musashino, Akishima-shi, Tokyo Japan 196-8558
http://www.j-resonance.com
http://www.jeol.co.jp/

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4 SUPPORTED ENVIRONMENTS

Supported PCs

JEOL guarantees operation of this software for PCs of the following specifications and on corresponding JEOL products.

- PC: HP Z4 Workstation
- Processor: Intel® Xeon® processor W-2102 (2.9 GHz)
- Memory: 8 GB DDR4 SDRAM (2666 MHz)
- Hard disk drive: 500 GB 7200 rpm SATA
- Graphic adapter: NVIDIA® Quadro® P400 2 GB
- Optical drive: DVD writer (slimline)
- OS: Windows® 10 IoT Enterprise 2016 LTSB
- Monitor: 23-inch IPS LCD

Delta is a 64-bit application and does not run on a 32-bit Windows® environment.

Supported spectrometers

- JNM-ECZ series spectrometers
- JNM-ECZL series spectrometers

For information on upgrading NMR application software to Delta V6.1.0, consult your local JEOL Ltd. branch or agency.

5 ADDITIONS AND IMPROVEMENTS OF FUNCTIONS

The new functions added to Delta V6.1.0 are as follows.

Category	Item	
Software	Added some searchable items to the file search tool	☞ Section 5.1
Software	Added a function to send measurement data by email	☞ Section 5.2
Software	Added a category display for local folders	☞ Section 5.3
Measurement	Added an alarm when refrigerant level drops	☞ Section 5.4
Measurement	Added a sort function for sample define	☞ Section 5.5
Measurement	Improved the refrigerant filling screen	☞ Section 5.6
Measurement	Added a quantitative NMR measurement function for JASON	☞ Section 5.7
Measurement	Changed the multinuclear nuclide from selective to individual placement	☞ Section 5.8
Measurement	Changed the display contents of the Method panel in Smart mode	☞ Section 5.9
Measurement	Added and modified the pulse sequences, etc.	☞ Section 5.10
Data processing	Added a Normalize Region	☞ Section 5.11

5.1 Added Searchable Items to the File Search Tool

New searchable items have been added to the file search tool.

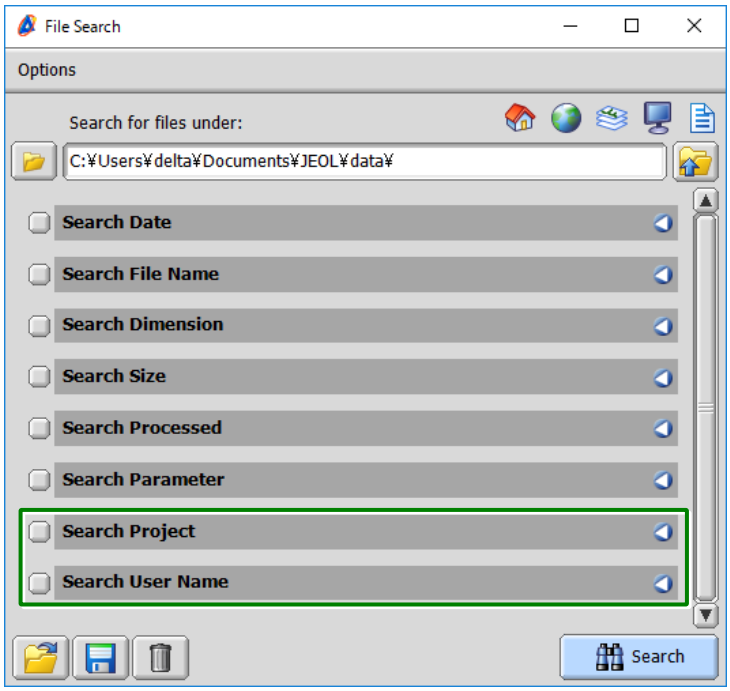


Figure 5.1 New items added to the File Search tool

■ Search Project

Search for files in the search folder by the name of the project.

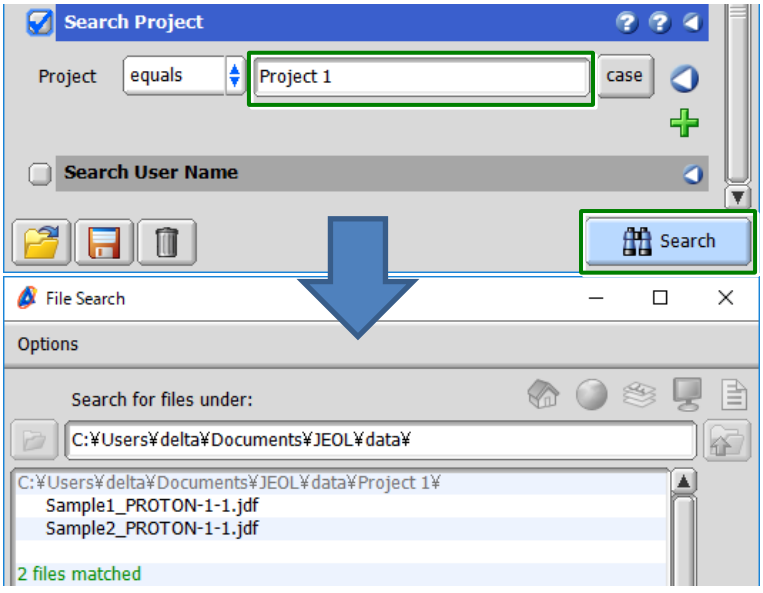


Figure 5.2 Search results in Search Project

Search condition list

Search Condition	Search Result
contains	Search for files that contain the name of the project. Input example: pro
equals	Search for files that match the project name. Input example: project 1
excludes	Search for files that do not match the project name. Input example: project 2 All results except “project 2” matches.
GLOB	Use wildcards to search for matching files. Input example: projec*, project ?, project [123], project [1-9] , project [123], project [1-9]
REGEXP	The entered character string is treated as a regular expression to search for files. Input example: ._project Matches any single character. Project names such as “a_project” and “b_project” are matched. [ab]_project Matches one character contained in parentheses. “a_project” and “b_project” matches, but “c_project” does not. [^b]_project Any project name other than “b_project” that matches “._projec” is matched.

case button

Click this button to search in a case-sensitive manner.

Default button

Clears all search conditions and entered project names and returns to the default state.

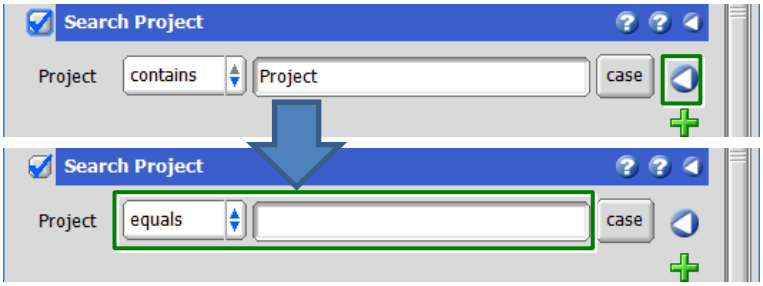


Figure 5.3 Default button

Add button

Click this button to add search conditions.

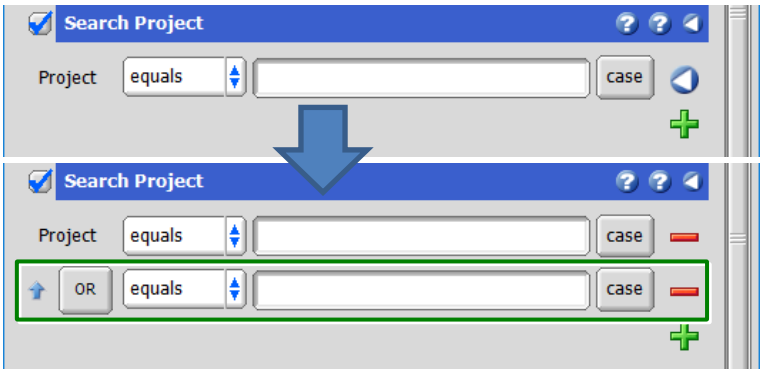


Figure 5.4 Adding search conditions

When you click the **OR** button, it changes to an **AND** button, and the file search is performed with the AND condition.

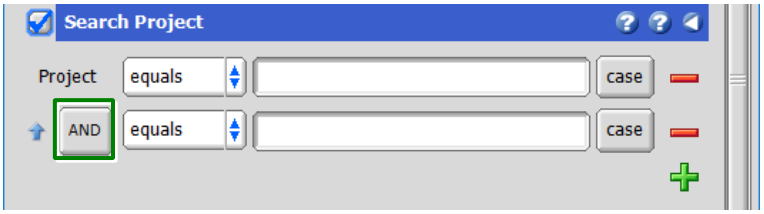


Figure5.5 OR condition and AND condition for the search condition

You can swap the added search conditions with the arrow buttons.

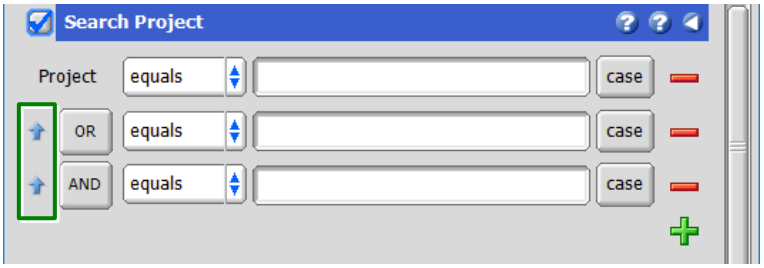


Figure 5.6 Swapping search conditions

■ Search User Name

Search the file by the user name who made the measurement.

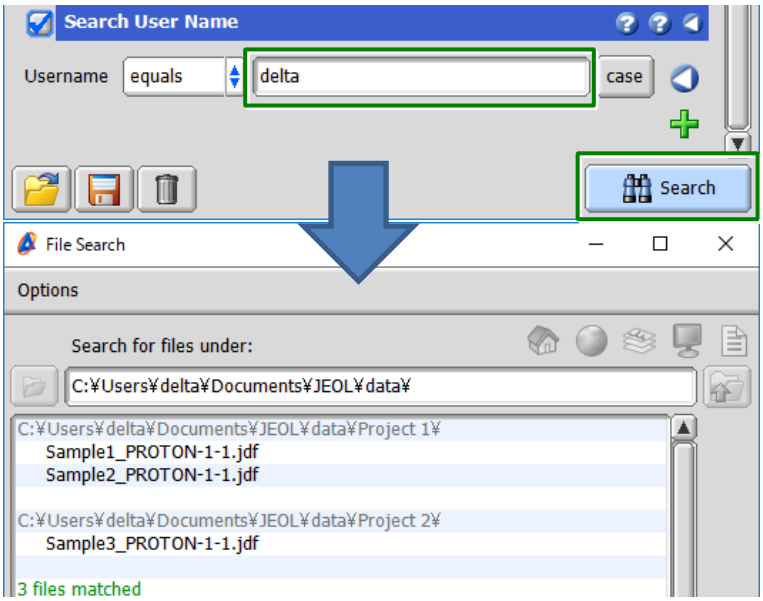


Figure 5.7 Search results by Search User Name

☞ The search conditions are the same as in Section 5.1 “■ Search Project”. For details, refer to Section 5.1 “■ Search Project”.

5.2 Added a Function to Send Measurement Data by Email

A function has been added to send the measurement data by e-mail when the measurement is completed.

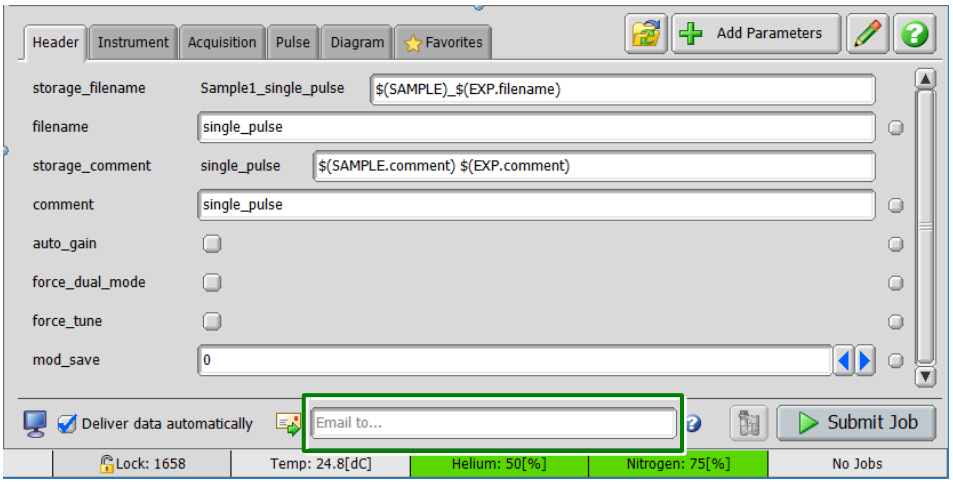


Figure 5.8 Email address input field

■ Function activation

This function is displayed when you enter an item related to e-mail in the **Preferences** - **Environment** tab of the spectrometer control window.

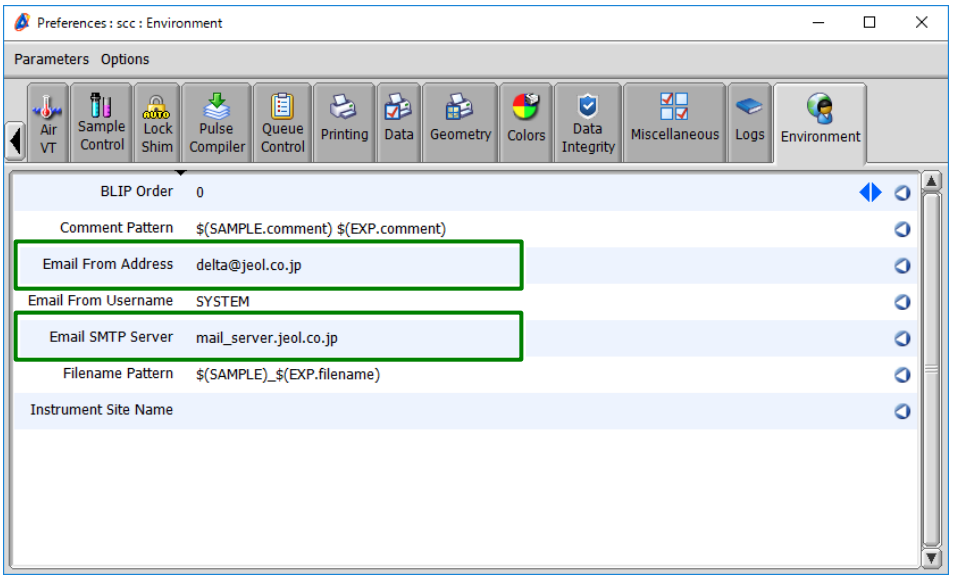


Figure 5.9 Email activation

- The displayed e-mail address and SMTP server name are input examples.
- Check your e-mail address and SMTP server name or IP address with your network administrator.
- The spectrometer must be connected to the network environment to send e-mail.

■ How to enter your email address

Enter the recipient email address.
Example: user1@jeol.co.jp

When sending to multiple recipients, separate the email addresses with a “; (semicolon)”.
Example: user1@jeol.co.jp;user2@jeol.co.jp;user3@jeol.co.jp

Figure 5.10 Example of entering multiple email addresses

5.3 Added a Category Display for Local Folders

An item has been added in the options menu to change the category display for the files stored in the local folder (C:\Users\username\Documents\JEOL\Delta 6.1).

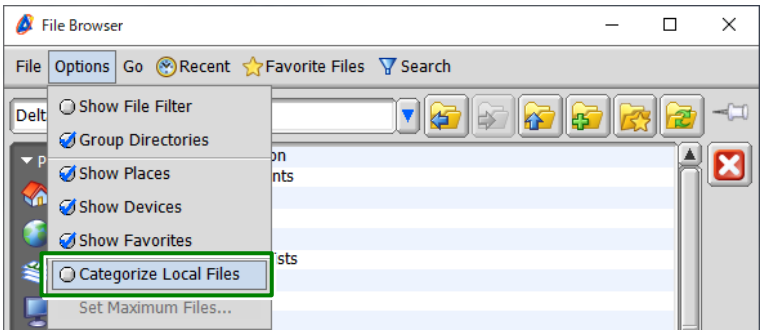


Figure 5.11 File Browser Options menu

When the option is turned on, the display is changed to categorize the local files.

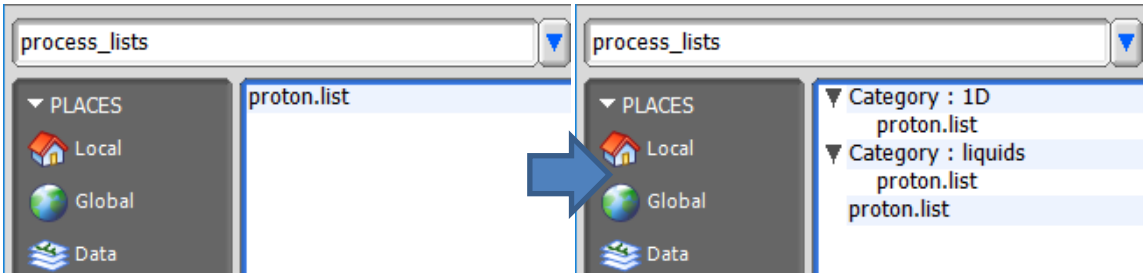


Figure 5.12 Switching to category display

5.4 Added an Alarm when Refrigerant Level Drops

A function has been added to display a warning message and generate an alarm sound from the speaker of the control PC when the remaining amount of refrigerant (liquid helium or liquid nitrogen) falls below a certain percentage.

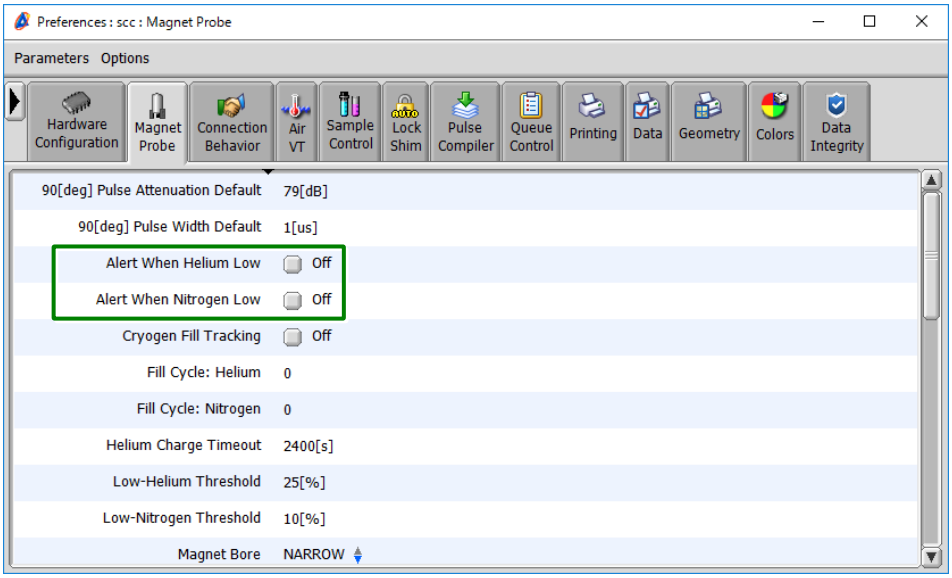


Figure 5.13 Alarm function when the refrigerant level drops

The control PC and the spectrometer must be connected via a network for the alarm to sound.

■ Parameters that control the remaining amount of refrigerant

The parameter that monitor the remaining amount of refrigerant exists in the **Magnet & Probe** tab.

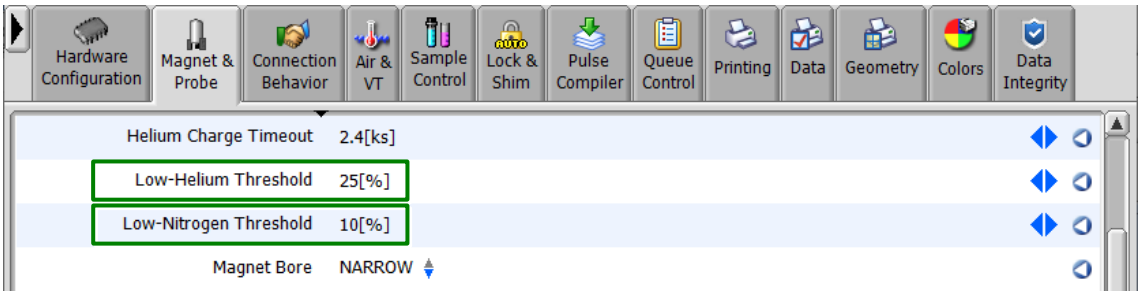


Figure 5.14 Monitoring parameters for the remaining amount of refrigerant

- Low-Helium Threshold:
  A parameter that monitors the remaining amount of liquid helium.
  If the value is less than the entered percentage, a warning message and alarm sound is generated.
- Low-Nitrogen Threshold:
  A parameter that monitors the remaining amount of liquid nitrogen.
  If the value is less than the entered percentage, a warning message and alarm sound is generated.

■ How to display warning messages

To display warning messages and activate alarms, turn ON the “Alert When Helium Low” parameter and the “Alert When Nitrogen Low” parameter.

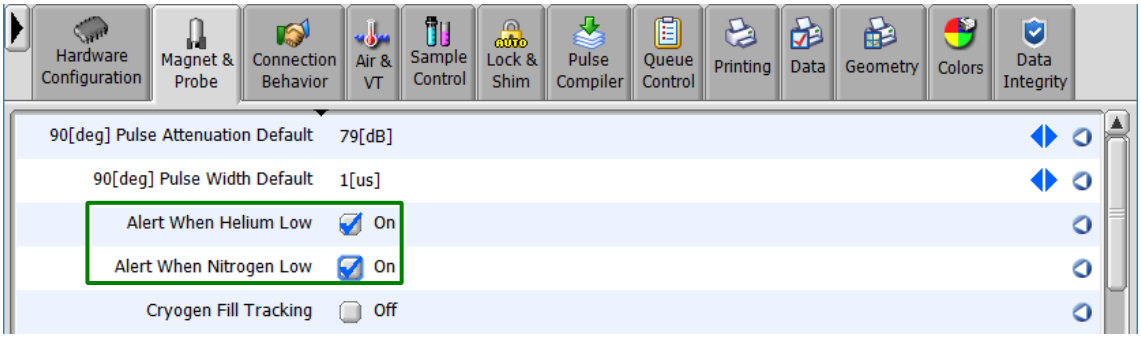


Figure 5.15 Activating the alarm function

When the remaining amount of refrigerant becomes less than the percentage set in the “Low-Helium Threshold” or “Low-Nitrogen Threshold” parameter, a warning message for the remaining amount of refrigerant appears and an alarm sounds at the same time.

Figure 5.16 Warning message

The control PC and the spectrometer must be connected via a network to display warning messages for the alarm to sound.

The warning message and alarm sound will continue until you click the **Acknowledge** button. Warning messages and alarm sounds are output after the spectrometer is selected and connected.

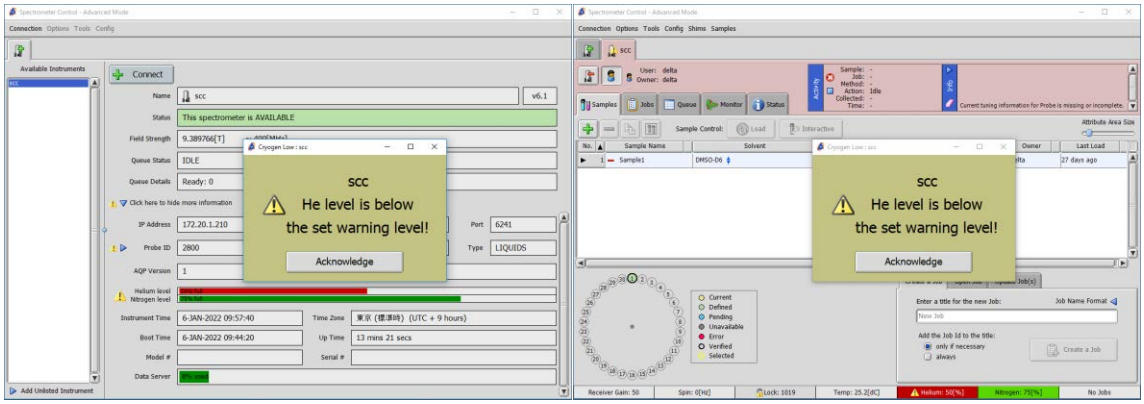


Figure 5.17 Warning message display and alarm sound

To prevent the warning message and alarm sound from being output, it is necessary to fill the refrigerant or turn off the “Alert When Helium Low” parameter.

■ How to output the alarm sound

Separate settings are required to sound the alarm.
In the Delta console, select the **Preferences** - **Sounds** tab and turn on the “Enable Sounds” parameter.

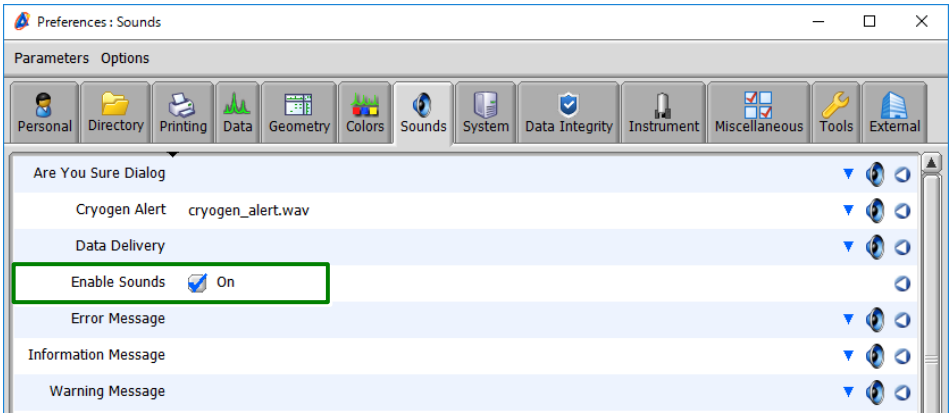


Figure 5.18 Delta console preferences

The speaker of the control PC is muted at the time of shipment.
Click the **Windows speaker** icon to cancel the mute setting.

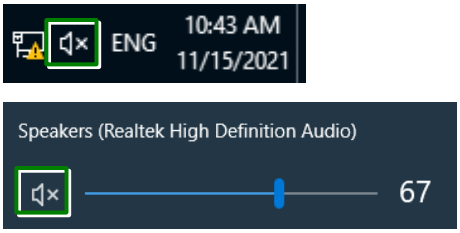


Figure 5.19 Unmute on Windows

5.5 Added a Sort Function to Sample Define

A function has been added so that you can sort the samples registered in the sample definition.
Sorting is performed in ascending or descending order based on the slot number.

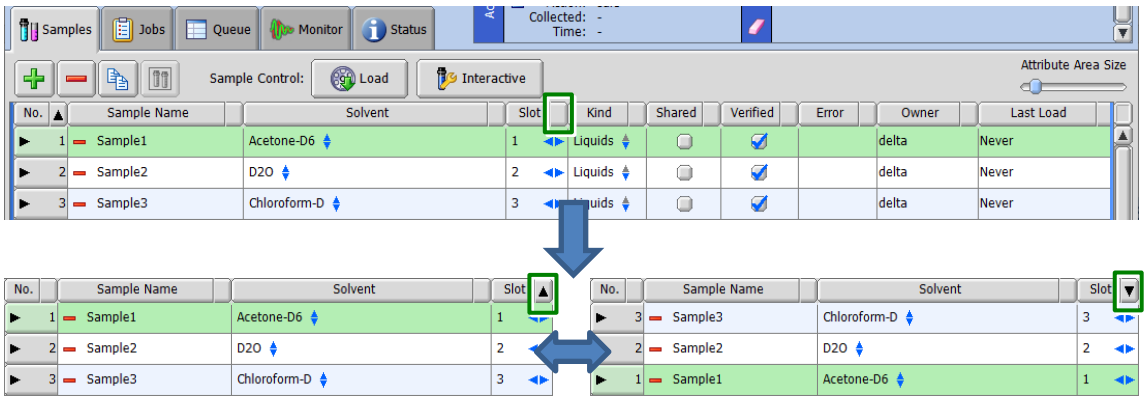


Figure 5.20 Sorting of sample definitions

5.6 Improved the Refrigerant Filling Screen

The elapsed time since the refrigerant filling screen appeared is now displayed.

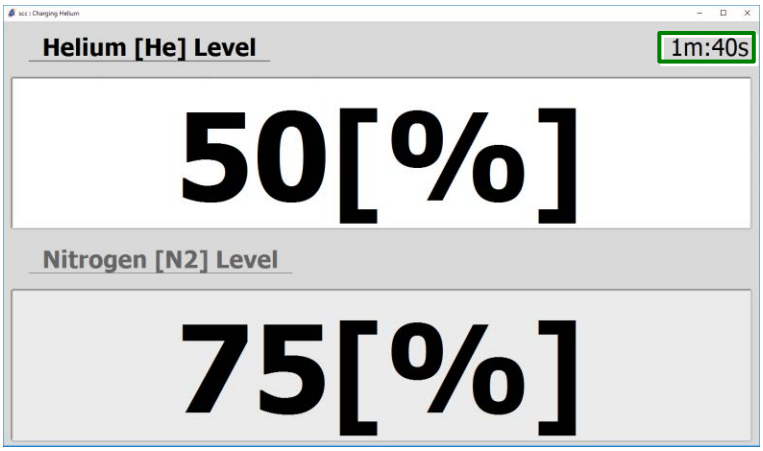


Figure 5.21 Timer of refrigerant filling screen

In addition, a warning button automatically appears to inform you that the filling window will close in less than two minutes.
If you click the warning button, the filling screen will not close automatically.

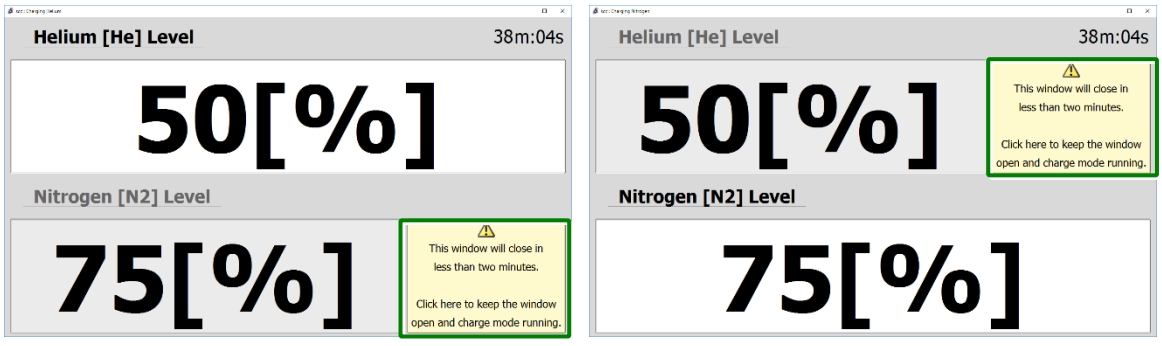


Figure 5.22 Warning button on the refrigerant filling screen

Click the warning button to hide the button.
When the time has elapsed up to two minutes before the time set in the “Helium Charge Timeout” parameter, the warning button is appeared again.

About the time to automatically close the refrigerant filling screen

The time that the refrigerant filling screen closes automatically can be set in the environment setting parameters of the spectrometer.
Set the time to close the refrigerant filling screen for “Helium Charge Timeout” on the **Settings** menu- **Preferences** - **Magnet & Probe** tab of the spectrometer control window.

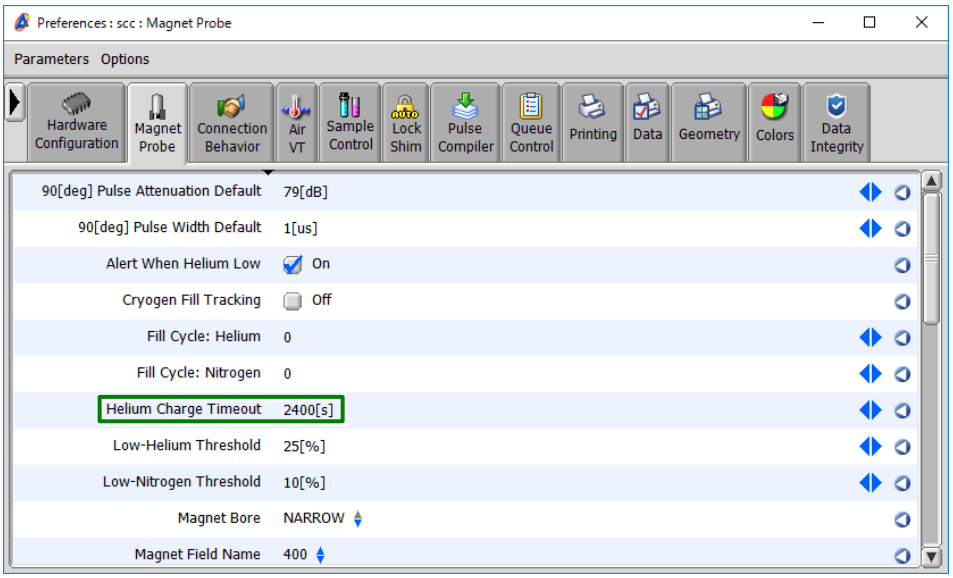


Figure 5.23 Automatic closing time parameter

Set a maximum of 3,600 seconds (1 hour) in seconds.

5.7 Added a Quantitative NMR Measurement Function for JASON

A function has been added to link with the quantitative analysis plug-in (SmileQ) of the NMR data analysis software “JASON”. This function requires JASON and SmileQ.

SmileQ will be released in February 2022.

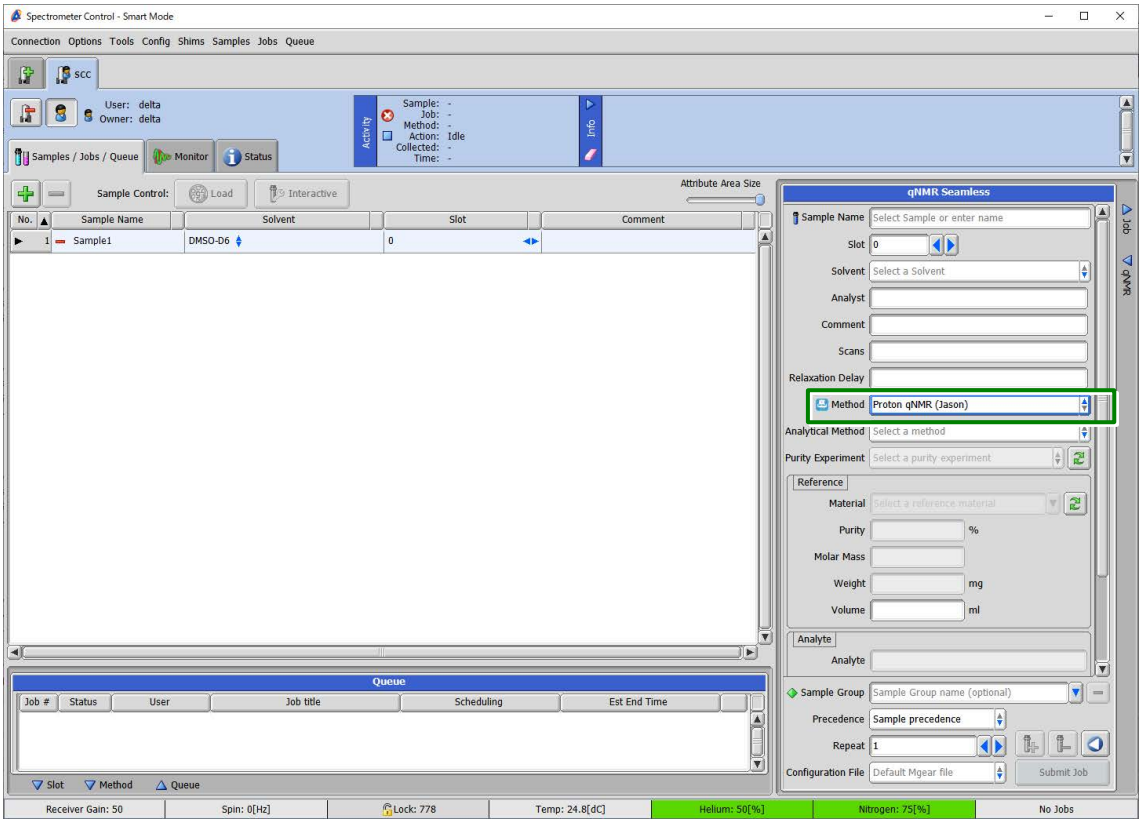


Figure 5.24 Functions that link with the quantitative analysis plugin (SmileQ)

5.8 Changed the Multinuclear Nuclide from Selective to Individual Placement

The nuclide of the multinuclear was selected from the list box, but it has been changed to be placed individually in the list of available methods.

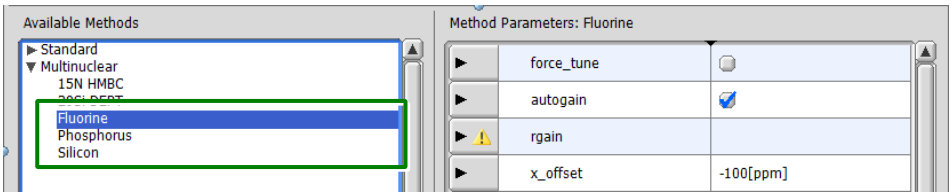
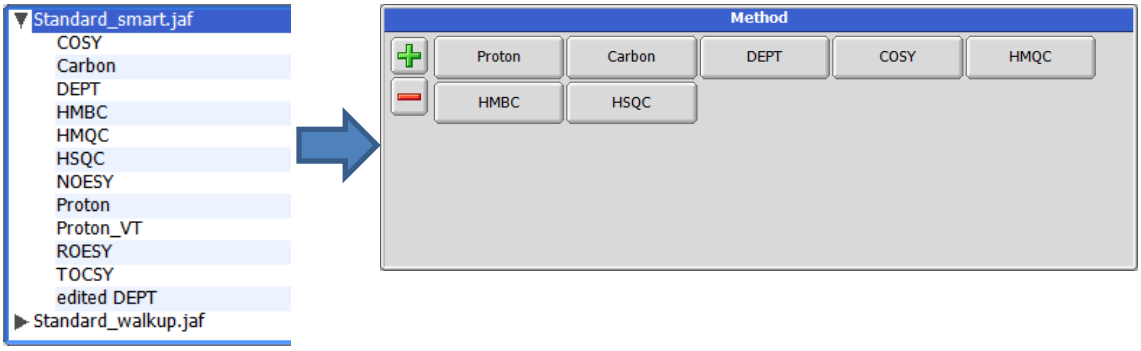


Figure 5.25 Multinuclear nuclide placement change

5.9 Changed the Display Contents of the Method Panel in Smart Mode

Smart mode has the following standard sequences, but in the default state, all the sequences were not displayed in the Method panel.



The display contents of the Method panel have been updated to display all the sequences.

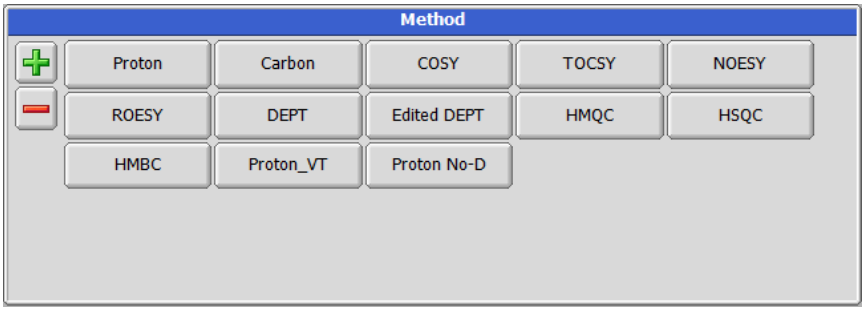


Figure 5.26 Smart mode Method panel

5.10 Added and Corrected Items such as Pulse Sequences

■ Added files

● Pulse sequences

solids - cpmas
- cpmas_pass.jxp
- matpass.jxp
- matpass_dec.jxp
- single_pulse_dec_pass.jxp
- single_pulse_pass.jxp

liquid_advanced - 2d

j resolved
- clean_gserf.jxp
- gserf.jxp

hsqc
- hsqcad.jxp

hsqc - water_suppression
- hsqcad_wgh.jxp

tocsy
- 19f_tocsy_burbop.jxp

Process lists

solids

- pass.list

Automatic measurement scripts

- pip_experiment.jaf
  PIP_HSQMBC

Corrected files

Pulse sequences

liquid_standard
1d
- carbon.jxp

2d
- tocsy.jxp

liquid_advanced
1d - single_pulse
- single_pulse_dec_wet.jxp

2d - hsqc
- ghsqcad.jxp

2d - hector
- hetcor_tocsy_phase.jxp

Automatic measurement scripts

- Noah.jaf
  NOAH hsqc cosy
  NOAH hsqc hmbc cosy

Noise files (decoupling files)

- cm.noise
- spinal64_vp.noise
- swftppm.noise
- tppm.noise

5.11 Added a Normalize Region

A “Normalize Region” option has been added to the processing commands displayed for the 1D processor and nD processor. “Normalize Region” can normalize a specific integral or integral range.

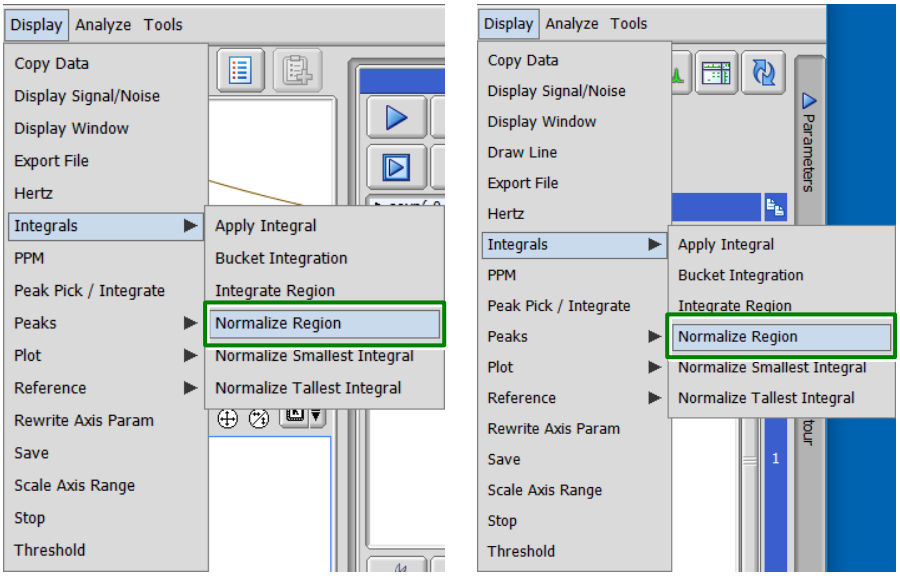


Figure 5.27 Normalize Region

The parameters that can be entered are as follows.

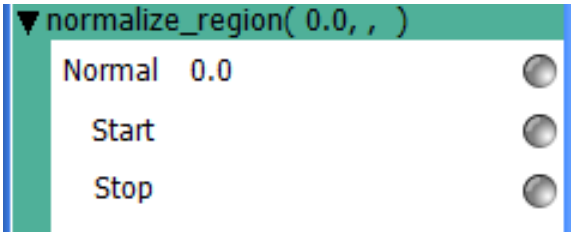


Figure 5.28 Normalize Region parameters

- Standard: Enter the value to be standardized for the sum of the integrals in the region.
- Start: Enter the start position of the region to be standardized.
- End: Enter the end position of the region to be standardized.

How to use the command

To execute the Normalize Region, first add some **Integrate - Integrate Region** items from the **Display** menu and enter the parameters.

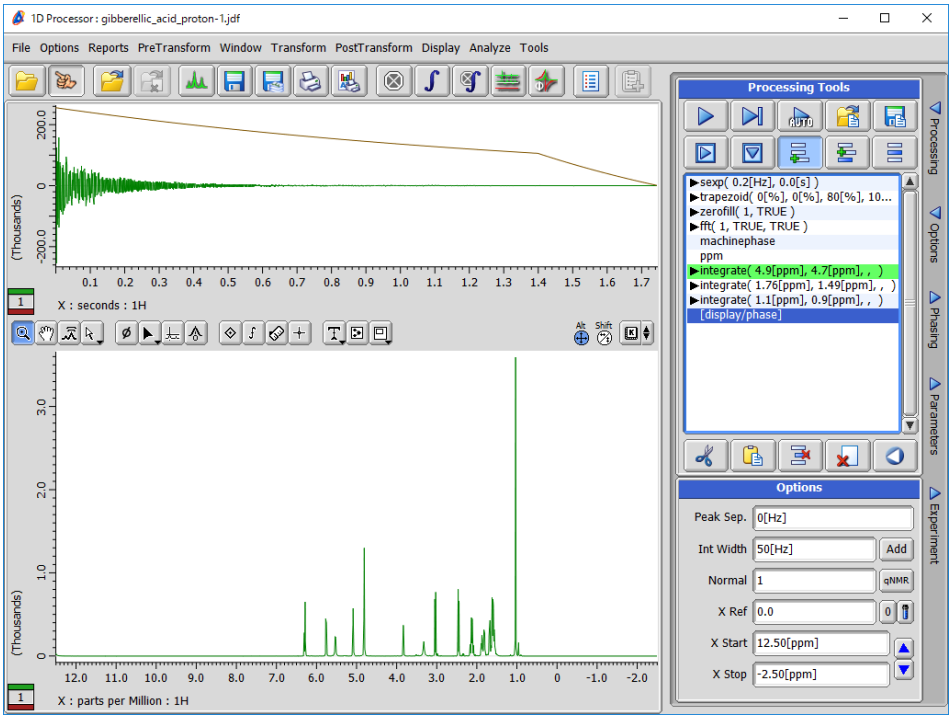


Figure 5.29 Addition of Integrate Region

Next, add **Integrate - Normalize Region** from the **Display** menu and enter the parameters.

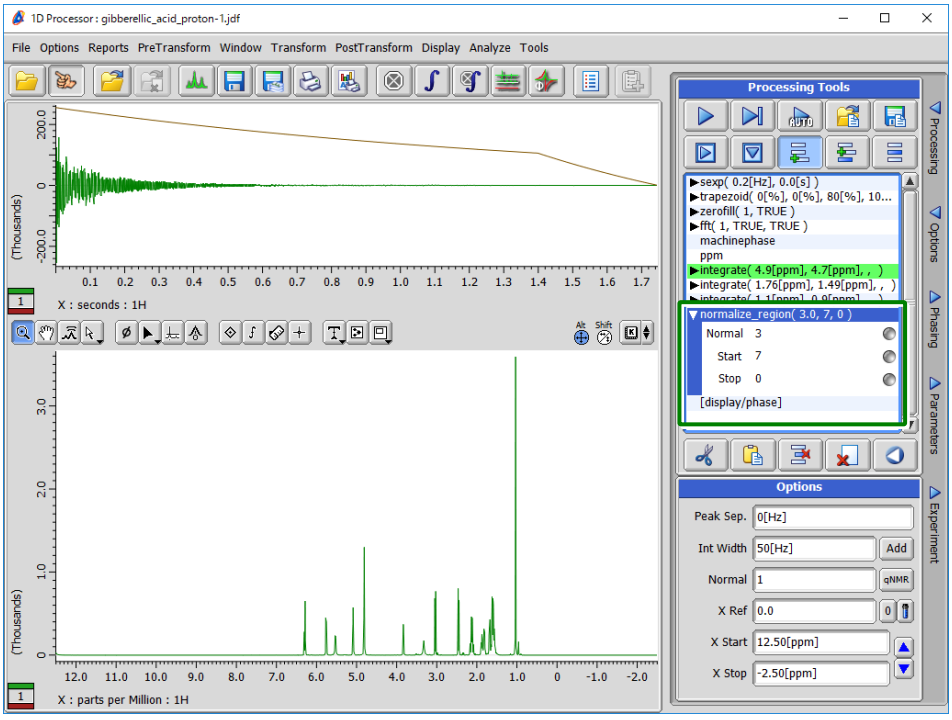


Figure 5.30 Addition of Normalize Region

When you click the  button to execute the process, normalization is performed on the sum of the integrals in the input region.

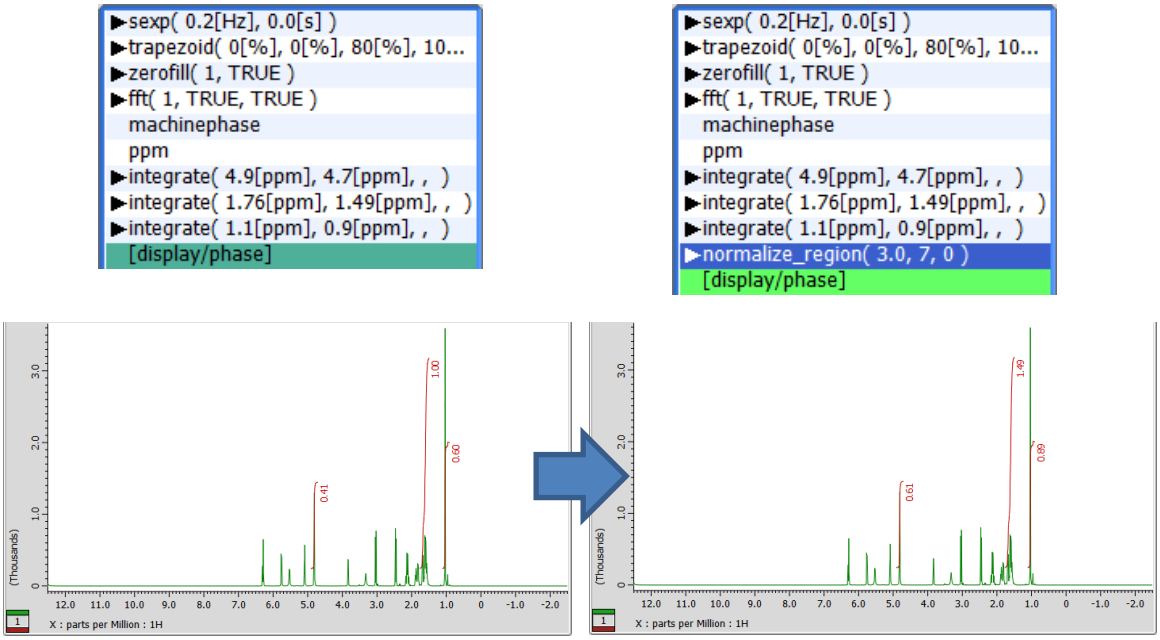


Figure 5.31 Comparison before and after execution of Normalize Region

6 BUG FIXES

The bug fixes supported by Delta V6.1.0 are as follows.

Item
Fixed an issue where the Delta console menu would disappear
Fixed an issue where files in subdirectories could not be displayed
Fixed an issue where Machine Log rollover might not occur
Fixed an issue where files remained in the data folder
Modified the data conversion process to JCAMP-DX format
Modified the data conversion process to Galactic format
Improved memory leak
Fixed an issue where the Customize Sample Parameters function caused an error
Fixed an issue where a warning message appeared even though the solvent temperature parameter was not exceeded
Fixed an issue where custom sample parameters were not reflected
Fixed an issue where copying job parameters failed when copying the job
Fixed an issue where the expected end time was not displayed correctly
Fixed the HMBC method in Walkup mode
Fixed an issue where Storage_filename was not working in Smart mode
Fixed an issue where added parameters are not reflected during measurement
Fixed an issue where the font size was smaller when changing parameters
Fixed an issue where the paste function was not working properly
Fixed an issue where the measurement time was not displayed correctly when updating multiple jobs
Fixed an issue where PIP windows might not be deleted
Fixed an issue where axis information was not displayed correctly
Fixed an issue where panel information could not be displayed in a separate window