

Delta V6



Measure Updated functions

Operating System

64 bits OS native

Measurement

New	Smart mode for solid state
	Spin and temperature monitoring
	Japanese Walkup mode
Improve	GLP Tool
	Shape Viewer
	Data Integrity compliance
	NUS scheduling

Data processing / analysis

New	Chemometrics analysis
	Bundle store of multiple spectra
Improve	Level tool
	DOSY analysis
	Diffusion coefficient analysis
	Copy integral tool
	NUS processing

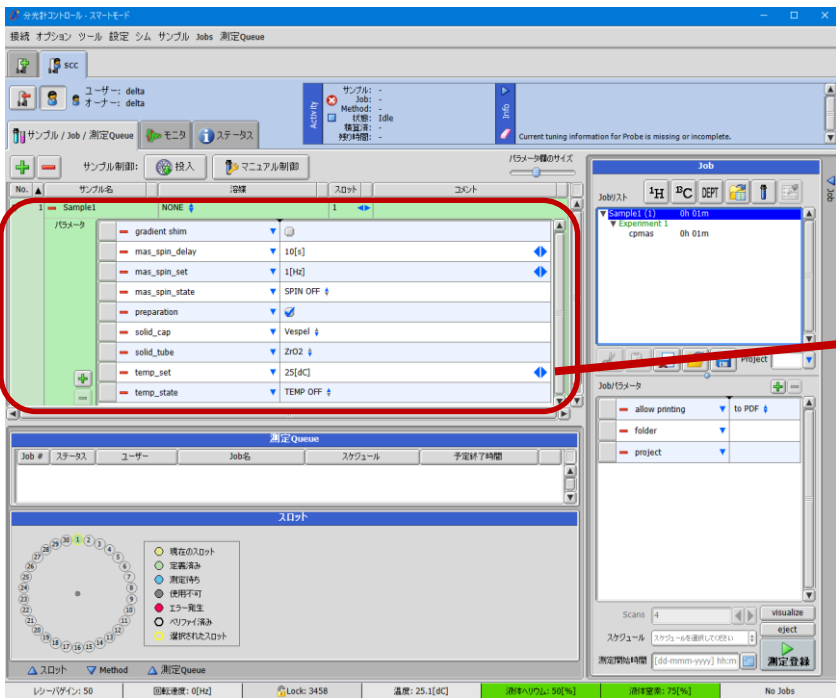
Delta V6.0.0

Measurements

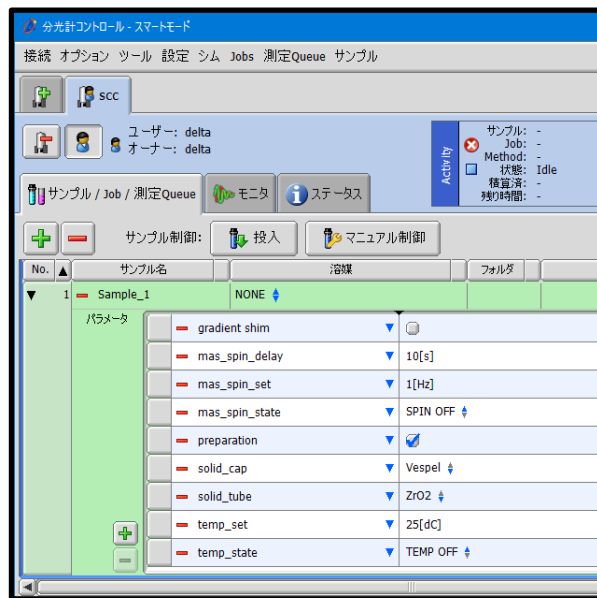


Smart mode for Solid State NMR

Smart mode allows you to set and check sample and measurement conditions on a single screen. This mode is convenient for routine measurement when conditions are fixed.



Smart mode interface

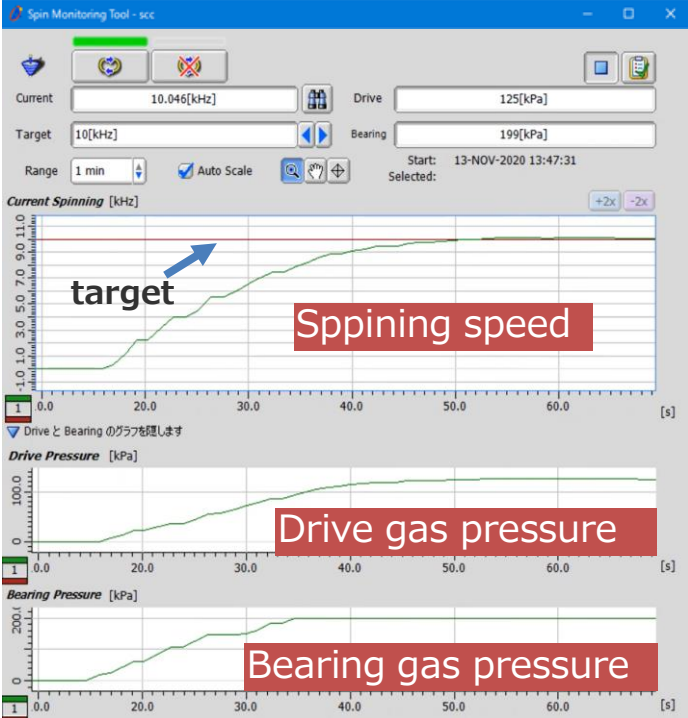


Sample parameter setting

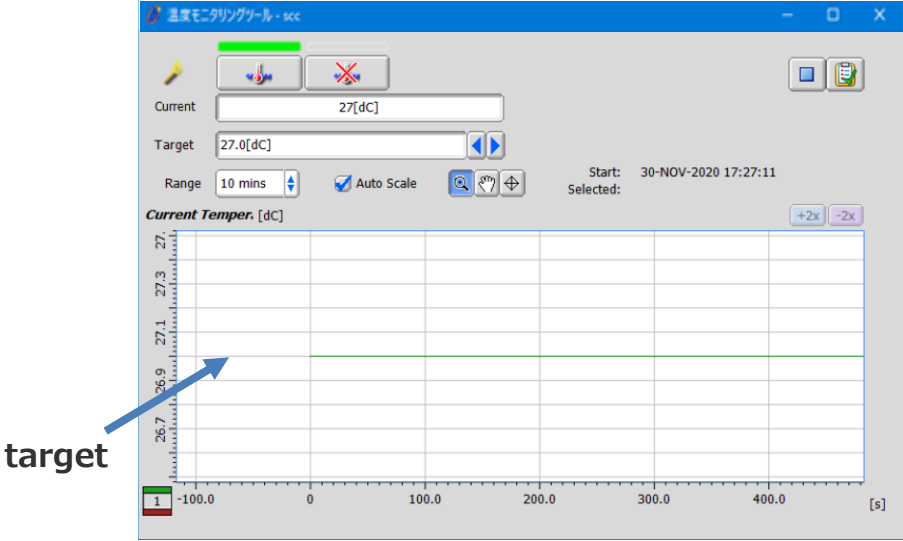
When combined with the Auto MAS probe, automatic solid measurement is also possible with the same ease of operation as solution measurement.

Spin / Temperature monitoring tool

In the case of solids measurement or variable temperature measurement, this tool allows you to check the status of equipment settings in real time.



Spin monitoring tool



Temperature monitoring tool
For confirming stable operation
and for use in remote work

GLP tool

An evaluation tool to verify that the equipment is maintaining proper performance.

	標準テスト		オプション
1	1H Signal to Noise	1	19F Signal to Noise
2	13C Signal to Noise	2	13C Signal to Noise
3	1H 90 degree Pulse Width Calibration	3	31P Signal to Noise
4	13C 90 degree Pulse Width Calibration	4	15N Signal to Noise
5	1H Lineshape	5	1H 90 degree Spin Lock Calibration
6	1H Stability	6	1H 90 degree Gauss Calibration
7	Gradient Power Test	7	19F 90 degree Pulse Width Calibration
		8	31P 90 degree Pulse Width Calibration
		9	15N 90 degree Pulse Width Calibration
		10	1H Decoupler Pulse Width Calibration
		11	13C Decoupler Pulse Width Calibration
		12	1H RF Homogeneity
		13	13 Degree Phase Stability Test
		14	Center band Suppression
		15	1H Beat Test
		16	13C Beat Test
		17	Gradient Linearity Test
		18	Gradient Recovery Test



Status:

PASSED

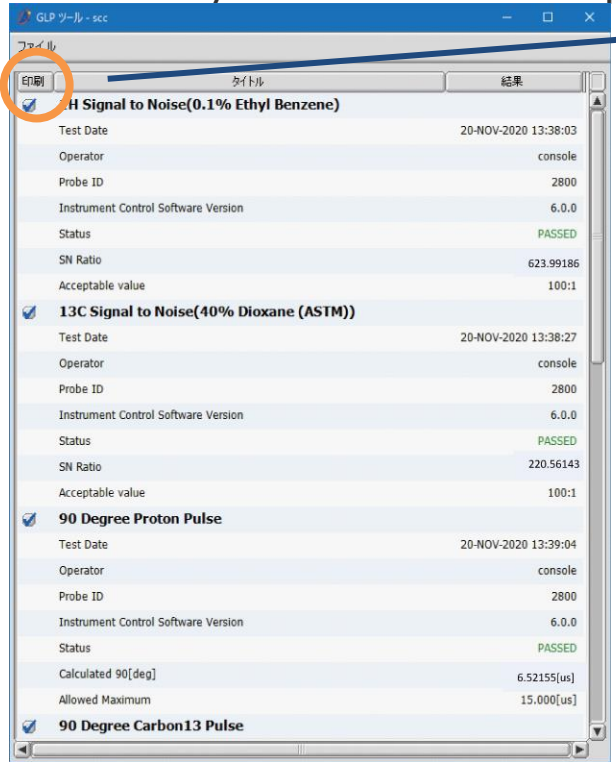
A GLP reports example. ¹H sensitivity

GLP Total 25 items (Standard tests:7 items, Optional tests:18 items)

GLP Tool

GLP report tool

: Results are easy to check and output.



```

GLP Test Report
Created Date       : 10-DEC-2020 18:54:10
Created by        : Administrator
Instrument         : scc

-----
1H Signal to Noise(0.1% Ethyl Benzene)
-----
Test Date                20-NOV-2020 13:38:03
Operator                 console
Probe ID                 2800
Instrument Control Software Version 6.0.0
Status                   PASSED
SN Ratio                 623.99186
Acceptable value        100:1

-----
13C Signal to Noise(40% Dioxane (ASTM))
-----
Test Date                20-NOV-2020 13:38:27
Operator                 console
Probe ID                 2800
Instrument Control Software Version 6.0.0
Status                   PASSED
SN Ratio                 220.56143
Acceptable value        100:1

-----
90 Degree Proton Pulse
-----
Test Date                20-NOV-2020 13:39:04
Operator                 console
Probe ID                 2800
Instrument Control Software Version 6.0.0
Status                   PASSED
Calculated 90[deg]      6.52155[us]
Allowed Maximum         15[us]

-----
90 Degree Carbon13 Pulse
-----
Test Date                20-NOV-2020 13:39:39
Operator                 console
Probe ID                 2800
Instrument Control Software Version 6.0.0
Status                   PASSED
Calculated 90[deg]     10.10618[us]
Allowed Maximum         15[us]

```

Report output example

For use in equipment condition management and failure reporting

GLP tool result confirmation view

Delta V6.0.0

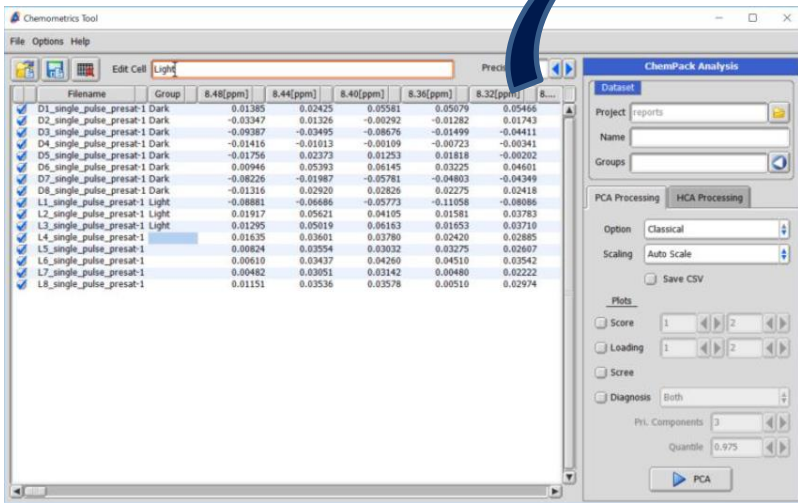
Data processing and analysis



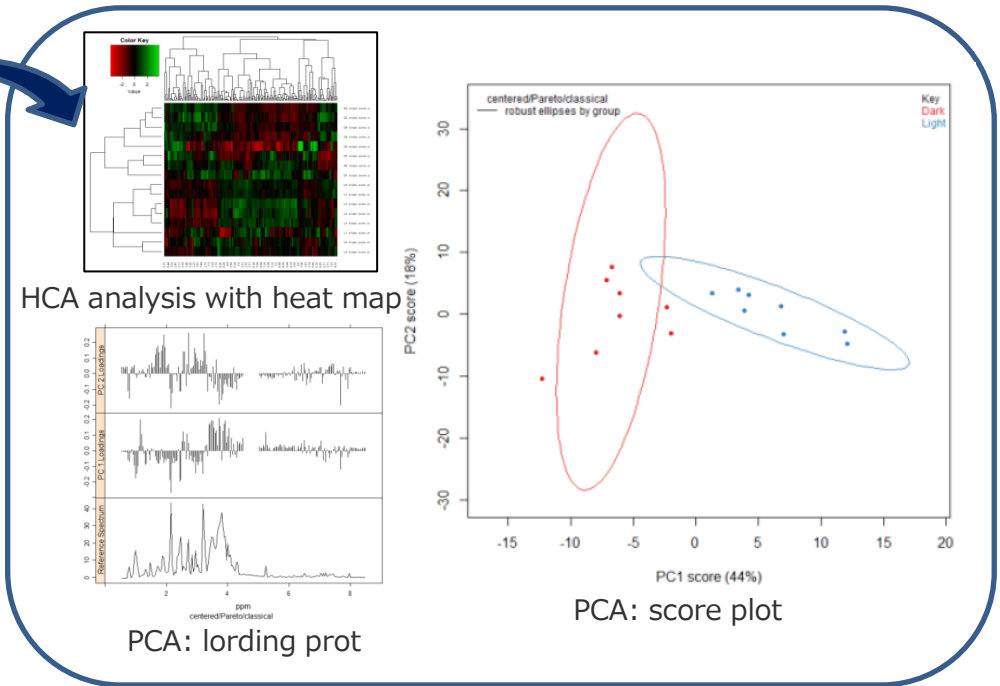
Chemometrics analysis tool

Delta and the statistical analysis language "R" work together.

* "R" is a free software and available from the Comprehensive R Archive Network (CRAN) website.



Chemometrics analysis tool (Delta)

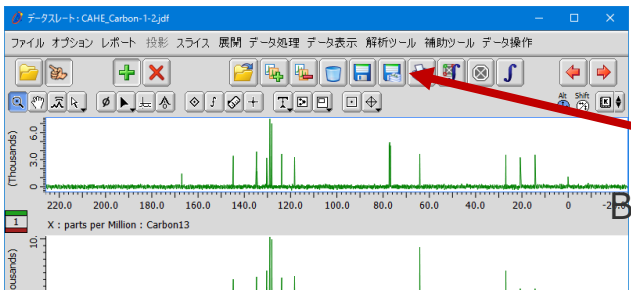


Analyses results (R)

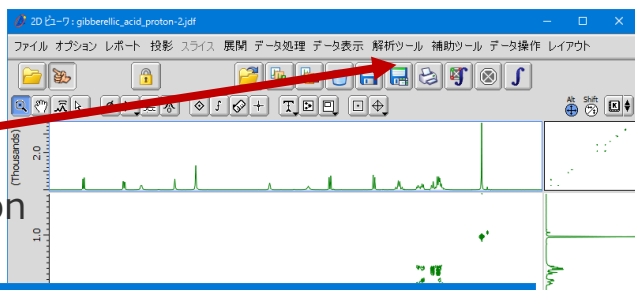
Exploratory multivariate analysis using multiple NMR spectra seamlessly

Bundle store function of multiple spectra

New function to store multiple one-dimensional data, data slates containing PIP, and two-dimensional data pasted with high-resolution data.



Bundle store button



Filename extension (.jda)

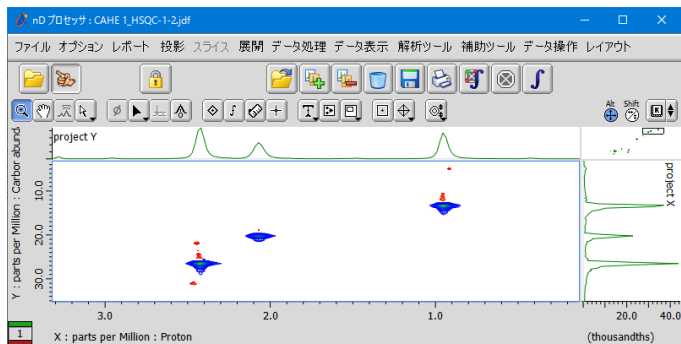
Data slate

Filename extension (.jda)

2D viewer

Processing and analysis results can be saved and read directly

Level tool



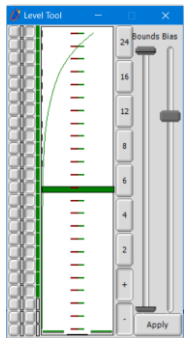
下限 1.935E-03 上限 3.967E-02 係数 1.115 レベル 21 色 Blue-Green

ポジティブ

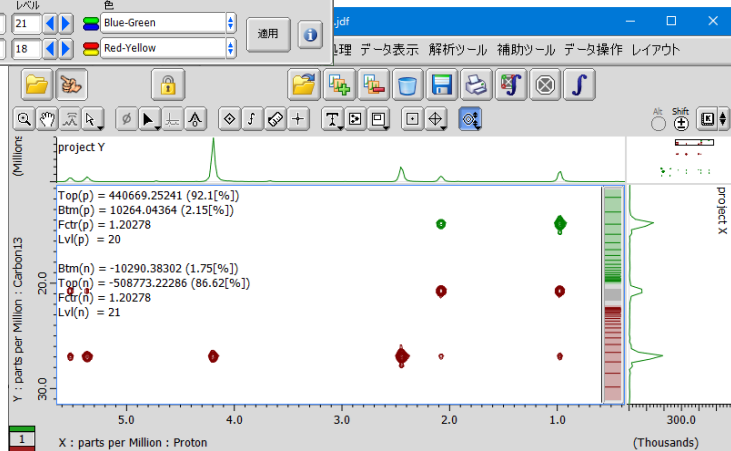
ネガティブ -9.35E-04 -2.035E-03 2.0 18 色 Red-Yellow

適用

- numerical setting of upper/lower bounds and bias of contour
- contour level list is implemented
- read/write contour level information -> applicable to other data
- embedded in a data -> save/load directly



Conventional Level Tool



Level tool interface on 2D viewer

Info: CAHE_1_HSQC-1-2.jdf

ジオメトリ情報

Minimum: -0.00197452
 Maximum: 0.04394065
 Magnitude: 0.04394065
 Baseplane: 0.00000235
 Positive thresh: 0.00276472
 Negative thresh: -0.00276002
 Noise level: 0.0022099

等高線レベルリスト

ポジティブレベル:		ネガティブレベル:	
No.	レベル	No.	レベル
1	3.967E-02	1	-9.35E-04
2	3.529E-02	2	-9.35E-04
3	3.136E-02	3	-9.35E-04
4	2.784E-02	4	-9.351E-04
5	2.468E-02	5	-9.351E-04
6	2.184E-02	6	-9.353E-04
7	1.929E-02	7	-9.355E-04
8	1.701E-02	8	-9.361E-04
9	1.496E-02	9	-9.371E-04
10	1.312E-02	10	-9.393E-04
11	1.147E-02	11	-9.436E-04
12	9.989E-03	12	-9.522E-04
13	8.661E-03	13	-9.694E-04
14	7.469E-03	14	-1.004E-03
15	6.4E-03	15	-1.072E-03
16	5.441E-03	16	-1.21E-03
17	4.58E-03	17	-1.485E-03
18	3.807E-03	18	-2.035E-03
19	3.115E-03		
20	2.493E-03		
21	1.935E-03		

Detailed level tool

Contour levels can be easily reproduced

Others -1

1. Japanese Walkup mode
Japanese localization of the spreadsheet-type interface for setting up and running measurements.
2. Shape Viewer Tool
A tool to identify excitation profile, creation, and implementation of arbitrary shape pulse. Adiabatic, BOP, Decoupling pulse, constant adiabatic pulse, time reverse, frequency reverse, save function, etc. are improved.
3. Data Integrity compliance
A system has been introduced whereby data files cannot be saved or printed without stating the reason for the change, all operations on the spectrometer are logged, and old log files can be deleted from Delta. All operations on the spectrometer are logged, and old log files can be deleted from Delta.
4. NUS scheduling function
In addition to Linear sampling and manual sampling (generated by the user using the sampling scheduler), automatic scheduling is now available. Simply specify the compression ratio and the measurement will be automatically generated and executed at the start of the measurement.

Others -2

5. DOSY analysis
Implemented ILT based on maximum entropy regularization (MAXENT) and Lp-norm regularization (LPNORM).
6. Diffusion coefficient analysis
The calculation method now includes multi-component support and NUG (Non-Uniform Gradient), which can compensate for the effect of non-uniform FG intensities depending on the sample position.
7. Transfer Integral function
In addition to the conventional method, we have added two new methods: 1) setting the center position and specifying the width of the integral range, and 2) specifying the width of each side (low field side and high field side) from the specified position.
8. NUS processing
Reconstruction of 5D NUS data (NUS dimensions is 4) is implemented.

Delta Ver 6.1.0 introduction



Delta Ver6.1.0

■ Support both ECZL series and ECZ series

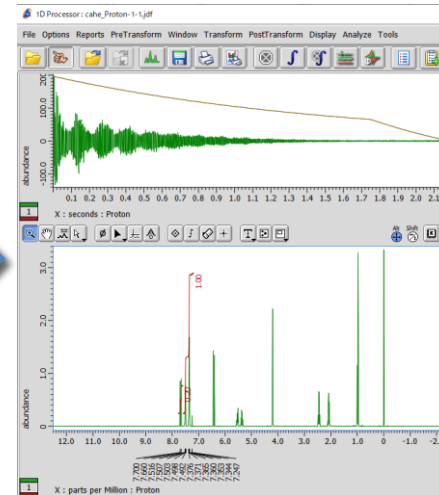
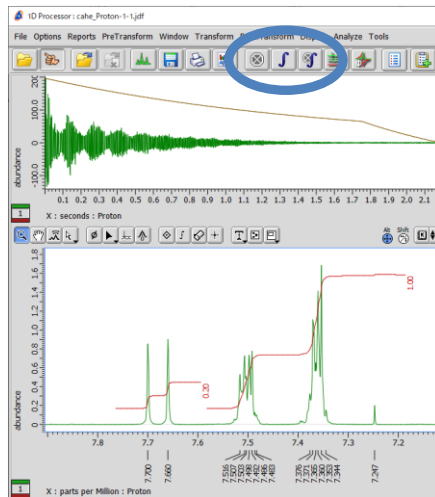
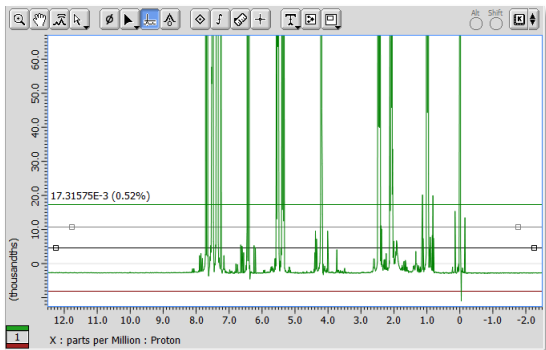
- 3D Shimming speed enhanced for ECZL series
- MFDS (**M**ulti **F**requency **D**rive **S**ystem): Standard 2 CH configuration ECZL spectrometer can run triple or more resonances experiments e.g. $\{^1\text{H}, ^{13}\text{C}, ^{15}\text{N}\}$

■ Additional Experiments

- Automation of Sapphire Pureshift (including method, pulse program, processing command, process list)
 - Suppressing decoupling side band
- Automation of PIP HSQMBC (pip_experiment.jaf)
 - parameter setting, automatic file math process
- Pulse program and process list of PASS (Phase Adjusted Spinning Sideband)
- Automation of solid state CPMAS (solids_cpmas.jaf)
 - automatic relaxation delay calibration depends on duty cycle for CPMAS

■ Usability enhancement

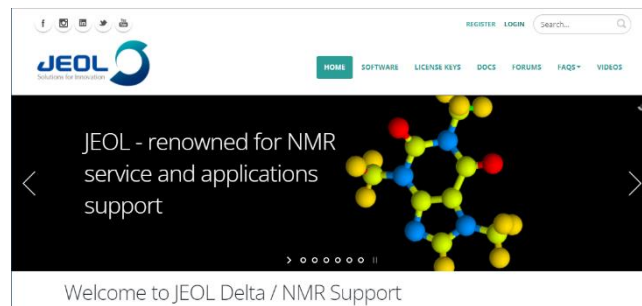
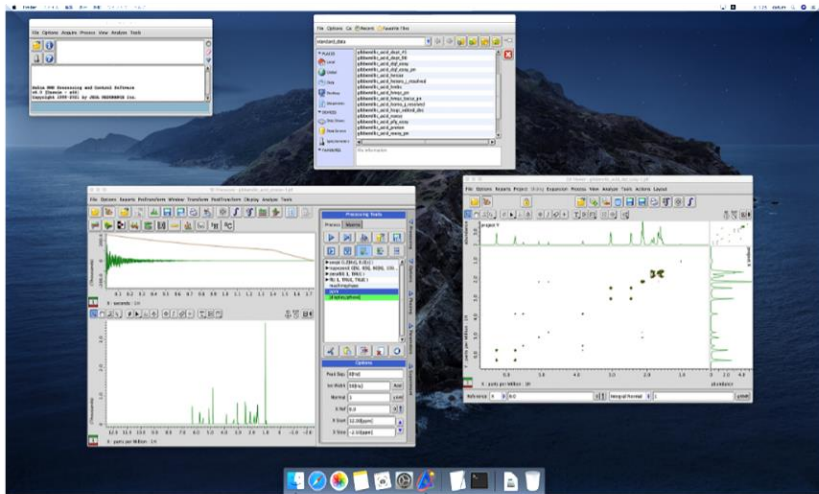
- Cryogen alert improvement
 - Sound, alert level setting, elapsed-time
 - Threshold/noise/baseline display improvement
 - Numerical indication of Threshold / noise / baseline level
 - Easy to apply to the other data
 - Automatic peak picking/integration at specific region
 - Experiment parameters can be display on Queue tab
- Etc.



Delta Ver 6.0.0 for Mac



Delta V6.0.0 for Mac



- ✓ Recent macOS support
macOS 10.14(Mojave) ~ 12(Monterey)
- ✓ Intel, Apple Silicon support
Apple Silicon require Rosetta2
- ✓ Same function with Windows version

Downloadable from NMR support site
<https://nmrsupport.jeol.com/>

Delta NMR software Ver 6.2.0



■ Implementation of Phase Covariance

- Processing function of PCW (Phase Covariance Weighted) method is implemented.

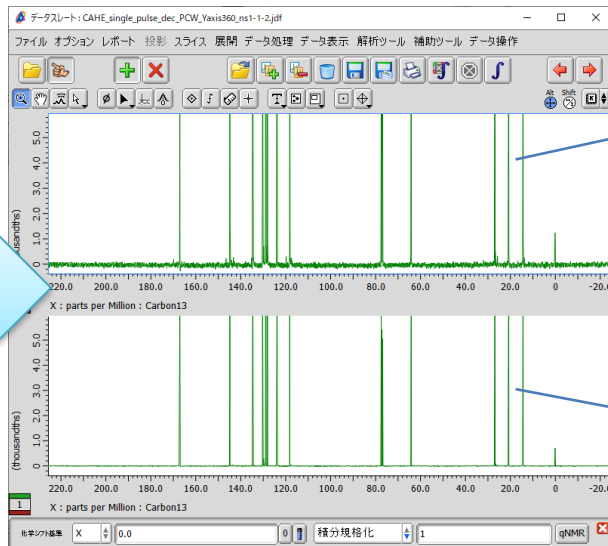
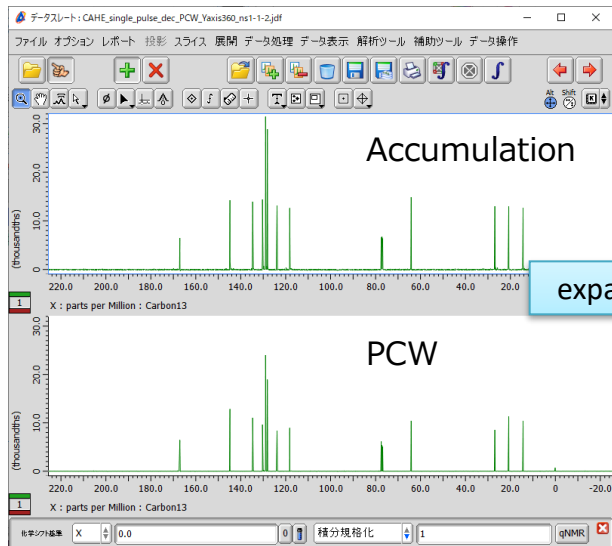
■ Usability improvement

- Automatic Cooling/VT port control function of MASCONT
- Improved spectrometer account setting
- Spectrometer announcement function etc.

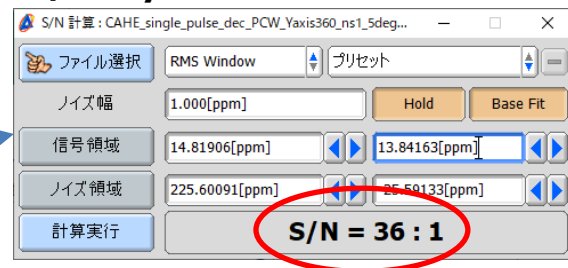
■ New function “Phase Covariance” is implemented.

- Additional PCW(Phase Covariance Weighted) processing function
S/N improvement with covariance calculation

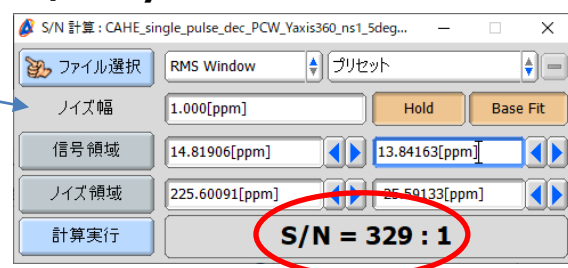
Only works on ECZL series spectrometer



S/N by accumulation



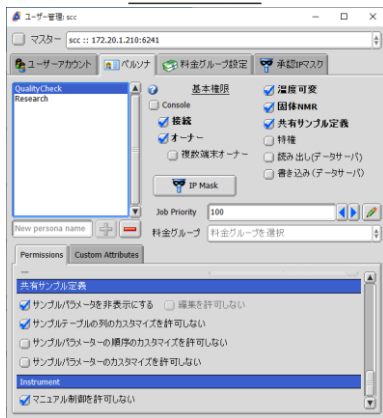
S/N by PCW



■ Usability improvement

- Automatic Cooling/VT port control function of MASCONT
Automatic open/close 'Cooling port' when attaching/detaching Solid probe
Automatic open/close 'VT port' when start/stop VT control
(when the VT gas is supplied by MASCONT)
Spin/VT control available by Set_State_MAS method in Utilities.jaf
- Improved spectrometer account setting
Detailed setting for each account is available by using new Persona function.
- Spectrometer announcement function etc.

Persona



Spectrometer Announcement function

