



Scientific / Metrology Instruments  
Nuclear Magnetic Resonance System

Solutions for Innovation

**JNM-ECZL series**

**NMR spectrometer ECZ Luminous**



JEOL Ltd.

Brand new ECZ, beyond ECZ  
Higher performance, smaller, easier!

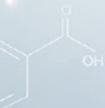
## NMR spectrometer “ECZ Luminous” JNM-ECZL series

The JNM-ECZL series is an FT NMR system equipped with state-of-the-art digital and high-frequency technologies.

The highly integrated Smart Transceiver System, a high-speed, high-precision digital high-frequency control circuit, enables further miniaturization and ensures the stability of spectrometer. It is capable of performing state-of-the-art high-field and solid-state NMR measurements while maintaining the size of a routine solution-state NMR system.

The new Multi Frequency Drive System enables multi-resonance measurements in a standard configuration, providing a wider range of solutions. Welcome to the world of ECZ Luminous.





## Major Features

### Three ECZL models

There are three series in the lineup. The G Series combines a compact footprint with full expandability to support the widest range of cutting-edge applications, including advanced solid-state and biomolecular experiments. In addition, the G series can support functional expansion after installation, which has been difficult in the past. The S series is an entry-level 400 MHz system for solution-state measurements that shares the advanced architecture of the other ECZL models. Sitting between the G and S Series is the R Series, which provides compatibility with 400-600 MHz magnets and can be expanded to support solid-state NMR measurements.

### High-stability, high-speed and high-sensitivity

In order to maintain the high stability required to acquire high-quality spectra, all circuits that can be effectively digitized, such as the high-frequency transceiver circuit and lock circuits, are digitized. The STS (Smart Transceiver System), which is the culmination of our technological expertise, enables ultra-fast control of frequency, phase, and amplitude modulation with a time resolution of 5 ns. The excellent stability of the STS ensures outstanding performance in critical applications such as solvent suppression and difference spectroscopy. The newly designed SiGe preamplifier enhances the sensitivity and makes it possible to obtain a wide variety of high-quality spectra more quickly and easily.

### Multi-resonance experiments in standard configuration

Even with the standard 2-channel configuration, the system can support multi-resonance measurements involving multiple nuclides such as HFX and HCN. However, the newly developed MFDS (Multi Frequency Drive System), the excellent probe technology and unique multi-sequencer architecture, enables multi-resonance measurements without the need for additional oscillators and power amplifiers. (Patent 2021-176250)

### Remote access and automation

The ECZL system that flexibly supports the networking realizes various user environments. The spectrometer, which operates independently of the operating terminal, can be accessed from any computer on the network, enabling NMR data collection, processing and analysis to be performed remotely. When combined with an auto sample changer, compatible for both of solution and solid-state NMR, fully automated remote operation is possible. In addition, the new auto-tuning unit improves the measurement throughput.



# World Best FT NMR system

## Lineup of ECZ Luminous

**ECZ Luminous is available in three different models to meet a wide variety of user needs. All models feature high performance digital high frequency technology and user-friendly Delta software.**

### ECZL G series

This is a flagship model that supports diversified, cutting-edge applications. The footprint of the spectrometer has been reduced to less than 60% of that of ECZR, while maintaining the expandability needed to support a wide range of applications. It is flexible in terms of expansion, with support for three or more channels, high power amplifiers, and high power magnetic field gradients, allowing for future functional expansion even when installed in the minimum configuration. It is an adaptable FT-NMR system that can respond to changes in user applications and the introduction of the latest applications.



Dual rack configuration



### ECZL R series

This model is a compact spectrometer that is compatible with magnetic fields of up to 600 MHz. The footprint is less than 50% of that of ECZR, and it can also be used for solid-state measurements.



### ECZL S series

This is an entry-level model dedicated to 400 MHz solution NMR while incorporating the high performance digital high frequency technology of the ECZL series.





## More compact spectrometer

ECZ Luminous has achieved a significant reduction in size while enhancing the performance of the spectrometer. The volume of the R series has been reduced to about 1/3 of that of the previous equivalent.



ECZ R series



ECZ Luminous R series

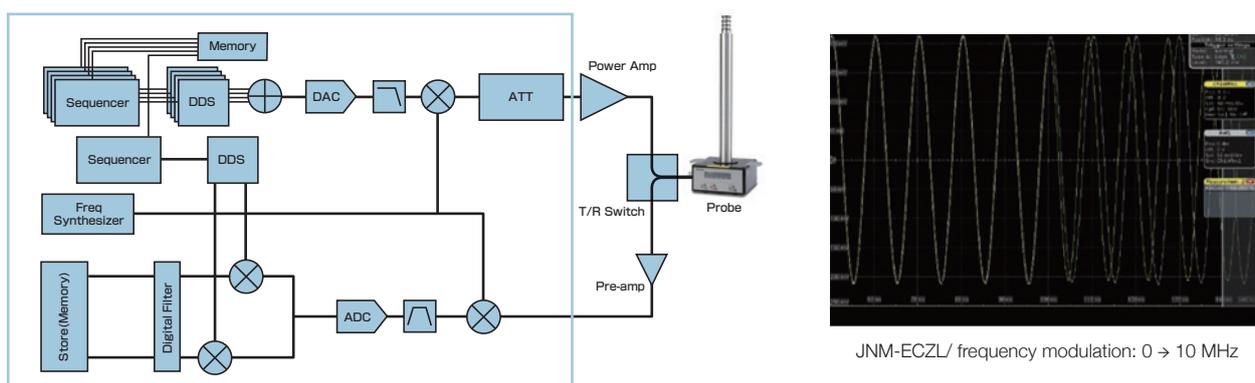
Size comparison with previous models with equivalent performance

	ECZL G series	ECZL R series	ECZL S series
Frequency	400 MHz to 1.3 GHz	400 MHz to 600 MHz	400 MHz
Sample type	solution/solid	solution/solid	solution
Number of channels	2 (standard)	2	2
	Expandable up to 8 channels		
High frequency power amplifier	100 W (standard) 200/500/1000 W (as option)	100 W	50 W
Low frequency power amplifier	300 W (standard) 500/1000/2000 W (as option)	300 W	150 W
Magnetic field gradient amplifier	10 A (standard)	10 A	10 A
	30/50 A (as option)		
Console size (W*D*H)	600*855*1,279 mm	536*730*855 mm	536*730*855 mm

## STS (Smart Transceiver System)

ECZ Luminous inherits the STS (Smart Transceiver System) digital high integration and high frequency technology used in the previous ECZ series. The sequencer, DDS (Direct Digital Synthesizer), FSU (Frequency Synthesizer Unit), transmitter, receiver, acquisition unit, and gate control unit are all integrated on a single RF (Radio Frequency) transmitter/receiver board. Two 4-frequency source units (one each for HF and LF) and one receiver are configured on a single RF transmitter/receiver board. The standard configuration has a total of eight frequency sources and one receiver. The ECZ Luminous can be expanded to four RF transmitter/receiver boards to support up to 32-frequency sources and four receivers\*. In addition, the transmitter/receiver system in the STS has a hybrid of direct conversion oversampling and superheterodyne undersampling technologies, which allows for flexible frequency conversion and efficient and optimal signal transmission/reception depending on the target frequency. (Patent: EP297779B1/US10295632, Patent: EP2977780B1/US10338168).

\*:In the maximum case of ECZL G series

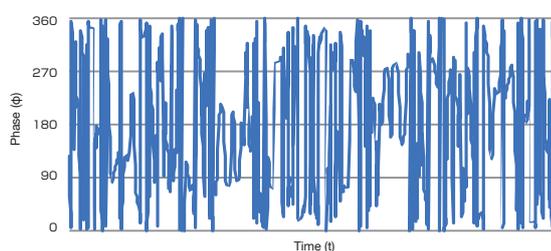


## High-speed, high-precision digital control

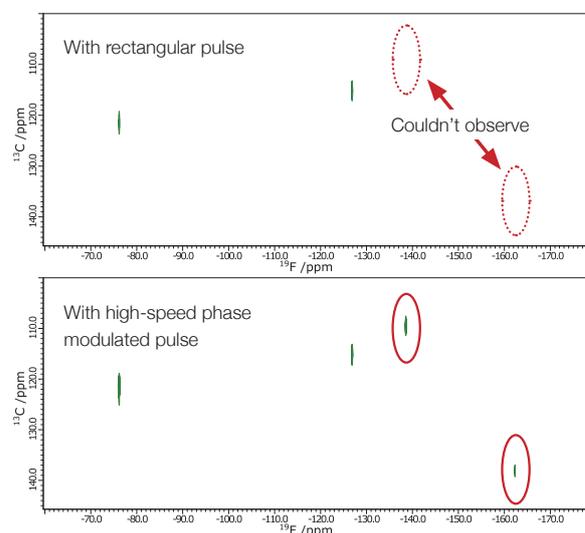
The ECZ Luminous sequencer provides fast control of frequency, phase and amplitude modulation with a minimum control time resolution of 5 ns. In addition, the ECZ Luminous is equipped with a digital quadrature detection (DQD) circuit that enables dynamic frequency and phase modulation synchronously or asynchronously in both the transmitter and receiver systems. This enables signal processing with high functionality and a high degree of freedom, and is expected to be applied to cutting-edge solid-state NMR measurements, which have become increasingly important in recent years. In addition, a unique streaming transfer technology is used for the sequence memory (Patent: EP2977781B1/US10302721), which has a quasi-infinite memory capacity. At the same time, the same control performance is provided for various gating and synchronization operations with external systems. These high-speed, high-accuracy digital control technologies provide the best solution for a wide variety of requirements to realize a wide range of advanced NMR measurements.

In case that observe nucleus has a wide range of chemical shifts, such as  $^{19}\text{F}$ , some signals may not be observed due to the limited bandwidth of conventional rectangular pulses. In such a case, high-speed phase modulation pulses excite much wider ranges and are very useful.

Example of phase by PM-BEBOP 180 pulse modulation



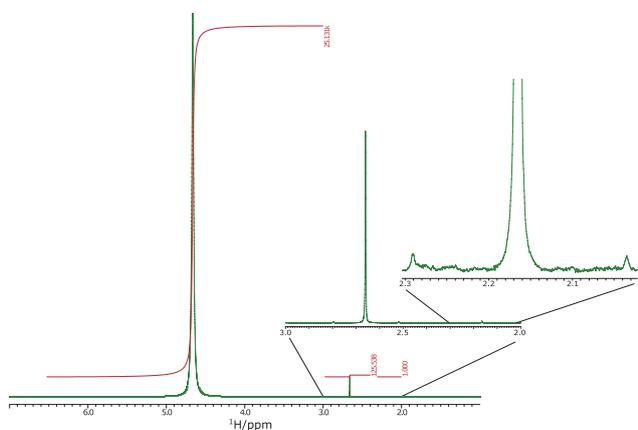
$^1\text{H}$  decoupled  $^{19}\text{F}$ - $^{13}\text{C}$  HMQC spectrum



## Wide dynamic range

The receivers in the ECZ Luminous are sequencer controlled and can be independently and dynamically frequency and phase modulated for sampling. DQD (Digital Quadrature Detection) with 16-bit 100Msps high-speed A/D conversion not only improves the effective dynamic range against quantization noise by high-rate oversampling, but also reduces unwanted signals such as intermodulation distortions (IMDs) to the utmost limit. The digital filter is optimized for NMR and ensures quantitative performance over a wide bandwidth.

The high dynamic range of ECZ Luminous allows you to clearly capture small signals in presence of large ones, such as from a non-deuterated solvent.



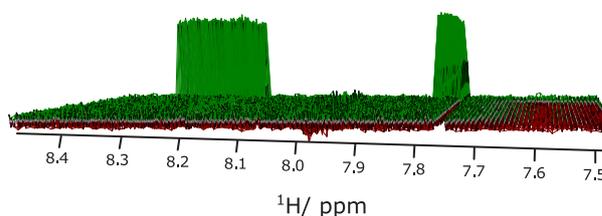
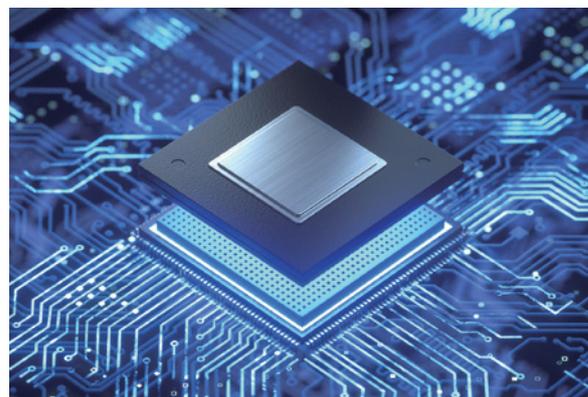
A small  $^{13}\text{C}$  satellite signal (about 4.6 millionths) of the acetone signal in a mixed sample:  $\text{H}_2\text{O}:\text{DMSO}:\text{Acetone}=25131:125:1$  (about 10 %  $\text{D}_2\text{O}$ ) is clearly visible.

## Digital lock circuit for stability

ECZ Luminous uses STS technology to digitally control the  $^2\text{H}$  lock with high speed and high accuracy. The excellent response control of the digital feedback circuit suppresses the effects of magnetic field fluctuations more efficiently. The high speed and high precision digital lock feedback function enables stable and long time measurement.

## Low noise wideband SiGe preamplifier

Newly developed low-noise wideband SiGe preamplifier improves sensitivity. In combination with ROYALPROBE™ and ROYALPROBE™ HFX, the sensitivity has been improved.



Stability test data over 12 hours

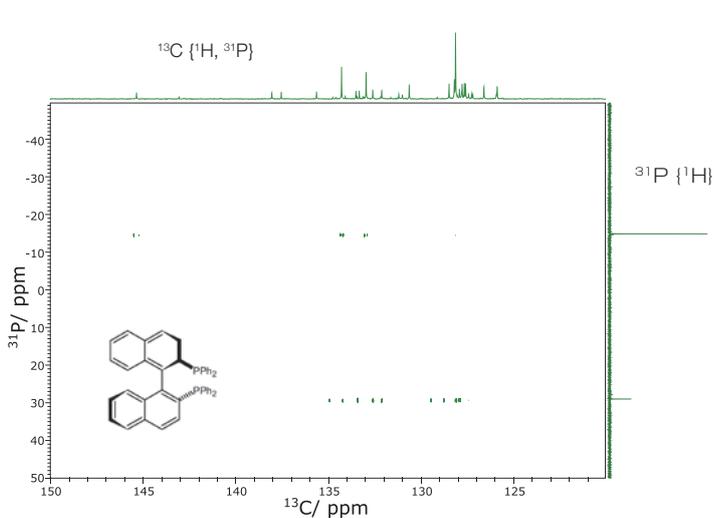
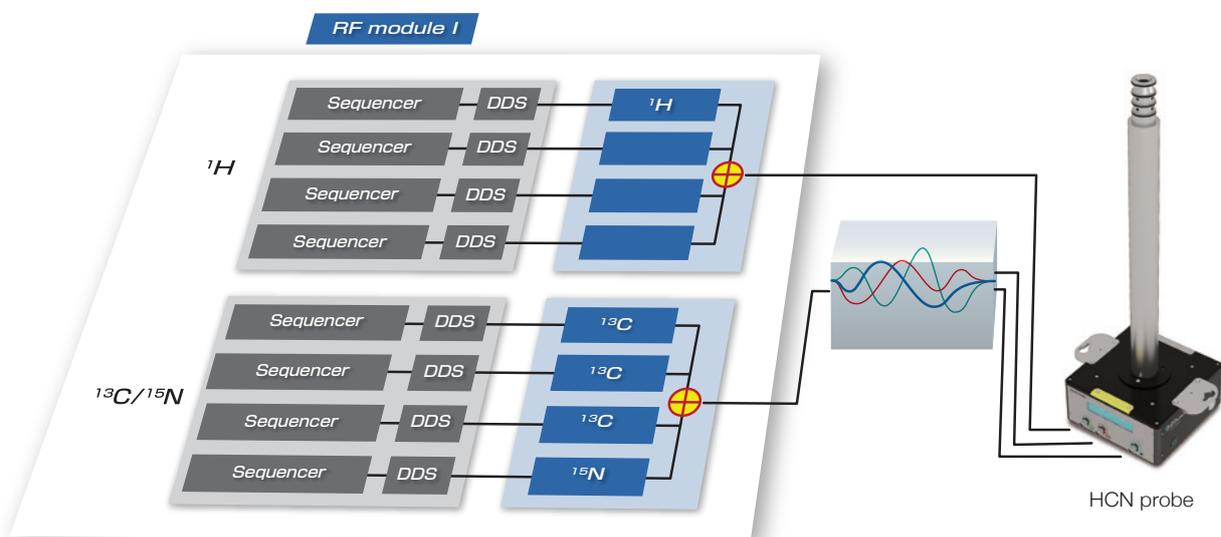
1D  $^1\text{H}-^{13}\text{C}$  HMQC observes the signals from  $^{13}\text{C}$ -coupled  $^1\text{H}$  (left and right signals), while suppressing the  $\sim 100\times$  larger signals from  $^1\text{H}$  attached to  $^{12}\text{C}$ . Reliable suppression of the  $^{12}\text{C}$ -attached  $^1\text{H}$  signals demands a high level of short-term and long-term instrument stability.

## MFDS (Multi Frequency Drive System)

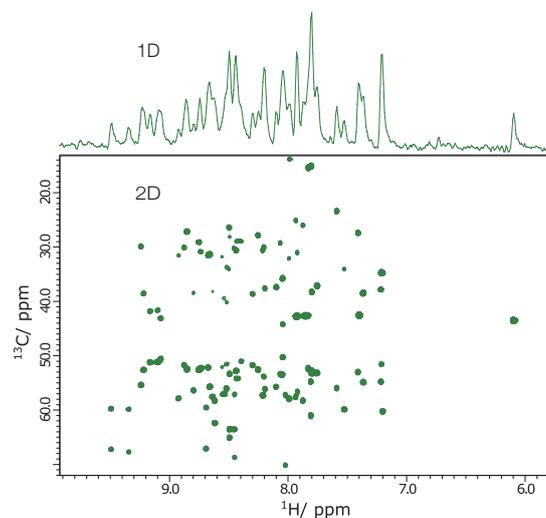
We have developed a new Multi Frequency Drive System. Expanding on the design concept of the HFX system, the ECZ Luminous system enables multiple resonance measurements using triple-resonance probes such as HCN and HPX probes on a standard two-channel spectrometer. Conventional triple-resonance measurements, which require pulse irradiation of three or more nuclides with different frequencies, traditionally require costly expansion of channels and installation space. With ECZ Luminous, the multi-sequencer architecture with STS and the newly-developed MFDS (Multi Frequency Drive System) enable triple-resonance measurements with a two-channel spectrometer. It opens the door of multiple-resonance experiments to more users.

### ■ When HCN probe is equipped

ECZ Luminous system



HCP triple-resonance experiment with a two-channel spectrometer  
( $^{13}\text{C}$ - $^{31}\text{P}$   $\{^1\text{H}\}$  shift correlation experiment)

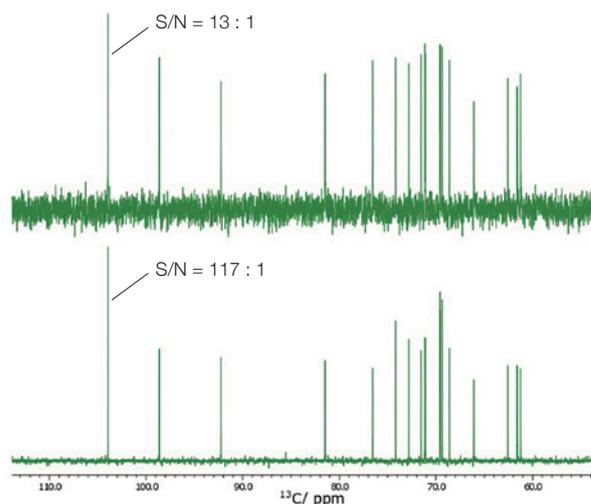


HCN triple-resonance experiment with a two-channel spectrometer  
(CBCACONH experiment)

## Dramatic S/N improvement

The PCW (Phase Covariance Weighted) method, which can improve the S/N of a spectrum using covariance processing, is now available in ECZ Luminous (Patent: EU2388611/US8798949). Multiple data with different acquisition phases are acquired, then the covariance between the phase of the measurement data and the acquisition phase is calculated, and it is applied to the spectrum to improve the S/N. It is expected to improve S/N for about 10 times and reduce the time required for accumulation.

\*1: The extent of S/N improvement depends on the spectrum.



<sup>13</sup>C-NMR spectra of raffinose recorded conventionally (top) and using the PCW method (bottom). Both spectra were recorded using the same number of scans.

## Easy to adjust resolution

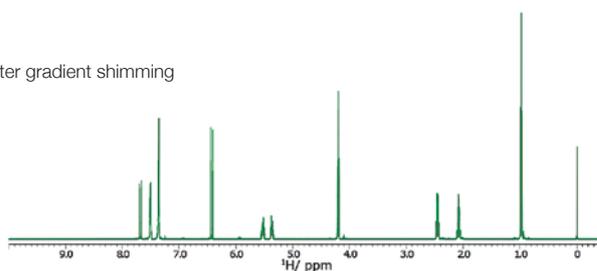
ECZ Luminous includes a digital matrix shim system (25 shims) for 400 MHz, and a Lagrange shim system (44 shims) for higher-field instruments requiring higher resolution. Gradient shimming is a technique that uses magnetic field gradients to measure the magnetic field distribution in the sample space, and then immediately calculates and applies the appropriate shim values. Gradient shimming allows rapid and automatic optimization of the shims, even for samples with small volumes or different solvent systems, to obtain NMR spectra with the highest resolution.

ECZ Luminous can perform gradient shimming by observing nuclei other than <sup>2</sup>H (D) and <sup>1</sup>H nuclei. For example, if you want to perform NMR measurements on a sample that is only soluble in fluorinated solvents, you can adjust the resolution by gradient shimming on <sup>19</sup>F. The accelerated 3D gradient shimming (3 axes) measures the 3D magnetic field map of the sample and calculates and applies the optimal shim value for the radial terms, making it easy to optimize resolution in various conditions.

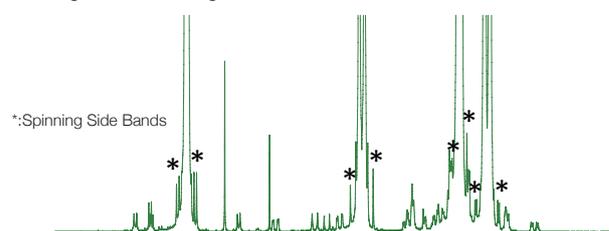
Before gradient shimming



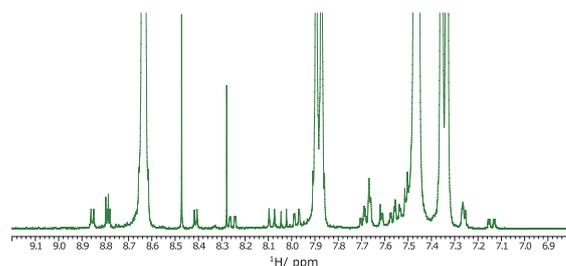
After gradient shimming



Before 3D gradient shimming



After 3D gradient shimming



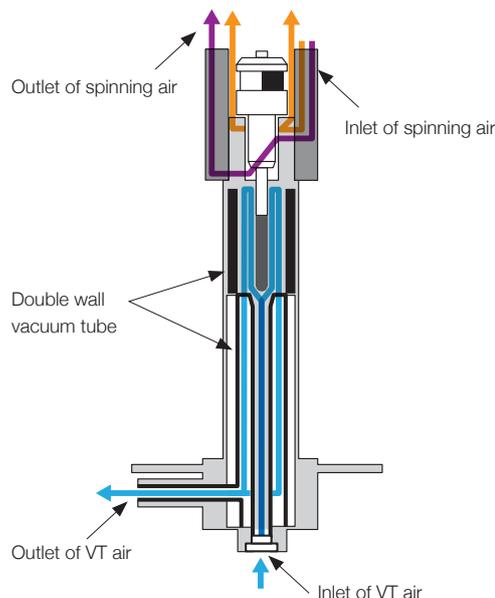
Poorly adjusted radial shims under sample rotation (top) and corrected with 3D gradient shimming (bottom)

## Sample temperature control system

The temperature control system of JEOL's solution NMR probe enables stable measurements even under temperature control by enhancing the coordination with a highly responsive heater.

The variable temperature (VT) gas that heats up or cools down the sample passes through the vacuum double tube from the bottom of the probe to the sample, and then returns through the vacuum double tube to the gas outlet at the bottom of the probe. In this way, the variable temperature gas does not affect the spinner housing or the room temperature shim system by heating or cooling, and thus stable and reliable variable temperature measurement is possible.

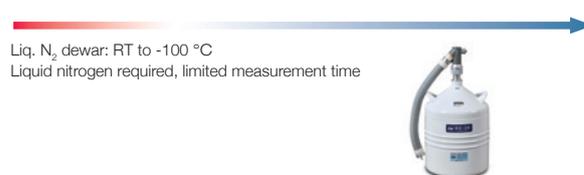
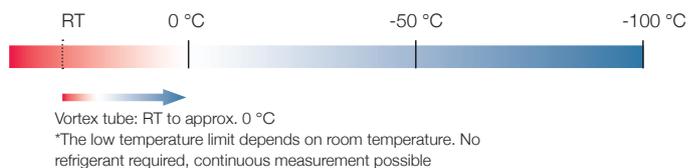
When performing high temperature measurement, there is no need to use an inert gas such as dry nitrogen, and the air supplied from the compressor can be used for measurement up to 250 °C\*.



\*Please refer to the probe specifications for the temperature range that can be used.

## Low temperature options

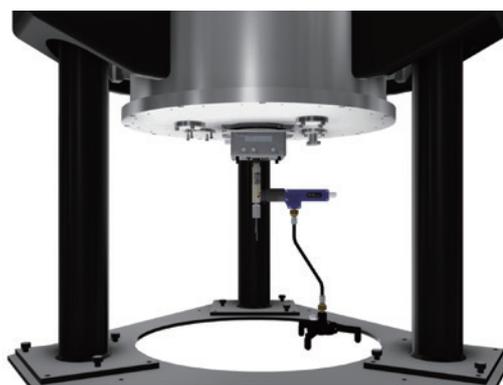
By supplying cooling gas, low temperature measurement is possible. A variety of units are available to suit different temperature ranges and measurement times.



## Vortex tube

Compressed air is fed through a vortex tube (Rank-Hirsch vortex tube) to generate cold air. The air is supplied to the probe at temperature about 25 °C lower than room temperature\*<sup>2</sup>. Since there are no mechanical parts, this device is maintenance free and requires no refrigerant such as liquid nitrogen.

\*<sup>2</sup> Depends on the performance of the compressor used.



## Superconducting magnets of JJ Series

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The magnets of JJ Series are compact, low helium-consumption magnets equipped with newly designed superconducting wires and cryostats. The JJ Series has a smaller footprint and lower ceiling height requirements than the previous models. The consumption of liquid helium has been reduced and the filling interval has been extended. In addition, the JJ superconducting magnets are equipped with an extra coil that provides the highest level of isolation from fluctuations of external magnetic fields. Therefore, even if external magnetic field fluctuates, the magnetic field at the center of the magnet is virtually unaffected and extremely stable.

## Earthquake-resistant magnets

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The superconducting magnets of JJ Series can be transported with liquid nitrogen or liquid helium in the cryostat, i.e., in a cooled state (cold shipment). In order to make cold-shipment possible, the strength of the composite reinforced rods that support the He and N<sub>2</sub> vessels inside the SCM has been increased. These rods are designed to withstand the vibrations during transportation, and can withstand large vibrations during earthquakes.

JEOL's magnets comprise a highly reliable vibration isolator that prevented SCMs from tipping over in major earthquakes in the past. The combination of the low center of gravity with the base plate and non-contact anchor bolts minimize damage in the event of a disaster.

## 400JJYH superconducting magnet

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In the 400 MHz class of superconducting magnets, year-hold time (365 days or more of helium retention) is now the standard. The 400JJYH superconducting magnet significantly reduces the burden on NMR maintenance.

## Nitrogen replenishment system

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The liquid nitrogen recycler NR-50 replaces the periodic refills of liquid nitrogen. The NR-50 uses a small, air-cooled cryogenic refrigerator that operates on single-phase AC 100 V, and hence saves space and minimizes running costs.

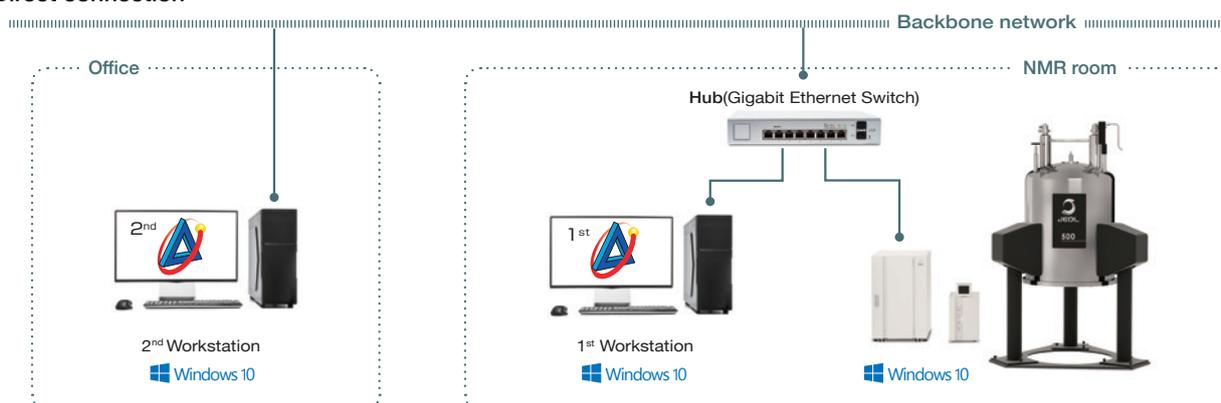


# Remote access and automation

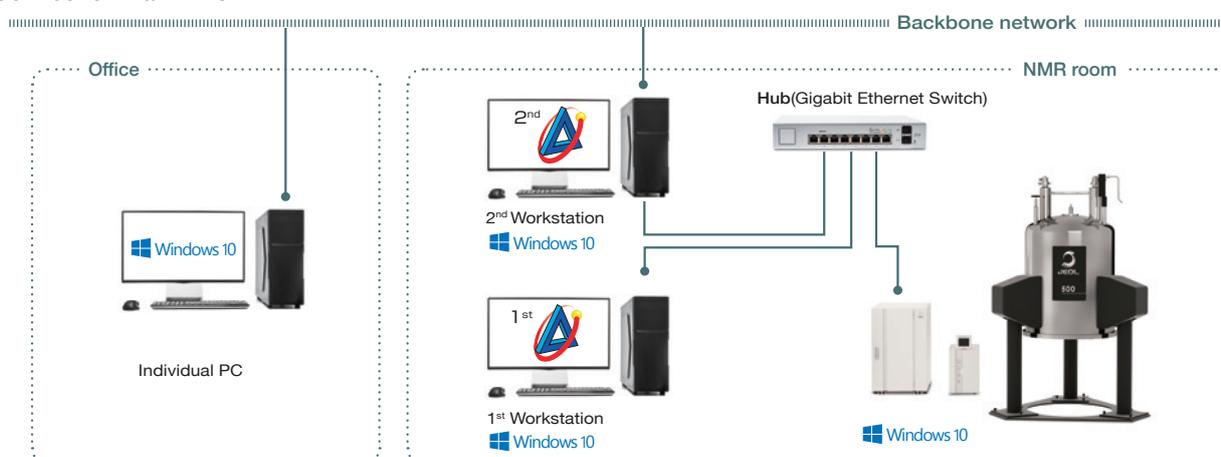
## Adaptation for networking

ECZ Luminous is an NMR system that supports remote access through network operation, allowing users to access the NMR system from a remote location, such as office or home. In addition to remote operation by connecting the workstation directly to the spectrometer via a network, a second PC can be installed to create a comfortable and safe NMR remote operation environment without exposing the important equipment to external danger.\*<sup>1</sup> ECZ Luminous has a built-in spectrometer control computer (SCC) that controls the spectrometer. Since the SCC is a high-performance computer with a large hard disk, it can execute pulse sequences, store data, and perform other operations independently. The measurement data is always written to the hard disk in the SCC. Therefore, even if the workstation or the network fails during continuous measurement, all the pre-scheduled measurements will be executed normally and the measurement data will be automatically written to the hard disk in the SCC.

### Direct connection



### Connection via 2nd PC



\*1 Connection to the backbone network is recommended via a second PC.

Network and VPN connections are not guaranteed in all network environments. Please connect within the scope of user's responsibility.

Operation of the network connection is the responsibility of the user.



## New high-speed auto-tuning unit



The auto-tuning unit, developed by JEOL as a world pioneer and supplied since 1985, is now in its fourth generation. The 4<sup>th</sup> generation of JEOL auto-tuning unit contributes to further improvement in throughput. With the new algorithm, the average tuning time has been reduced to about 40% of the previous model. In addition, while the previous auto-tuning unit required an extension unit to perform triple-resonance measurements, the new auto-tuning unit can perform triple-resonance measurement without the need for an additional unit. JEOL's auto-tuning unit can be used for all probes that support the auto-tuning function. Since the dial information is stored in the probe, there is no need for the pre-tuning procedure when changing probes. In addition, a quick coupler is used to connect the probe to the unit, freeing the user from troublesome connection and disconnection work.

## Versatile auto sample changers

JEOL's auto sample changers are designed not to touch the NMR sample tube, and hence can safely transport sample tubes of various diameters and special sample tubes. We offer two types of auto sample changers: the JackBean, which sets the sample at waist height and uses a manipulator to transport it, and the ASC24, which is mounted on the top of a magnet. The JackBean, which is compact and closely attached to the magnet, eliminates the need to go up and down stairs when changing samples. For customers who wish to cool or preheat their samples, we have a lineup of pre-cooled and pre-heated models. These auto sample changers can be used in combination with not only solution probes, but also with compatible solid-state NMR probes, such as AUTOMAS, to enable continuous automated measurements, further contributing to high throughput.

Type	Option
ASC24	
JackBean-ASC30	Pre-Cool Pre-Heat
JackBean-ASC64	
JackBean-ASC100	



ASC24



ASC30



ASC100

# High sensitivity NMR probes

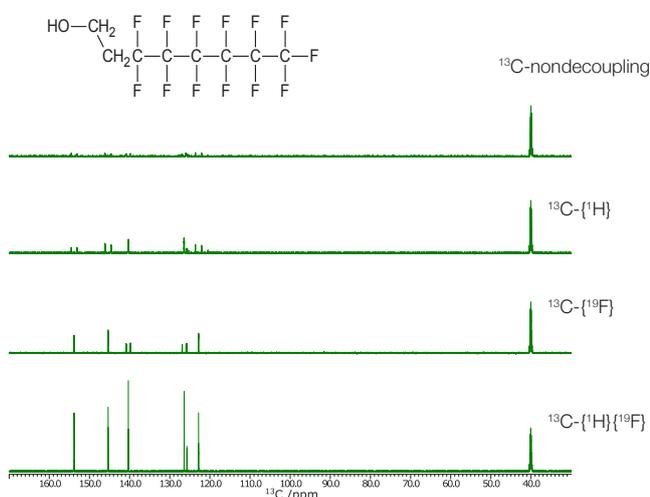
## ROYALPROBE™ and ROYALPROBE™ HFX

The ROYALPROBE™ (Reverse Optimally Autotune Liquid Probe), which is a standard component of ECZ Luminous, is a probe with optimized sensitivity for both HF and LF nuclear observations using JEOL's probe technology. Conventionally, two types of probes have been used: a tunable probe suitable for direct observation of low frequency nuclides and an inverse probe with high  $^1\text{H}$  sensitivity. The high  $^1\text{H}$  sensitivity of the ROYALPROBE™ is equivalent to that of the inverse probe. ECZ Luminous provides the performance of both types of probes without the need for cumbersome probe exchanges, while maintaining the same ease of use through the use of the ROYALPROBE™ as standard, resulting in lower detection limits and shorter measurement times.

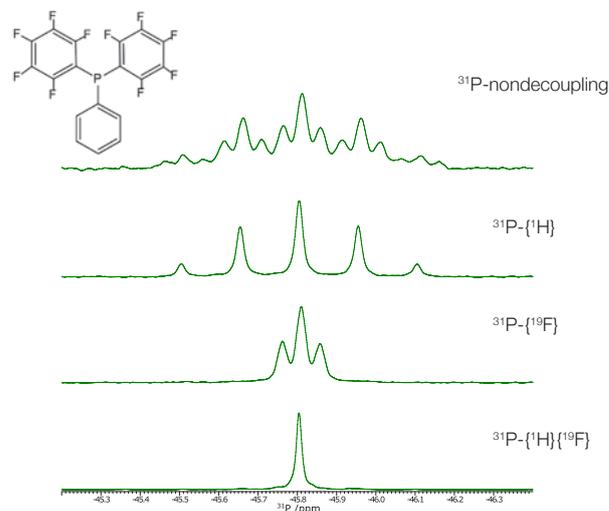


In addition, the ROYALPROBE™ HFX is capable of automatically switching between the double-resonance and triple-resonance modes. In the double-resonance mode, the probe can be used as the highly sensitive ROYALPROBE™. The triple-resonance mode of the ROYALPROBE™ HFX is a triple-resonance probe that allows the high-frequency coil to be tuned to frequencies of  $^1\text{H}$  and  $^{19}\text{F}$  simultaneously. In the analysis of fluorine-containing compounds, which are becoming increasingly important in new materials and pharmaceuticals, it is necessary to simultaneously decouple both  $^1\text{H}$  and  $^{19}\text{F}$  during  $^{13}\text{C}$  measurements. Conventional NMR instruments require three independent channels to irradiate  $^1\text{H}$ ,  $^{19}\text{F}$  and  $^{13}\text{C}$  pulses. ECZ Luminous can perform triple-resonance experiments even in a two-channel configuration.

With the ECZ Luminous, a  $^{13}\text{C}$  spectrum with simultaneous  $^1\text{H}$  and  $^{19}\text{F}$  decoupling can be obtained by simply combining the ROYALPROBE™ HFX with a standard two-channel spectrometer without the need for the 3<sup>rd</sup> channel.



$^{13}\text{C}$  spectra of 1,1,2,2-tetrahydroperfluoro-1-octanol measured with JNM-ECZL400S (with one RF module) and ROYALPROBE™ HFX.

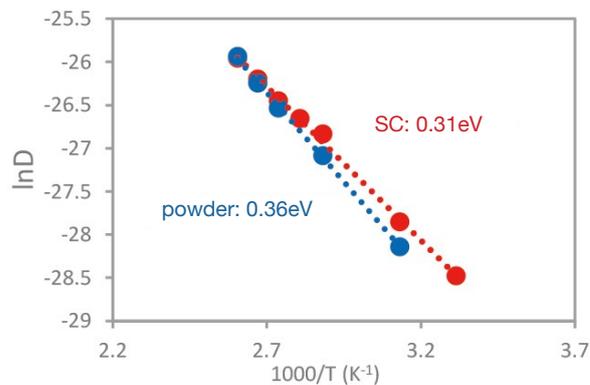


Variants of  $^{31}\text{P}$  NMR experiments



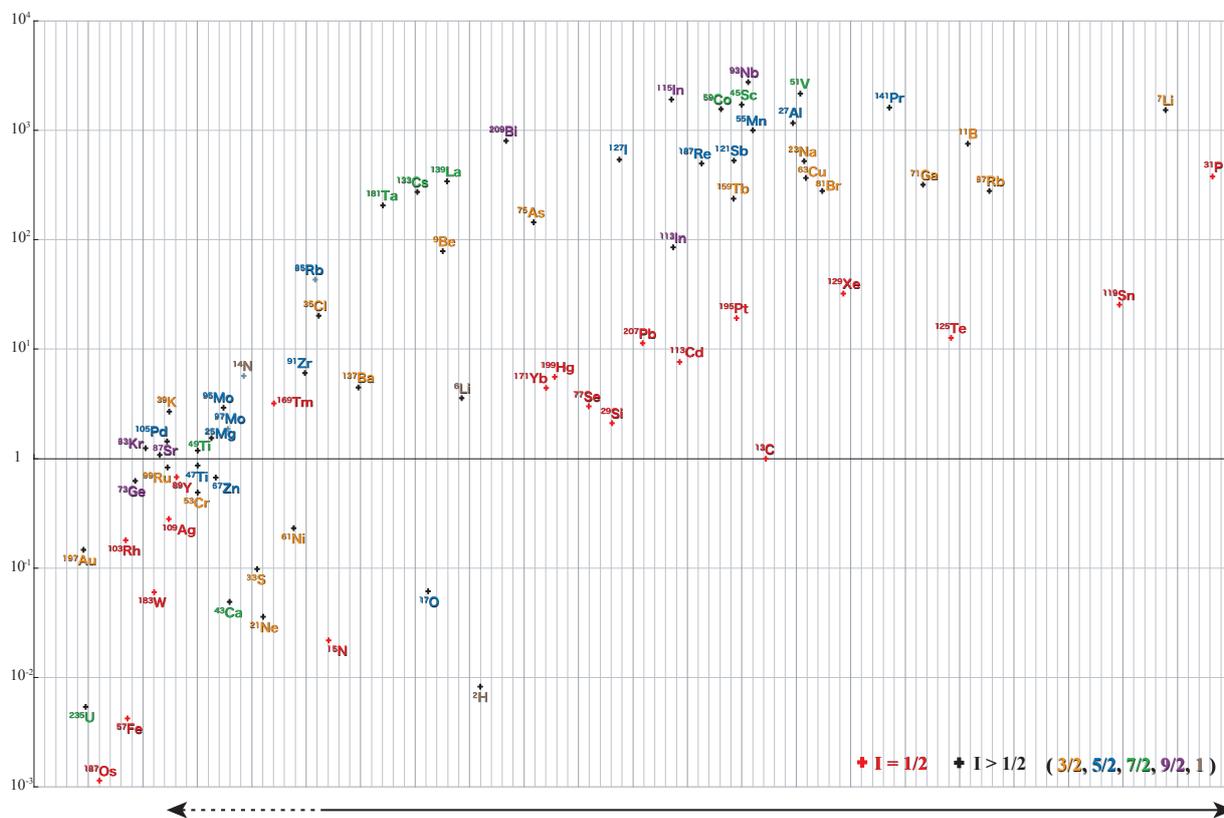
## Diffusion Probe

The new Diffusion Probe is a special probe for measurement of self-diffusion and DOSY (Diffusion Ordered SpectroscopY) by applying large magnetic field gradient pulses. By improving the design around the coil, the new Diffusion Probe has a much shorter recovery time after the magnetic field gradient pulse than the previous model. It is ideal for analyzing the dynamics of large molecules with small diffusion coefficients, nuclides with small gyromagnetic ratios, and ions in solid electrolytes, which have been actively developed in recent years. In combination with the new 50 A magnetic field gradient power supply, the system is capable of generating a maximum intensity of 2,000 G/cm in a narrow-bore configuration.



Activation energy of diffusion motion (Arrhenius plot of diffusion coefficient)

## Resonance frequencies and overall relative sensitivity of various nuclides



\*Relative sensitivity ratio to  $^{13}\text{C}$  taking into account the natural abundance ratio. (Logarithmic scale)  
Horizontal axis is gyromagnetic ratio.

## UltraCOOL for ultra-high sensitivity and SuperCOOL for low running cost

The detection coil and preamplifier are cooled to cryogenic temperature to reduce thermal noise to an extremely low level, enabling measurement with sensitivity several times higher than that of conventional room temperature probes. Automatic tuning and matching is supported, so a wide variety of continuous measurements can be performed in combination with the auto-tuning unit. JEOL offers three types of cryogenic probes for solution NMR: UltraCOOL probe, SuperCOOL open type (SCO) and SuperCOOL circulation type (SCC). All probes are capable of controlling the sample temperature over a very wide range from  $-40\text{ }^{\circ}\text{C}$  to  $+150\text{ }^{\circ}\text{C}$ . The Probe Lifter and Probe Arm are available as optional accessories to alleviate probe exchange.

### UltraCOOL probe

The UltraCOOL probe is capable of ultra-sensitive measurement, which is a feature of cryogenic probes, as well as stable high-temperature measurement, which is necessary for analysis of polymers and other materials. It also supports the new high-speed automatic tuning and matching.



### SuperCOOL probe

The SuperCOOL probe is available in two cooling methods: open type using a liquid nitrogen tank and circulating type using an air-cooled refrigerator. The open type does not require a refrigerator, so it is superior in terms of running cost. The circulating type, which has a higher cooling capacity and better sensitivity, does not require replenishment of the refrigerant and has a higher continuous operating capacity.



- SuperCOOL open type
- Reasonable installation and running costs
  - Uses liquid nitrogen as coolant
  - Liquid nitrogen can be refilled during NMR measurement



- SuperCOOL circulation type
- Higher sensitivity than the open type
  - About 1/4 of the running cost of UltraCOOL probe
  - Uses He gas as coolant
  - No need to fill the cooling system with liquid nitrogen

### Probe Arm and Probe Lifter

Cryogenic probes cannot be raised or lowered by hand in the cooled state due to safety concerns, and hence it might be necessary to warm up cryogenic probes to room temperature before manipulating with them. However, you can replace the UltraCOOL probe or SuperCOOL probe in cooled state by using the probe arm or lifter. Also, though UltraCOOL and SuperCOOL probes are heavier than room temperature probes due to their design, they can be easily exchanged using the Probe Arm or the Probe Lifter.



Probe Arm



Probe Lifter

## From automation to advanced solid-state NMR measurements

JEOL's solid-state NMR probes are available in a variety of sample tube diameters, from high-sensitivity large-volume to small-volume for high-speed rotation, in a wide temperature range, and in top-loading for automatic measurement. With ECZ Luminous, solid-state NMR probes can be easily exchanged with solution NMR probes by using the probe files, and the operation is the same, making it suitable for solid-state and solution NMR applications. In addition, ECZ Luminous is capable of continuous automatic measurement of solid-state NMR experiments as easy as solution NMR. The combination of automatic resolution adjustment by Magic Shimming, automatic rotation speed control by the Magic Angle Spinning (MAS) controller, auto sample changer and auto-tuning unit makes it easy to perform a series of automatic solid-state NMR experiments.



Video on High Throughput Solid State NMR System



### AUTOMAS probe for wide temperature range and automatic measurement

The AUTOMAS probe can be combined with the Auto Sample Changer and Auto-Tuning Unit, which are common to solution NMR, to automatically exchange solid samples using the ROTORCARRIER™, tune and match the probe, control MAS rate and temperature. This automation makes it possible to use nights and weekends more efficiently.

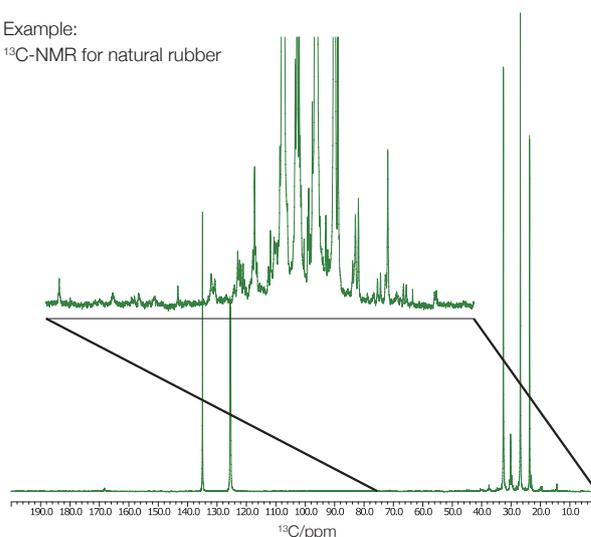


### The new MAS controller

It is a high-precision controller that automatically reaches and maintains the desired speed, and can be controlled online from Delta.

\* The MAS controller is externally mounted.

Example:  
<sup>13</sup>C-NMR for natural rubber



### Magic Shimming

By automatically correcting the shim terms of Y1, X2, and Z3, it is possible to acquire solid-state NMR spectra with high resolution with very little effort. (Patent: EP2551693B1/US9389187B2)

## Delta

Delta is the spectrometer control and data processing software used by ECZ Luminous. The spectrometer control software comes with pulse programs for a wide range of basic and advanced experiments, and has the capability to support new pulse programs. In addition, three measurement modes are available to flexibly meet the different needs of users. The data processing software includes not only general NMR data processing and analysis functions, but also dedicated tools for various applications.

## Delta's three measurement modes

The Delta has three measurement modes: Walkup mode, Smart mode, and Advanced mode.

### Walkup mode

The user interface is as simple as a photocopier, and five simple steps are all that is required to obtain data through the automatic measurement.

- (1) Load the sample into the auto sample changer
- (2) Enter the sample information
- (3) Select the solvent
- (4) Select the measurement method
- (5) Click "Submit".

### Smart mode

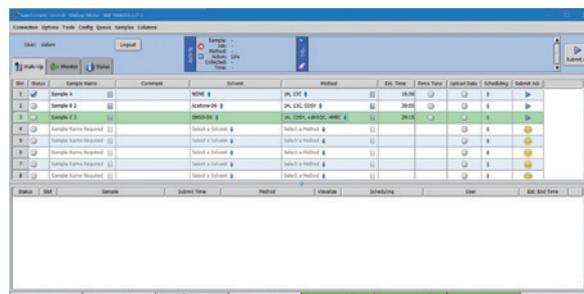
It is a simple measurement mode with improved operability, allowing you to optimize even the most detailed condition settings while maintaining the easy operability that rivals Walkup mode. A wide range of measurements, from basic solution NMR measurements to solid-state NMR measurements, can be automated by selecting the experiment with the touch of a button.

### Advanced mode

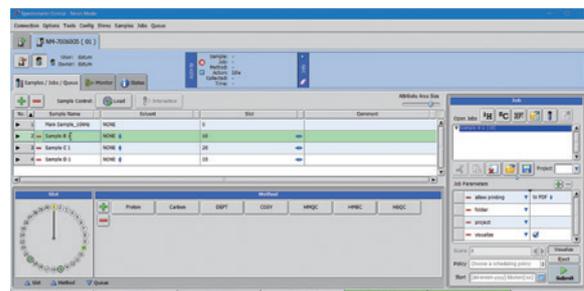
This mode is recommended for users who want to take full advantage of the various functions of ECZ Luminous.

## Spectrometer control

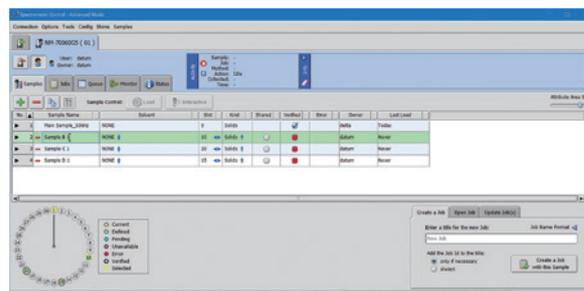
The Delta has an excellent automatic measurement function that does not require any complicated operation. After loading the sample, entering the sample information, selecting the measurement, and clicking the button, Delta performs everything from sample loading, probe tuning, resolution adjustment, measurement, data processing, and printing of the results. Automatic measurement functions include basic one- and two-dimensional measurements, including  $^1\text{H}$  and  $^{13}\text{C}$ , as well as variable temperature, multi-nuclear NMR, and time-specified measurements. In addition, a variety of NMR measurements can be freely customized to provide a measurement environment that meets your needs. You can leave your routine NMR measurements to Delta.



Walkup mode measurement screen



Smart mode measurement screen

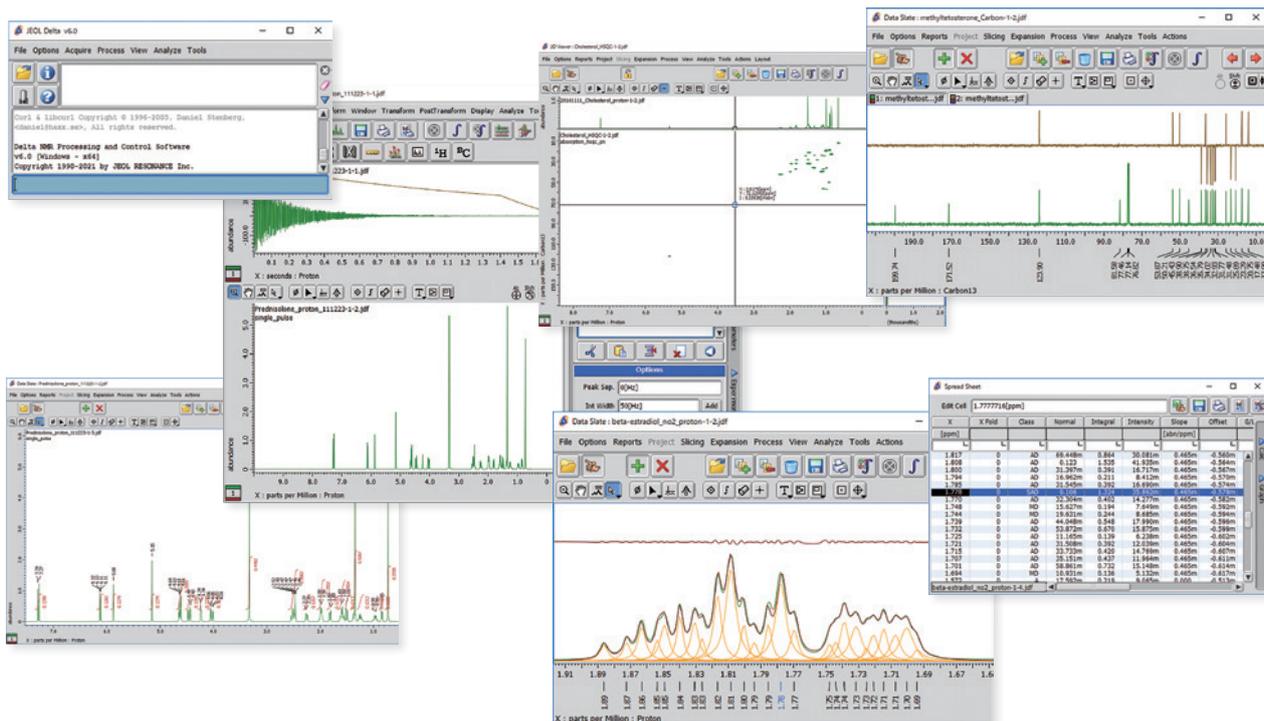


Advanced mode measurement screen



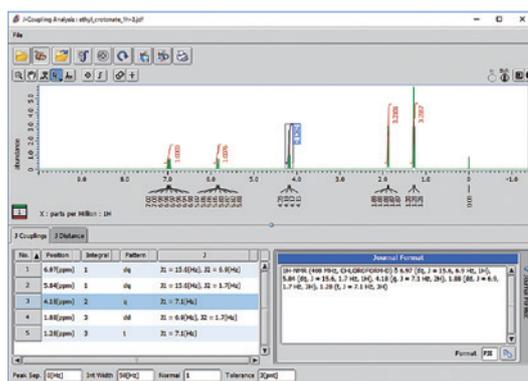
## Data processing

Delta's versatile and convenient analysis tools help users reduce the time required for data analysis. The ease of use is standardized among the tools, allowing users to perform a variety of analyses with a consistent feel.



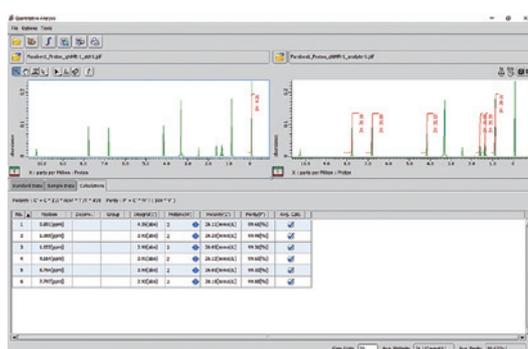
## J-coupling analysis tool

This is a tool that instantly analyzes splitting patterns and *J*-coupling constants. It allows you to perform analysis based on peak picking and integration, and is easy to modify manually after the automatic analysis. It can be copied as a text file to fit various paper formats.



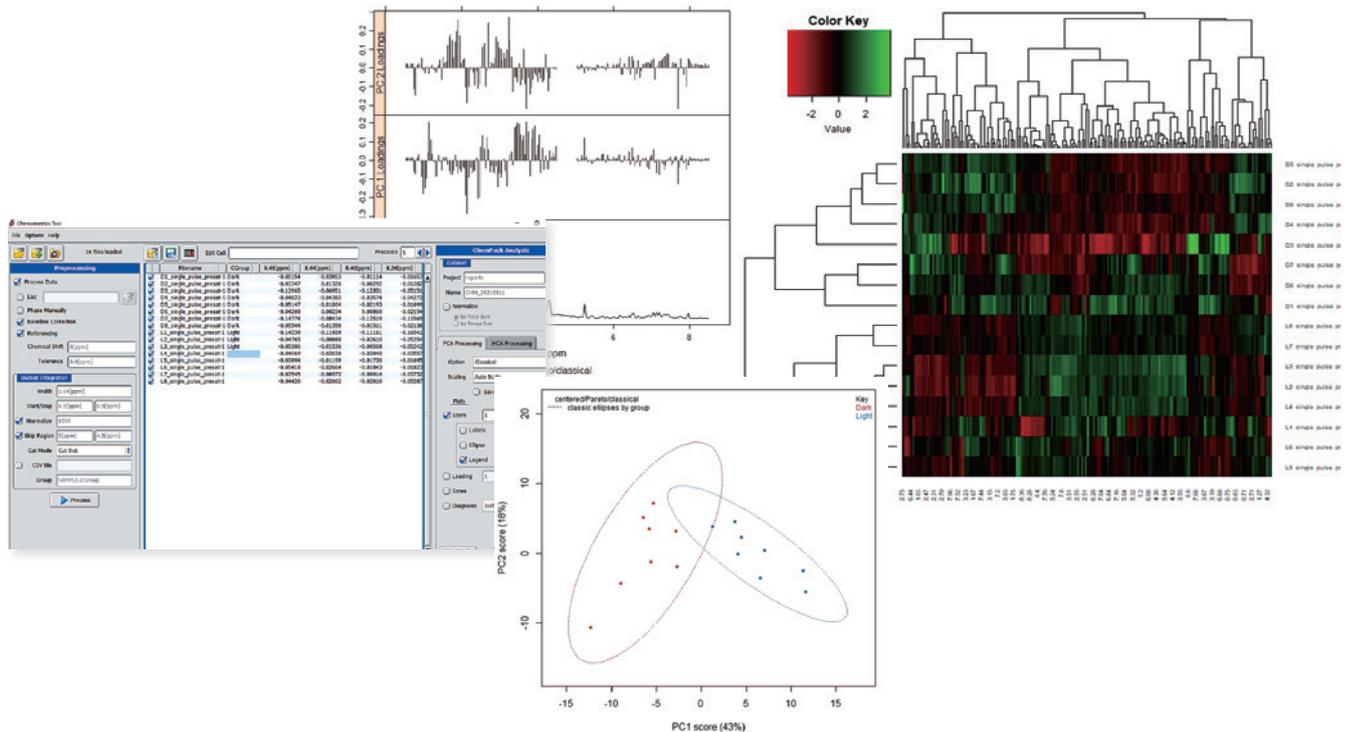
## Quantitative analysis tool

It is a tool for quantitative NMR analysis, and can handle both internal standard methods such as AQARI and external standard methods such as PULCON. The tool will assist you in preparing reports.



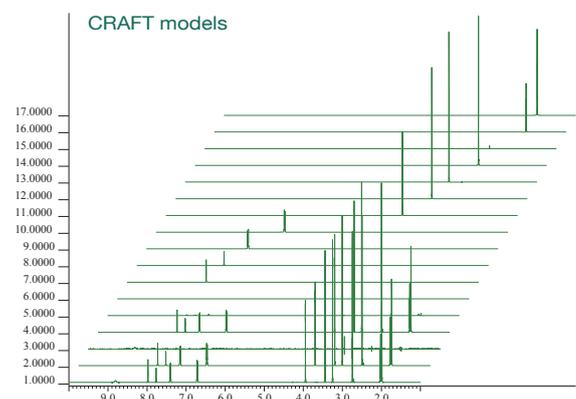
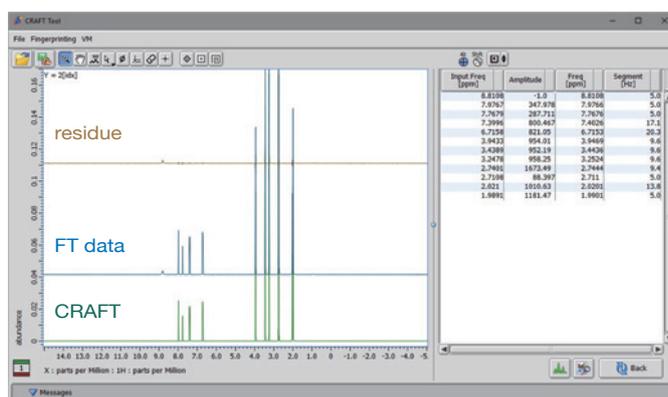
## Chemometrics tool

NMR is a spectroscopic method with excellent quantitative performance and reproducibility, and the sample preparation is simple and the sample is analyzed non-destructively. Taking advantage of these features, NMR spectra of a series of samples, such as biological samples, are used as input for data mining using multivariate analysis and other methods. The Chemometrics tools of Delta software 1) converts a set of NMR spectra into a data matrix, and 2) supports multivariate analysis on the data matrix.



## CRAFT (Complete Reduction to Amplitude Frequency Table)

CRAFT is a new concept for analysis of high-resolution NMR data that directly transforms NMR time-domain data (FID data) into a spreadsheet consisting of the frequencies and amplitudes of each component, based on Bayesian analysis. In conventional analysis using Fourier transform, the frequency spectrum is converted into quantitative information through window function processing, Fourier transform, phase correction, baseline correction, integration, etc. CRAFT converts the time domain data into the frequency and amplitude information directly without these processes and user's intervention, and can be used as an alternative to conventional methods. CRAFT can also be used in combination with chemometrics tools for exploratory data analysis.



## Data integrity (DI) support for JEOL Delta

JEOL's NMR systems were released in May 2004 with Delta ver. 4.3, which included FDA 21 CFR Part 11-compliant functions and supported the principle of data integrity in handling electronic data under GMP. Since then, all subsequent versions have continued to support data integrity with improved functionality. In ECZ Luminous, the computer at the measurement terminal and the control computer built into the spectrometer are completely independent, allowing extremely safe operation for data management. The ECZ Luminous NMR data (Delta format) is extremely easy to manage, as all metadata such as measurement parameters, data processing details, audit trail, and digital signature are contained in a single file.



■ A system for allowing unique user accounts to be created for each user or manager of the system with appropriate permissions or restrictions as necessary.



■ An electronic record according to the guidelines on each regulator has to be automatically recorded during the use of the instrument including measurement and processing of data.



■ Data and all records have to be kept in a browsable condition through the whole life cycle of data.

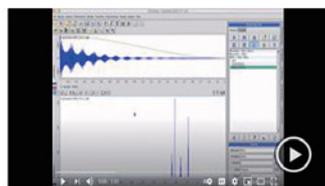


■ A function to put electronic signature into each data according to guidelines on each regulator has to be implemented.

ECZ Luminous provides records that meet the ALCOA-plus principles (Attributable, Legible, Contemporaneous, Original, Accurate, Completeness, Consistent, Enduring, Available) required by data integrity guidance.

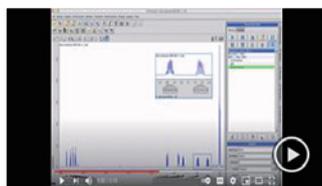
## Delta free download

Delta, the world's first free downloadable NMR data processing software, was launched in 2007 and has become the most downloaded NMR data processing software in the world. Delta, the standard data processing software for the ECZ Luminous, can be downloaded free of charge from the JEOL Delta/NMR support site ([nmrsupport.jeol.com](http://nmrsupport.jeol.com)). A wide variety of data processing functions can be realized on your own PC. Manuals are available, and tutorial movies are available on the JEOL website ([jeolusa.com](http://jeolusa.com)). A variety of data formats are supported, so you can analyze NMR data from the comfort of your desk.



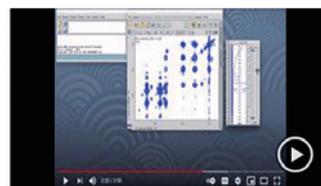
Delta Tutorials: Annotations  
January 26, 2021

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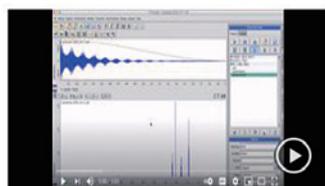
Delta Tutorials: Picture in Picture Part 1  
January 26, 2021

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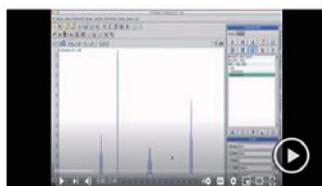
Delta Tutorials: 2D Contours and Zooming  
January 26, 2021

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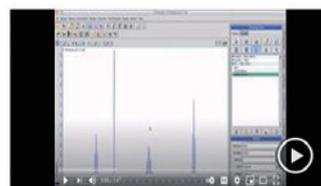
Delta Tutorials: Zoom Cursor Part 1  
January 26, 2021

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Delta Tutorials: Peak Picking Part 1  
January 26, 2021

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Delta Tutorials: Integration Part 1  
January 26, 2021

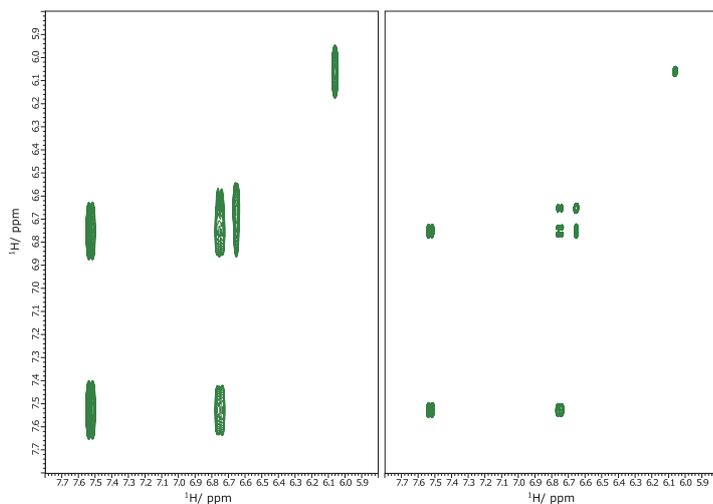
250



# Experience the world of ECZ Luminous!

## NUS (Non Uniform Sampling)

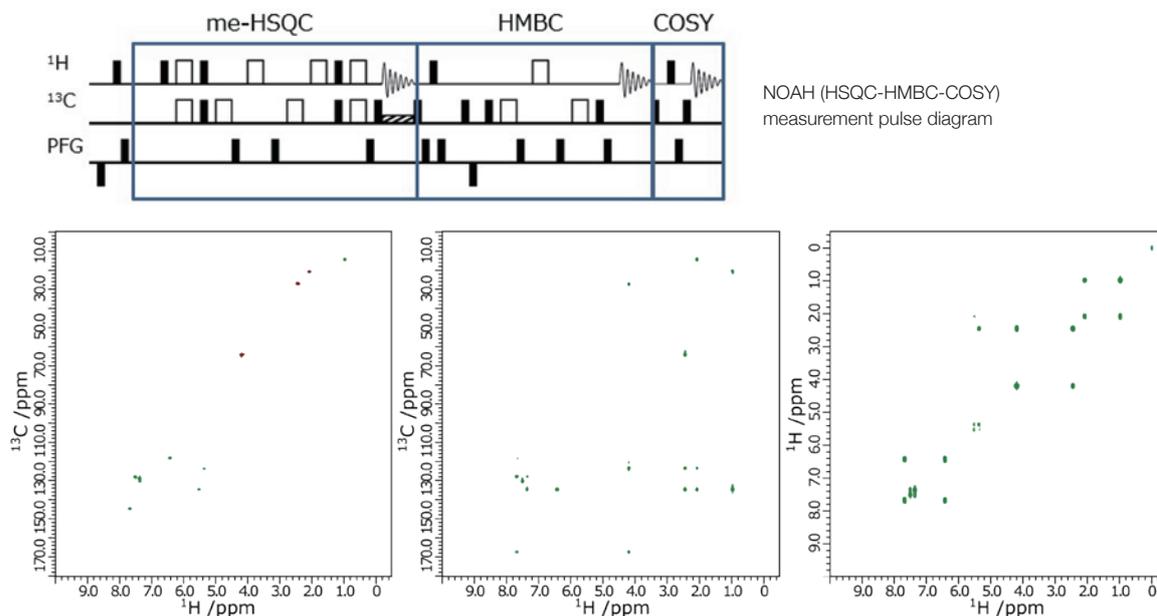
With NUS, the data points of the indirect ( $F_1$ ) dimension of a multidimensional NMR data set are nonlinearly reduced and measured. The resulting sparse data is reconstructed using a special processing algorithm. Even with a small number of acquired data points, data with no degradation in digital resolution can be obtained. Since the measurement time is proportional to the number of data points in the indirect observation axis, the measurement time can be greatly reduced.



Aromatic region of COSY spectrum of 4-methylumbelliferone  
Left: Normal measurement 1024 x 128 points  
(zero filled to 1024 x 2048)  
Right: NUS measurement 1024 x 128 points  
(reconstructed to 1024 by NUS and then zero filled to 1024 x 2048)

## NOAH (NMR by Ordered Acquisition using $^1\text{H}$ -detection)

This method combines several 2D NMR measurement methods such as COSY, HSQC, and HMBC into a single pulse sequence. This method is effective for 2D NMR measurements of relatively small molecules, and allows a variety of different spectroscopic information to be obtained in a short time. It can be particularly useful when a minimum amount of 2D data is required in a limited amount of time.



NOAH (HSQC-HMBC-COSY)  
measurement pulse diagram

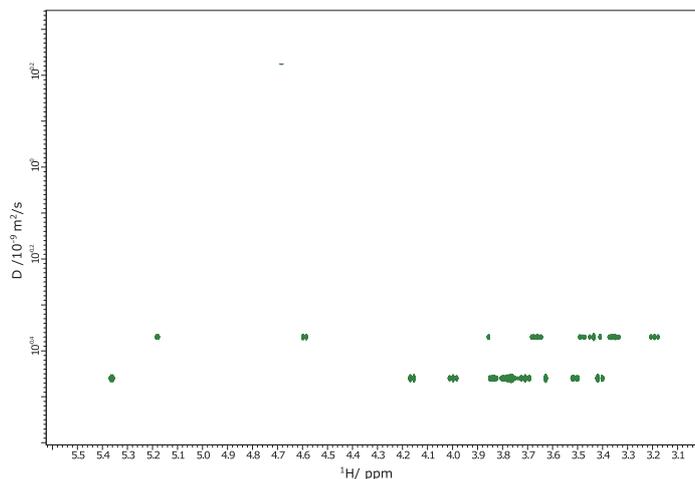
Spectra obtained by NOAH



## DOSY (Diffusion Ordered Spectroscopy)

DOSY is a powerful method for the analysis of mixtures. In DOSY, signals from different components are separated according to their diffusion coefficient. Additives and impurities in the sample, reaction intermediates that cannot be isolated, and differences in the degree of polymerization of polymers can be analyzed without any chemical or physical effects on the sample. ECZ Luminous is equipped with high-linearity magnetic field gradient power supply, which is critical for DOSY, and the rich algorithms and analysis functions of the Delta software make it possible to achieve separations that were previously considered difficult. The gradient amplifier power output can be selected from 10 A and 30 A<sup>\*3</sup>, and even in combination with the standard ROYALPROBE™ (30 G/cm@10 A, 90 G/cm@30 A), the DOSY method can be used for samples with a wide range of molecular weights, from small molecules to large molecules.

\*3: In combination with a diffusion probe, a 50 A model is also available.



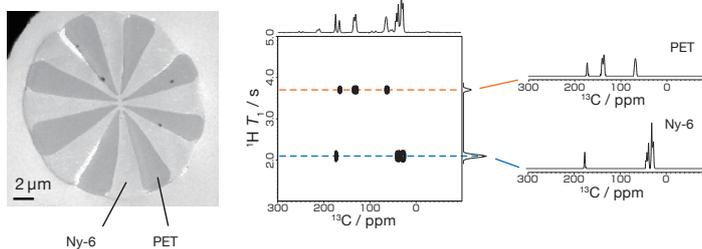
DOSY spectrum of  $\alpha$ -dextrin and glucose

## ROSY (Relaxation Ordered Spectroscopy)

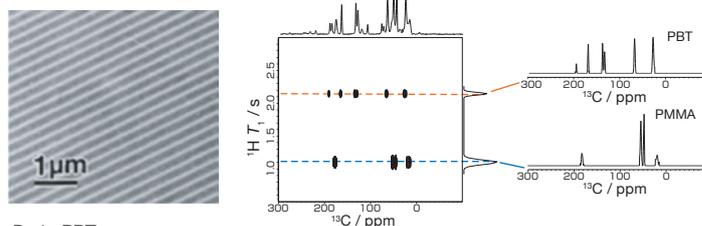
We propose JEOL's proprietary ROSY method for the analysis of mixtures in solid-state, which is equivalent to the DOSY method for solution samples. (Patent: EP2166369B1/US8072213B2) Using the property that the <sup>1</sup>H longitudinal relaxation time  $T_1$  of a solid sample becomes uniform within a domain, the ROSY method separates the signals in the <sup>13</sup>C-CPMAS spectrum by the difference in the <sup>1</sup>H  $T_1$  relaxation time for each domain. Similar to the DOSY method, the ILT method<sup>\*4</sup> is used to separate the relaxation times. ROSY is expected to be applied to the analysis of crystal polymorphism, crystal and non-crystal, etc. as an experiment to analyze solid mixtures.

\*4: Inverse Laplace Transformation

### PET/Ny-6 Compound Fiber



### PBT/PMMA Nanolayer Film

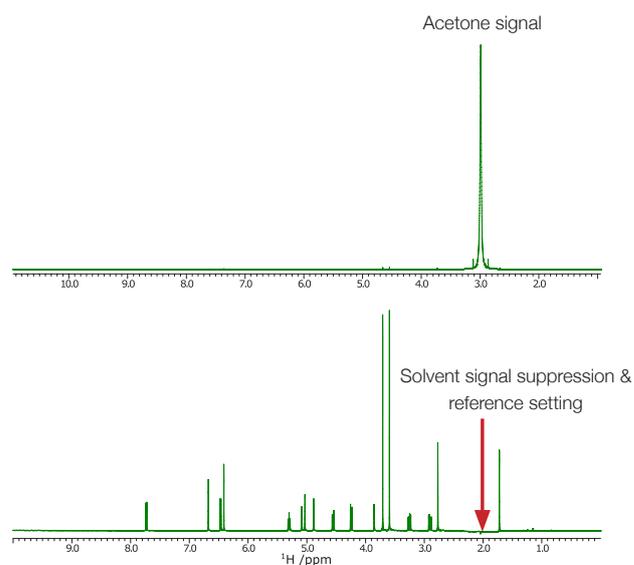


Dark: PBT  
Light: PMMA

Samples courtesy of Teijin Limited

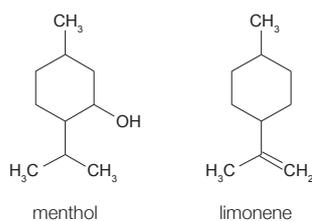
## No-D NMR

No-D NMR, which stands for "No-Deuterium Proton NMR," is a solution NMR technique to measure samples dissolved in non-deuterated solvents. Since expensive deuterated solvents are not used, the cost can be reduced, and the pretreatment time required for solvent replacement before NMR measurement can be greatly reduced. In addition, the possibility of sample decomposition during the solvent replacement process can be avoided, making it ideal for measuring unstable samples. ECZ Luminous features a comprehensive suite of No-D NMR methods for fully automated NMR measurements in the absence of deuterated solvents, including a  $^1\text{H}$ -selective gradient shimming method that uses the protonated solvent signal, automatic detection and suppression of the light solvent signal (or multiple solvent signals, if appropriate). ECZ Luminous offers the same ease of use for automated No-D NMR measurements as it has for automated measurements with deuterated solvents.

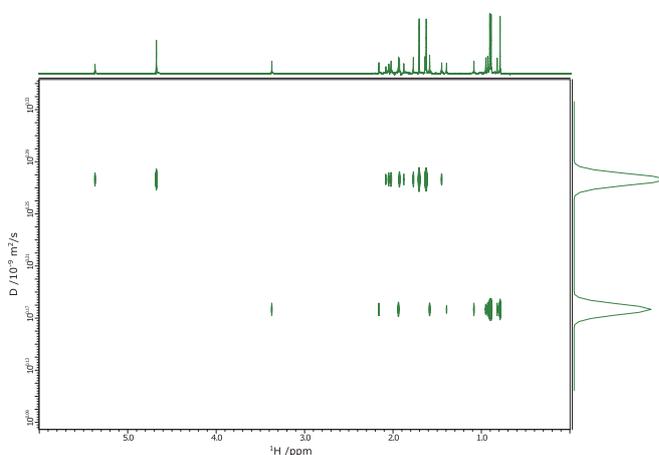
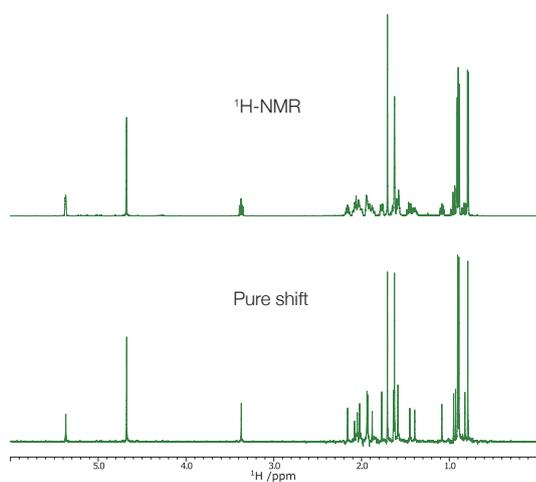


## Pure shift

Pure shift is a powerful class of NMR methods that greatly reduce signal overlap by removing homonuclear  $J$ -splittings in the spectrum to give single lines instead of broad multiplets for each peak. It can also be applied to multidimensional measurements to reduce signal overlap in two-dimensional spectra. With ECZ Luminous, a variety of pure shift measurements is available on a standard configuration system.



Examples of pure shift NMR measurements on a mixed sample of menthol and limonene  
Left: Normal  $^1\text{H}$ -NMR spectrum (upper panel) and pure shift spectrum (lower panel)  
Right: Pure shift DOSY spectrum



Spectrometer: JNM-ECZL500R, ROYALPROBE™ HFX



Link to tutorial videos.

# JASON (JEOL Analytical Software Network)



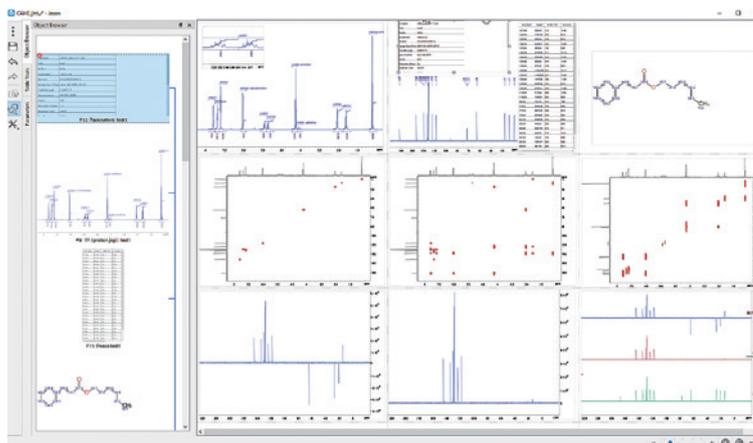
# JASON



JASON is next-generation software with special emphasis on the automated processing, analysis and reporting of NMR data. The intuitive interface facilitates basic NMR analysis. In addition to basic 1D/2D-NMR data processing, the software offers <sup>1</sup>H and <sup>13</sup>C chemical shift prediction, automatic assignment, multiplet analysis, deconvolution, spin simulation, and molecular structure drawing.

### Flexible interface

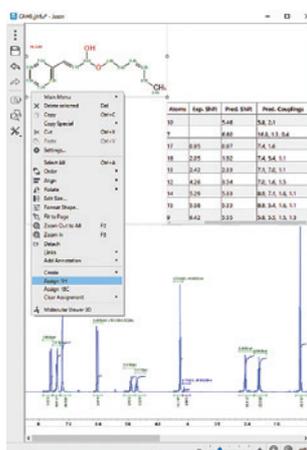
One of the distinguishing features of JASON is the data canvas. As data files are opened, they are displayed on the canvas, which can be extended both horizontally and vertically to accommodate as much data as the computer's working memory can deal with. Navigating the canvas is done using the mouse to scroll and zoom or by specific data objects using the object browser. Related data sets and objects can be linked together with a shared cursor for spectral analysis.



JASON canvas with various data and information displayed

### Auto assignment

JASON has the function to automatically assign <sup>1</sup>H and <sup>13</sup>C NMR signal from chemical structure formula. If you have an NMR spectrum and an estimated chemical structure formula, simply select "Assign <sup>1</sup>H" or "Assign <sup>13</sup>C" from the menu, and JASON will perform the signal assignment fully automatically.

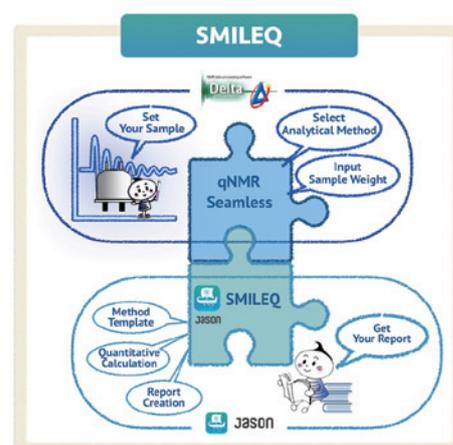


Auto assignment for <sup>1</sup>H-NMR signals



# SMILEQ

JASON can extend the application. The SMILEQ (Spectrum Management Interface Launching Engine for QNMR) is a plug-in software for quantitative NMR analysis and can perform purity or molar concentration analysis using internal standard methods. By linking with Delta, quantitative analysis can be performed seamlessly from measurement to analysis and reporting.



## Standard configuration

---

	ECZL400S	ECZL400R / 400G	ECZL500R / 500G	ECZL600R / 600G
Console (output of power amplifier)	HF 50 W / LF 150 W	HF 100 W / LF 300 W		
Superconducting magnet	9.39 T	9.39 T	11.74 T	14.09 T
Probe	ROYALPROBE™			
Software	Delta ver. 6.1			

S series/ R series



G series



## Primary options

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High power amplifier  
 Channel extension  
 Auto-tuning unit  
 Auto sample changer  
 Probe arm/ Probe lifter  
 Low temperature unit  
 Nitrogen replenishment system  
 High power field gradient amplifier  
 MAS controller

Probes for Solution NMR  
 5 mm ROYALPROBE™ HFX  
 5 mm HCN probe  
 5 mm HPX probe  
 3 mm probe  
 10 mm probe  
 10 mm probe (<sup>29</sup>Si low-background)  
 Diffusion probe  
 High sensitivity cryogenic probe UltraCOOL/ SuperCOOL (Closed)/ SuperCOOL (Open)

Probes for Solid-state NMR  
 AUTOMAS probe  
 HXMAS probe 0.75 mm/1 mm/2 mm/3.2 mm/4 mm/8 mm  
 HXYMAS probe  
 Wide VT HXMAS probe  
 FGMAS probe  
 High sensitivity cryogenic probe (Cryocoil MAS probe)

High sensitivity DNP system

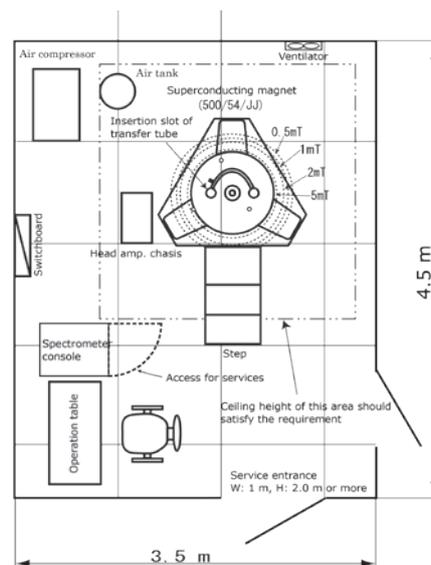
## Installation requirements

### Power supply facilities

Spectrometer (S)	Single phase, 100 to 240 V $\pm$ 10% (less than 250 V) 50/60 Hz 15 A
Spectrometer (R)	Single phase, 100 to 240 V $\pm$ 10% (less than 250 V) 50/60 Hz 20 A
Spectrometer (G)	Single phase, 200 to 240 V $\pm$ 10% (less than 250 V) 50/60 Hz 20 A
Data system	Single phase, 100 to 240 V, 50/60 Hz 1 kVA
Spare	Single phase, AC100/120 V, 50/60 Hz 3 kVA
Grounding work	$\leq 100 \Omega$
Nitrogen replenishment system	Single phase, AC100 V, 50/60 Hz 20 A

### Example of installation room for 500MHz SCM

Permissible range of humidity	70% or below
Ceiling height	2.83 m or higher
0.5 mT position	Vertical direction: 1.15 m, Horizontal direction: 0.60 m (from the field center)

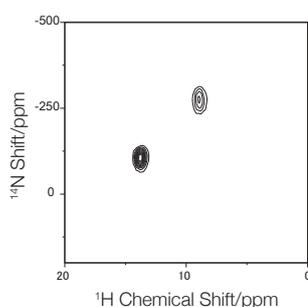


Example of installation for 500 MHz

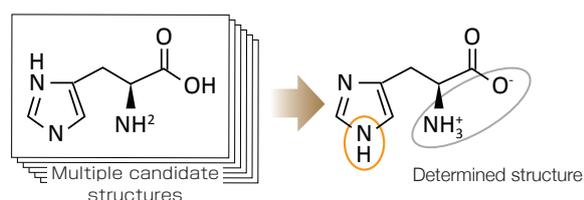
## Complex structure analysis by combining MicroED/3DED and solid-state NMR

MicroED/3DED is a technique to visualize the three-dimensional structure of molecules using electron diffraction (ED: Electron Diffraction). While the use of electron beams has the advantage of being able to measure nano-sized microcrystals, it is sometimes difficult to obtain accurate proton position information and attribute heteroatoms. To solve this problem, for example, the protonation of zwitterionic compounds, as shown in the figure below, can be determined from solid-state NMR spectra to supplement the structural information obtained by MicroED/3DED.

$^1\text{H}$ - $^{14}\text{N}$  solid-state NMR spectrum



$^1\text{H}$  positional information obtained from solid-state NMR



C. Guzmán-Afonso, ..., Y. Nishiyama\*, Nat. Commun. 10 (2019) 3537.  
N.T. Duong, ..., Y. Nishiyama\*, Molecules 26 (2021) 4652.

## Integrated platform for electron diffraction structure analysis Synergy-ED

Synergy-ED is an integrated platform for structural analysis using MicroED/3DED that combines the core technologies of both Rigaku Corporation and JEOL. By seamlessly integrating the workflow from sample selection (nanocrystals) to data collection and analysis, Synergy-ED has made structural analysis by electron diffraction easily accessible to users who do not have specialized knowledge in electron microscopy and crystallography.

For inquiries about Synergy-ED, please e-mail to [info-gsm@rigaku.co.jp](mailto:info-gsm@rigaku.co.jp).



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JEOL Ltd.

3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577  
www.jeol.com ISO 9001 • ISO 14001 Certified

• **AUSTRALIA & NEW ZEALAND** /JEOL (AUSTRALASIA) Pty.Ltd. Suite 1, L2 18 Aquatic Drive - Frenchs Forest NSW 2086 Australia • **BELGIUM** /JEOL (EUROPE) B.V. Planet II, Gebouw B Leuvensesteenweg 542, B-1930 Zaventem Belgium  
• **BRAZIL** /JEOL Brasil Instrumentos Cientificos Ltda. Av. Jabaquara, 2958 5º andar conjunto 52 : 04046-500 Sao Paulo, SP Brazil • **CANADA** /JEOL CANADA, INC. 3275 1ere Rue, Local #8 St-Hubert, QC J3Y-8Y6, Canada • **CHINA** /JEOL (BEIJING) CO., LTD. Zhongkeziyuan Building South Tower 2F, Zhongguancun Nanshanjie Street No. 6, Haidian District, Beijing, P.R.China • **EGYPT** /JEOL SERVICE BUREAU 3rd Fl. Nile Center Bldg, Nawal Street, Dokki, (Cairo), Egypt • **FRANCE** /JEOL (EUROPE) SAS Espace Claude Monet, 1 Allée de Giverny 78290, Croissy-sur-Seine, France • **GERMANY** /JEOL (GERMANY) GmbH Gute Aenger 30 85356 Freising, Germany • **GREAT BRITAIN & IRELAND** /JEOL (U.K.) LTD, Silver Court, Watchmead, Welwyn Garden City, Hertfordshire AL7 1LT, U.K. • **INDIA** /JEOL INDIA PVT. LTD, Unit No.305, 3rd Floor, ABW Elegance Tower, Jasola District Centre, New Delhi 110 025, India /JEOL INDIA PVT. LTD, Hyderabad Office 422, Regus Solitaire Business centre, 1-10-39 to 44, level 4, Gumidelli Towers, Old Airport Road, Begumpet, Hyderabad - 500016, India • **ITALY** /JEOL (ITALIA) S.p.A. Palazzo Pacinotti - Milano 3 City, Via Ludovico il Moro, 6/A 20079 Basiglio(MI) Italy • **KOREA** /JEOL KOREA LTD, Dongwoo Bldg, 7F, 1443, Yangjae Daero, Gangdong-Gu, Seoul, 05355, Korea • **MALAYSIA** /JEOL (MALAYSIA) SDN.BHD. 508, Block A, Level 5, Kelana Business Center, 97, Jalan SS 7/2, Kelana Jaya, 47301 Petaling Jaya, Selangor, Malaysia • **MEXICO** /JEOL DE MEXICO S.A. DE C.V. Arkansas 11 Piso 2 Colonia Napoles Delegacion Benito Juarez, C.P. 03810 Mexico D.F., Mexico • **QATAR** /Mannai Trading Company W.L.L. ALI Emadi Complex, Salwa Road P.O.Box 76, Doha, Qatar • **RUSSIA** /JEOL (RUS) LLC Office 351, floor 3, 23, Novoslobodskaya St, Moscow 127055, Russia • **SCANDINAVIA** /SWEDEN JEOL (Nordic) AB Hammarbacken 6A, Box 716, 191 27 Sollentuna Sweden • **SINGAPORE** /JEOL ASIA PTE.LTD, 2 Corporation Road #01-12 Corporation Place Singapore 618494 • **TAIWAN** /JIE DONG CO., LTD, 7F, 112, Chung Hsiao East Road, Section 1, Taipei, Taiwan 10023 (R.O.C.) • **THE NETHERLANDS** /JEOL (EUROPE) B.V. Lireweg 4, NL-2153 PH Nieuw-Vennep, The Netherlands • **USA** /JEOL USA, INC, 11 Dearborn Road, Peabody, MA 01960, U.S.A.

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