

Solutions for Innovation

# **JNM-ECZR series**

# NMR spectrometer Z





# World's Latest • Next Generation NMR Spectrometer

# NMR spectrometer Z

**JNM-ECZR** series

The JNM-ECZR NMR spectrometer (JNM-ECZR series), a member of the JNM-ECZ series of instruments, is a new research system that fully incorporates the latest digital and high frequency technologies.

Highly reliable, yet in a more compact size made possible by incorporating advanced integrated circuits, it supports even greater expandability options than past models for multi-channel operation, high power amplifiers and other accessories.

The bus line for control of attachments has been upgraded to even higher speed and enables highly accurate and rapid control.





### **Major Features**

#### Two JNM-ECZs

The JNM-ECZ series has two models; the high-end model (JNM-ECZR) offering wide expandability, and the entry level model (JNM-ECZS) with the same characteristics but in an ultra-compact chassis. Please discuss with your local JEOL representative to select which model is optimized for your purpose.

#### Highly stable spectrometer enabling high speed and high accuracy

The JNM-ECZ NMR spectrometer is equipped with JEOL RESONANCE's newly-developed Smart Transceiver System (STS), which uses a fusion of the latest integrated digital circuit and high frequency technologies. By fully implementing the multi-sequencer which has been cultivated from earlier models, it can manage 8 frequency sources as standard. All frequency sources are freely and simultaneously controllable for phase, amplitude and frequency at high switching speeds.

The single board STS employed in the JNM-ECZ series provides long-term reliability of spectrometer, measurement stability, high digital accuracy of all transmitter and receiver frequencies, as well as contributing to the substantial downsizing of the spectrometer. It can not only execute all pulse programs used in routine work, but also execute very complex pulse programs with ease. Pulse sequence editing is also possible for pulse programs developed in the future.

#### **Excellent Expandability**

The STS transceiver consists of a single circuit board that can be described as an NMR system by itself, and can transmit 8 frequencies. However, in the JNM-ECZR model, the STS itself can be expanded to control more than 30 frequencies and yet is still contained within the compact spectrometer chassis. This high degree of expandability gives JNM-ECZR the ability to accommodate future hardware requirements.

#### An NMR in the Network Age

With the JNM-ECZ series, the spectrometer and workstation each have their own independent computers, being connected through a network. Therefore, measurements are possible by any authorized computer and user on the network. Since the spectrometer computer executes all measurements and initial data storage, it does not have any problem in continuing measurement and storage in the event of a network failure.

#### Hardware

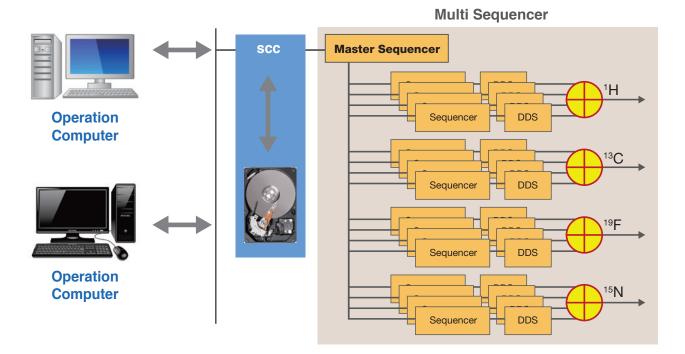
# Spectrometer Control Computer

The JNM-ECZ spectrometer control computer (SCC) is a high performance computer with large capacity hard disc, and is used for execution of pulse sequences, signal-to-noise calculation during measurement, storage of data, data processing, etc. are all possible and independent of the workstation.

All measured data is written to the SCC hard disc without fail, thus the SCC also serves as a data server.

Even if there is any kind of failure to the workstation computer or network during sequential measurements, all measurements that were submitted will be executed normally and the results will be written to the SCC's disc.

Even in a multi-user environment where many users require different measurements and processing, stable operation of the instrument is assured.



#### Multi-Sequencer

The sequencer controls RF, lock and PFG channels during pulse sequence execution. The JNM-ECZR spectrometer can use multiple slave sequencers which control each of these channels, and a master sequencer which synchronizes all slave sequencers. Individual slave sequencers can execute pulse sequences irrespective of synchronous or asynchronous fashion. Thus, by controlling several slave sequencers by the master sequencer, any NMR pulse sequence can be carried out.

Hence, the JNM-ECZR spectrometer can accommodate up to 8 nuclei, 32 frequency sources and PFG simultaneously. It can compile and execute any complex pulse sequence, even those that may be developed in the future.

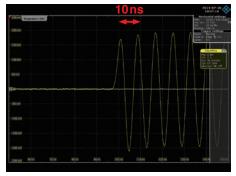
# STS (Smart Transceiver System)

The Smart Transceiver System (STS) is a highly advanced integration of RF sequencer, DDS (Direct Digital Synthesizer), FSU (Frequency Synthesizer Unit), transmitter, receiver, acquisition unit and gate control unit into a single transceiver board. This is equivalent to integrating the basic composition of an NMR system onto one board. The standard instrument composition is one source with 2 nuclei, 8 frequencies and one receiver.

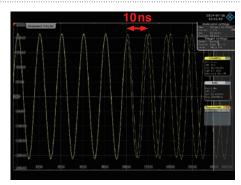
The JNM-ECZR spectrometer can accommodate up to four RF transceiver boards, and so can support 8 nuclei, 32 frequencies and 4 receivers.

# Highly Precise Digital Control

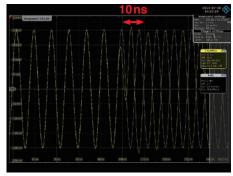
The STS used in the JNM-ECZR spectrometer realizes control at the highest speed for frequency, phase and amplitude modulation, with a control time resolution of just 5 ns. This high speed digital control is extremely useful for high speed phase modulation pulses which are required for the most recent NMR pulse sequences. The same time control performance is offered for various external systems.



JNM-ECZ Amplitude modulation 0 → 100 %



JNM-ECZ Frequency modulation 0 ( without modulation) → 10 MHz (with modulation)



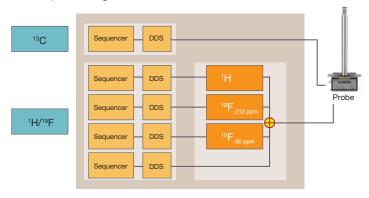
JNM-ECZ Phase modulation 0 → 180 °

## High Performance DDS

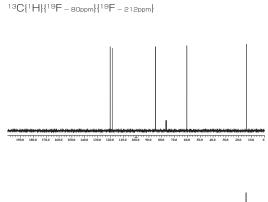
The DDS (Direct Digital Synthesizer) unit of the JNM-ECZ spectrometer available from the STS, can create a very wide offset range.

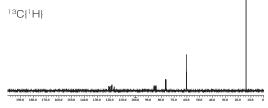
Using an appropriate probe, this enables a triple-resonance measurement with the standard instrument. For example, <sup>13</sup>C{<sup>1</sup>H}{<sup>19</sup>F} measurement is possible with the standard configuration of JNM-ECZ spectrometers.

Example of configuration for ROYALPROBE™ HFX



<sup>1</sup>H and <sup>19</sup>F RF pulses can be output at the same time.





 $^{13}C$  spectra of CF3CH(F)CF2OCH2CH3 measured on JNM-ECZ400R (one RF module only) and ROYALPROBETM HFX.

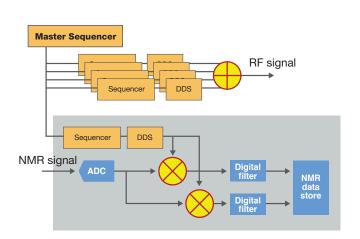
#### Receiver

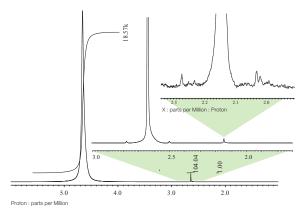
The receiver of the JNM-ECZ spectrometer is controlled by the sequencer. A reference frequency generated in the receiver can be dynamically modulated for phase and amplitude even during FID sampling.

DQD (Digital Quadrature Detection) by high speed A/D conversion at 16 bit 100 Msps, not only improves the effective dynamic range for quantization noise, but also reduces unwanted signals such as IMD (InterModulation Distortion), by over-sampling at high rates.

In addition, the digital receiver filter optimized for NMR ensures accurate quantitative results.

The high dynamic range of the JNM-ECZ spectrometer enables the observation of very small signals. The  $^{13}$ C satellite signals of acetone in a mixed sample of  $H_2O$ : DMSO: acetone = 18,570: 104: 1 (with small amount of  $D_2O$ , ca 10%) are clearly observed which corresponds to a dynamic range of approx. 1: 3,400,000.



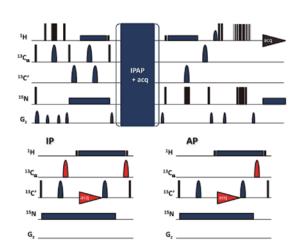


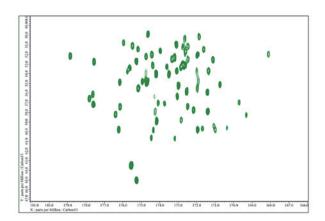
As the natural abundance of  $^{13}$ C is 1.1%, and hence the intensity of each  $^{13}$ C satellite is 0.55%, the figure shows that a dynamic range of approximately 1:3,400,000 has been achieved.

JNM-ECZR spectrometers have one receiver as standard. However, as receiver is a part of RF module, by installing additional RF module(s), JNM-ECZR spectrometers may have 2-4 receivers.

Importantly, JNM-ECZR spectrometers can control multiple receivers flexibly.

The figure shows an example of one experiment that collects 2D <sup>13</sup>C-detected data and 3D <sup>1</sup>H-detected data simultaneously.





Pulse sequence for parallel 2D (H)CACO / 3D (H)CA(CO)NH experiment  $^{\star 1}.$ 

<sup>13</sup>C detected 2D (H)CACO spectrum of <sup>13</sup>C /<sup>15</sup>N labelled ubiquitin acquired in parallel with 3D (H)CA(CO)NH spectrum.

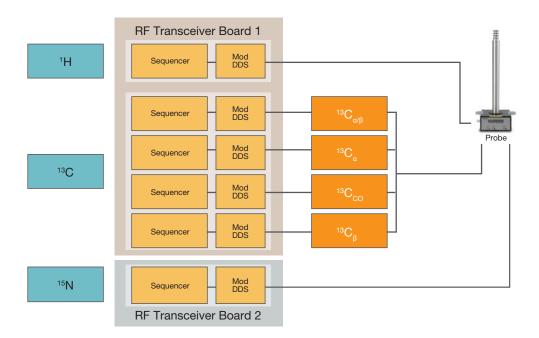
Spectrometer: JNM-ECZ900R

Sample: 1 mM <sup>13</sup>C/<sup>15</sup>N labelled ubiquitin in 90% H<sub>2</sub>O / 10% D<sub>2</sub>O

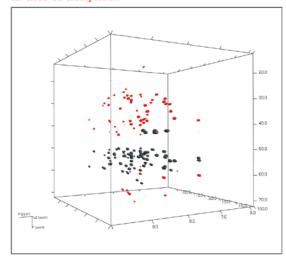
\*1 Kupce E., Kay L. E., Freeman R., J. Am. Chem. Soc., 132, 18008-18011(2010).

# Multi-sequencer and Multi-dimensional NMR measurement

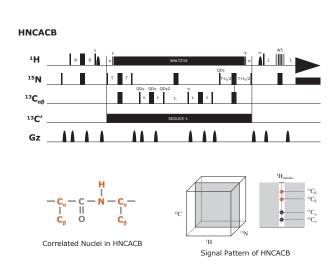
The JNM-ECZR spectrometer can control up to four RF sources, thus 8 nuclei and 32 frequencies, using the multi-sequencer method, with each RF source controlling 2 nuclei and 8 frequencies. Intelligent control of multiple RF sources enables not only highly precise execution of complex multi-dimensional NMR measurements, but allows the use of parallel expressions within the pulse sequence. In addition, by using conditional statements within a pulse sequence, more than one experiment is possible using the same pulse sequence program.



#### HNCACB 3D cube spectrum



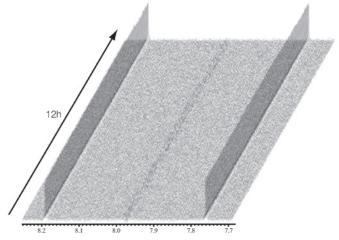
 $^{13}C/^{15}N$  doubly enriched ubiquitin 90%  $H_2O\,/\,10\%\,D_2O$ 



# Digital NMR Lock Circuit

Application of STS technology provides high precision and high speed digital control of the <sup>2</sup>H lock. This new digital feedback circuit offers extremely efficient control of the magnetic field against external modulation.

The precise digital lock feedback mechanism thus enables highly stable operation for protracted measurements.



Hetero spin echo measurement of 1 % chloroform.

### Shimming

Gradient shimming uses pulsed field gradients to determine magnetic field distribution inside NMR sample and instantaneously calculates optimal shim values.

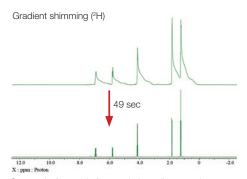
The higher order shim adjustment, which conventionally takes a few hours of manual shimming to a skilled service engineer, can be optimized in a very short period of time.

Even for samples of various height or samples dissolved in various solvents, gradient shimming runs automatically and always delivers high-resolution NMR spectra.

In the case of solvents which have more than one signal, such as methanol- $d_4$  and toluene- $d_8$ , gradient shimming employs selective pulses. In addition to  ${}^2\text{H}$  signal, gradient shimming can also use other nuclei, such as  ${}^1\text{H}$  and  ${}^{19}\text{F}$ . Therefore, high resolution can automatically be adjusted on samples dissolved in non-deuterated solvents.

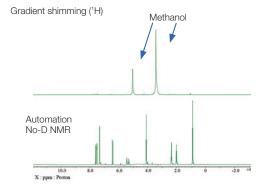
The 3D gradient shimming, which was firstly implemented into Delta V5.2, can be used to optimize both axial and radial shims.

For this reason, it has become possible to adjust high resolution easily no matter how poor starting condition is.

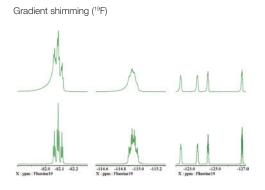


Spectra before and after resolution adjustment by gradient shimming.

High resolution has been achieved in 49 sec.



No-D NMR measurement using resolution adjustment by selective pulse gradient shimming where the solvent has multiple signals (top). Solvent signal is automatically suppressed by the 'WET' method (bottom).

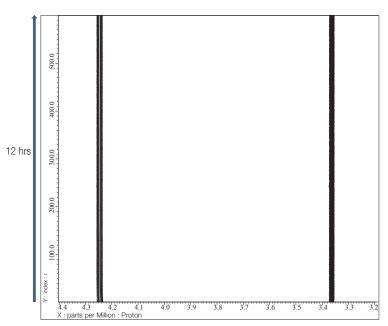


Resolution adjustment is possible by gradient shimming in the same manner as <sup>2</sup>H, by selecting the <sup>19</sup>F signal.

# Temperature Control System

The temperature control system enables stable measurements using a newly-designed heater with improved response. The JNM-ECZ spectrometer allows faster and more stable operation of peripheral devices using the new high speed bus control line.





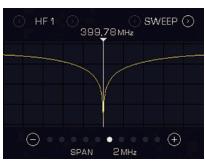
Chemical shift change of CH2 group and OH group of ethylene glycol with time (40  $^{\circ}\text{C}$  ).

# **Head Amplifier Chassis**

The head amplifier chassis has various functions related to probe and the superconducting magnet. A touch-panel display is located on top of the head amplifier chassis, offering an intuitive user interface. During probe tuning, reflection dip and reflection value are indicated, whilst during cryogen refilling, the actual level of cryogen in the magnet is indicated in real time. It makes the routine maintenance related to probes and superconducting magnet convenient and efficient.



Head Amplifier Chassis



Indication of reflection dip when probe tuning.



Indication of remaining quantity when refilling Helium.

## **Power Amplifier**

The Power Amplifier amplifies the RF pulse and outputs it to the probe. Various models are available depending on the purpose but all power amplifiers exhibit excellent linearity and response performance.

The JNM-ECZ spectrometer is designed so that the power amplifier keeps constant thermal stability, regardless of output / non-output of RF pulses. Thus stable RF output is achieved for every kind of measurement, regardless of number of pulses, pulse widths, intervals etc. used within the pulse sequence.

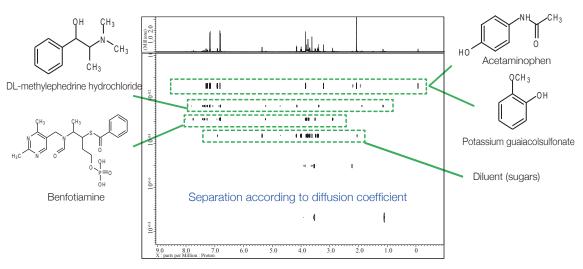
HF (High Freq.)	LF (Low Freq.)	Remarks
100 W	300 W	Standard PA for liquids & solids
200 W	500 W	Middle PA for liquids & solids
500 W	1,000 W	High PA for advanced solids

## PFG (Pulsed Field Gradient)

PFG (Pulsed Field Gradient) control by STS (Smart Transceiver System) technology offers technical advantages. The new PFG control offers higher precision and stability for measurements that require highly precise control such as DOSY, etc.

#### **PFG** Amplifier

For the JNM-ECZR series, two models of PFG amplifier with different power outputs, 10 A and 30 A, are available. Please discuss with your local JEOL representative which is more suitable for your application.



DOSY spectrum of a readily available cold medicine

# Superconducting Magnet "JJ series"

The JJ series of superconducting magnets are compact, low-cryogen-consumption magnets made with newly-developed superconducting wire and cryostat. Compared to alternative products, the footprint is smaller and the minimum ceiling height is reduced. The consumption of liquid helium has also been reduced and the interval for refill is correspondingly longer. The shield coil used in the JJ series not only blocks magnetic leakage from inside to outside, but also prevents magnetic field modulation from outside to inside, thus minimizing any impact on measurement. Magnets installed on JEOL's anti-vibration mounts have proven to be completely reliable in reducing damage to a minimum in different types of disaster.

400JJYH is a year-hold 400 MHz magnet which reduces the frequency of helium refill to just once each year.

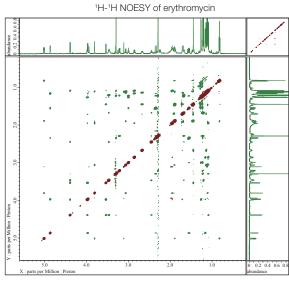


# World's First Practical Realization, Zero Boil-off Superconducting Magnet "ZB series"

The world's first practical NMR system using a **zero boil-off** superconducting magnet, free from cryogen refills, has been achieved. This magnet prevents evaporation of the superconducting magnet cryogen by condensing and re-circulating the helium. In addition, the use of JEOL's unique anti-vibration mechanism removes any vibration from the refrigeration unit so ensures that the magnet can be used for any measurements in the same way as a conventional superconducting magnet.

Available for 400 MHz and 600 MHz.





Magnet: ZB600

## Versatile Auto Sample Changers

At laboratories where many samples are measured daily, auto sample changers are essential for efficient sample management. Fully supported by the auto measurement function of Delta, a reliable, safe and powerful combination is established. As JEOL's auto sample changers are designed to be free from direct handling of the NMR sample tube, safe transfer of the sample tube of various diameters and forms is assured. The JackBean series (30, 64, or 100 samples) transfers the sample using a manipulator, whilst the ASC24 (24 samples) is located on top of an SCM. Safely and reliably operating 24/7 and without the need for a step ladder, the compact JackBean series perfectly complements JNM-ECZ spectrometers whilst positively contributing to laboratory safety.

#### JackBean series







ASC64 (64 samples model)



ASC100 (100 samples model)



ASC24 (24 samples model)

The ASC24 sample changer is a carousel type and is located on top of the SCM, so no additional installation area is required. The exchangeable sample trays allow advance preparation of multiple trays of samples.



#### Pre-Cool ASC30

Pre-Cool ASC30 keeps samples at a low temperature of around 4 °C in order to prevent unstable samples from degradation.

It is a must-have accessory for food and biological samples requiring storage at low temperature.

### JEOL's High Sensitivity Probes

The JNM-ECZ series is compatible with many types of probes:

The standard room temperature solution NMR probe is the ROYALPROBE™ which delivers optimum sensitivity for both ¹H and ¹³C.

The brand-new ROYALPROBE<sup>TM</sup> HFX is the world's first state-of-the-art probe which can be switched between double-resonance and triple-resonance modes. This probe is essential to researchers who extensively study fluorinated compounds.

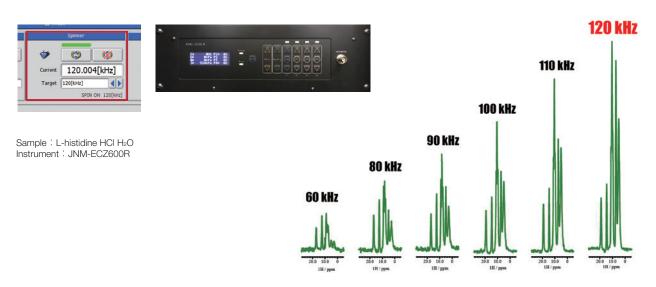
The JNM-ECZ series is also compatible with many optional probes, such as the UltraCOOL probe, a cryogenically cooled system giving highest sensitivity; the SuperCOOL probe, a liquid nitrogen cooled system that enables high sensitivity, and GR probe for experiments using high power gradient pulses.



# Solid-State NMR Measurements

Indeed, JNM-ECZR series can run not only solution-state NMR experiments but also various solid-state NMR experiments. It supports a wide variety of solid-state NMR probes, such as the world's fastest 0.75 mm (o.d.) probe, ultrafast 1 mm probe, easy-to-use 2 mm, 3.2 and 4 mm HXMAS probes, large-sample-volume 8 mm probe, FGMAS probe for semi-solid samples, and so forth.

The newly developed MAS controller can control sample spinning from low to very high spinning speed safely and stably. In combination with high-speed and high-accuracy RF control of JNM-ECZR spectrometers, any solid-state NMR experiment can be executed efficiently.



#### **AUTOMAS Probe**

The newly developed AUTOMAS probe and ROTORCARRIER™ bring the usability of solution NMR probes to solid-state NMR spectroscopy\*1.

The ROTORCARRIER $^{TM}$ , which is of similar shape as a sample holder for solution NMR, stores the solid-state NMR sample tube (rotor), and carries it from the top of SCM or ASC to the probe.

The AUTOMAS probe receives the sample tube from the rotor carrier and automatically adjusts Magic Angle.

As the AUTOMAS probe also has the automatic tuning function, all operations including sample loading, sample spinning, temperature control, probe tuning and experiment can be done in a fully automated way.

The innovative point of AUTOMAS probe and ROTORCARRIER™ is that solution and solid state can share the same auto sample changer\*2.







<sup>\*1</sup> Compatible with the JNM-ECZ series only. MASCONT improvements may be required in some cases.

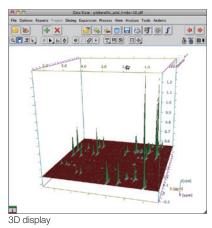
<sup>\*2</sup> Compatible Auto Sample Changers are ASC24 and JackBean 30, 64, 100 only.

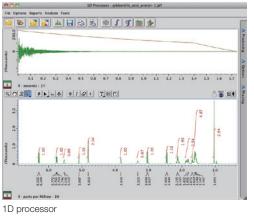
#### Software

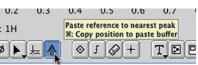
#### The most powerful NMR data processing software - "Delta"

Waveform separation

The control and data processing software "Delta" used by JNM-ECZ spectrometers is supplied with excellent and simple auto measurement functions. After setting the sample, enter simple information and click the button. Then, everything will be done by Delta and spectrometer, from sample transfer, tuning, resolution adjustment, measurement, data processing, to printing the result. The standard auto measurement functions provided have not only one dimensional measurements including <sup>1</sup>H, <sup>13</sup>C, etc., but also include two dimensional NMR measurements. Additional NMR measurements such as variable temperature, multi-nuclear NMR, and time-scheduled measurements can be customized with perfect freedom; therefore it is useful not only in day time, but highly effective at night and weekends. You can safely and confidently leave your daily NMR measurements with Delta.







Pop up help

# Overlay display Linked to the Natural Organic Compound NMR Database " CH-NMR-NP"

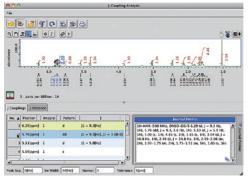
Delta is compatible with the natural organic compound NMR database "CH-NMR-NP" by Dr. Kikuko Hayamizu. With Delta, a direct comparison of the search result from CH-NMR-NP and the observed spectrum is possible. With data in Delta format, manual input of chemical shifts is not required.

\*CH-NMR-NP is an NMR database of natural organic compounds, and is available free of charge at the JEOL web site. (http://www.jeol.co.jp/en/)

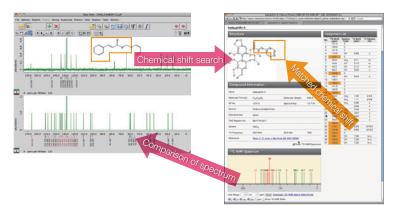
# Assistance for Reporting

The J-coupling analysis tool can analyze coupling patterns and determine J-coupling constants immediately once peak picking and peak integrals are loaded.

The result of multiplet analysis can be corrected within the tool, and the generated text can be copied to clipboard or saved in a text format.



J-coupling analysis tool



#### **Smart Mode**

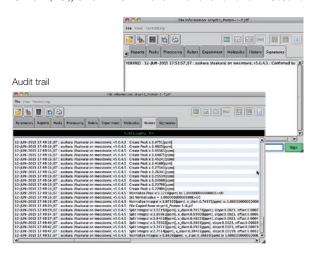
This is a measurement mode with exceptionally easy operation. Information of sample, slot, job, queue and method can be confirmed on one screen. It is suitable for many types of measurement including one dimensional experiments such as proton and carbon, and also fully supports routine two dimensional experiments.



Smart mode

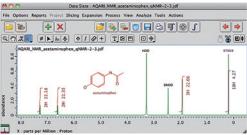
# Audit Trail & Electronic Signature

Delta is equipped with functions necessary for electronic recording and electronic signature compliant with ER/ES guidelines of the Ministry of Health, Labor and Welfare, ANNEX 11 of European Union (EU), and 21 CFR Part 11 of the F.D.A. in U.S.A.



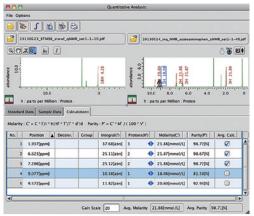
#### Various Quantitative NMR Methods

Delta is also equipped with the qNMR module. Once the number of protons for each signal is defined, the concentration ratio of each component is automatically calculated instead of displaying the more general integration value.



Spectrum of qNMR mode

The quantitative analysis tool supplied with Delta can easily calculate concentration and purity, not only using AQARI (Internal standard reference), but also using an external standard reference such as PULCON.



Quantitative analysis tool

#### Free Download

Delta, the standard data processing software of the JNM-ECZ NMR spectrometer, is free to download from the JEOL web site (http://www.jeol.co.jp/en/) \*1.

Available for both Windows® and Mac OS X, it is exactly the same software as that supplied with an instrument, and most data processing functions can be performed on your PC \*2. A soft copy of the user's manual is included and tutorial movies are also available from the web site. As Delta also supports various non-JEOL data formats, you can enjoy the analysis of NMR data at your own desk \*3.

- \*1 User registration (free of charge) on the web site is required for continuous operation. Free software is offered without support.
- \*2 Depending upon the many different configurations where Windows® or Mac OS X is installed, there is a possibility that Delta does not work properly depending on the configuration and performance of the PC used.
- \*3 For non-JEOL data, Delta software can apply basic FID data processing. Also, in data formats other than JEOL format, some special operations may be needed in processing the data.

Windows is either the registered trademark or trademark of Microsoft Corporation in the United States and/or other countries.

Mac and OS X are trademarks of Apole Inc.

#### Installation requirements

Unit Supply capacity, breaker and grounding Spectrometer Single-phase, AC 100-240 V, 50/60 Hz, 3 kVA Single-phase, AC 100-240 V, 50/60 Hz, 1 kVA Data system Air compressor (400 MHz) Single-phase, AC 100 V, 50/60 Hz, 15 A Air compressor (≥500 MHz) Three-phase, AC 200 V, 50/60 Hz, 15 A Auxiliary Single-phase, AC 100/120 V, 50/60 Hz, 3 kVA

Grounding 100  $\Omega$  or less (1x)

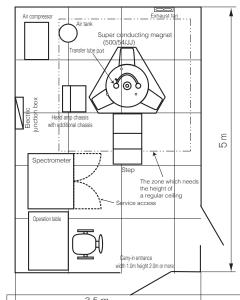
Note: Long-term low temperature air supplier (optional) requires separate power supply.

500 MHz Installation Room

Temperature Range 17 to 27 °C (±1 °C /h)

Humidity 70% or less Ceiling Height 2.87 m or more

0.5 mT (5 Gauss) position From SCM center, vertical 1.15 m; horizontal 0.6 m



Certain products in this 37c5nt/fe are controlled under the "Foreign Exchange and Foreign Trade Law" of Japan in compliance with international security export control. JEOL Ltd. must provide the Salan set in Conjunctual at with "Enclars spic Statement of Assurance" and "End-use Certificate" in order to obtain the export license needed for export from Japan. If the product to be exported is in this category, the end user will be asked to fill in these certificate forms.



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