



JEOL Delta acquisition and Jason processing

# New NMR software

13<sup>th</sup> June 2024

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JEOL UK Demo Lab

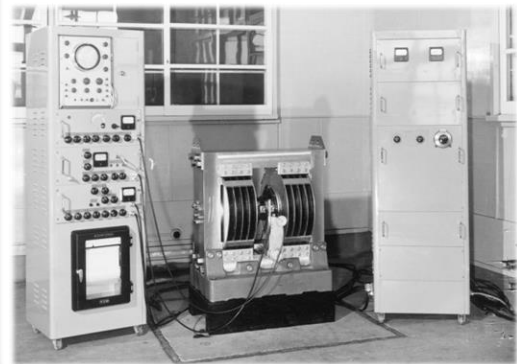
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# Some highlights of JEOL NMR history

**1956**

JNM-1 (32MHz commercial NMR)



**1972**

JNM-FX60 (Fourier Transformed NMR)



**1981**

JNM-GX400

(First automated NMR)



**1985:** First autotunable probe

**1996:** First Windows NMR software

**2005:** First Mac NMR software

**2016:** First liquid state autotunable probe with both double and triple resonance modes

**2002**

JNM-ECA series

(Modular NMR with sequencers and full automation)



**2014**

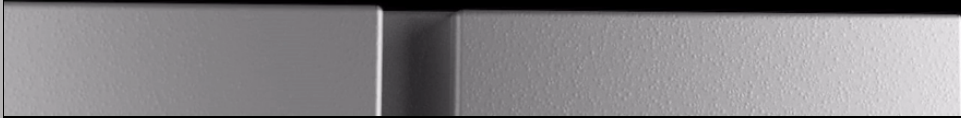
JNM-ECZ series

(Transceiver system)



And in 2021 ...

**JEOL ECZL**  
**spectrometer**  
see NMR in a new light



# User management



# Automation setup

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## **Flexible configuration of defaults and privileges**

### **for different users, including:**

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

# Automation setup

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## Flexible configuration of defaults and privileges

### for different users, including:

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

## Usage reports, logs, statistics and billing:

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

# Automation setup

## Flexible configuration of defaults and privileges

### for different users, including:

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

## Usage reports, logs, statistics and billing:

Detailed output:

* Breakdown of folder 'demo'														
Operation Began	Operation End	Duration	Duration/day	Username	Job Name	Experiment Began	Experiment End	Experiment Duration	Experiment Duration/day	Experiment	Project Name	Folder	Filename	Job Result
14-12-22 23:14	14-12-22 23:14	0 days 00:00:00	0.00037037	demo	Proton	14-12-22 23:14	14-12-22 23:14	0 days 00:00:18	0.000208333	proton.jpg		demo	test1_1H	FINISHED
15-12-22 10:19	15-12-22 10:19	0 days 00:00:00	0.000208333	demo	Proton	15-12-22 10:19	15-12-22 10:19	0 days 00:00:08	9.25926E-05	proton.jpg		demo	sample1_1H	FINISHED
21-01-23 21:46	21-01-23 21:46	0 days 00:00:00	0.000300926	demo	Proton	21-01-23 21:46	21-01-23 21:46	0 days 00:00:18	0.000208333	proton.jpg		demo	aa1_1H	FINISHED
* Breakdown of folder 'organometallic/PhD_1'														
Operation Began	Operation End	Duration	Duration/day	Username	Job Name	Experiment Began	Experiment End	Experiment Duration	Experiment Duration/day	Experiment	Project Name	Folder	Filename	Job Result
29-06-23 9:38	29-06-23 9:38	0 days 00:00:00	0.000243056	test	1H	29-06-23 9:38	29-06-23 9:38	0 days 00:00:10	0.000115741	proton.jpg		organome	sampl3_PROTON	FINISHED
* Breakdown of folder 'organometallic/PhD_2'														
Operation Began	Operation End	Duration	Duration/day	Username	Job Name	Experiment Began	Experiment End	Experiment Duration	Experiment Duration/day	Experiment	Project Name	Folder	Filename	Job Result
16-12-22 19:21	16-12-22 19:21	0 days 00:00:00	0.000196759	test2	1H	16-12-22 19:21	16-12-22 19:21	0 days 00:00:10	0.000115741	proton.jpg		organome	fds_PROTON	FINISHED



# Automation setup

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

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

## Usage reports, logs, statistics and billing:

JEOL Instrument:	Virtual_spectrometer			
Usage Log Report:	1-AUG-2022 - 18-AUG-2022			
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demo	<blank>	35	10.00	5.83
test	<blank>	2	0.00	0.00
		<b>300</b>		<b>5.83</b>

## Custom time limitations:

The screenshot shows the 'Time Limits' configuration window in the JEOL Scheduler tool. It features a 24-hour clock interface with a color-coded legend on the right. The legend includes options for 'Prohibited', '00:15', '00:30', '00:45', '01:00', '01:15', '01:30', '02:00', '03:00', '05:00', and 'Unrestricted'. A text box provides instructions: '1. Adjust the time limits in the legend on the right. 2. Select a desired time limit by clicking on the corresponding color button. 3. Click and drag the mouse on the twenty-four hour schedule area above to designate a portion of the day that will limit jobs by their expected duration. \* Policy changes will take effect when the Scheduler tool is closed.'

# Automation setup

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

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

**Usage reports, logs, statistics and billing:**

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

**Custom time limitations:**

1. Adjust the time limits in the legend on the right.  
2. Select a desired time limit by clicking on the corresponding color button.  
3. Click and drag the mouse on the twenty-four hour schedule area above to designate a portion of the day that will limit jobs by their expected duration.  
\* Policy changes will take effect when the Scheduler tool is closed.

**Fully customizable methods for each user**

**User 1**

Method: Proton assay  
QC check

Parameters: comment: 1:07

**User 2**

Method: 1. 1H  
2. 13C  
3. 1H & 13C  
4. 1H, 13C & COSY  
5. 1H, 13C, COSY & edHSQC  
6. 1H, 13C, COSY, edHSQC, HMBC  
7. 1H, COSY, edHSQC, HMBC  
8. Quantitative Carbon  
9. DEPT  
10. Edited Dept  
11. COSY  
12. DQF COSY  
13. TOCSY  
14. NOESY  
15. ROESY  
16. HMQC  
17. HSQC  
18. HMBC  
19. Selective NOESY 1D  
20. Selective TOCSY 1D  
21. Selective ROESY 1D

Parameters: 4:16

- calculate\_proton\_90
- force\_tune
- dual\_tuned
- autogain
- receiver\_gain: 0
- scans: 16
- dummy\_scans: 0
- tip\_angle: 45[deg]
- x\_offset: 5[ppm]
- x\_sweep: 15[ppm]
- data\_points: 32768
- relaxation\_delay: 4[s]

# Persona manager

Authorization Manager: ECZL400R

Master ECZL400R :: 192.168.1.65:6241

Authorized Users Personas Billing Rates Authorized IP Masks

demo  
gmp\_operator  
solids  
solids\_student

Base Privilege

- Variable Temperature
- Console
- Solids
- Connection
- Samples
- Owner
- Privilege
- Multiple Owner
- Read (Data Server)
- Write (Data Server)

IP Mask

Job Priority low

Billing Rate Standard

New persona name

Permissions Custom Attributes

Automation Scripts

- Load Automation scripts student\_solids.jaf
- Do not load the standard Automation script
- Do not auto-load global Automation scripts ("Load Scripts" Delta preference)
- Do not allow loading of additional Automation scripts
- Override Automation Walkup mode script student\_solids.jaf

Experiment View

- Hide experiment Header parameters tab  Prevent editing
- Hide experiment Instrument parameters tab  Prevent editing
- Hide experiment Acquisition parameters tab  Prevent editing
- Hide experiment Pulse parameters tab  Prevent editing
- Hide experiment Diagram tab
- Hide experiment Favorites tab

Experiments

- Disallow adding experiments to Jobs in Advanced mode
- Disallow adding experiments to Jobs in Smart mode
- Disallow adding parameters to Experiments

- Disallow adding parameters to Experiments

Jobs

- Disallow Automation Job and Experiment submission
- Disallow early termination of Jobs
- Disallow early termination of Experiments
- Disallow changing order of Jobs in queue
- Submit all Jobs with the specified policy Choose a scheduling policy

Samples

- Hide Sample table attributes  Prevent editing
- Disallow customization of the Sample table columns
- Disallow customization of the Sample attribute order
- Disallow Sample attribute customization

Instrument

- Disallow interactive Instrument control

# Persona manager

Authorization Manager: ECZL400R

Master ECZL400R :: 192.168.1.65:6241

Authorized Users | **Personas** | Billing Rates | Authorized IP Masks

demo  
gmp\_operator  
solids  
**solids\_student**

Base Privilege  Variable Temperature

Console  Solids

Connection  Samples

Owner  Privilege

Multiple Owner  Read (Data Server)

Write (Data Server)

IP Mask

Job Priority low

Billing Rate Standard

New persona name

Permissions | Custom Attributes

**Automation Scripts**

Load Automation scripts student\_solids.jaf

Do not load the standard Automation script

Do not auto-load global Automation scripts (\*Load Scripts' Delta preference)

Do not allow loading of additional Automation scripts

Override Automation Walkup mode script student\_solids.jaf

**Experiment View**

Hide experiment Header parameters tab  Prevent editing

Hide experiment Instrument parameters tab  Prevent editing

Hide experiment Acquisition parameters tab  Prevent editing

Hide experiment Pulse parameters tab  Prevent editing

Hide experiment Diagram tab

Hide experiment Favorites tab

**Experiments**

Disallow adding experiments to Jobs in Advanced mode

Disallow adding experiments to Jobs in Smart mode

Disallow adding parameters to Experiments

Disallow adding parameters to Experiments

**Jobs**

Disallow Automation Job and Experiment submission

Disallow early termination of Jobs

Disallow early termination of Experiments

Disallow changing order of Jobs in queue

Submit all Jobs with the specified policy Choose a scheduling policy

**Samples**

Hide Sample table attributes  Prevent editing

Disallow customization of the Sample table columns

Disallow customization of the Sample attribute order

Disallow Sample attribute customization

**Instrument**

Disallow interactive Instrument control

Authorization Manager: ECZL400R

Master ECZL400R :: 192.168.1.65:6241

Authorized Users | **Personas** | Billing Rates | Authorized IP Masks

Username	Persona	Priority	Privilege
console			<input type="checkbox"/> Console
default		low	<input checked="" type="checkbox"/> Connection
delta		low	<input checked="" type="checkbox"/> Owner
demo	demo	low	<input type="checkbox"/> Multiple Owner
student_ss1	solids_student	low	<input checked="" type="checkbox"/> Variable Temperature

Solids

Samples

Privilege

Read (Data Server)

Write (Data Server)

New user name

IP Mask Set Password

Persona No Persona

Default Folder No special folder  Login Moniker

Job Priority low Billing Rate Billing rate not set

Email Email address

Alert Email Email address for alerts

Subject w/ Alert Email

# Announcement editor

The screenshot shows a window titled "Spectrometer Announcements" with two announcement entries and a control bar at the bottom. Each entry includes fields for "Event Begin", "Event End", "Show" (days in advance), "Title", and "Message".

Event Begin	Event End	Show (days in advance)	Title	Message
05-JUL-2023	26-JUL-2023	0	Temperature regulation is not allowed	n for any of your experiments, come and see Adolfo
13-JUL-2023	13-JUL-2023	7	Helium refill	No usage during morning. No 2D experiments during

Control bar buttons: Erase Seen List, Add, Save, Close.



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

Push this button to show again.

# Announcement editor

Spectrometer Announcements

Event Begin: 05-JUL-2023  
Event End: 26-JUL-2023  
Show: 0 days in advance  
Title: Temperature regulation is not allowed  
Message: n for any of your experiments, come and see Adolfo

Event Begin: 13-JUL-2023  
Event End: 13-JUL-2023  
Show: 7 days in advance  
Title: Helium refill  
Message: No usage during morning. No 2D experiments during

Erase Seen List Add Save Close

Spectrometer Control - Walkup Mode

Connection Options Tools Config

Available Instruments: ECZL400R

Connect

Name: ECZL400R v6.2

Status: This spectrometer is AVAILABLE

Field Strength: 9.389766[T] ~ 400[MHz]

Queue Status: IDLE

Queue Details: Ready: 0

Click here to hide more information

IP Address: 192.168.1.65 Port: 6241

Probe ID: 2800 Type: LIQUIDS

AQP Version: 1 AQP4 Specs: 16 bits @ 100[MHz]

Helium Level: [Green bar] Unspecified 12-OCT-2022

Nitrogen Level: [Green bar]

Instrument Time: 5-JUL-2023 13:04:20 Time Zone: GMT Daylight Time (UTC + 1 hours)

Boot Time: 5-JUL-2023 12:29:38 Up Time: 34 mins 42 secs

Model # Serial #

Data Server: 97% used

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

Push this button to show again.

# Manual use

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~~Manual use???~~

---

Non-routine use



# Easy multiple decoupling setup

irr_decoupling	
irr_noe	<input checked="" type="checkbox"/>
irr_decoupling	<input checked="" type="checkbox"/>
irr_domain	Proton
irr_noise	WALTZ
irr_atn_noe	26.9[dB] <input type="text" value="irratn_lo"/>
irr_offset	5[ppm] <input type="text" value="irr_offset_default"/>

tri_decoupling	
tri_noe	<input type="checkbox"/>
<b>tri_decoupling</b>	<input checked="" type="checkbox"/>
tri_domain	Fluorine19
tri_noise	WURST_40
tri_atn_noe	26[dB] <input type="text" value="triatn_lo"/>
tri_offset	-200[ppm]

qua_decoupling	
qua_noe	<input type="checkbox"/>
<b>qua_decoupling</b>	<input checked="" type="checkbox"/>
qua_domain	Fluorine19
qua_noise	GARP
qua_atn_noe	26[dB] <input type="text" value="quaatn_lo"/>
qua_offset	-50[ppm]

Just choose nuclei and offsets (and decoupling schemes)  
No need to recalculate pulses

# HMBC $^1\text{H}$ - $^{13}\text{C}$ to HMBC $^1\text{H}$ - $^{11}\text{B}$

y_domain	Carbon13
y_offset	100[ppm]
y_sweep	250[ppm]
default_y_resolution	100[Hz]
y_points	256 <input type="text" value="y_points_default"/>
x_acq_time	0.21345[s]
x_resolution	4.68495[Hz]
y_acq_time	10.02733[ms]
y_resolution	99.72748[Hz]
y_pulse	5[us] <input type="text" value="y90"/>
y_atn	1[dB]
grad_selection	Carbon13 = 1.98847 : 1.98847 : 1

Only change the nucleus.

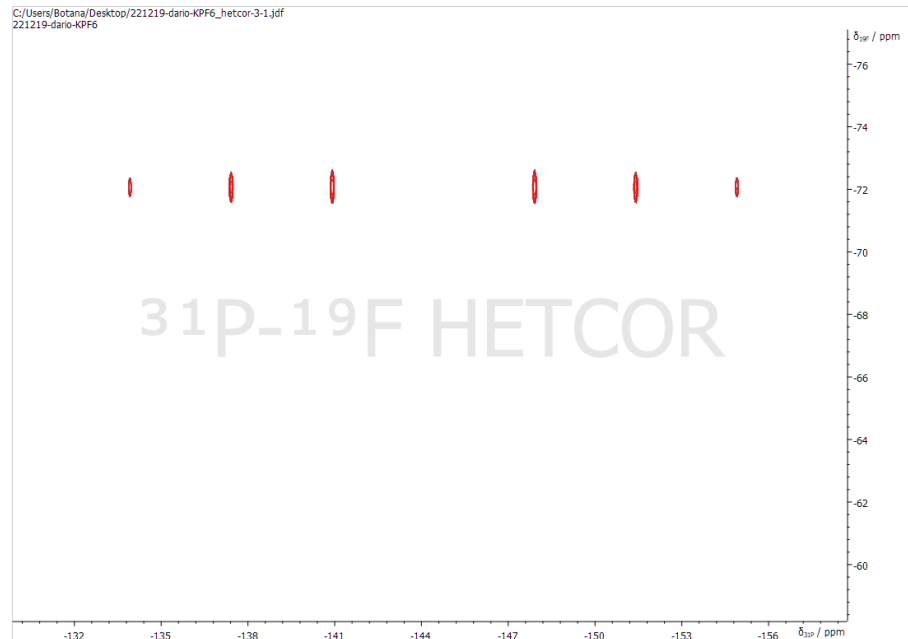
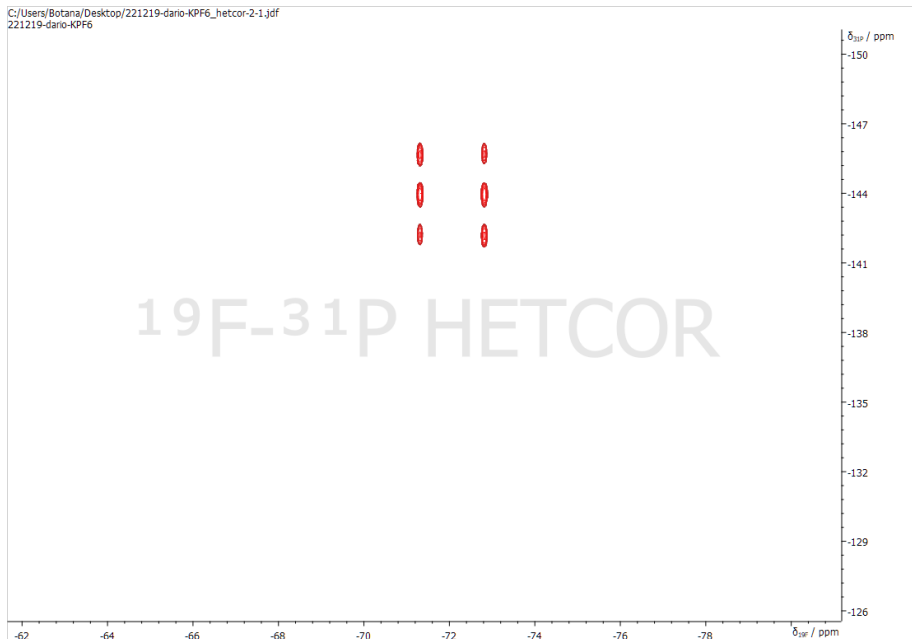
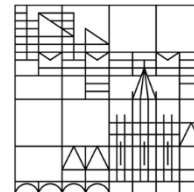
Other related parameters will be automatically calculated!

y_domain	Boron11
y_offset	0[ppm]
y_sweep	250[ppm]
default_y_resolution	100[Hz]
y_points	512 <input type="text" value="y_points_default"/>
x_acq_time	0.21345[s]
x_resolution	4.68495[Hz]
y_acq_time	10.01044[ms]
y_resolution	99.89574[Hz]
y_pulse	7[us] <input type="text" value="y90"/>
y_atn	2[dB]
grad_selection	Boron11 = 1.55841 : 1.55841 : 1

# $^{19}\text{F}$ - $^{31}\text{P}$ and $^{31}\text{P}$ - $^{19}\text{F}$ HETCOR!

Data kindly provided by Dario Rothauer and Ulrich Haunz,  
University of Konstanz

Universität  
Konstanz



# Automation use

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# Spectrometer control Interfaces

## Walkup

- User accessible Methods defined by administrator
- Select slot, put sample information, select the method, and then Go!

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Price Rate	Upload Date	Email Data	Email PCB
1	Sample Name Required			Select a Solvent	Select a Method					
2	Chilled	Chilled		Select a Solvent	Select a Method	25:59				
3	Sample Name Required			Select a Solvent	Select a Method					
4	Sample Name Required			Select a Solvent	Select a Method					
5	Sample Name Required			Select a Solvent	Select a Method					
6	Sample Name Required			Select a Solvent	Select a Method					
7	Sample Name Required			Select a Solvent	Select a Method					
8	Sample Name Required			Select a Solvent	Select a Method					
9	Sample Name Required			Select a Solvent	Select a Method					
10	Sample Name Required			Select a Solvent	Select a Method					

## Smart

- Method shortcuts defined by user as buttons
- Define sample information, select the method, and then Go!

Slot	Sample Name	Solvent	Method
1	linshape	Acetone-D6	3
2	fluoround	DMSO-d6	4
3	fluoround	D2O	15
4	cube	Chloroform-D	2
5	fluoround	DMSO-d6	5

## Advanced

- Easy access to all functions
- Suitable both for continuous work on a sample and for sample batch submission

Slot	Sample Name	Solvent	Slot	End	Shared	Verified	Comp	User	Last Used
1	linshape	Acetone-D6	4	Locals: 4		✓		delta	0 days ago
2	fluoround	DMSO-d6	4	Locals: 4		✓		delta	Recently
3	fluoround	D2O	15	Locals: 6		✓		delta	25 days ago
4	cube	Chloroform-D	2	Locals: 6		✓		delta	2 days ago
5	fluoround	DMSO-d6	5	Locals: 4		✓		delta	Recently

# Walkup mode

Spectrometer Control - Walkup Mode - adolfo-pc

Connection Options Tools Config Queue Samples Columns

User: test1 Logout

Activity Sample: - Job: - Method: - Action: Idle Collected: - Time: - Info

Walk-Up Monitor Status

Current tuning information for Probe is missing or incomplete.

Slot	Status	Sample Name	Solvent	Method	Est. Time	Scheduling	Submit Job
1	⊘						
2	☐	Sample Name Required	Select a Solvent	Select a Method			⊘
3	☐	Sample Name Required	Select a Solvent	Select a Method			⊘
4	☐	Sample Name Required	Select a Solvent	Select a Method			⊘
5	☐	Sample Name Required	Select a Solvent	Select a Method			⊘
6	☐	Sample Name Required	Select a Solvent	Select a Method			⊘
7	☐	Sample Name Required	Select a Solvent	Select a Method			⊘

Status Slot Sample Submit Time Method Visualize Scheduling User Est. End Time

NOAH

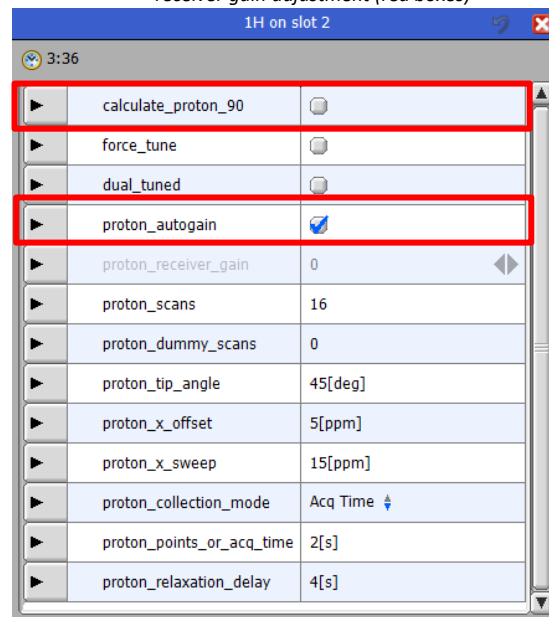
Receiver Gain: 50 Spin: 0[Hz] Lock: 1332 Temp: 25.1[dC] Helium: 50[%] Nitrogen: 75[%] EJECTED No Jobs

# On-the-Fly Parameter Optimization

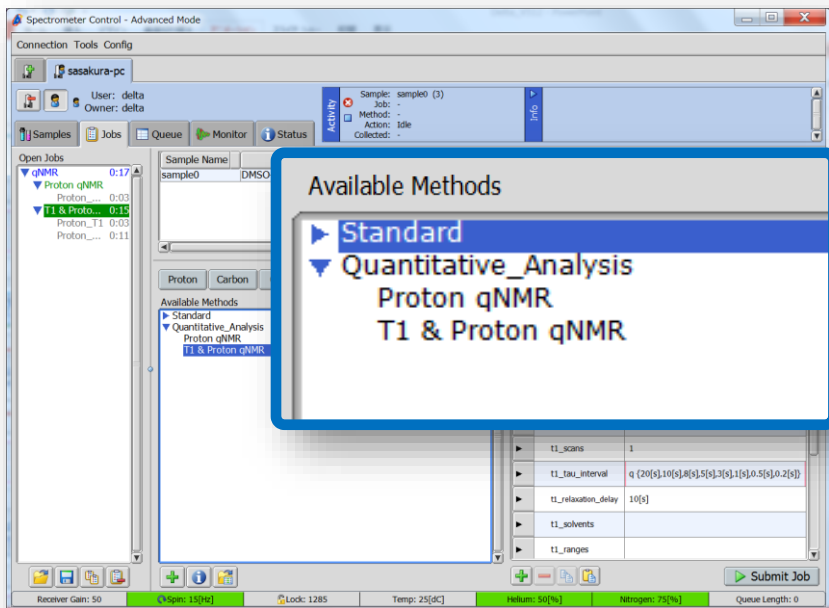
JEOL Delta acquisition software provides a variety of tools for on-the-fly parameter optimization of acquisition parameters, including:

- Fully automated probe tuning and gradient shimming
- Automatic adjustment of receiver gain (autogain)
- Automatic calibration of 90-degree pulse for each sample
- Automatic optimization of  $F_1/F_2$  spectral windows in 2D methods
- Automatic optimization of offset (e.g. for presaturation) in solvent suppression methods
- Automatic determination of signal-to-noise ratio in 1D carbon experiments

*Parameter panel for  $^1\text{H}$  method showing calculate 90-degree pulse and automatic receiver gain adjustment (red boxes)*



# Automation scripts



**T<sub>1</sub> & qNMR (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, etc.)**  
Automatic 90 pulse calibration,  
T<sub>1</sub> measurement first, then  
automatically extract the T<sub>1</sub>  
values to set the relaxation  
delay of the qNMR experiment

**<sup>1</sup>H T<sub>1</sub> & CPMAS**  
Run T<sub>1</sub> measurement first (IR  
or SR), then automatically  
extract the T<sub>1</sub> value to set  
the relaxation delay of  
CPMAS



# Automation for both solid and liquid samples

- **Use the same sample changer for solids and liquids**
- Routine SS-NMR measurements, same as solution NMR.
- Compatible with Narrow Bore Magnets
- **-100°C to +220°C**
- **Auto tuning and magic angle adjustment**
- Up to 100 samples
- **1 mm (0.8uL @ 80kHz) , 3.2 mm (49uL @ 22 kHz) and 8 mm (~600uL @8kHz)**



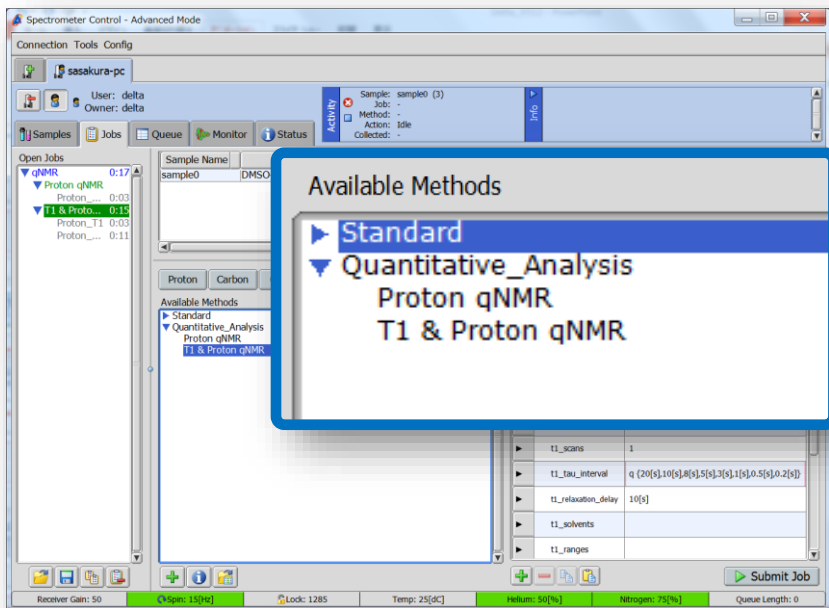
Introducing rotor in rotorcarrier



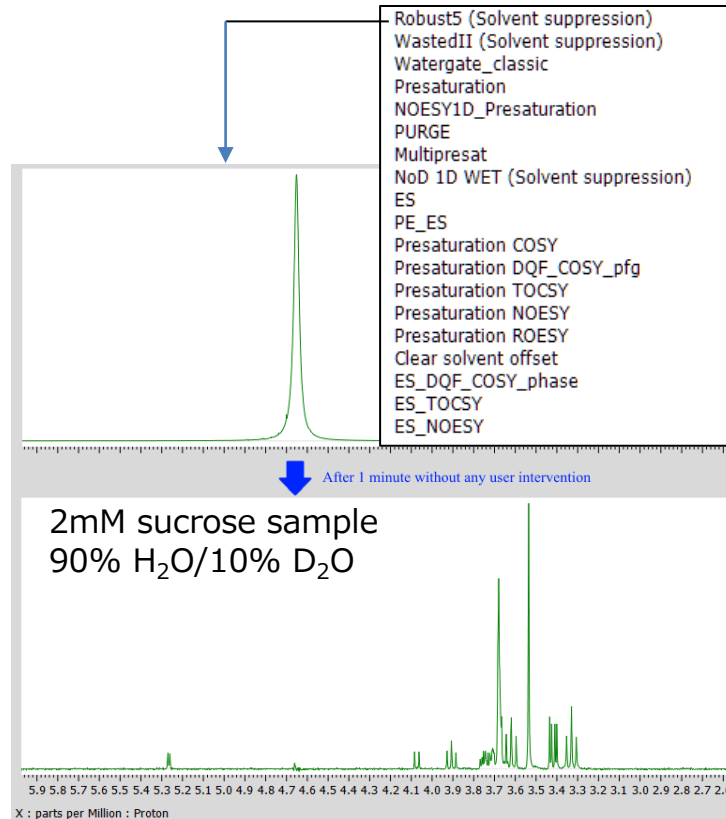
Bench spinner



# Automation scripts



## Solvent suppression

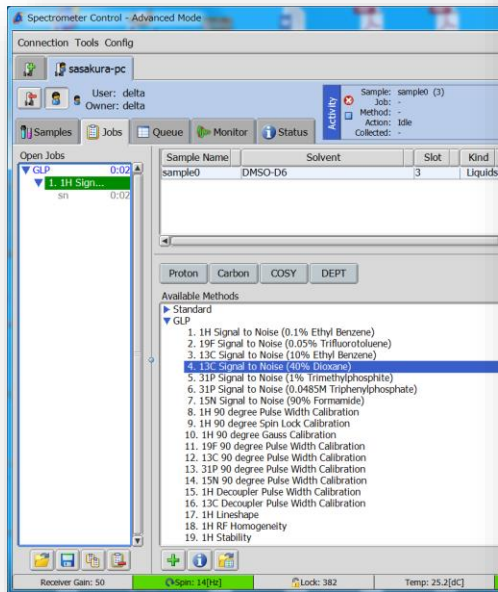


**T<sub>1</sub> & qNMR (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, etc.)**  
 Automatic 90 pulse calibration,  
 T<sub>1</sub> measurement first, then  
 automatically extract the T<sub>1</sub>  
 values to set the relaxation  
 delay of the qNMR experiment

**<sup>1</sup>H T<sub>1</sub> & CPMAS**  
 Run T<sub>1</sub> measurement first (IR  
 or SR), then automatically  
 extract the T<sub>1</sub> value to set  
 the relaxation delay of  
 CPMAS

# System suitability (GLP) tests

The GLP methods can verify the performance of the NMR machine periodically



## Available Methods

### GLP

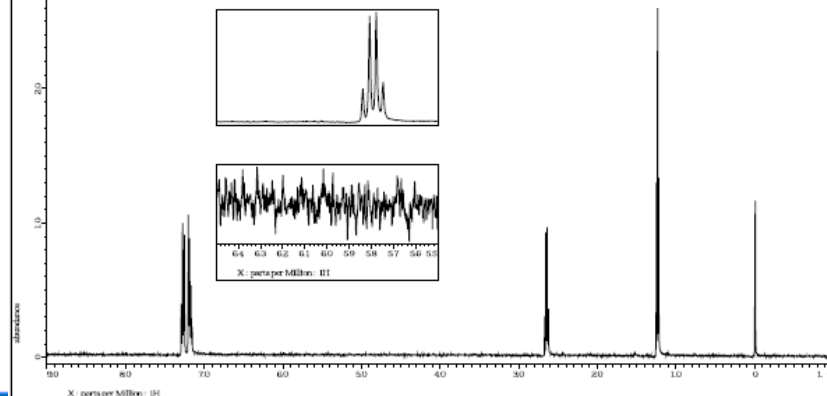
1. 1H Signal to Noise (0.1% Ethyl Benzene)
2. 19F Signal to Noise (0.05% Trifluorotoluene)
3. 13C Signal to Noise (10% Ethyl Benzene)
4. 13C Signal to Noise (40% Dioxane)
5. 31P Signal to Noise (1% Trimethylphosphite)
6. 31P Signal to Noise (0.0485M Triphenylphosphate)
7. 15N Signal to Noise (90% Formamide)
8. 1H 90 degree Pulse Width Calibration
9. 1H 90 degree Spin Lock Calibration
10. 1H 90 degree Gauss Calibration
11. 19F 90 degree Pulse Width Calibration
12. 13C 90 degree Pulse Width Calibration
13. 31P 90 degree Pulse Width Calibration
14. 15N 90 degree Pulse Width Calibration
15. 1H Decoupler Pulse Width Calibration
16. 13C Decoupler Pulse Width Calibration
17. 1H Lineshape
18. 1H RF Homogeneity
19. 1H Stability
20. 13 Degree Phase Stability Test
21. Center band Suppression
22. Quad Image
23. 1H Beat Test
24. 13C Beat Test
25. 1H Transmitter Phase Linearity
26. 1H Receiver Phase Linearity
27. 13C Transmitter Phase Linearity
28. 13C Receiver Phase Linearity
29. Gradient Linearity Test
30. Gradient Power Test
31. Gradient Recovery Test

## GLP Test Report

Operator: aabe  
 Site: ECA500 (5th BLD)  
 Test Date: 4NOV2004 15:05:03

Test Performed: 1H Signal to Noise  
 Filename: 1h\_sn3.jdf  
 Comment: glp  
 Probe ID: 2692

Signal: 0.9626  
 Noise: 0.0018  
 SN Ratio: 261.2168  
 Signal area(From): 2.5000[ppm]  
 Signal area(To): 3.0000[ppm]  
 Noise area(From): 6.5000[ppm]  
 Noise area(To): 5.5000[ppm]  
 Noise width: 200.0000[Hz]  
 Noise area: Window determined  
 Acceptable value: 100:1  
 Status: PASSED



# DOSY steps (automatic\_setup)

1. Automatic setting of chosen sample parameters (temperature, temperature delay, shimming, tuning\*,...)
2. Automatic estimation of diffusion coefficient using SEGWE with the **solute MW**



▶	dosy_scans	16
▶	dosy_relaxation_delay	3[s]
▶	solute_MW	300
▶	calculate_proton_90	<input type="checkbox"/>
▶	convection_check	<input checked="" type="checkbox"/>
▶	<b>automatic_setup</b>	<input checked="" type="checkbox"/>
▶	diffusion_time	0.1[s]
▶	smallDelta	2[ms]
▶	predefined_array	<input checked="" type="checkbox"/>
▶	g	5[T/m], 0.28993[T/m], 0.3[T/m]}
▶	array_type	Linear ↕
▶	g_max	0.3[T/m]
▶	g_min	0.03[T/m]
▶	g_points	16
▶	log_base	2

# Self-Diffusion and molecular weight (SEGWE)

- Approximation for the correlation between molecular weight and self-diffusion coefficient
- More advanced than previous estimations such as  $r_H \propto \sqrt[3]{MW}$
- Takes into account the molecular interactions of solvent and solutes
- **Calculator available, input: temperature, solvent and MW or D**

$k_B$  : Boltzmann constant

$T$ : temperature

$\eta$ : viscosity

$\rho_{\text{eff}}$ : effective density of the molecule  
(packing effects, geometry,  
solvation and flexibility)

$MW$ : molecular weight of the  
molecule

$MW_S$ : molecular weight of the solvent

$N_A$ : Avogadro number

$$D = \frac{k_B T \left( \frac{3 \sqrt[3]{\frac{MW_S}{MW}}}{2} + \frac{1}{1 + \sqrt[3]{\frac{MW_S}{MW}}} \right)}{6\pi\eta \sqrt[3]{\frac{3MW}{4\pi\rho_{\text{eff}} N_A}}}$$

R. Evans et al, *Angew. Chem. Int. Ed.* (2013), 52: 3199–3202

R. Evans et al, *Anal. Chem.* (2018), 90 (6), 3987–3994

R. Evans, *Prog Nucl Magn Reson Spectrosc* (2020), 117, 33-69

<https://www.nmr.chemistry.manchester.ac.uk/?q=node/432>

# Calculating DOSY parameters (Stejskal-Tanner equation)

$$S = S_0 e^{-D\gamma^2\delta^2 G^2 \Delta'}$$

$$\delta = \sqrt{-\frac{\ln S/S_0}{D\gamma^2 G^2 \Delta'}}$$

$S$  : signal amplitude [0.1  $S_0$ ]

$S_0$  : signal amplitude without diffusion [ $S_0$ ]

$D$  : diffusion coefficient [SEGWE]

$\gamma$  : gyromagnetic ratio (dependent on  $x\_domain$ ) [ $\gamma_H$ ]

$\delta$  : gradient pulse width (**delta** or **smallDelta**)

$G$  : gradient amplitude (**g**) [maximum usable gradient strength]

$\Delta'$  : corrected diffusion time

$\Delta$  : diffusion time (**diffusion\_time**) [0.1 s]

# DOSY steps (automatic\_setup)

1. Automatic setting of chosen sample parameters (temperature, temperature delay, shimming, tuning\*,...)
2. Automatic estimation of diffusion coefficient using SEGWE with the **solute MW**
3. Automatic determination of gradient length to achieve 90% signal attenuation (0.1 s diffusion time and maximum usable gradient strength)

**Info** Starting Job 'DOSY'  
Estimated Diffusion coefficient is 10.98386\*10E-10 m<sup>2</sup>/s  
Delta set to 1.8041[ms] to achieve 90% signal attenuation

4. Automatic determination of 90 degrees pulse and setup (**optional**)
5. Automatic determination of sample convection (**optional**), by evaluating if a delay imbalance of 30ms leads to a signal loss of more than 20%.

**Info** Post-experiment Default Initialization  
There is convection in this sample (signal ratio of 0.59402. Proceeding with convection compensated experiment  
Digital Filter Factor is 12

**Info** Post-experiment Default Initialization  
Convection test indicates there is no significant convection in this sample (signal ratio of 0.98005)  
Digital Filter Factor is 12

6. Automatic acquisition of DOSY with/without convection compensation
7. Automatic DOSY plot automatically generation

▶	dosy_scans	16
▶	dosy_relaxation_delay	3[s]
▶	solute_MW	300
▶	calculate_proton_90	<input type="checkbox"/>
▶	convection_check	<input checked="" type="checkbox"/>
▶	automatic_setup	<input checked="" type="checkbox"/>
▶	diffusion_time	0.1[s]
▶	smallDelta	2[ms]
▶	predefined_array	<input checked="" type="checkbox"/>
▶	g	5[T/m], 0.28993[T/m], 0.3[T/m]}
▶	array_type	Linear ↕
▶	g_max	0.3[T/m]
▶	g_min	0.03[T/m]
▶	g_points	16
▶	log_base	2

# Results from automatic\_setup (Quinine + Geraniol + Camphene)

MW set to 324

Info

Reached Lock State 'AUTOLOCK'  
Estimated Diffusion coefficient is  $7.78834 \times 10^{-10} \text{ m}^2/\text{s}$   
Delta set to 2.14247[ms] to achieve 90% signal attenuation

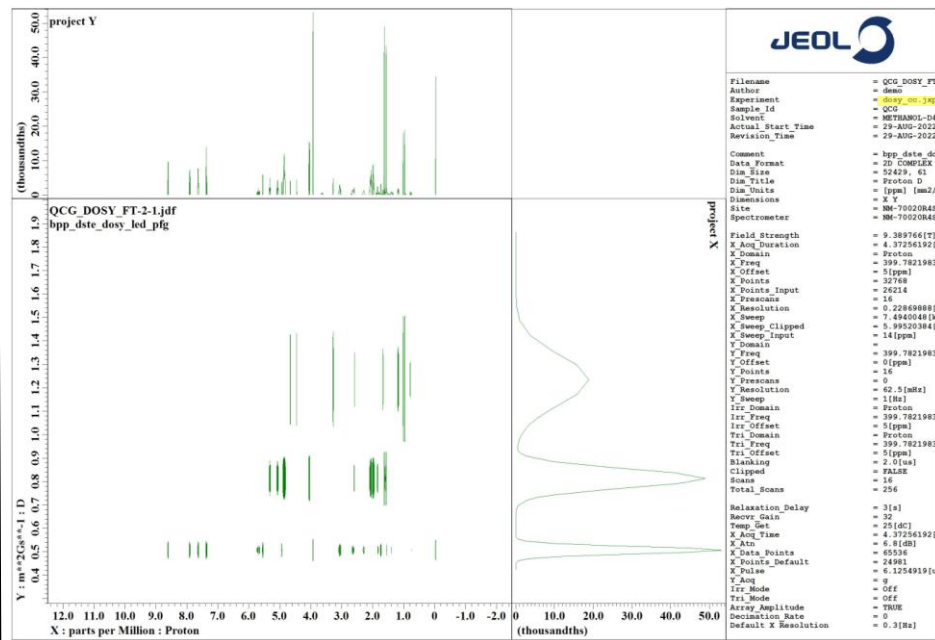
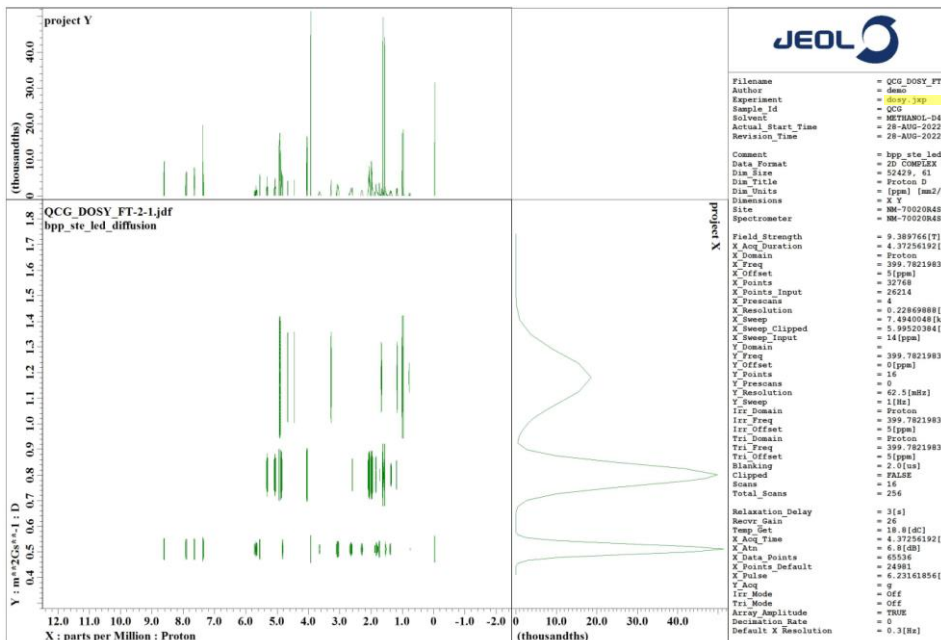
1H 90 degree pulse width for QCG estimated as 6.12549[us]

## Room temperature

Convection test indicates there is no significant convection in this sample (signal ratio of 0.9784)

## 25C

There is convection in this sample (signal ratio of 0.35024).  
Proceeding with convection compensated experiment



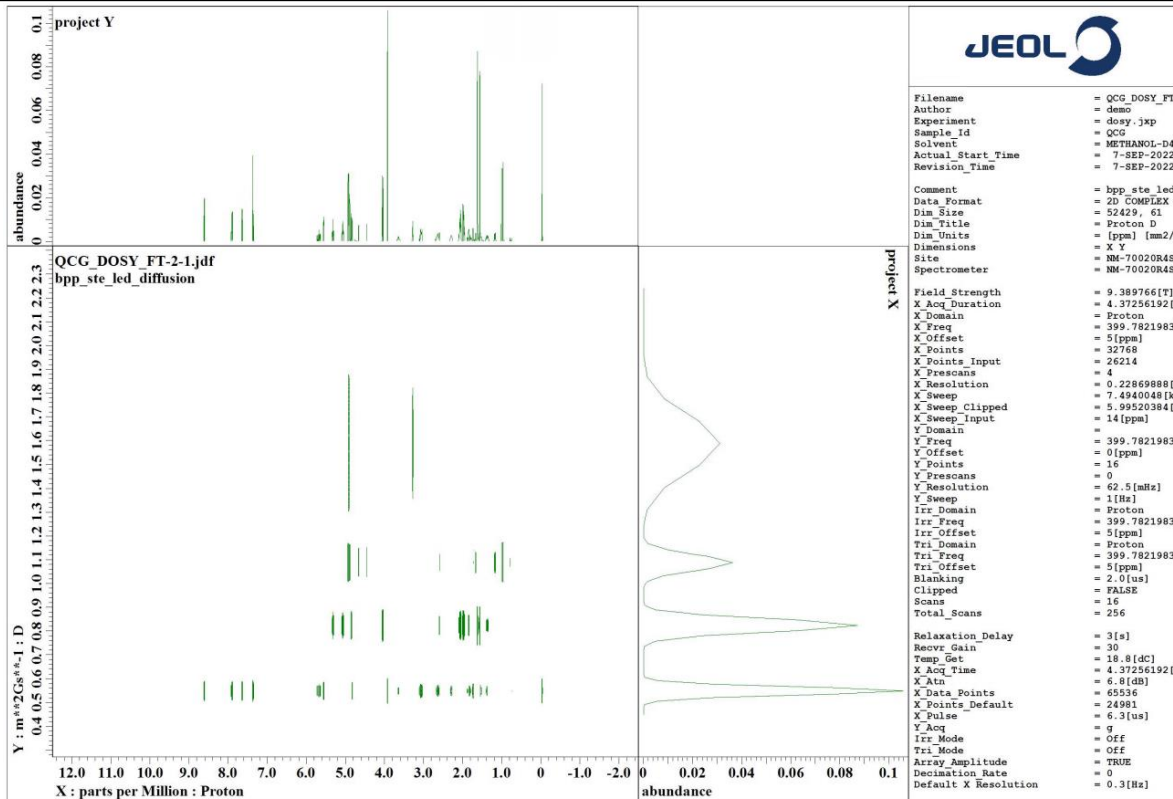


# Results from automatic\_setup (Quinine + Geraniol + Camphene)

MW set to 136

Info

Reached Lock State 'AUTOLOCK'  
 Estimated Diffusion coefficient is  $11.71103 \times 10^{-10} \text{ m}^2/\text{s}$   
 Delta set to 1.74719[ms] to achieve 90% signal attenuation



PDF automatically generated after clicking the Submit Job button with the DOSY automation method

Note PDF printout is generated using multivariate analysis, results can be misleading

**Further analysis with other methods is recommended, particularly for more complex samples**

# JEOL Diffusion probe

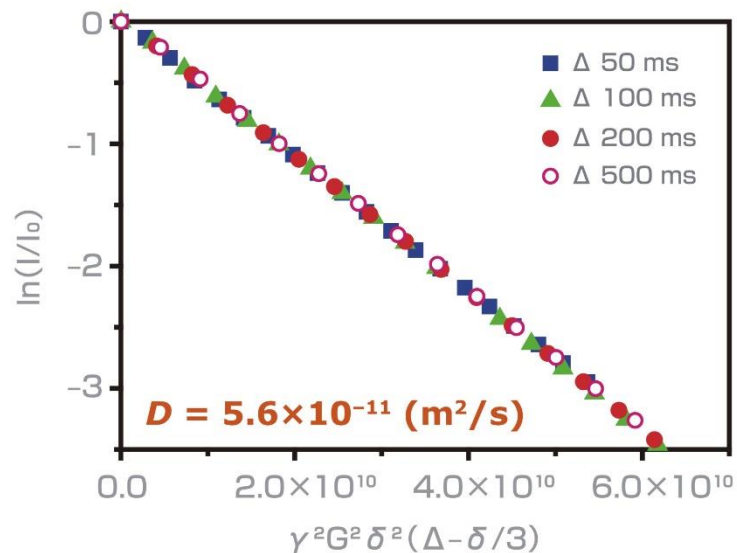


- Narrow bore
- Air cooled
- -70 to 120 °C
- 1200G/cm at 30A
- 2000G/cm at 50A

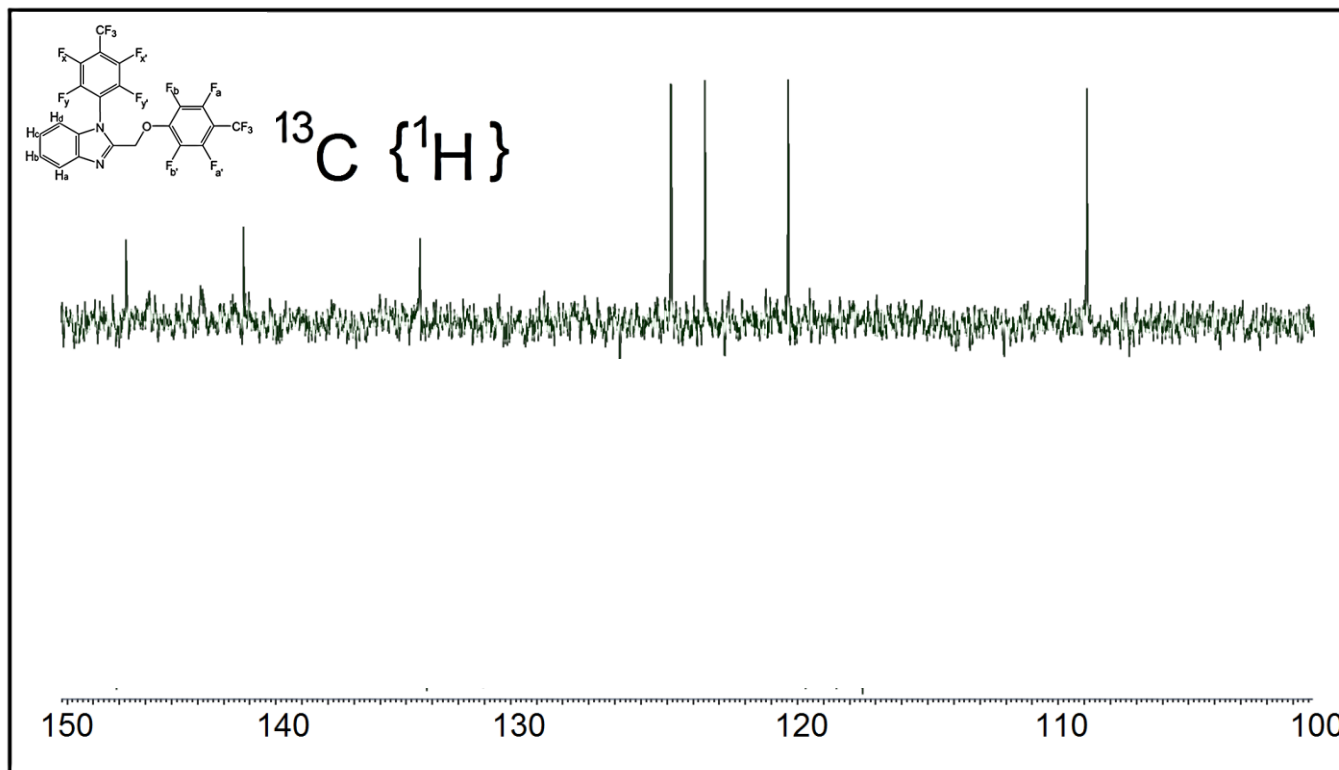


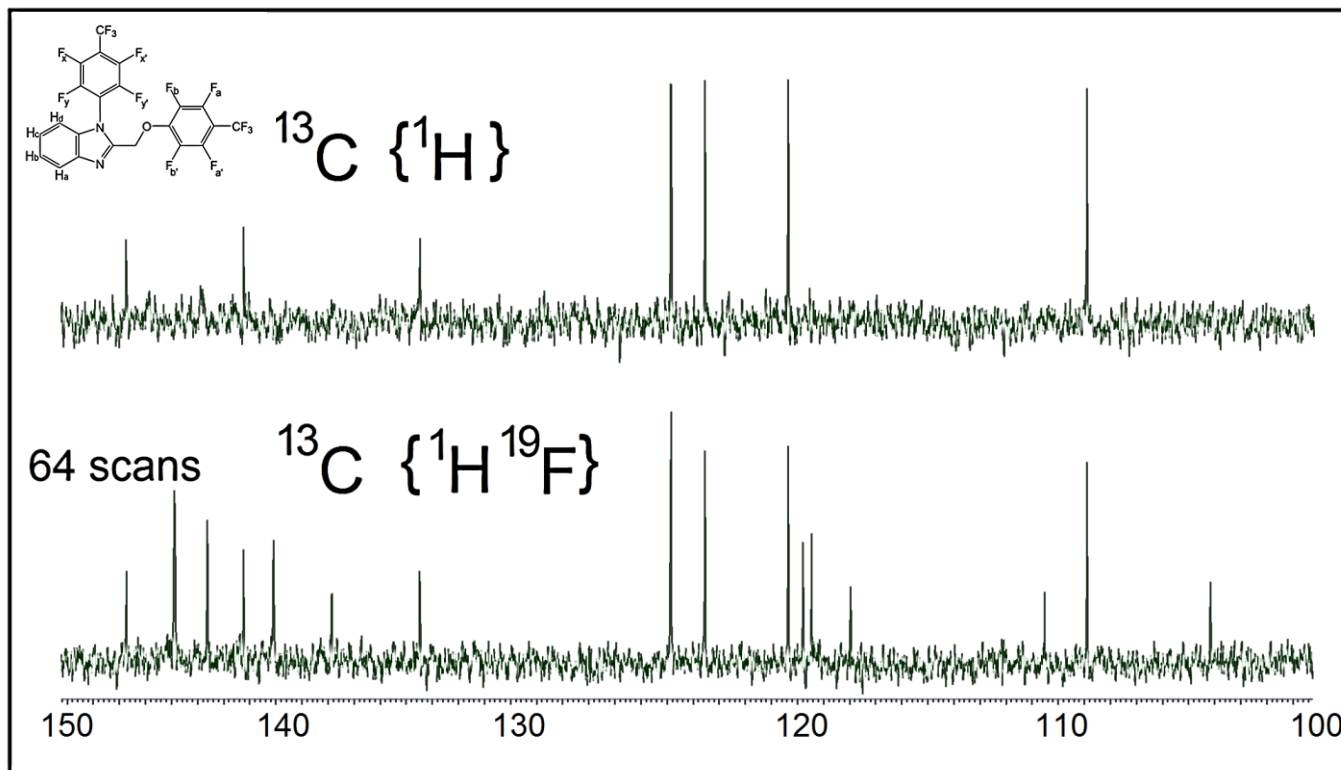
50A PFG amplifier

## Analysis of Li diffusion in solid-state electrolyte

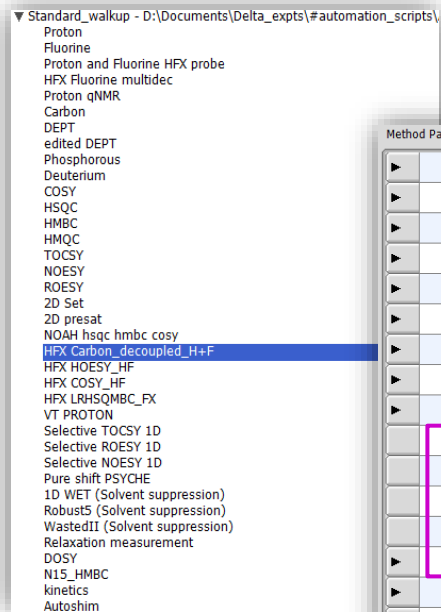


Data courtesy:  
Y. Hashimoto, N. Horiike, and H. Shobukawa, Asahi Kasei Corp





# HFX experiments in automation



Method combining expts multiple  $^1\text{H}$ ,  $^{19}\text{F}$  and  $^{13}\text{C}$  spectra with/out decoupling

Method Parameters: HFX Carbon_decoupled_H+F	
H_scans	16
H_offset	6[ppm]
H_sweep	16[ppm]
H_relaxation_delay	2[s]
F_scans	32
F_offset	-100[ppm]
F_sweep	300[ppm]
F_relaxation_delay	2[s]
F_peaks	1
Carbon_HFdec	<input checked="" type="checkbox"/>
Carbon_Hdec	<input type="checkbox"/>
Carbon_Fdec	<input type="checkbox"/>
Carbon_noddec	<input type="checkbox"/>
carbon_scans	32
sn_ratio	50
force_tune	<input checked="" type="checkbox"/>

1. Runs  $^1\text{H}$

2. Runs  $^{19}\text{F}$

3. Runs  $^{19}\text{F}\{^1\text{H}\}$  centered on “F\_peaks”  
tallest fluorine signals

4. Runs  $^1\text{H}\{^{19}\text{F}\}$  with decoupling centered on  
tallest fluorine peak

5. Runs choice of  $^{13}\text{C}\{^1\text{H},^{19}\text{F}\}$ ,  $^{13}\text{C}\{^1\text{H}\}$ ,  $^{13}\text{C}\{^{19}\text{F}\}$ ,  $^{13}\text{C}$  (with  
decoupling centered on tallest fluorine peak)

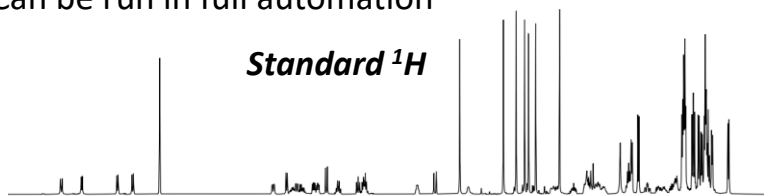
# More single click experiments

## PSYCHE PURE SHIFT (homonuclear broadband decoupling)

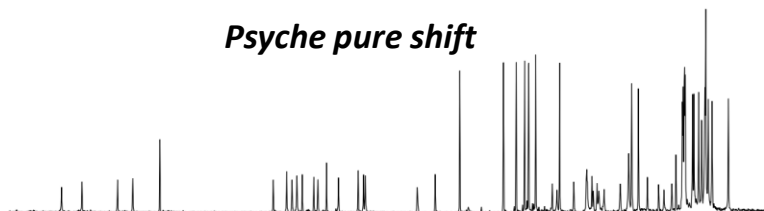
A single line for each peak in the spectrum

Can be run in full automation

*Standard  $^1\text{H}$*

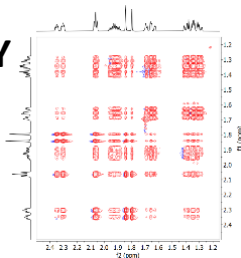


*Psyche pure shift*

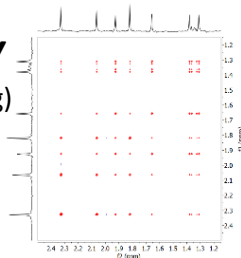


8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5  
ft (ppm)

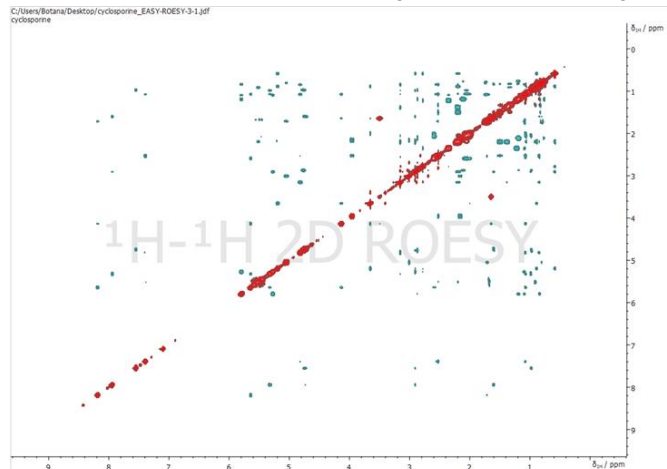
**TOCSY**



**PSYCHE- TOCSY**  
(covariance processing)



## Off-resonance ROESY (EASY-ROESY)



Automatically:

- Set spin-lock RF field dependent on magnet field strength
- Set spin-lock angle to 60 degrees
- Calculate off-resonance shift as per spin-lock RF strength, angle and magnet field
- Set offset frequency of spin-lock pulses

# IPAP-HSQMBC: Measurement of long-range heteronuclear coupling constants

Spectrometer Control - Walkup Mode - ECZL400R

Connection Options Tools Config Queue Samples Columns

User: demo Logout

Activity Sample: sample\_X (1)  
Job: -  
Method: -  
Action: Idle  
Collected: -  
Time: -

Info Starting Collection  
Building Output File : 3 MB  
Sending file to data server  
Experiment Completed  
Post-experiment Default Initialization  
Completed Job 'ROESY'

Walk-Up Monitor Status Submit All

Slot	Status	Sample Name	Comment	Solvent	Method	Est. Time	Force Tune	Scheduling	Submit Job
1		sample_X		Chloroform-D	Select a Method				
2		Sample Name Required		Select a Solvent	Select a Method				
3		Sample Name Required		Select a Solvent	Select a Method				
4									
5		Sample Name Required		Select a Solvent	Select a Method				
6		Sample Name Required		Select a Solvent	Select a Method				
7									
8		Sample Name Required		Select a Solvent	Select a Method				

Status Slot Sample Submit Time Method Visualize Scheduling User Est. End Time

Receiver Gain: 50 Spin: 16[Hz] Lock: 175 Temp: 25.1[dC] Helium: 50[%] Nitrogen: 75[%] LOADED (1) No Jobs

# IPAP-HSQMBC: Measurement of long-range heteronuclear coupling constants

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*Two complementary in-phase (IP) and anti-phase (AP) data are separately recorded from a modified HSQMBC experiment and then added/subtracted to provide spin-state-selective  $\alpha/\beta$ -HSQMBC spectra. The magnitude of  $^nJ_{XH}$  can be directly determined by simple analysis of the relative displacement between  $\alpha$ - and  $\beta$ -cross-peaks.*

*S. Gil et al./Journal of Magnetic Resonance 207 (2010) 312–321*

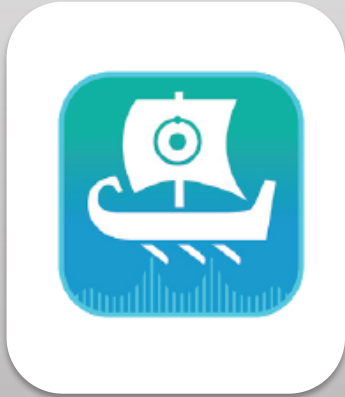
What the automation is doing:

```
EXPERIMENT pip_hsqmbc_ip IS
  COLLECT "pip_hsqmbc";
  SET ipap_flg          = FALSE;
END EXPERIMENT;

EXPERIMENT pip_hsqmbc_ap IS
  COLLECT "pip_hsqmbc";
  SET ipap_flg          = TRUE;
END EXPERIMENT;

SET pip_hsqmbc_add = pip_hsqmbc_ip + pip_hsqmbc_ap;
SET pip_hsqmbc_sub = pip_hsqmbc_ip - pip_hsqmbc_ap;
```





## Jason software

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- **Vendor agnostic**
- Easy reports
- Windows and Mac OS X versions
- Subscription based
- Agile release cycle (new release every 3 months)
- Automated structure verification

# JASON Software Development Team



Vadim  
Zorin



Iain  
Day



Yibiao  
Li



Hiroshi  
Endo



Yuko  
Igarashi



Naoto  
Seki



Nikolay  
Larin



Peter  
Kiraly



Rachel  
Brignall



Nader  
Amin



1 Customer Support  
1 Developer



Ronil  
Sedani



Maximillian  
Reinhart



Saeko  
Suzuki

# Very Agile team

## The request:

Forward



Wed 08/05/2024 23:21

I am trying to link both the y axis and x-axis on a proton - proton correlated 2D spectrum to a 1D proton spectrum.

On a proton-proton correlation like a noesy and linking the noesy to the proton, moving the cursor on the noesy spectrum along the x axis shows the cursor on the relevant proton peak on the proton spectrum. However, moving it in the Y-axis direction and keep it stationary on the x-axis position quite understandably does not move the cursor on the proton spectrum.

## The response:

Forward



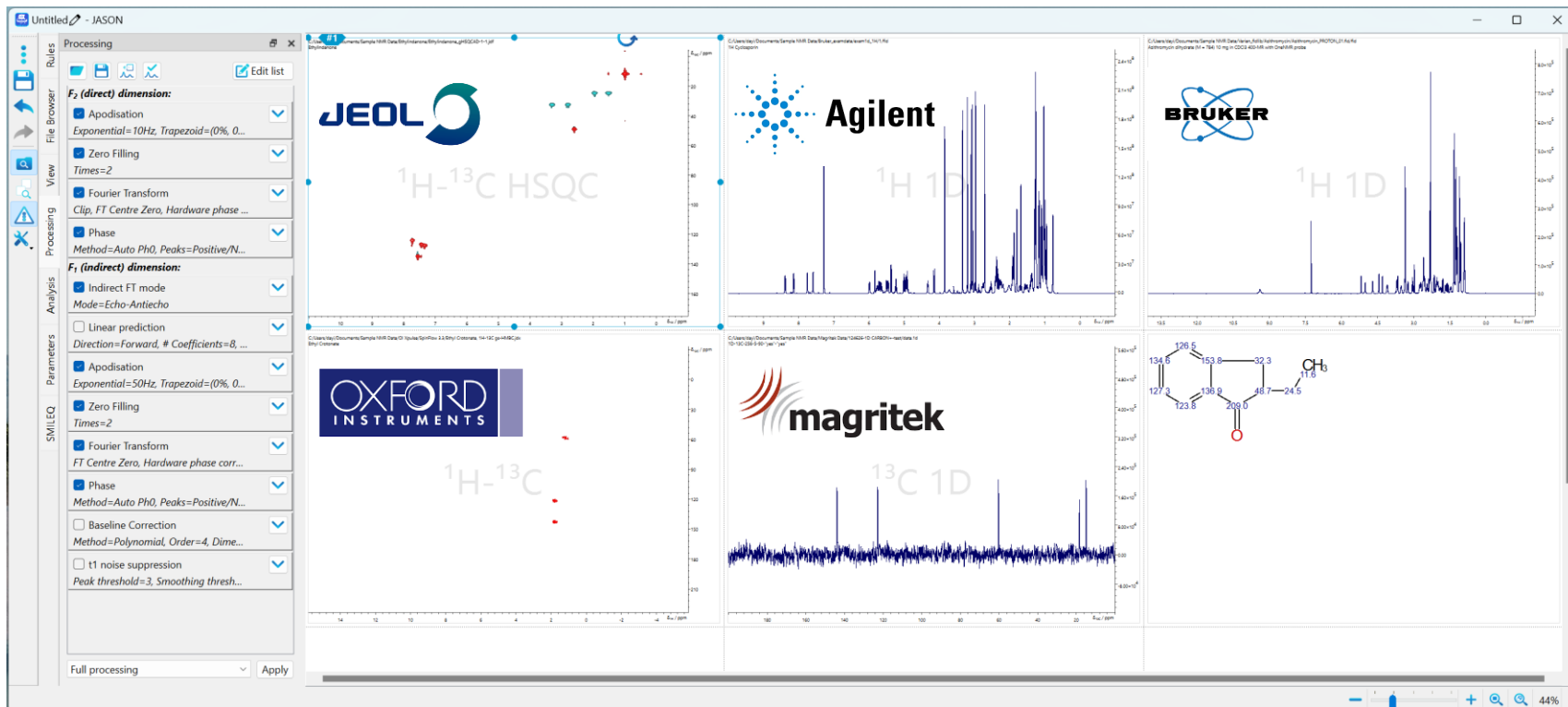
Thu 09/05/2024 14:54

Thanks again for your email. We had a quick discussion and Vadim has already added this feature to the development version of [JASON!](#) It should be available from version 4.1.7300

# Vendor Agnostic

- Redeploy and synchronize any data/reports around the **WYSIWYG canvas**

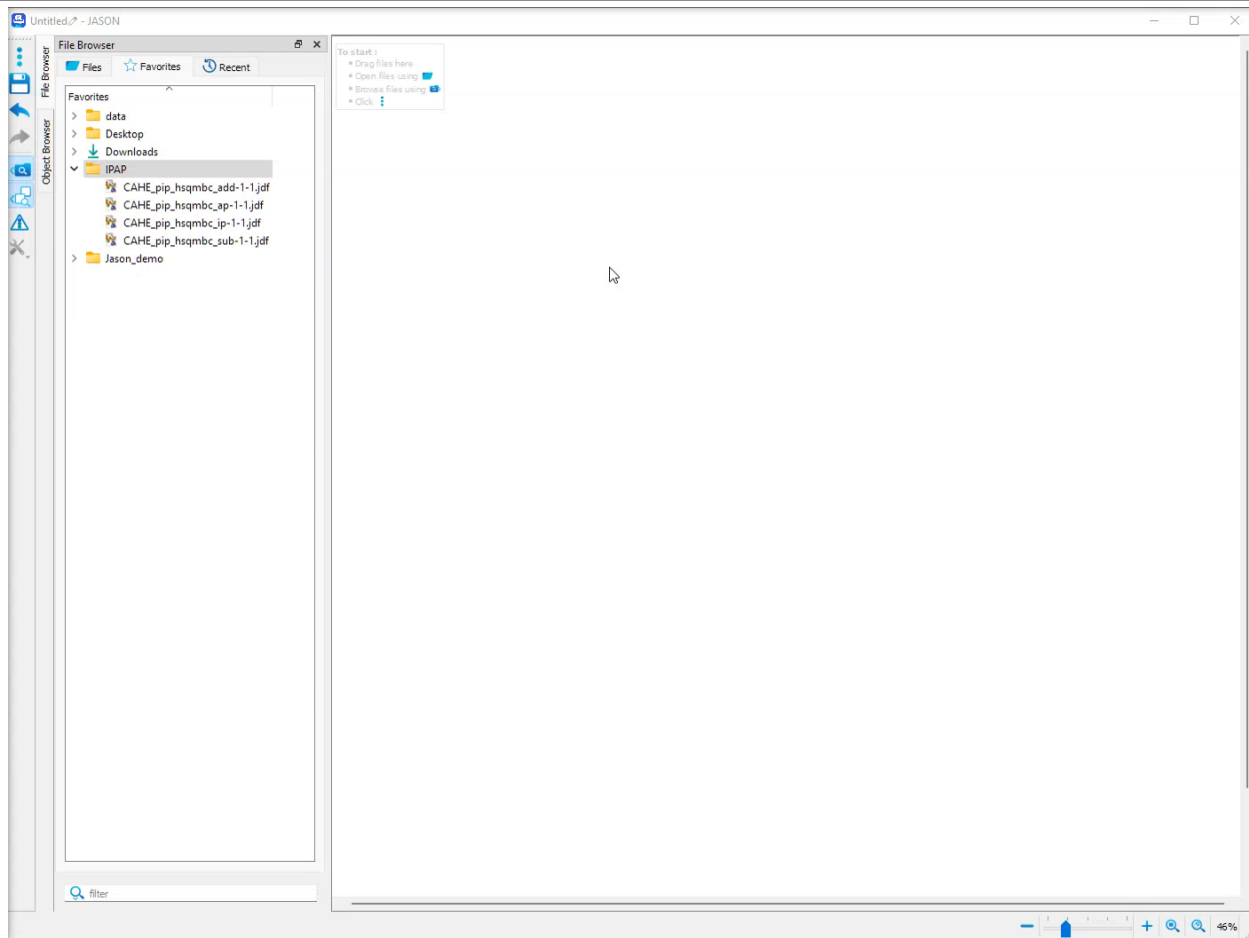
- Data and metadata stored in standard **HDF-5 format**, accessible with any HDF-5 reader.



**Findable, Accessible, Interoperable, Reusable**

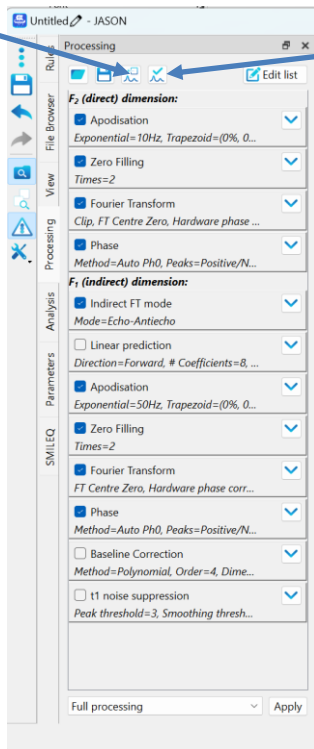
# Stacking IPAP-HSQMBC spectra

- IPAP-HSQMBC experiments acquired in Delta Walkup mode
- Addition and subtraction datasets automatically obtained in Delta automation. If not present, they can be generated with Jason.
- Overlay or stack vertically, horizontally or diagonally multiple 1D or 2D spectra
- Easily change layout and colours
- Easily measure distances



# Powerful Processing Engine

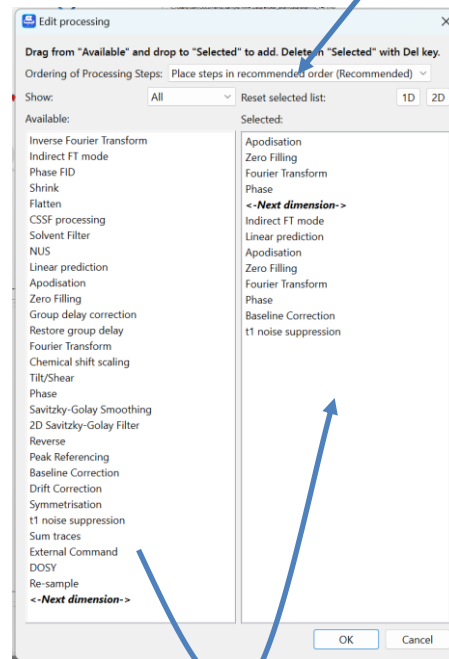
Raw data



Recommended processing

**Automatic experiment recognition**

Expert vs guided mode



Drag and drop



- External command enables further processing with other programs such as scripts made in Python, R or Matlab
- BeautifulSoup enables calling a background instance of Jason from your Python scripts to integrate the power of Jason in your workflows
- Free tool:

`pip install beautifuljason`



# Beyond Python

## The problem

Dear Application Team,

I have been faced with a task that seems to have been beyond my field of expertise. After two days of struggle, I'm slowly losing hope for completion. It requires me to convert several thousands of <sup>1</sup>H NMR spectra into a suitable format, which will then be used as an input for machine learning. The format I need at this stage is a vector containing only normalized intensities for individual points.

The first step is to process the spectra into a form in which each spectrum will have the same range of chemical shifts (for example, from 10 ppm to -1 ppm) and an identical number of points so that each point in each vector always corresponds to

## Solution: Step 1

<input checked="" type="checkbox"/> Re-sample	
From:	-1.0000 ppm
To:	14.0000 ppm
Points kept:	131072

**From** and **To** specifies the range of the spectrum which will be kept. If the spectrum doesn't contain datapoints in some part of the requested region then zero intensity points will be used in place of the missing data. Values of from and to are automatically swapped internally if needed, a region can be specified in any order.

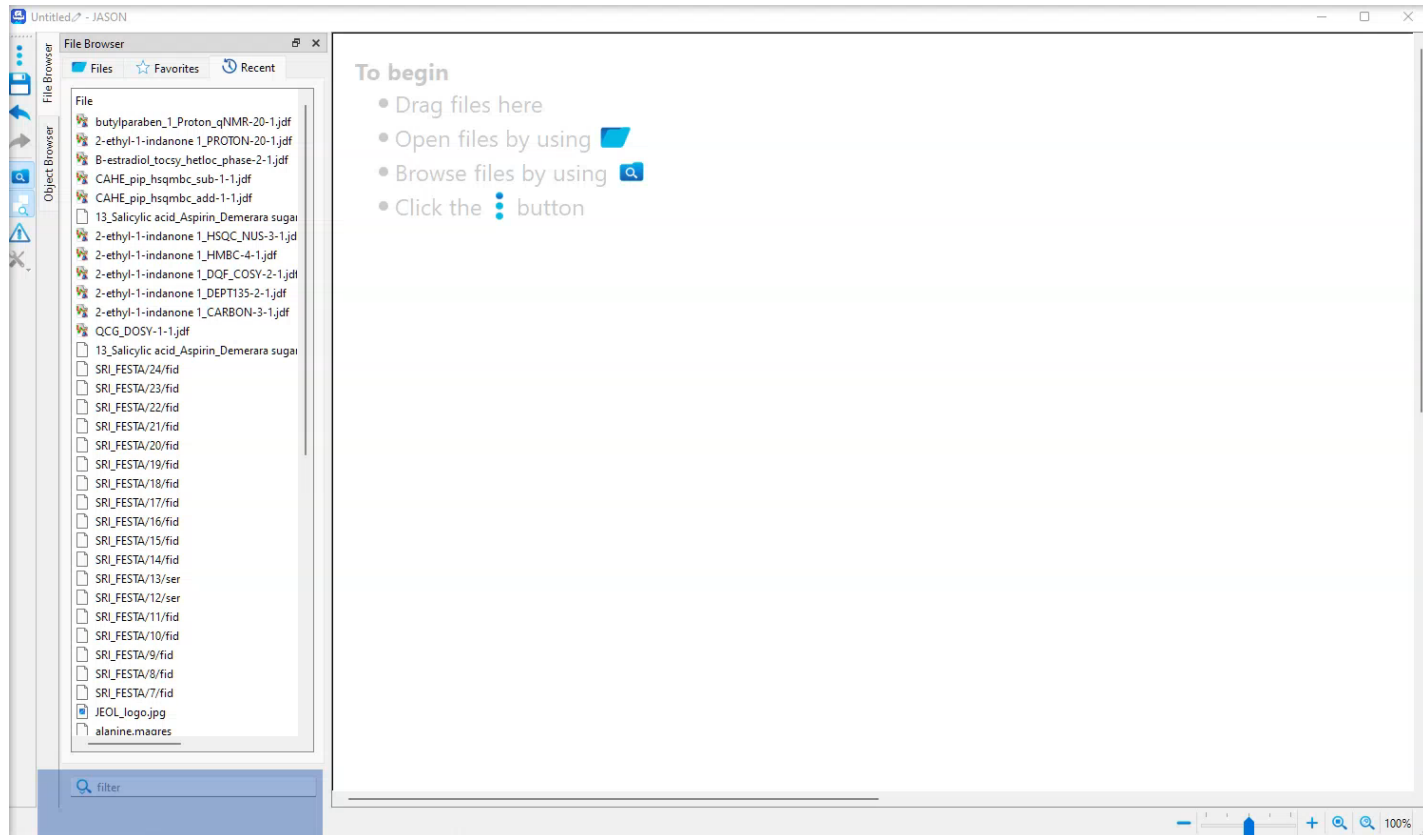
**Points kept** defines the exact number of points which will be used within the above specified region. Linear interpolation is used to convert the existing data points to the new digital resolution of the spectrum.

## Solution: Step 2

```
24 for %%f in (*.jdf) do (  
25   %jason_path% --headless "%path%\%%f" "%path%\kp_process1d.jjp" -s "%path%\%%~nf.jjh5" -s "%path%\%%~nf.csv"  
26 )
```

# Automated structural assignment

- **Molecular drawing tools**  
(Reads/writes .mol and .sdf files)
- $^1\text{H}$  and  $^{13}\text{C}$  (for now) **chemical shift prediction** on the fly
- Hybrid approach:
  - Neural Network based on NMRShiftDB and JEOL Natural product DB
  - HOSE code-like approach for unfamiliar molecules
- **Automatic structural assignment** and drag-and-drop manual assignment
- Accurate simulate systems with up to 20 spins coupled
- Automatic peak picking, integration, J-coupling analysis, multiplet analysis. Drag-and-drop manual reformulation of multiplets







# Reporting

The screenshot displays the JEOL JSMILEQ software interface. The main window shows an NMR spectrum with a chemical structure of CH1D and a "Multiplet Report" overlaid on the spectrum. The report includes the following chemical shift ranges and integrations:

- 7.340-7.350 ppm (1.0000)
- 7.300-7.310 ppm (1.0000)
- 7.250-7.260 ppm (1.0000)
- 7.200-7.210 ppm (1.0000)
- 7.150-7.160 ppm (1.0000)
- 7.100-7.110 ppm (1.0000)
- 7.050-7.060 ppm (1.0000)
- 7.000-7.010 ppm (1.0000)
- 6.950-6.960 ppm (1.0000)
- 6.900-6.910 ppm (1.0000)
- 6.850-6.860 ppm (1.0000)
- 6.800-6.810 ppm (1.0000)
- 6.750-6.760 ppm (1.0000)
- 6.700-6.710 ppm (1.0000)
- 6.650-6.660 ppm (1.0000)
- 6.600-6.610 ppm (1.0000)
- 6.550-6.560 ppm (1.0000)
- 6.500-6.510 ppm (1.0000)
- 6.450-6.460 ppm (1.0000)
- 6.400-6.410 ppm (1.0000)
- 6.350-6.360 ppm (1.0000)
- 6.300-6.310 ppm (1.0000)
- 6.250-6.260 ppm (1.0000)
- 6.200-6.210 ppm (1.0000)
- 6.150-6.160 ppm (1.0000)
- 6.100-6.110 ppm (1.0000)
- 6.050-6.060 ppm (1.0000)
- 6.000-6.010 ppm (1.0000)
- 5.950-5.960 ppm (1.0000)
- 5.900-5.910 ppm (1.0000)
- 5.850-5.860 ppm (1.0000)
- 5.800-5.810 ppm (1.0000)
- 5.750-5.760 ppm (1.0000)
- 5.700-5.710 ppm (1.0000)
- 5.650-5.660 ppm (1.0000)
- 5.600-5.610 ppm (1.0000)
- 5.550-5.560 ppm (1.0000)
- 5.500-5.510 ppm (1.0000)
- 5.450-5.460 ppm (1.0000)
- 5.400-5.410 ppm (1.0000)
- 5.350-5.360 ppm (1.0000)
- 5.300-5.310 ppm (1.0000)
- 5.250-5.260 ppm (1.0000)
- 5.200-5.210 ppm (1.0000)
- 5.150-5.160 ppm (1.0000)
- 5.100-5.110 ppm (1.0000)
- 5.050-5.060 ppm (1.0000)
- 5.000-5.010 ppm (1.0000)
- 4.950-4.960 ppm (1.0000)
- 4.900-4.910 ppm (1.0000)
- 4.850-4.860 ppm (1.0000)
- 4.800-4.810 ppm (1.0000)
- 4.750-4.760 ppm (1.0000)
- 4.700-4.710 ppm (1.0000)
- 4.650-4.660 ppm (1.0000)
- 4.600-4.610 ppm (1.0000)
- 4.550-4.560 ppm (1.0000)
- 4.500-4.510 ppm (1.0000)
- 4.450-4.460 ppm (1.0000)
- 4.400-4.410 ppm (1.0000)
- 4.350-4.360 ppm (1.0000)
- 4.300-4.310 ppm (1.0000)
- 4.250-4.260 ppm (1.0000)
- 4.200-4.210 ppm (1.0000)
- 4.150-4.160 ppm (1.0000)
- 4.100-4.110 ppm (1.0000)
- 4.050-4.060 ppm (1.0000)
- 4.000-4.010 ppm (1.0000)
- 3.950-3.960 ppm (1.0000)
- 3.900-3.910 ppm (1.0000)
- 3.850-3.860 ppm (1.0000)
- 3.800-3.810 ppm (1.0000)
- 3.750-3.760 ppm (1.0000)
- 3.700-3.710 ppm (1.0000)
- 3.650-3.660 ppm (1.0000)
- 3.600-3.610 ppm (1.0000)
- 3.550-3.560 ppm (1.0000)
- 3.500-3.510 ppm (1.0000)
- 3.450-3.460 ppm (1.0000)
- 3.400-3.410 ppm (1.0000)
- 3.350-3.360 ppm (1.0000)
- 3.300-3.310 ppm (1.0000)
- 3.250-3.260 ppm (1.0000)
- 3.200-3.210 ppm (1.0000)
- 3.150-3.160 ppm (1.0000)
- 3.100-3.110 ppm (1.0000)
- 3.050-3.060 ppm (1.0000)
- 3.000-3.010 ppm (1.0000)
- 2.950-2.960 ppm (1.0000)
- 2.900-2.910 ppm (1.0000)
- 2.850-2.860 ppm (1.0000)
- 2.800-2.810 ppm (1.0000)
- 2.750-2.760 ppm (1.0000)
- 2.700-2.710 ppm (1.0000)
- 2.650-2.660 ppm (1.0000)
- 2.600-2.610 ppm (1.0000)
- 2.550-2.560 ppm (1.0000)
- 2.500-2.510 ppm (1.0000)
- 2.450-2.460 ppm (1.0000)
- 2.400-2.410 ppm (1.0000)
- 2.350-2.360 ppm (1.0000)
- 2.300-2.310 ppm (1.0000)
- 2.250-2.260 ppm (1.0000)
- 2.200-2.210 ppm (1.0000)
- 2.150-2.160 ppm (1.0000)
- 2.100-2.110 ppm (1.0000)
- 2.050-2.060 ppm (1.0000)
- 2.000-2.010 ppm (1.0000)
- 1.950-1.960 ppm (1.0000)
- 1.900-1.910 ppm (1.0000)
- 1.850-1.860 ppm (1.0000)
- 1.800-1.810 ppm (1.0000)
- 1.750-1.760 ppm (1.0000)
- 1.700-1.710 ppm (1.0000)
- 1.650-1.660 ppm (1.0000)
- 1.600-1.610 ppm (1.0000)
- 1.550-1.560 ppm (1.0000)
- 1.500-1.510 ppm (1.0000)
- 1.450-1.460 ppm (1.0000)
- 1.400-1.410 ppm (1.0000)
- 1.350-1.360 ppm (1.0000)
- 1.300-1.310 ppm (1.0000)
- 1.250-1.260 ppm (1.0000)
- 1.200-1.210 ppm (1.0000)
- 1.150-1.160 ppm (1.0000)
- 1.100-1.110 ppm (1.0000)
- 1.050-1.060 ppm (1.0000)
- 1.000-1.010 ppm (1.0000)
- 0.950-0.960 ppm (1.0000)
- 0.900-0.910 ppm (1.0000)
- 0.850-0.860 ppm (1.0000)
- 0.800-0.810 ppm (1.0000)
- 0.750-0.760 ppm (1.0000)
- 0.700-0.710 ppm (1.0000)
- 0.650-0.660 ppm (1.0000)
- 0.600-0.610 ppm (1.0000)
- 0.550-0.560 ppm (1.0000)
- 0.500-0.510 ppm (1.0000)
- 0.450-0.460 ppm (1.0000)
- 0.400-0.410 ppm (1.0000)
- 0.350-0.360 ppm (1.0000)
- 0.300-0.310 ppm (1.0000)
- 0.250-0.260 ppm (1.0000)
- 0.200-0.210 ppm (1.0000)
- 0.150-0.160 ppm (1.0000)
- 0.100-0.110 ppm (1.0000)
- 0.050-0.060 ppm (1.0000)
- 0.000-0.010 ppm (1.0000)

Below the spectrum is a "Peak Table" with the following columns: Pos (ppm), Start (ppm), End (ppm), Normalized, H (Hz), Type, J (Hz), Sum Integrate, Peak Area, and  $\sigma$  Sum Integrate.

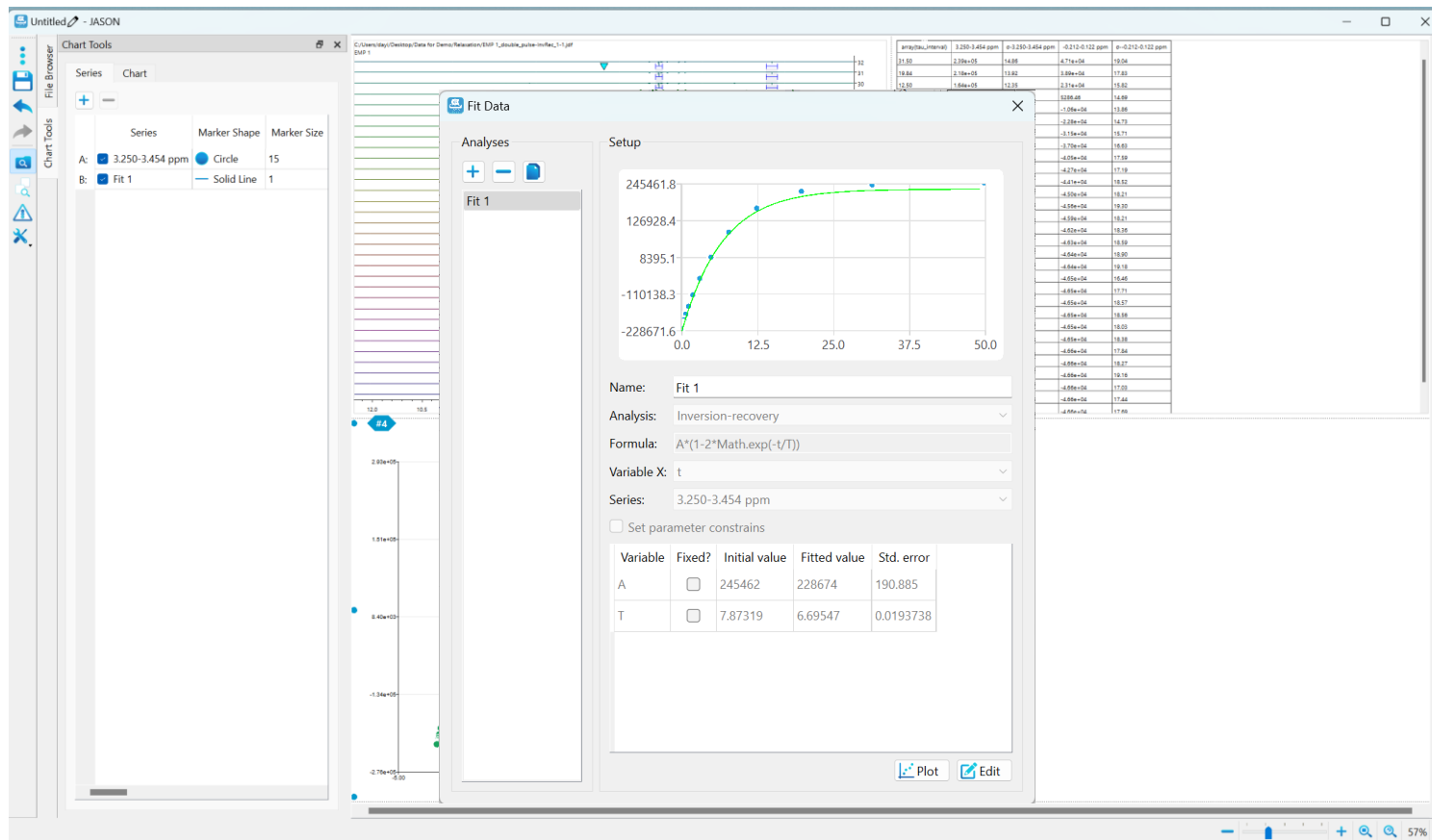
Pos (ppm)	Start (ppm)	End (ppm)	Normalized	H (Hz)	Type	J (Hz)	Sum Integrate	Peak Area	$\sigma$ Sum Integrate
7.733	7.713	7.754	0.782	1	m		2.68e+04	2.58e+04	8.16
7.581	7.566	7.596	1.000	1	m		3.63e+04	3.49e+04	11.09
7.447	7.434	7.467	0.940	1	m		3.33e+04	3.20e+04	9.90
7.344	7.317	7.372	1.001	1	m		3.00e+04	2.83e+04	10.00
7.204	7.201	7.248	1.236	1	dd	17.2478807383	4.24e+04	4.08e+04	13.32
7.010	7.070	7.007	1.000	1	dd	17.4433027110	4.33e+04	4.33e+04	13.04
6.800	6.840	6.800	1.000	1	dd	16.1186444438	3.67e+04	3.50e+04	12.78
1.980	1.904	2.001	1.041	1	dd	18.6873334534	4.00e+04	3.80e+04	15.42
1.837	1.804	1.879	0.933	0	d	5.67	4.33e+04	1.687e+04	16.20
1.531	1.480	1.580	1.040	1	dd	18.68810733610	4.00e+04	3.80e+04	15.42
1.239	1.209	1.272	0.954	0	d	4.7570	4.33e+04	1.687e+04	16.20
1.133	1.127	1.141	0.887	0	d	0.60	4.33e+04	1.687e+04	16.20
0.994	0.969	1.015	0.702	0	d	7.4322	1.27e+05	1.19e+05	10.71
0.807	0.800	0.807	0.932	0	d	0.00	7.90e+03	4.91e+03	7.22

Peak Table

Multiplet/Integral Table

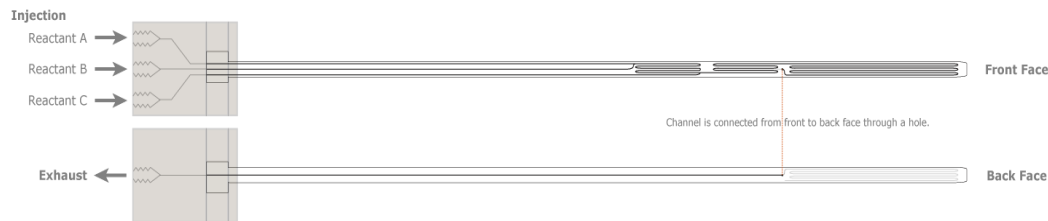
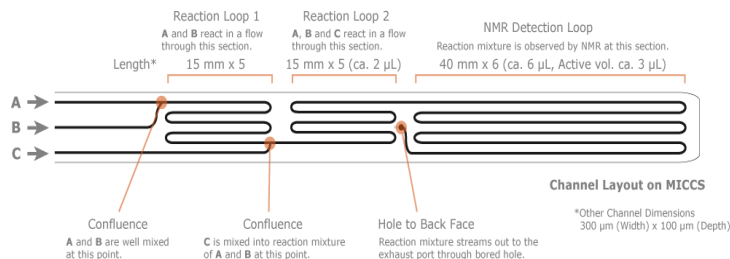


# Charts and Fitting

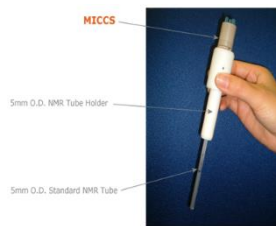


# Reaction monitoring with MICCS

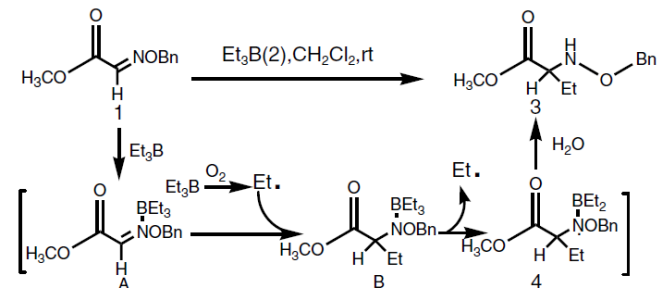
## Micro Channeled Cell for Synthesis monitoring



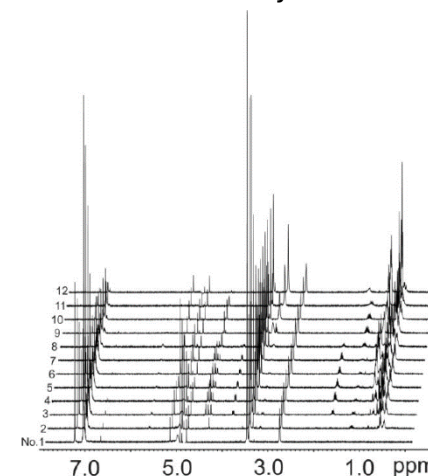
Micro Channeled NMR Cell Design



MICCS Inserted into 5 mm NMR Tube w/ Holder



Oxime ether and triethylborane reaction



Takahashi et al., *Anal. Sci.* 2007 Apr;23(4):395-400

# DOSY Processing

**Processing**

**F<sub>2</sub> (direct) dimension:**

- Apodisation: Exponential=0.15Hz, Trapezoid=(0%, 0%, 80%, 10...
- Zero Filling: Times=2
- Fourier Transform: Clip, FT Centre Zero, Hardware phase correction, ...
- Phase: Method=Auto Ph0
- Baseline Correction: Method=Polynomial, Order=4, Dimensions=This...
- Drift Correction: Calculate automatically

**F<sub>1</sub> (indirect) dimension:**

- DOSY

**Expert mode**

- Use: Integrals
- Lowest D: 0.8e-10
- Highest D: 0.5e-8
- Digitisation: 128
- Sequence: Bipolar

**Gradient parameters**

- T/m factor: 0.001
- Pulse [s]: 0.0015
- Array list: array(g)
- Shape: Rectangular
- Use shape factor: 1
- InterPulseDelay [s]: 0.002012 s

**Diffusion delay parameters**

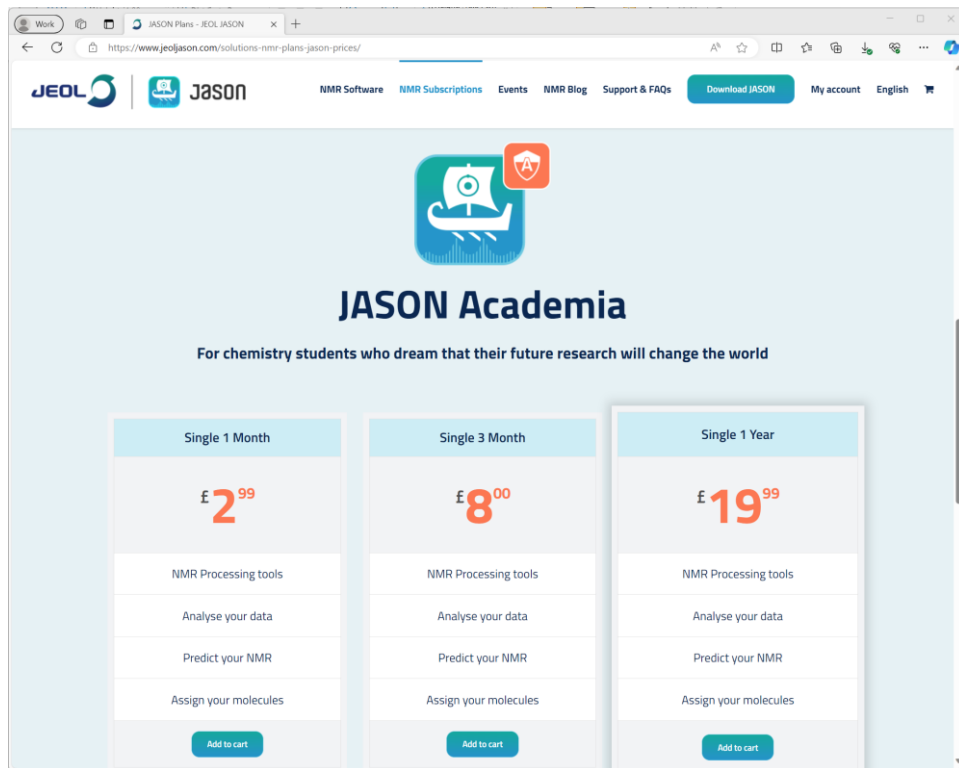
- Δ [s]: 0.1
- Auto: Δ' [s]: 0.098494 s
- γ [rad s<sup>-1</sup> T<sup>-1</sup>]: 267522128

**Table:**

array(g)	0.041-0.020	-0.041-0.0	0.067-0.030	0.087-0.030	0.067-0.030	0.118-0.208	0.0-1.98	0.00
ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
600.00	253.31	2.94	133.64	5.26	45.28	4.79		
588.18	295.18	2.89	126.73	8.43	43.28	4.87		
575.99	353.13	3.11	122.78	5.47	46.40	5.06		
563.24	418.38	3.02	131.18	5.31	36.91	4.82		
549.00	465.48	2.80	149.81	5.10	17.88	4.56		
536.24	565.94	2.82	169.43	5.33	45.58	4.78		
521.82	655.32	2.86	208.24	6.40	82.23	4.82		
506.68	737.06	2.89	235.88	3.27	96.79	4.71		
490.72	881.89	3.02	299.71	5.52	114.64	4.93		
473.81	1065.79	2.88	360.41	5.46	124.54	4.68		
455.80	1252.84	3.01	434.23	8.48	157.82	4.80		
436.47	1517.11	3.04	536.40	5.54	183.76	4.95		
415.99	1825.42	3.19	680.57	6.82	230.20	5.20		
392.64	2181.92	3.30	829.81	6.02	303.50	5.39		
367.17	2615.03	3.39	1030.89	5.64	405.28	5.24		
339.23	3134.17	3.06	1240.84	5.58	627.12	4.98		
304.27	4277.38	3.14	1537.02	6.73	882.70	5.11		
262.11	5660.88	3.34	2064.40	6.09	1364.43	5.44		
203.13	7790.32	3.14	3.05e+04	5.73	3011.54	5.12		
150.00	1.24e+04	3.38	2.69e+04	6.50	7315.51	5.81		

# JASON Licensing

- JASON uses a subscription model
- Benefits for the user include:
  - Frequent updates
    - Bug fixes every month
    - New features every 3 months
  - Easier support, you always have the latest version
- Pricing around “consumables” level
- Discounts for large userbase and campus licences



The screenshot shows the JEOL JASON website. The main heading is "JASON Academia" with the tagline "For chemistry students who dream that their future research will change the world". Below this, there are three pricing cards for different subscription durations:

Subscription Duration	Price	Features
Single 1 Month	£ 2 <sup>99</sup>	NMR Processing tools, Analyse your data, Predict your NMR, Assign your molecules
Single 3 Month	£ 8 <sup>00</sup>	NMR Processing tools, Analyse your data, Predict your NMR, Assign your molecules
Single 1 Year	£ 19 <sup>99</sup>	NMR Processing tools, Analyse your data, Predict your NMR, Assign your molecules

Each card has an "Add to cart" button at the bottom.

~ 41 NZD

# Plugins

## MAGRES for solid state NMR / NMR crystallography

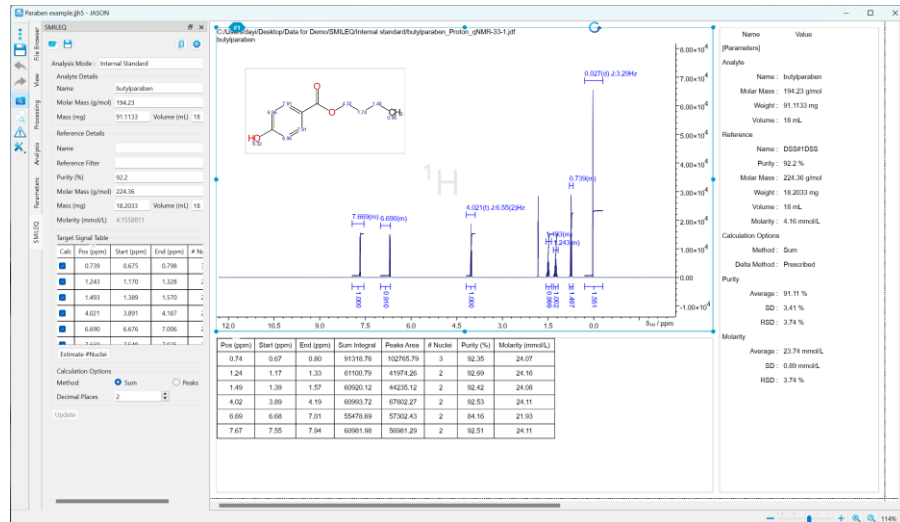
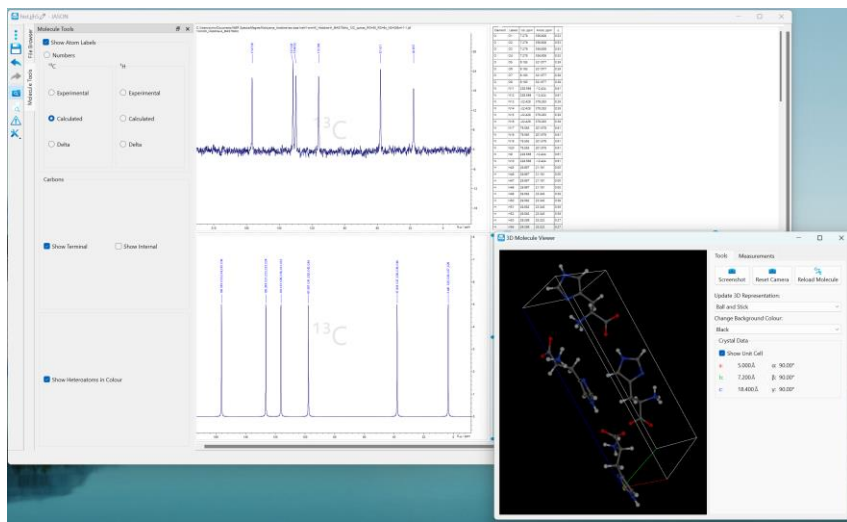
- Reads .magres output from CASTEP or QuantumESPRESSO
- View crystal structure
- Create 1D and 2D simulated spectra
- Option to include 2<sup>nd</sup>-order quadrupolar shift
- RMSD alignment with experimental data
- 3D visualization, easy distance and angle measurements

Free!

## qNMR with SMILEQ

- Internal or External standard methods
  - PULCON and SOLCOR corrections
- Report generation
- Batch mode for multiple repetitions
- ISO 24583 compliant uncertainty reporting
- Seamless integration with JEOL Delta

207 NZD /year





# JEOL webinars

([https://www.jeol.co.jp/en/news/seminar/webseminar/movie\\_index.html](https://www.jeol.co.jp/en/news/seminar/webseminar/movie_index.html))

Webinar	Link
An Introduction to NMR: Practical Aspects	<a href="https://attendee.gotoweinar.com/register/6221243905175906829">https://attendee.gotoweinar.com/register/6221243905175906829</a>
Speeding up NMR: NUS and NOAH	<a href="https://attendee.gotoweinar.com/register/5215973618176042256">https://attendee.gotoweinar.com/register/5215973618176042256</a>
An Introduction to Pure Shift NMR	<a href="https://attendee.gotoweinar.com/register/7480233097627308048">https://attendee.gotoweinar.com/register/7480233097627308048</a>
Introduction to JEOL Delta: Processing of 1D NMR data	<a href="https://attendee.gotoweinar.com/register/3743196484819939856">https://attendee.gotoweinar.com/register/3743196484819939856</a>
An Introduction to Solid-State NMR	<a href="https://attendee.gotoweinar.com/register/1588889267810221067">https://attendee.gotoweinar.com/register/1588889267810221067</a>
Natural Products identification through JEOL systems	<a href="https://attendee.gotoweinar.com/register/987608140196536078">https://attendee.gotoweinar.com/register/987608140196536078</a>
An Introduction to JEOL Delta pulse programming	<a href="https://attendee.gotoweinar.com/register/4684449906779482894">https://attendee.gotoweinar.com/register/4684449906779482894</a>
Main aspects and applications of FAST MAS Solid-State NMR	<a href="https://attendee.gotoweinar.com/register/3947946440960288782">https://attendee.gotoweinar.com/register/3947946440960288782</a>
Elucidating nano-crystalline structure by combining microED and solid-state NMR	<a href="https://attendee.gotoweinar.com/register/5151154110240940816">https://attendee.gotoweinar.com/register/5151154110240940816</a>
Delta processing part 2: quantitative NMR	<a href="https://attendee.gotoweinar.com/register/591245194184783115">https://attendee.gotoweinar.com/register/591245194184783115</a>
Assignment strategies in NMR pt1: 1D NMR and coupling	<a href="https://attendee.gotoweinar.com/register/7874168324236508685">https://attendee.gotoweinar.com/register/7874168324236508685</a>
NMR application in battery research	<a href="https://attendee.gotoweinar.com/register/7305723011972237583">https://attendee.gotoweinar.com/register/7305723011972237583</a>
Gradient Shimming: Theory and Practice	<a href="https://attendee.gotoweinar.com/register/5291489178361927691">https://attendee.gotoweinar.com/register/5291489178361927691</a>
A Synergy between Cryo-EM and NMR	<a href="https://attendee.gotoweinar.com/register/7623552241737432588">https://attendee.gotoweinar.com/register/7623552241737432588</a>
Assignment strategies in NMR pt2, 2D NMR	<a href="https://attendee.gotoweinar.com/register/2012768594452261388">https://attendee.gotoweinar.com/register/2012768594452261388</a>
Solid-State NMR Tutorial: Sample Packing, Standard Samples & Sample Spinning	<a href="https://attendee.gotoweinar.com/register/8621407423140093454">https://attendee.gotoweinar.com/register/8621407423140093454</a>
Ethyl Indanone: a user's perspective of the new JASON software	<a href="https://attendee.gotoweinar.com/register/3360923782708443918">https://attendee.gotoweinar.com/register/3360923782708443918</a>
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Solid-State NMR Tutorial: Setting up CPMAS Probe	<a href="https://attendee.gotoweinar.com/register/477678849452440848">https://attendee.gotoweinar.com/register/477678849452440848</a>
Quantitative 13C NMR	<a href="https://attendee.gotoweinar.com/register/2577550346473705743">https://attendee.gotoweinar.com/register/2577550346473705743</a>
A Practical Introduction to Diffusion-Ordered Spectroscopy	<a href="https://attendee.gotoweinar.com/register/4225933783914972175">https://attendee.gotoweinar.com/register/4225933783914972175</a>

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Webinar	Link
Solving the Structures of Small Molecules Using Fluorine's Unique NMR Properties	<a href="https://connect.acspubs.org/CENWebinar_JEOL_10_22_19">https://connect.acspubs.org/CENWebinar_JEOL_10_22_19</a>
Advances in Liquid Nitrogen Cold Probe Technology	<a href="https://connect.acspubs.org/CENWebinar_JEOL_11_19_19">https://connect.acspubs.org/CENWebinar_JEOL_11_19_19</a>
NMR without deuterated solvents – principles and applications of No-D NMR	<a href="https://connect.acspubs.org/CENWebinar_JEOL_4_21_20">https://connect.acspubs.org/CENWebinar_JEOL_4_21_20</a>
Core principles of precise qNMR – Common Pitfalls and Solutions	<a href="https://connect.acspubs.org/CENWebinar_JEOL_6_24_20">https://connect.acspubs.org/CENWebinar_JEOL_6_24_20</a>
Introduction to Solid-State Nuclear Magnetic Resonance Spectroscopy and Applications	<a href="https://connect.acspubs.org/CENWebinar_JEOL_5_26_21">https://connect.acspubs.org/CENWebinar_JEOL_5_26_21</a>
Main Aspects and Applications of FAST MAS Solid-State NMR	<a href="https://connect.acspubs.org/CENWebinar_JEOL_7_14_21">https://connect.acspubs.org/CENWebinar_JEOL_7_14_21</a>
Proton, Fluorine and X: Practical Aspects and Real Life Applications	<a href="https://go.jeolusa.com/Webinar_031">https://go.jeolusa.com/Webinar_031</a>
AutoMAS Solid State NMR for Improved Sample Throughput	<a href="https://connect.acspubs.org/CENWebinar_JEOL_10_5_21">https://connect.acspubs.org/CENWebinar_JEOL_10_5_21</a>
An Introduction to JASON NMR Processing Software using a number of worked examples	<a href="https://connect.acspubs.org/CENWebinar_JEOL_11_10_21">https://connect.acspubs.org/CENWebinar_JEOL_11_10_21</a>
An Introduction of Delta NMR Data Processing Software ver.5	<a href="https://vimeo.com/755875413/1e71d583b0">https://vimeo.com/755875413/1e71d583b0</a>
Fluorinated Small Molecules at NMR -Simplifying Structure Elucidation of Fluorinated Small Molecules-	<a href="https://vimeo.com/755891713/a56376c521">https://vimeo.com/755891713/a56376c521</a>
Introduction to Quantitative NMR —Easy and Reliable Assay—	<a href="https://vimeo.com/755891839/c906767e0b">https://vimeo.com/755891839/c906767e0b</a>
Introduction to solid-state MAS NMR	<a href="https://vimeo.com/755877206/48ed7afcb5">https://vimeo.com/755877206/48ed7afcb5</a>
JASON a novel NMR tool	<a href="https://vimeo.com/755877511/17ebb853b4">https://vimeo.com/755877511/17ebb853b4</a>
To analyze the motion of molecule (ion) by NMR	<a href="https://vimeo.com/755879143/d15bc3a1c4">https://vimeo.com/755879143/d15bc3a1c4</a>
Tackling complex mixture by NMR	<a href="https://vimeo.com/755879270/6d88566cc4">https://vimeo.com/755879270/6d88566cc4</a>
SMILEQ Plugin in JASON Software for Automated Quantitative NMR System	<a href="https://vimeo.com/755880107/efb95e2646">https://vimeo.com/755880107/efb95e2646</a>
NMR Techniques to Determine Local Structure and Ion Dynamics in Lithium Ion Batteries	<a href="https://www.bigmarker.com/azonetwork/NMR-Techniques-to-Determine-Local-Structure-and-Ion-Dynamics-in-Lithium-Ion-Batteries">https://www.bigmarker.com/azonetwork/NMR-Techniques-to-Determine-Local-Structure-and-Ion-Dynamics-in-Lithium-Ion-Batteries</a>
Solid-state NMR to elucidate the atomic level structures: basic principles and applications	<a href="https://www.jeol.com/events_seminars/webinars/2023/20230213_01_movie.php">https://www.jeol.com/events_seminars/webinars/2023/20230213_01_movie.php</a>
Introduction to solid-state NMR: half-integer quadrupolar nuclei	<a href="https://www.jeol.com/events_seminars/webinars/2023/20230707_01_movie.php">https://www.jeol.com/events_seminars/webinars/2023/20230707_01_movie.php</a>
What makes solid-state NMR broadened and how to overcome it	<a href="https://vimeo.com/936545870/9a33a89f95">https://vimeo.com/936545870/9a33a89f95</a>

# Thank you

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  - Free natural products database
  - Application notes
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