The way to NMR facility managers' hearts

24th June 2024

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JEOL UK Demo Lab nmrapps@jeoluk.com

Service support

Spare Parts Policy

Spares

We have a local dedicated stock department.
We hold spares for our current range and legacy range of instrumentation.
We have a total spares stock of ~5M€. Stock control is also computerised and centralised, so, when required, spares can immediately be located, even if they are in Europe (should we not have them locally), with same-day shipment.

And..

Our European spares support is backed up by our International Parts Centre in Japan that has a Web based ordering system. Dispatch within two days- delivery to customer is usually within a week (depending on customs clearance).

(Please note, priority is given to warranty/contract based customers)

Response Times

Normally, a qualified service engineer will contact you on the same working day that a fault is reported.

Often, problems can be resolved over the telephone, email or through remote login.

In the event that a site visit is required, we aim to have an engineer on site within 48 hrs (working). We currently achieve this for more than 80% of breakdowns.

Lab Design Consultancy

- Architectural consultancy available
- 25 years experience, 20 years with accreditation
- Full environmental surveying & characterisation
  - Seismic surveys
  - a.c. field gradients and spectrum analysis
  - d.c. field shift
  - acoustic noise spectrum analysis
  - air conditioning
  - building design
  - water cooling
  - data logging

With proven solutions.

Fault Reporting

As well as your personal contacts for direct support of Applications and Engineering, you can also log calls via: uk.svc@jeoluk.com

www.jeoluk.com

+44(0)1707 377117

This is regardless of any service agreement. All faults are logged locally with full details for easy tracking.

JEOL (UK) Support Level	NO CONTRACT	STANDARD	PREMIER	LIFETIME WARRANTY	ELITE
Telephone support	☐	☐	☐	☐	☐
Routine planed maintenance		☐	☐	☐	☐
Unlimited labour		☐	☐	☐	☐
Unlimited spare parts			☐	☐	☐
Parts (consumables)					☐

UK NMR Applications Team

Dr Adolfo Botana

Dr Paul Bowyer

Dr Claire Dickson

Dr Michal Malon

Satoshi Sakurai

Welwyn Garden City, UK

Onsite, remote and in-house customer training

JEOL NMR user meetings

JASON Software Development Team

Vadim
Zorin

Iain
Day

Yibiao
Li

Hiroshi
Endo

Yuko
Igarashi

Naoto
Seki

Nikolay
Larin

Peter
Kiraly

Rachel
Brignall

Nader
Amin

Ronil
Sedani

Maximillian
Reinhart

Saeko
Suzuki

1 Customer Support
1 Developer

Very responsive support

The request:

orward

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:

rward

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

Collaborations

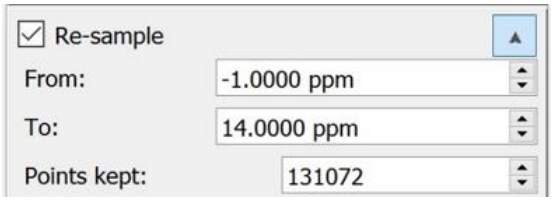
The problem

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 1H 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



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

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

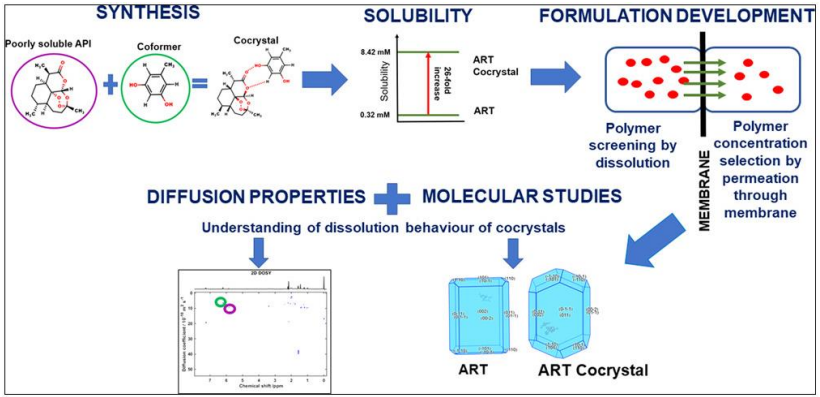
Other collaborations

molecular pharmaceutics

Artemisinin Cocrystals for Bioavailability Enhancement. Part 1: Formulation Design and Role of the Polymeric Excipient

Manreet Kaur, Vanessa Yardley, Ke Wang, Jinit Masania, Adolfo Botana, Randolph R. J. Arroo , and Mingzhong Li*

Cite this: *Mol. Pharmaceutics* 2021, 18, 12, 4256−4271
Publication Date: November 1, 2021
https://doi.org/10.1021/acs.molpharmaceut.1c00384

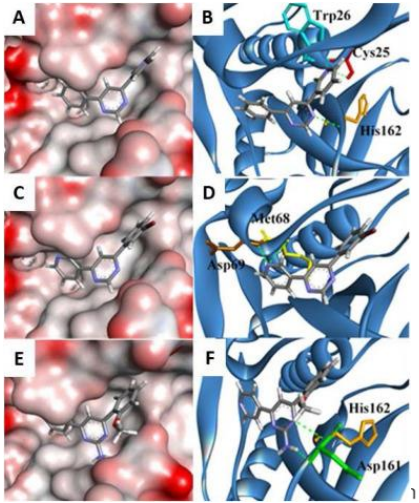


European Journal of Medicinal Chemistry
Volume 209, 1 January 2021, 112871

Research paper

The discovery of novel antitrypanosomal 4-phenyl-6-(pyridin-3-yl)pyrimidines

William J. Robinson [a], Annie E. Taylor [a], Solange Lauga-Cami [a], George W. Weaver [b], Randolph R.J. Arroo [c], Marcel Kaiser [d, e], Sheraz Gul [f, g], Maria Kuzikov [f, g], Bernhard Ellinger [f, g], Kuldip Singh [h], Tanja Schirmeister [i], Adolfo Botana [j], Chatchakorn Eurtivong [k], Avninder S. Bhambra [a]



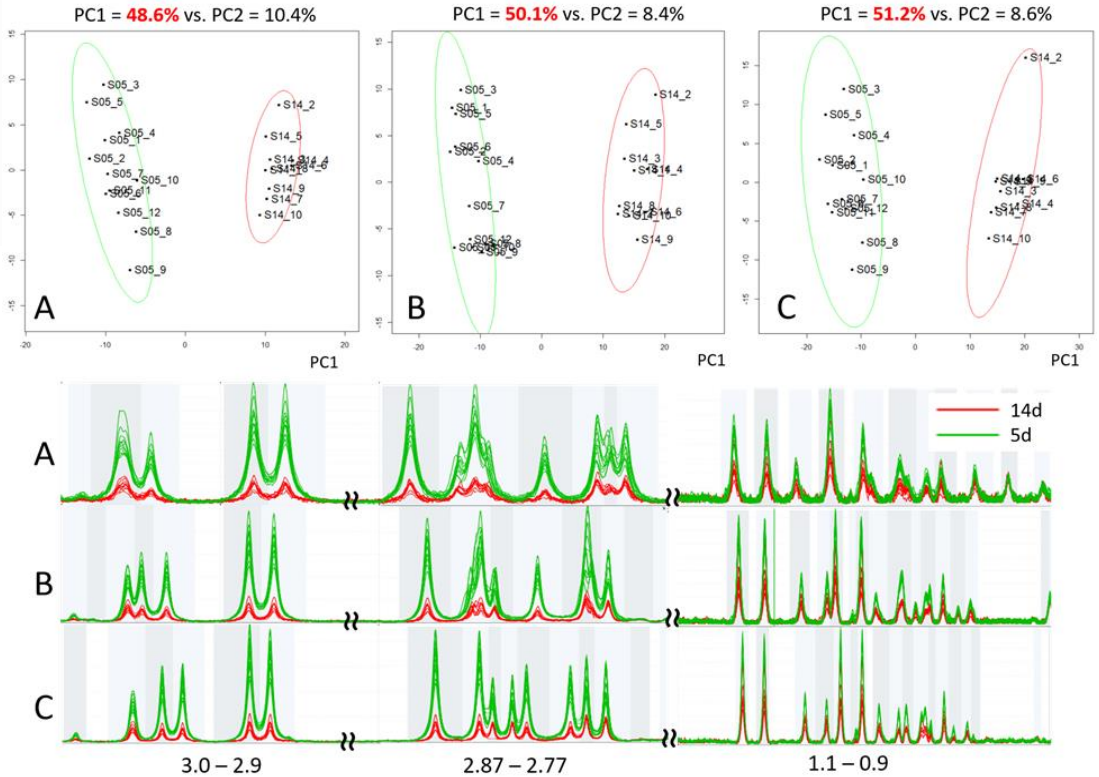
Inter-laboratory collaborations

Review Article | Open Access | Published: 26 February 2019

Optimizing 1D ^{1}H-NMR profiling of plant samples for high throughput analysis: extract preparation, standardization, automation and spectra processing

Catherine Deborde, Jean-Xavier Fontaine, Daniel Jacob, Adolfo Botana, Valérie Nicaise, Florence Richard-Forget, Sylvain Lecomte, Cédric Decourtil, Kamar Hamade, François Mesnard, Annick Moing & Roland Molinié

Metabolomics **15**, Article number: 28 (2019) | Cite this article



A: JEOL 400
B: Bruker 500
C: Bruker 600

Green: 5 days after flowering

Red: 14 days after flowering

Tools for NMR administrators

Automation setup

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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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
		300		**5.83**

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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	Experime	Project Na	Folder	Filename	Job Result
14-12-22 23:14	14-12-22 23:14	0 days 00:(	0.00037037	demo	Proton	14-12-22 23:14	14-12-22 23:14	0 days 00:00:18	0.000208333	proton.jxp		demo	test1_1H	FINISHED
15-12-22 10:19	15-12-22 10:19	0 days 00:(	0.000208333	demo	Proton	15-12-22 10:19	15-12-22 10:19	0 days 00:00:08	9.25926E-05	proton.jxp		demo	sample1_1H	FINISHED
21-01-23 21:46	21-01-23 21:46	0 days 00:(	0.000300926	demo	Proton	21-01-23 21:46	21-01-23 21:46	0 days 00:00:18	0.000208333	proton.jxp		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	Experime	Project Na	Folder	Filename	Job Result
29-06-23 9:38	29-06-23 9:38	0 days 00:(	0.000243056	test	1H	29-06-23 9:38	29-06-23 9:38	0 days 00:00:10	0.000115741	proton.jxp		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	Experime	Project Na	Folder	Filename	Job Result
16-12-22 19:21	16-12-22 19:22	0 days 00:(	0.000196759	test2	1H	16-12-22 19:21	16-12-22 19:22	0 days 00:00:10	0.000115741	proton.jxp		organome	fds_PROTON	FINISHED

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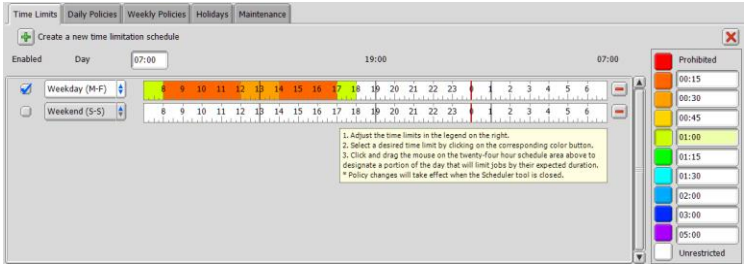
Custom time limitations:



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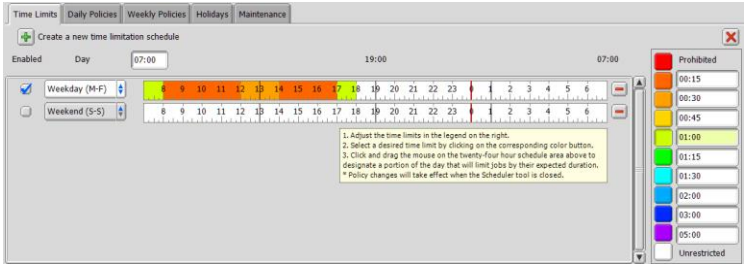
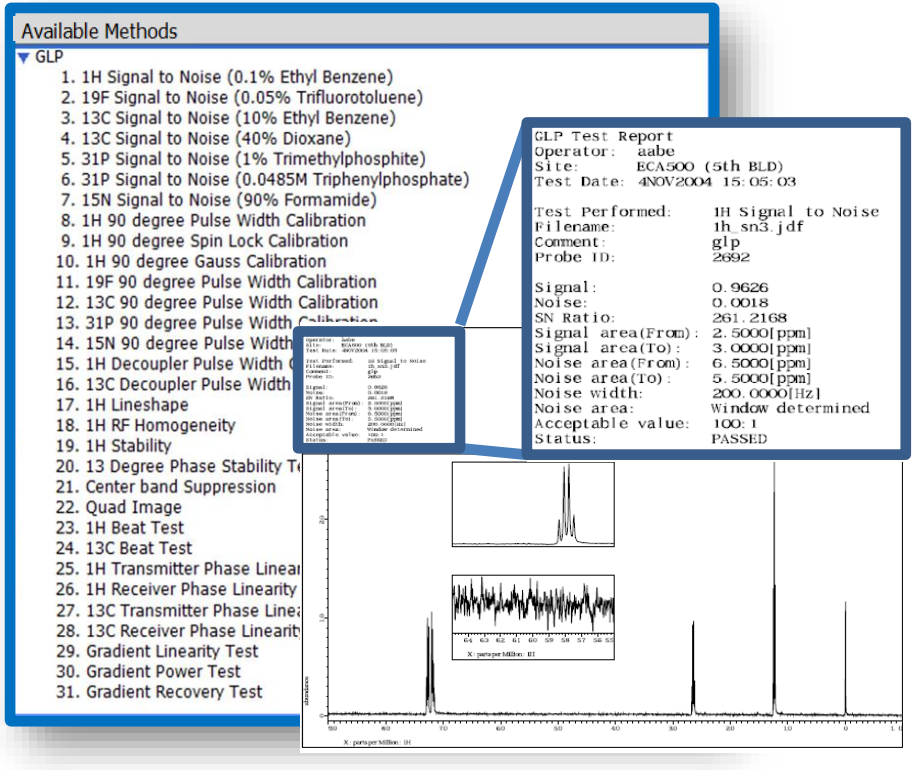


Automatic spectrometer calibration tools by default



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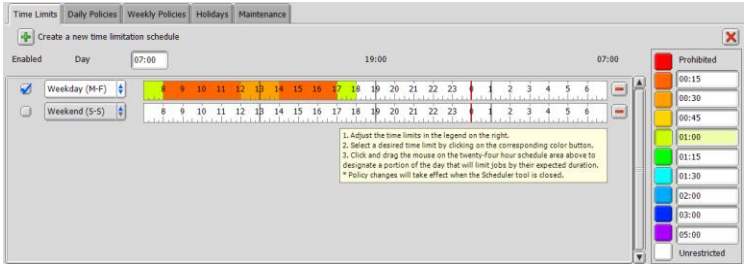
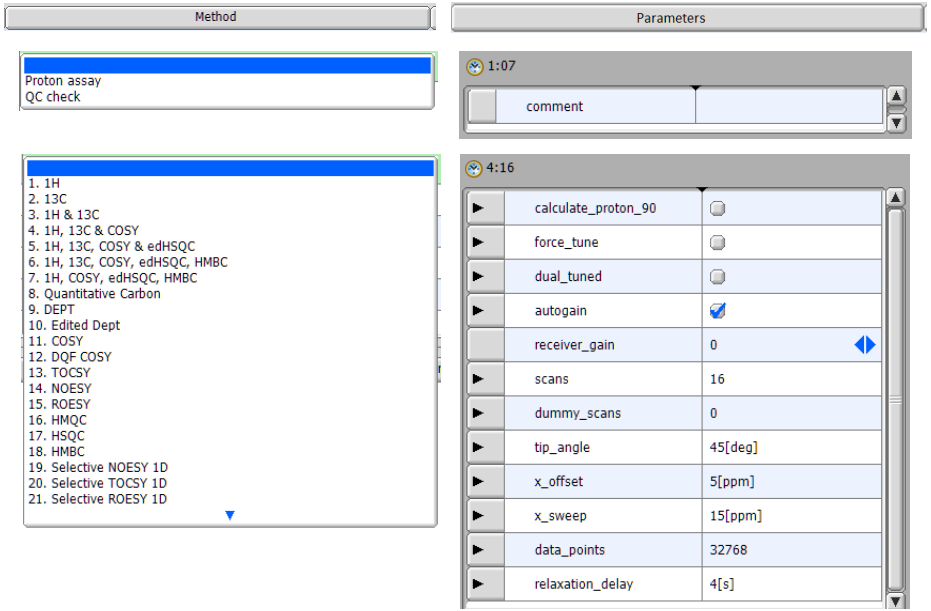


Automatic spectrometer calibration tools by default

Fully customizable methods for each user



JEOL webinars (https://www.jeol.co.jp/en/news/seminar/webseminar/movie_index.html)

Webinar	Link
An Introduction to NMR: Practical Aspects	https://attendee.gotowebinar.com/register/6221243905175906829
Speeding up NMR: NUS and NOAH	https://attendee.gotowebinar.com/register/5215973618176042256
An Introduction to Pure Shift NMR	https://attendee.gotowebinar.com/register/7480233097627308048
Introduction to JEOL Delta: Processing of 1D NMR data	https://attendee.gotowebinar.com/register/3743196484819939856
An Introduction to Solid-State NMR	https://attendee.gotowebinar.com/register/1588889267810221067
Natural Products identification through JEOL systems	https://attendee.gotowebinar.com/register/987608140196536078
An Introduction to JEOL Delta pulse programming	https://attendee.gotowebinar.com/register/4684449906779482894
Main aspects and applications of FAST MAS Solid-State NMR	https://attendee.gotowebinar.com/register/3947946440960288782
Elucidating nano-crystalline structure by combining microED and solid-state NMR	https://attendee.gotowebinar.com/register/5151154110240940816
Delta processing part 2: quantitative NMR	https://attendee.gotowebinar.com/register/591245194184783115
Assignment strategies in NMR pt1: 1D NMR and coupling	https://attendee.gotowebinar.com/register/7874168324236508685
NMR application in battery research	https://attendee.gotowebinar.com/register/7305723011972237583
Gradient Shimming: Theory and Practice	https://attendee.gotowebinar.com/register/5291489178361927691
A Synergy between Cryo-EM and NMR	https://attendee.gotowebinar.com/register/7623552241737432588
Assignment strategies in NMR pt2, 2D NMR	https://attendee.gotowebinar.com/register/2012768594452261388
Solid-State NMR Tutorial: Sample Packing, Standard Samples & Sample Spinning	https://attendee.gotowebinar.com/register/8621407423140093454
Ethyl Indanone: a user's perspective of the new JASON software	https://attendee.gotowebinar.com/register/3360923782708443918
Practical aspects of high-resolution 1H solid-state NMR at moderate MAS rate	https://attendee.gotowebinar.com/register/3873886639811883023
Your data in JASON: file formats and external access	https://attendee.gotowebinar.com/register/2441061364881739019
Selective Excitation of Overlapping Multiplets	https://attendee.gotowebinar.com/register/3213601326619561742
NMR Crystallography of Dynamically Disordered Solids	https://attendee.gotowebinar.com/register/3995403572903868683
Solid-State NMR Tutorial: Setting up CPMAS Probe	https://attendee.gotowebinar.com/register/477678849452440848
Quantitative 13C NMR	https://attendee.gotowebinar.com/register/2577550346473705743
A Practical Introduction to Diffusion-Ordered Spectroscopy	https://attendee.gotowebinar.com/register/4225933783914972175

JEOL webinars (https://www.jeol.co.jp/en/news/seminar/webseminar/movie_index.html)

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

Thank you

Email: nmrapps@jeoluk.com

JEOL webinars announced in social media:

@JEOLEUROPE

You can discover more about JEOL NMR at:

- **http://www.jeol.com/ (Products -> NMR)**
  - Description of our products
  - Free natural products database
  - Application notes
  - Webinar recordings
  - And more
- **http://nmrsupport.jeol.com/**
  - Free processing software Delta
- **https://jeoljason.com/**
  - Subscription-based software
  - JEOL blog

JEOL ECZL
NMR spectrometer

Pulse on several nuclides at once with a single channel

Our Logo is a ship, based on the Argo, from Jason and the Argonauts

JASON

Read any NMR data (Bruker, Varian, OI…)

Easy report design

Automatic structural assignment