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<https://nomad-nmr.uk>

# NOMAD - NMR Online Management And Datastore

UKMRM 2025  
London

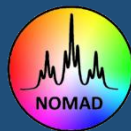


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<https://nomad-nmr.uk>

**Make Automation Great Again**

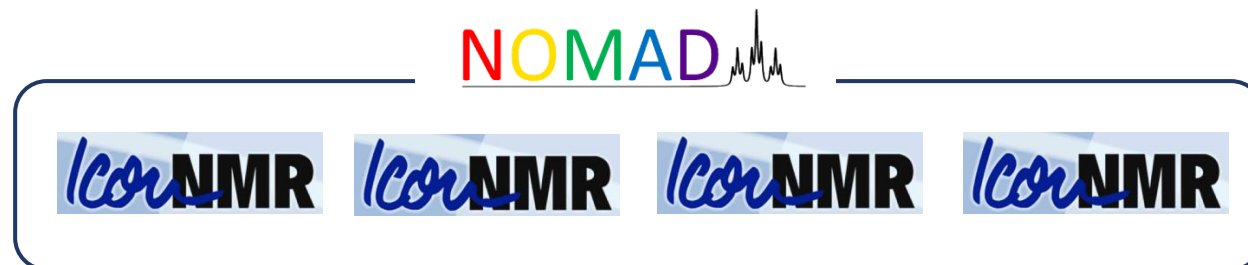
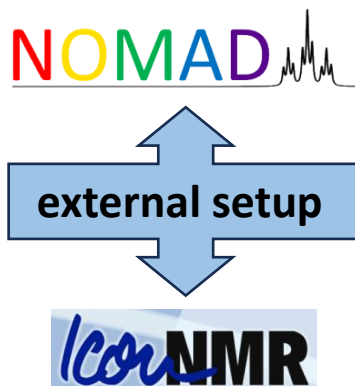


## Make Automated NMR Great Again

Year	1994	2004	2024
Number of instruments in the lab	1	5	6
Number of autosamplers	0	2	6
Experiments per year	~ 3 500	~ 18 500 *	65 276 *
Average experiments per year & instrument	~ 3 500	~ 9 250 *	10 879 *

\* acquired under automation only

NOMAD is using IconNMR API  
(external setup) to improve and  
extend its functionality



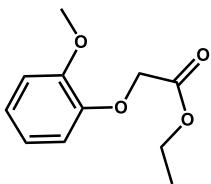
NOMAD is IconNMR orchestrator

## Next Step in Evolution of NMR data handling

## digitalisation trend of NMR data handling & information content & value

1994

### Publication strings

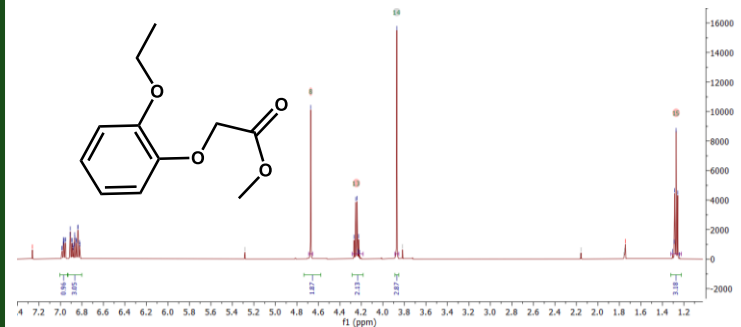


<sup>1</sup>H NMR (500 MHz): δ 1.27 (3H, t, *J* = 7.14 Hz), 3.87 (3H, s), 4.25 (2H, q, *J* = 7.14 Hz), 4.67 (2H, s), 6.97 (1H, ddd, *J* = 8.26, 7.32, 1.65 Hz), 6.83 (1H, dd, *J* = 7.91, 1.71 Hz), 6.87 (1H, ddd, *J* = 9.32, 8.05, 1.74 Hz), 6.90 (1H, dd, *J* = 8.01, 1.71 Hz).

**paper S.I.**

2004

### Images of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra



2024

### F.A.I.R NMR data

Findable



## Accessible



## Interoperable



## Reusable



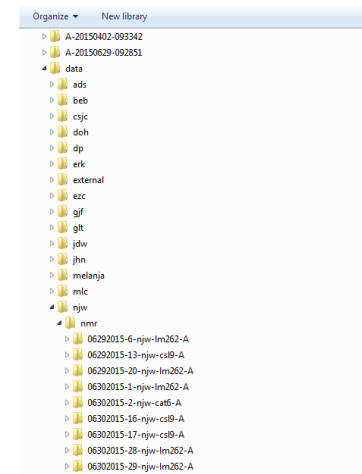
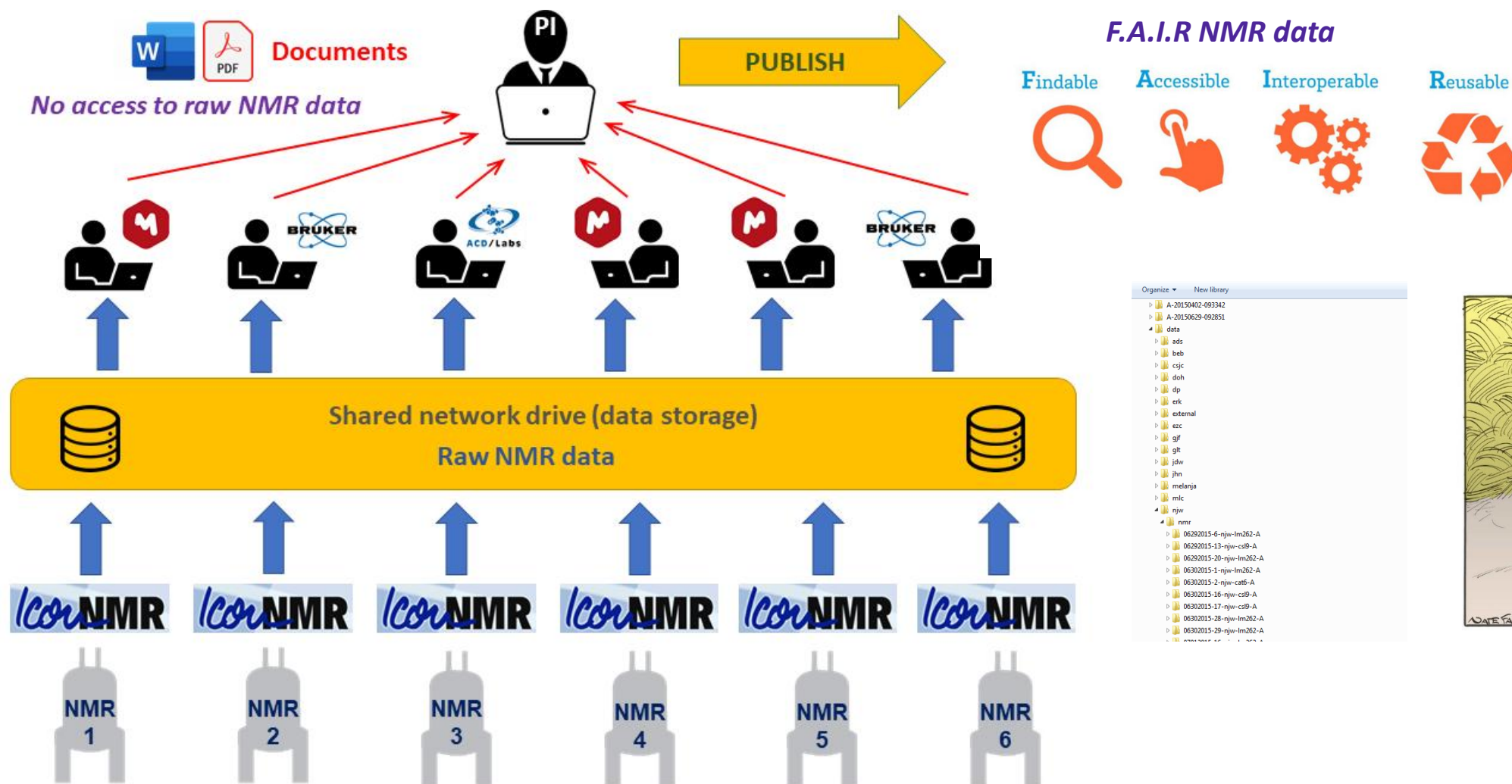
**digital S.I.**

## Why deposition of digital S.I. is still cumbersome?



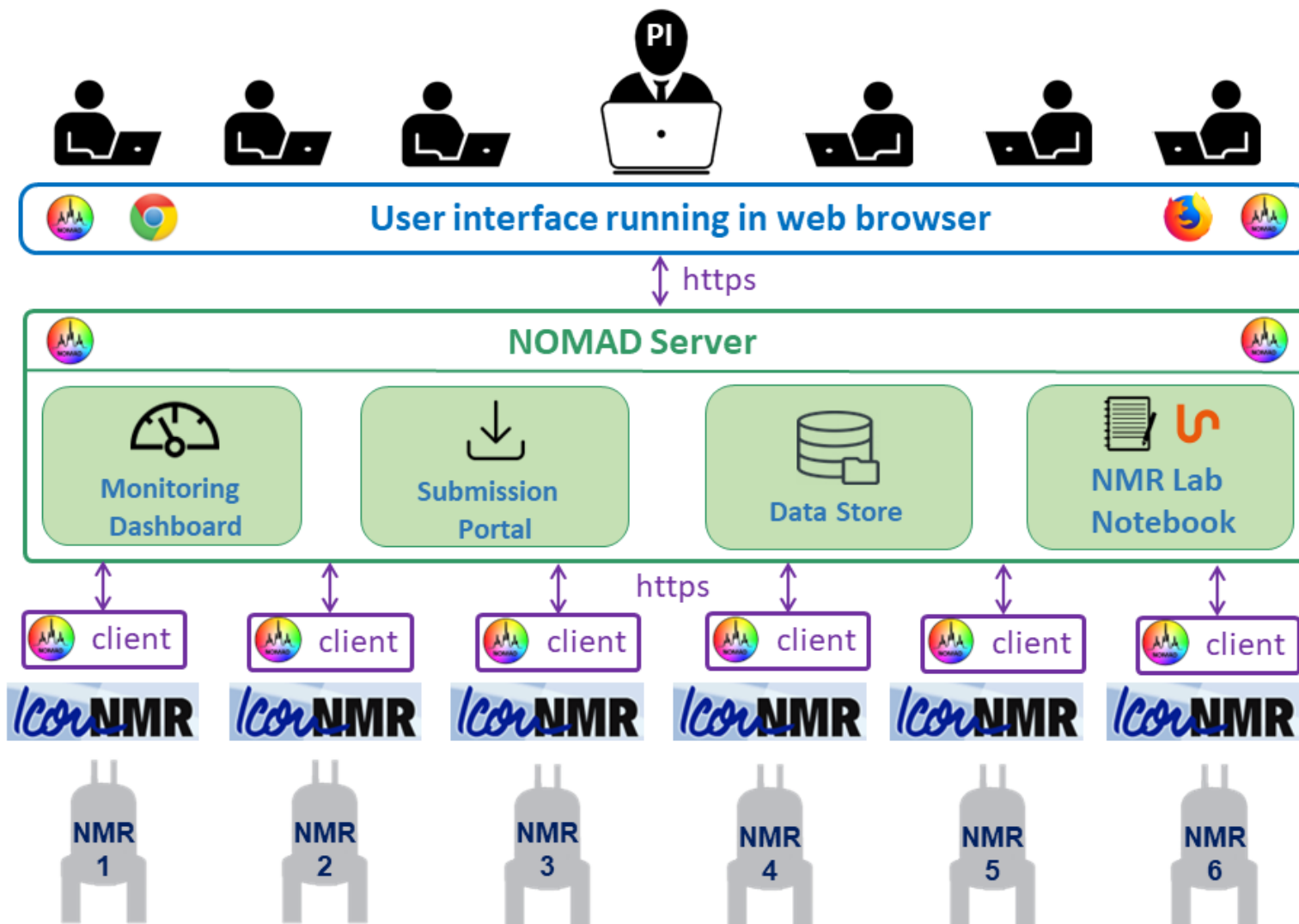


## Established Data Workflow in Multiuser NMR Lab





# Complete Solution for NMR Laboratory Data Management










# NMR Lab Management Features








Central dashboard for monitoring and controlling of all IconNMR instances in the lab




➤ Both users and administrators can see status of automation queues from anywhere










 Dashboard
 


 Cards On
 4
  1
  3


 Book New Job
  Batch Submit
  Datastore
 


A


 **Alec**  
 Bruker AVIII 500  
 [Prodigy BBFO]



 **Felix**  
 Bruker AVIII-HD 500  
 [BBFO+]



 **Hector**  
 Bruker AVIII-HD 700  
 [Prodigy TCI]



 **Ishbel**  
 Bruker Neo 400  
 [BBF-H-D iProbe]



 **Marcus**  
 Bruker AVII 400  
 [BBFO]



 **Noah**  
 Bruker AV 400  
 [BBFO]



Busy until: Mon 17:40  
 Expt Queue    Allowance  
 00:25    00:35  
 05:36    03:15

Busy until: Idle  
 Expt Queue    Allowance  
 00:00    00:25  
 00:00    03:15

Busy until: Mon 17:09  
 Expt Queue    Allowance  
 00:00    01:05  
 00:06    05:05

Busy until: Mon 17:06  
 Expt Queue    Allowance  
 00:01    00:25  
 02:04    03:25

Busy until: Mon 17:10  
 Expt Queue    Allowance  
 00:01    00:25  
 01:22    03:15

Busy until: Idle  
 Expt Queue    Allowance  
 00:00    00:25  
 02:29    03:15

Alec

Felix

Hector

Ishbel

Marcus

Noah

Delete



Resubmit

Reset

On

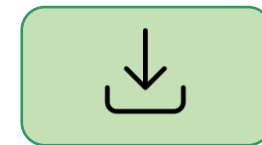
Busy until: Mon 17:09    Day Experiments: 00:00    Night Experiments: 00:06

22

Select	Holder	User	Group	Dataset Name	Exp Count	Solvent	Submitted At	ExpT	D/N	P	Status
+ <input type="checkbox"/>	2	tsh6	ezc	2506091459-5-2-tsh6	3	CD3CN	Mon 14:59	00:56:48			<span>Running</span>
+ <input type="checkbox"/>	1	tsh6	ezc	2506091459-5-1-tsh6	3	CD3CN	Mon 14:59	00:56:48			<span>Completed</span>





# NMR Lab Management Features




Central dashboard for monitoring and controlling of all IconNMR instances in the lab

➤ One central database of users for all instruments in the lab that is accessible from any computer






































Manage Users

Add
Delete

☐ Off

 Book New Job
 Batch Submit
 Datastore

 A

<input type="checkbox"/>	Username	Email	Full name	Group	Access level			Last login	Inactive Days	Actions
					Main	Data	Manual			
<input type="checkbox"/>	admin	tl12@st-andrews.ac.uk	Admin	admins	admin	admin		10 Jun 2025, 09:21	0	Active  
<input type="checkbox"/>	dm385	dm385@st-andrews.ac.uk	Dorian Moreau	raa	user	undefined		10 Jun 2025, 09:19	0	Active  
<input type="checkbox"/>	srs9	srs9@st-andrews.ac.uk	Siobhan Smith	admins	admin	admin		10 Jun 2025, 09:16	0	Active  
<input type="checkbox"/>	be34	be34@st-andrews.ac.uk	Balakumar Emayavaramban	cpj	user	undefined		10 Jun 2025, 09:11	0	Active  
<input type="checkbox"/>	lm432	lm432@st-andrews.ac.uk	Liam Mas	ezc	user	undefined		10 Jun 2025, 09:03	0	Active  
<input type="checkbox"/>	fp77	fp77@st-andrews.ac.uk	Ffion Platt	ads	admin-b	undefined		10 Jun 2025, 08:53	0	Active  
<input type="checkbox"/>	tl12	tl12@st-andrews.ac.uk	Tomas Lebl	tl	user-a	admin		10 Jun 2025, 08:53	0	Active  
<input type="checkbox"/>	al330	al330@st-andrews.ac.uk	Andrew Linz	cmc	user	undefined		10 Jun 2025, 08:44	0	Active  
<input type="checkbox"/>	lah27	lah27@st-andrews.ac.uk	Lucy Alexandra Hutton	erk	user	undefined		10 Jun 2025, 08:43	0	Active  
<input type="checkbox"/>	dc270	dc270@st-andrews.ac.uk	Daniel Cowpe	erk	user	undefined		10 Jun 2025, 08:43	0	Active  
<input type="checkbox"/>	jr294	jr294@st-andrews.ac.uk	Jiwu Rim	ak	user	undefined		10 Jun 2025, 08:42	0	Active  
<input type="checkbox"/>	jkj5	jkj5@st-andrews.ac.uk	Jaden Jones	external	user	undefined		10 Jun 2025, 08:31	0	Active  
<input type="checkbox"/>	as644	as644@st-andrews.ac.uk	Alice Sabey	anp	user	undefined		10 Jun 2025, 08:25	0	Active  
<input type="checkbox"/>	gh15	gh15@st-andrews.ac.uk	Guoxiong Hua	rem	user	undefined		10 Jun 2025, 08:20	0	Active  





# NMR Lab Management Features



Central dashboard for monitoring and controlling of all IconNMR instances in the lab

➤ Seamless accounting and usage statistics

Accounting

Set Instruments Costing

Set Grants

Download CSV

Book New Job

Batch Submit

Datastore

A

?

Grants

Groups

Users

Group: ads

Date Range: 2025-05-01 → 2025-05-31

Multiplier: ☐

Calculate Costs

✕

User Name	Group Name	Grant Code	Alec			Felix			Hector			Ishbel			Marcus			Noah			Total Cost [£]	
			Exp Time		Cost [£]	Exp Time		Cost [£]	Exp Time		Cost [£]	Exp Time		Cost [£]	Exp Time		Cost [£]	Exp Time		Cost [£]		
			Manual	Auto		Manual	Auto		Manual	Auto		Manual	Auto		Manual	Auto		Manual	Auto			
rkt4 - Raj Tak	ads	10-10022-424201-XEUK21AJ-RCEP-9999999	0	00:00:00	0	0	03:08:52	8.66	0	00:00:00	0	0	00:00:00	0	0	02:57:31	5.92	0	00:20:04	0.67	15.25	
sk341 - Sonia Kharb	ads	10-10022-424201-XEUK21AJ-RCEP-9999999	0	04:07:32	17.53	0	03:10:52	8.75	0	00:24:59	2.08	0	10:04:47	20.16	0	01:46:56	3.56	0	03:20:44	6.69	58.77	
ska8 - Shubham Agrawal	ads	10-10022-424201-XEUK21AJ-RCEP-9999999	0	01:10:18	4.98	0	00:24:40	1.13	0	00:00:00	0	0	00:11:07	0.37	0	02:20:21	4.68	0	02:38:41	5.29	16.45	
zz63 - Zhanyu Zhou	ads	10-10022-424201-XEUK21AJ-RCEP-9999999	0	00:00:00	0	0	06:49:41	18.78	0	00:15:13	1.27	0	00:05:31	0.18	0	02:08:03	4.27	0	01:59:28	3.98	28.48	
Total			0	12:04:56	51.35	0	21:32:42	59.26	0	01:20:50	6.74	0	50:29:31	100.99	0	18:13:40	36.46	0	46:14:46	92.49	347.29	




# NMR Lab Management Features

Three workflows for onboarding data to the datastore



- Walk-in automation (IconNMR)
- Smart traffic control for day/night queue scheduling


[Book New Job](#)
T

**Alec**  
 Bruker AVIII 500  
 [Prodigy BBFO]

Busy until: Idle  

Expt Queue	Allowance
☀ 00:00	00:35
🌙 00:00	03:15

**Felix**  
 Bruker AVIII-HD 500  
 [BBFO+]

Busy until: Idle  

Expt Queue	Allowance
☀ 00:00	00:25
🌙 00:00	03:15

**Hector**  
 Bruker AVIII-HD 700  
 [Prodigy TCI]

Busy until: Idle  

Expt Queue	Allowance
☀ 00:00	01:05
🌙 00:00	05:05

**Ishbel**  
 Bruker Neo 400  
 [BBF-H-D iProbe]

Busy until: Tue 11:28  

Expt Queue	Allowance
☀ 00:01	00:25
🌙 00:00	03:25

**Marcus**  
 Bruker AVII 400  
 [BBFO]

Busy until: Idle  

Expt Queue	Allowance
☀ 00:00	00:25
🌙 00:00	03:15

**Noah**  
 Bruker AV 400  
 [BBFO]

Busy until: Tue 11:37  

Expt Queue	Allowance
☀ 00:14	00:25
🌙 00:00	03:15

\* Instrument:

\* Number of samples:

[Book Slots](#)

[Cancel & return](#)

[Continue](#)

Total ExpT: 01:47:01



# NMR Lab Management Features

Three workflows for onboarding data to the datastore



- Batch/rack submission (teaching labs, temporary offline instruments, SampleJet)



Batch Submit

Open New Rack

Book

Submit

Cancel

Delete Rack

Datastore

A

NOAH - 10/06/2025

<input type="checkbox"/>	Slot	Username	Full Name	Group	Solvent	
+	<input type="checkbox"/>	dgg7	David Groves	cpj	CDCI3	DGG-2b-08X-SY
+	<input type="checkbox"/>	rh1	Reece Hoogesteger	cpj	CDCI3	RH-16-22
+	<input type="checkbox"/>	rh1	Reece Hoogesteger	cpj	CDCI3	RH-16-
+	<input type="checkbox"/>	rh1	Reece Hoogesteger	cpj	CDCI3	RH-16

Add Rack



Group

Instrument

\* Instrument:

\* Rack Title:

\* Number of Slots:

\* Start From Slot:

Edit Parameters: ☒

SampleJet Rack: ☐

Restrict Access: ☒

Restrict Access

Group:

Username:

Add



Group User : tl12

Cancel

OK

Actions

Reject

Reject

Reject

Reject



# NMR Lab Management Features



Three workflows for onboarding data to the datastore

- Uploading of NMR datasets/folders created by means of manual operation



Manual Claim

Show Archived  
Off

Claim Selected

Datastore

T

\* Instrument:

Felix

Get dataset folders



Select	Dataset Name	Date Created	Number of experiments
+ <input type="checkbox"/>	TestFelix	03-Jun-25 13:07	19
+ <input checked="" type="checkbox"/>	Demo	21-Apr-25 15:12	1
+ <input type="checkbox"/>	Si29 Calibration	01-Jun-23 14:02	2
+ <input type="checkbox"/>	TS-365-test	28-Apr-23 11:04	4



## Datastore Features

NMR Data F.A.I.R. from Inception to Publication



### NMR experiments



### NOMAD datasets



Digital S.I. item

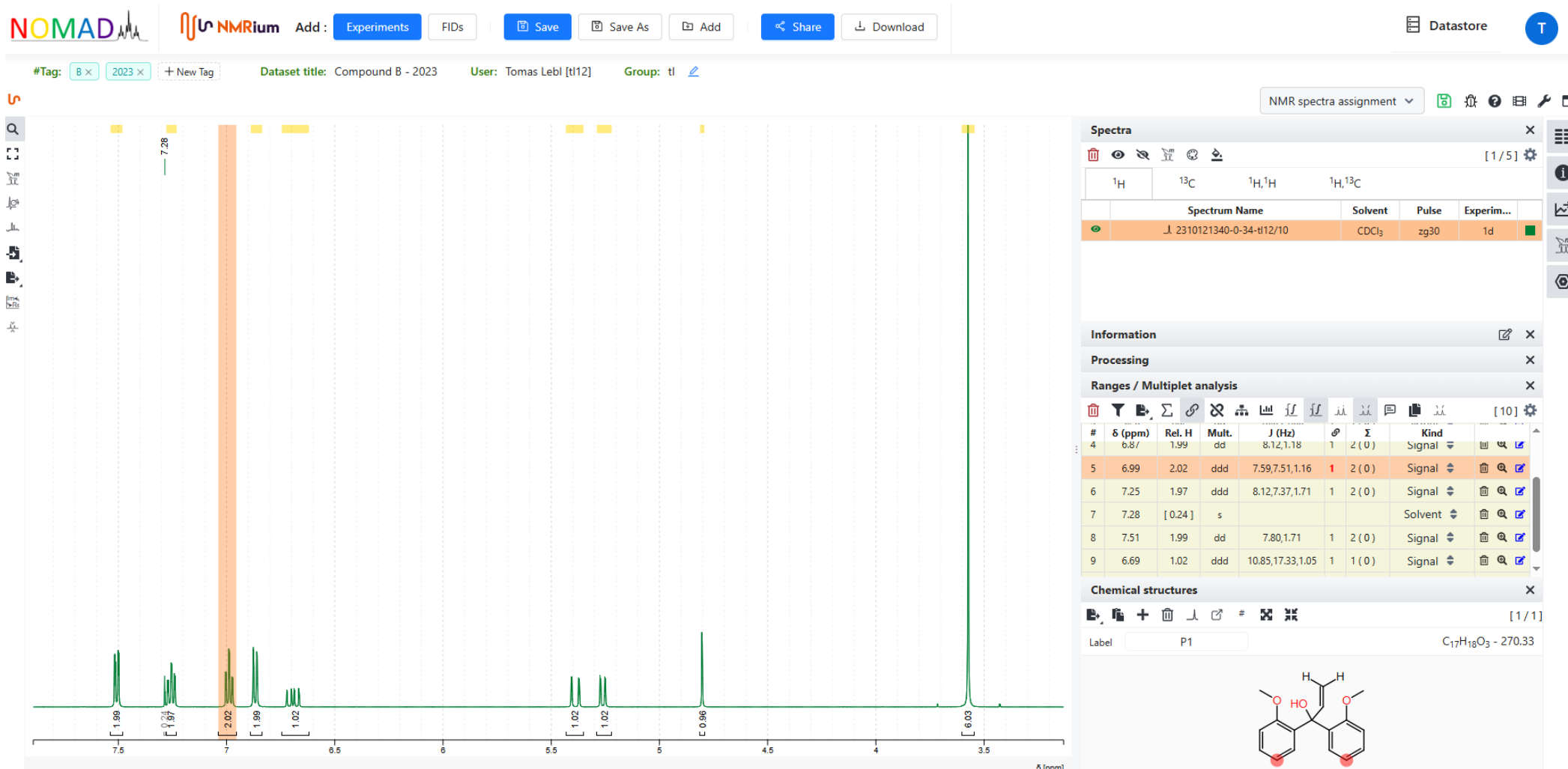






# Datastore Features

NMR Data F.A.I.R. from Inception to Publication





# Datastore Features

NMR Data F.A.I.R. from Inception to Publication







Table
 **Cards**

Add to:
 

Collection

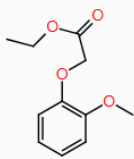
NMRium

Datasore
 

T

Tags: #Tags
 SMILES: C1(=CC=CC=C1)
 Substructure: **ON**
 Created Date Range: Start date → End date
 Last Updated Date Range: Start date → End date
 Title: Dataset Title
 Inactive: **OFF**
 Group: tl
 Inactive: **OFF**
 Username: [tl12] Tomas Lebl

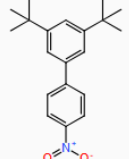
+ New Tag



Compound B - solved

☐
☐
☐
☐
☐

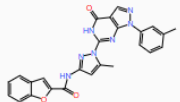
+ New Tag



Tutorial - A - processed

☐
☐
☐
☐
☐

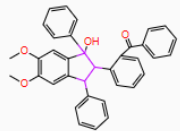
+ New Tag



HA031 tt 5-7

☐
☐
☐
☐
☐

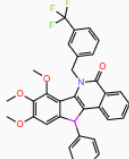
+ New Tag



FT383 - 60C full

☐
☐
☐
☐
☐

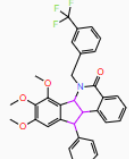
+ New Tag



MCDB\_049 - TL12

☐
☐
☐
☐
☐

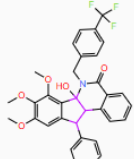
+ New Tag



MCDB\_040 - TL12

☐
☐
☐
☐
☐

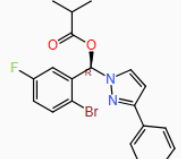
+ New Tag



MCDB\_041 - complete

☐
☐
☐
☐
☐

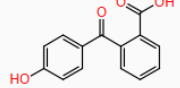
+ New Tag



Exp 9 - product

☐
☐
☐
☐
☐

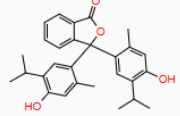
+ New Tag



Phenolphthalein Hydroxylamine - assigned

☐
☐
☐
☐
☐

+ New Tag

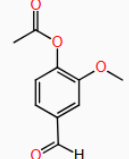


thymolphthalein

☐
☐
☐
☐
☐

workshop X

+ New Tag



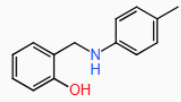
Vanillin demo

☐
☐
☐
☐
☐

C X

CH3431 X

+ New Tag



2-((p-tolylamino)methyl)phenol

☐
☐
☐
☐
☐



# Datastore Features

NMR Data F.A.I.R. from Inception to Publication

## NMR experiments



## NOMAD datasets



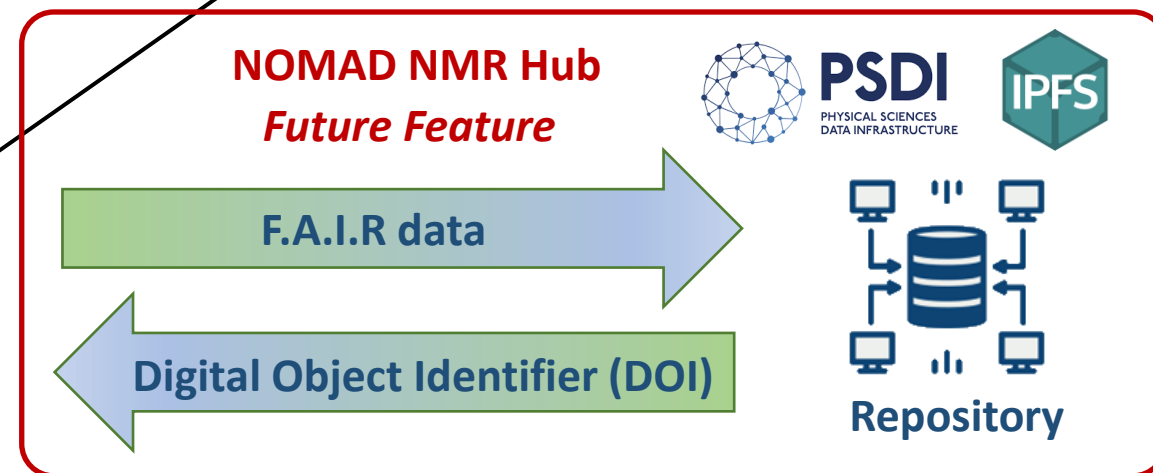
Digital S.I. item



## NOMAD collections



Digital S.I.





## NOMAD Evolution

### Version 1

Development: 2012 – 2016    Production: 2013 – May 2021

### Version 2

Development: 2016 – 2019    Production: 2017 – May 2022

private  
repositories

### Lindy Effect

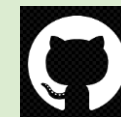
*The future life expectancy of a non-perishable thing is proportional to its current age.*

In simpler terms: if a system (like a piece of technology) has been around for a while, it's likely to stay around for a while longer.

### Version 3



open source



AGPL-3.0 license

In production since May 2021



## Collaborative and Community Driven Project



University of  
St Andrews | FOUNDED  
1413

Chemistry

6 instruments , ~ 350 users



Pharmacy

2 instruments , ~ 85 users

IMPERIAL

Chemistry



5 instruments , ~ 240 users



Chemistry

trial in teaching labs

1 instrument , ~ 750 users



Discord

Prospective funding opportunities



PSDI  
PHYSICAL SCIENCES  
DATA INFRASTRUCTURE





## Frequently Asked Questions

1. Do we need to liaise with IT services to install NOMAD server?
2. What version of IconNMR/TopSpin is required for connecting our instruments to NOMAD server?
3. Does NOMAD work with instruments of other vendors than Bruker?
4. Is NOMAD restricted for use in academia and non-profit organisations only?
5. Is it possible to run NOMAD alongside our existing data archiving solution?
6. Is it possible to use NOMAD without submission portal as datastore only solution?
7. Can we trial NOMAD without installing our own server?