

# Data station and sharing platform

A data repository for research groups  
and scientific communities



**Dr. Sina Kazemi**

Developer - Scientific Solutions

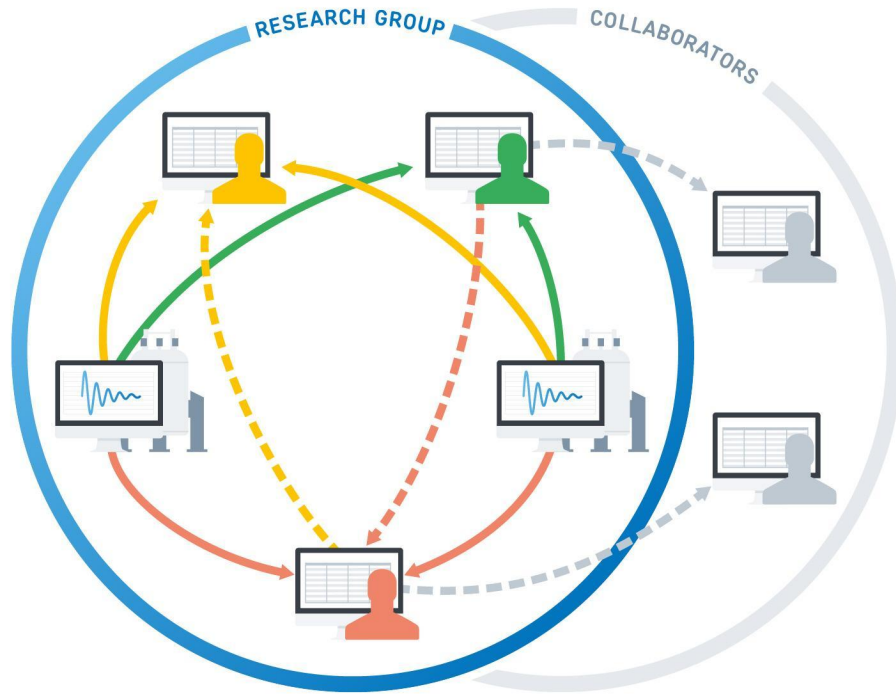
Sina.Kazemi@signals.company  
<http://logs-repository.com>

# Problem with current data management

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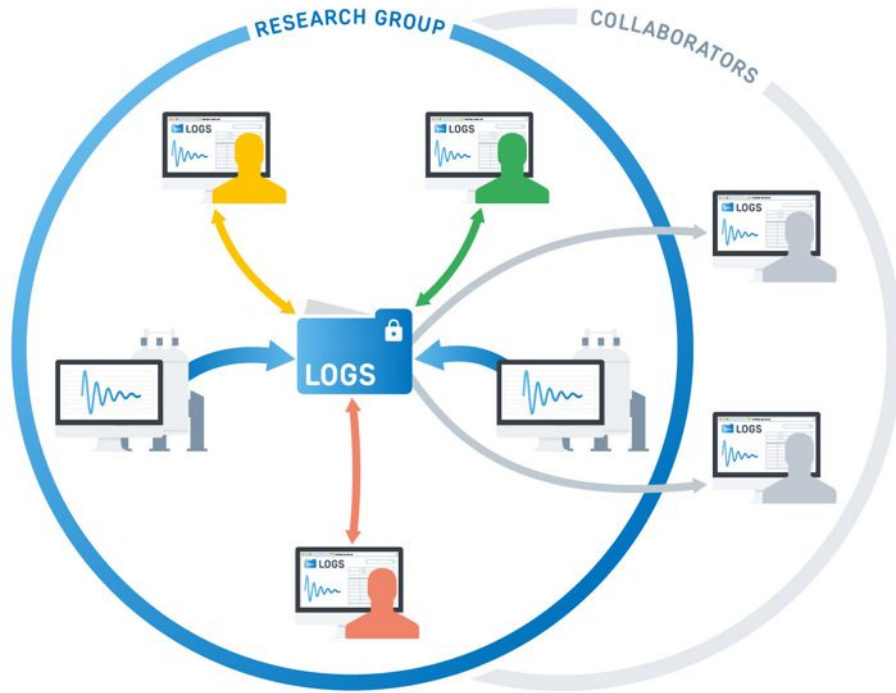
- No findability
- No accessibility
- No retrievability
- No reusability or reproducibility

# Problem Source: data pathways are unclear



- Data is acquired with multiple people, instruments, samples, experiments, etc.
- Data usually transferred personal storage
- High fluctuation of lab members
- No recording of metadata, e.g. experimental parameters.

# Problem Solution: data is saved in central hub



- LOGS checks the instruments periodically and uploads fresh data.
- Every piece of digital data related to do the experiment is saved, ensuring a maximum of automatically retained information.
- Enables and simplifies lab data administration
  - Transportability
  - Back-ups
  - Transparency

# The data repository for spectroscopists

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## Primary Data enters the system automatically

- Data inflow: Primary data automatically uploaded from instrument
- Monitor measurements, in the browser

# The data repository for spectroscopists



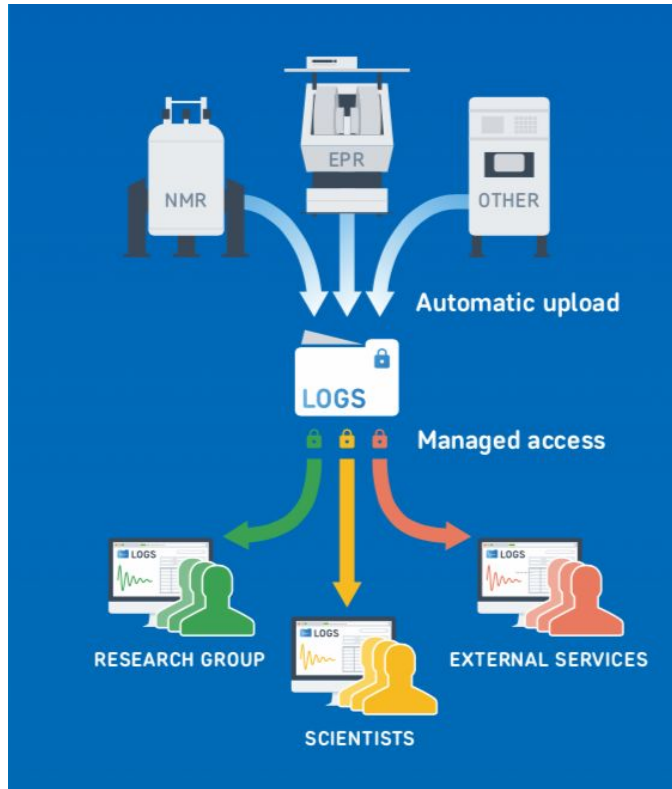
## Primary Data enters the system automatically

- Data inflow: Primary data automatically uploaded from instrument
- Monitor measurements, in the browser

## Users access, examine, filter, search, group or share data from LOGS

- Secure access
  - Search & filter and overview
  - Compare & display and download
- ... with the web browser!

# Distribution and communication of data to partners



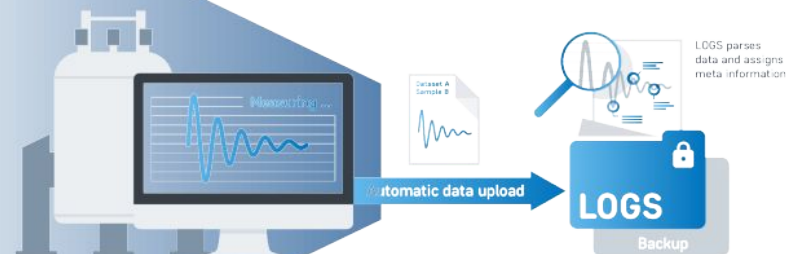
## LOGS workflows

- Download link generation
- Restricted users with limited access for partners and customers
- Data distribution and communication
- Used in e.g. service facilities; academic collaboration groups.

# LOGS speaks many formats

<b>CD (1)</b>	- Jasco
<b>EPR (4)</b>	- Bruker, Specman4EPR, Magnettech, fsc2 format
<b>EM (1)</b>	- EPMA (wip)
<b>FT-IR (1)</b>	- Bruker Opus
<b>HPLC (1)</b>	- Agilent
<b>ITC (2)</b>	- Malvern Analytical, MicroCal
<b>MPLC (2)</b>	- Äkta, NGC
<b>MS (3)</b>	- Bruker (MALDI-TOF, FT-ICR), JEOL (LIFDI MSAxel)
<b>Microscopy (1)</b>	- Zeiss
<b>NMR (4)</b>	- Bruker, Varian, JEOL (WIP), Magritek (WIP)
<b>Raman (1)</b>	- Acton
<b>TGA (1)</b>	- TA Instruments
<b>UV/Vis (3)</b>	- Jasco, Thermo Scientific, Varian
<b>XRD/XRD-VT (3)</b>	- Bruker
<b>Images</b>	- Formats *.png, *.tiff, *.jpg

**NMReData** - NMReDATA initiative



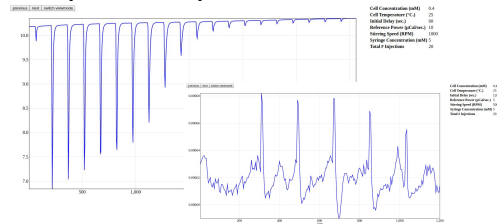
*The list of incorporated dataformats is continuously growing with users requests*



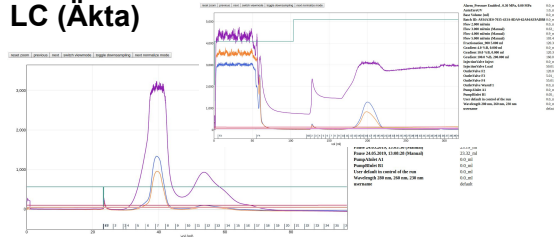
# LOGS as the ultimate data viewer



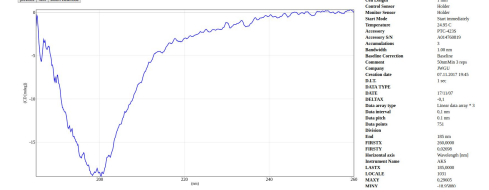
## ITC (MicroCal)



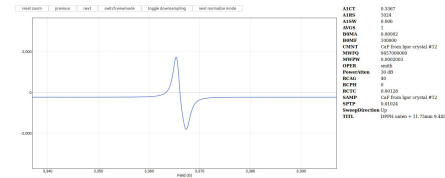
## LC (Äkta)



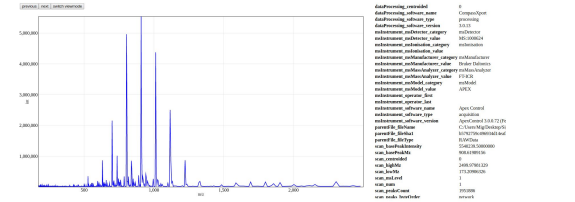
## CD (Jasco)



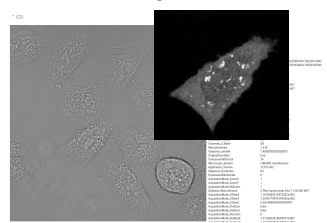
## EPR-CW (Bruker)



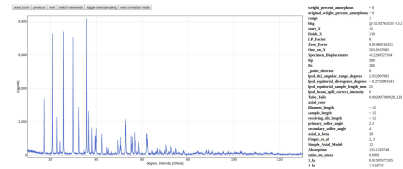
## ITC (MicroCal)



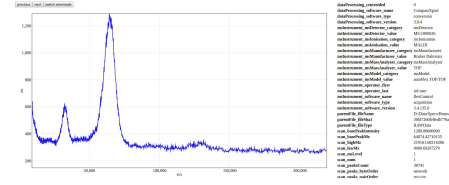
## Microscopy (Zeiss)



## XRD (Bruker)



## MALDI-TOF (Bruker)



# Dataset overview

DEVEL LOGS Projects Samples **Datasets** Documents Search More ▾

Sort by Session ▾

## Datasets

Upload Data ▾

**My datasets**

- All datasets
- Unclaimed (37+)
- Trash

**Filter by**

Project ▾

Operator ▾

Sample ▾

**Spectrometer** [Reset](#)

[NMR] 600 MHz Spec. ▾

Acquired After ▾

Acquired Before ▾

Experiment ▾

Dataset	Sample	Acquisition	Instrument Info
Sun, 15 May 2016 - 600 MHz Spec. (NMR) - Dr. Karl Otto (1 dataset)			
<input type="checkbox"/>	2-46 2D HSQC HC	2 Ubiquitin suffix	Sun 21:14 89HRS11-RDC/13 fhsqcf3gpph.jewoe
Wed, 11 May 2016 - 600 MHz Spec. (NMR) - Dr. Karl Otto (1 dataset)			
<input type="checkbox"/>	9-3 2D DARR	9 Terephthalic acid	Wed 18:38 89HRS11-Titration/10 fhsqcf3gpph
Sat, 10 May 2014 (2 days) - 600 MHz Spec. (NMR) - Ms. Anja Schneider (9 datasets)			
<input type="checkbox"/>	479-1 1D 1H	479 Tt S6	Sat 17:44 23HRS11/1 zgpr
<input type="checkbox"/>	479-2 2D HSQC HN	479 Tt S6	Sat 17:46 23HRS11/2 fhsqcf3gpph
<input type="checkbox"/>	482-1 2D HSQC HN	482 Tt S6 [15N] : AUUGCAC	Sat 17:53 23HRS11/3 fhsqcf3gpph
<input type="checkbox"/>	485-1 2D HSQC HN	485 Tt S6 [15N] : AUUGCAC	Sat 18:02 23HRS11/4 fhsqcf3gpph
<input type="checkbox"/>	480-5 2D HSQC HN	480 Tt S6	Sat 18:06 23HRS11/5 fhsqcf3gpph
<input type="checkbox"/>	480-4 3D HNCACB	480 Tt S6	Sat 19:04 23HRS11/9 hncacb3d
<input type="checkbox"/>	480-3 2D HSQC HN	480 Tt S6	Sat 19:21 23HRS11/6 fhsqcf3gpph

# Filter your datasets

The screenshot shows the LOGS web interface with the 'Datasets' tab selected. The interface includes a navigation bar with 'LOGS', 'Projects', 'Samples', 'Datasets', 'Media', 'Search', and 'More'. A search bar contains the text 'kotto'. The main content area is titled 'Datasets' and includes a 'Sort by Session' dropdown. On the left, there is a sidebar with 'My datasets' (All datasets, Unclaimed, Trash), a 'Filter by' section with dropdowns for Project, Operator, Sample, Spectrometer, Acquired After, and Acquired Before, and an 'Experiment' dropdown set to '2D HSQC HN' with a red arrow pointing to it and a 'Reset' link. Below the filters is a 'Measuring Method' dropdown set to 'NMR' with a 'Reset' link. The main table displays a list of datasets with columns for Dataset, Sample, Acquisition, and Instrument Info. The datasets are grouped by date and experiment name.

Dataset	Sample	Acquisition	Instrument Info
<b>Thu, 15 May 2014 - 700 MHz Spec. (NMR) - Mr. Fred Zimmermann (2 datasets)</b>			
442-2 2D HSQC HN	442 T1 L11-C	Thu 15:33	23HR511-RDC/12 fhsqc3gpph
442-3 2D HSQC HN	442 T1 L11-C	Thu 21:14	23HR511-RDC/13 fhsqc3gpph.jewoe
<b>Wed, 14 May 2014 (2 days) - 800 MHz Spec. (NMR) - Mr. Fred Zimmermann (7 datasets)</b>			
443-2 2D HSQC HN	443 T1 L11-N	Wed 11:57	23HR511-RDC/2 fhsqc3gpph
443-1 2D HSQC HN	443 T1 L11-N	Wed 19:27	23HR511-RDC/3 fhsqc3gpph.jewoe
443-5 2D HSQC HN	443 T1 L11-N	Thu 11:38	23HR511-RDC/4 fhsqc3gpph.jewoe
443-4 2D HSQC HN	443 T1 L11-N	Thu 11:44	23HR511-RDC/5 fhsqc3gpph
443-6 2D HSQC HN	443 T1 L11-N	Thu 11:50	23HR511-RDC/6 fhsqc3gpph.jewoe
472-2 2D HSQC HN	472 Hs U1A	Thu 15:33	23HR511-RDC/12 fhsqc3gpph
472-3 2D HSQC HN	472 Hs U1A	Thu 21:14	23HR511-RDC/13 fhsqc3gpph.jewoe
<b>Wed, 14 May 2014 - 900 MHz Spec. (NMR) - Dr. Karl Otto (2 datasets)</b>			
468-2 2D HSQC HN	468 Gs S4	Wed 11:57	23HR511-RDC/2 fhsqc3gpph
468-1 2D HSQC HN	468 Gs S4	Wed 19:27	23HR511-RDC/3 fhsqc3gpph.jewoe

# Get your data easily

x 3 datasets selected Download Share Edit Trash

## Datasets

Sort by Session ▾

Upload data ▾

**My datasets**  
[All datasets](#)  
[Unclaimed \(39+\)](#)  
[Trash](#)

**Filter by**

Project ▾

Operator ▾

Sample ▾

Spectrometer ▾

Acquired After ▾

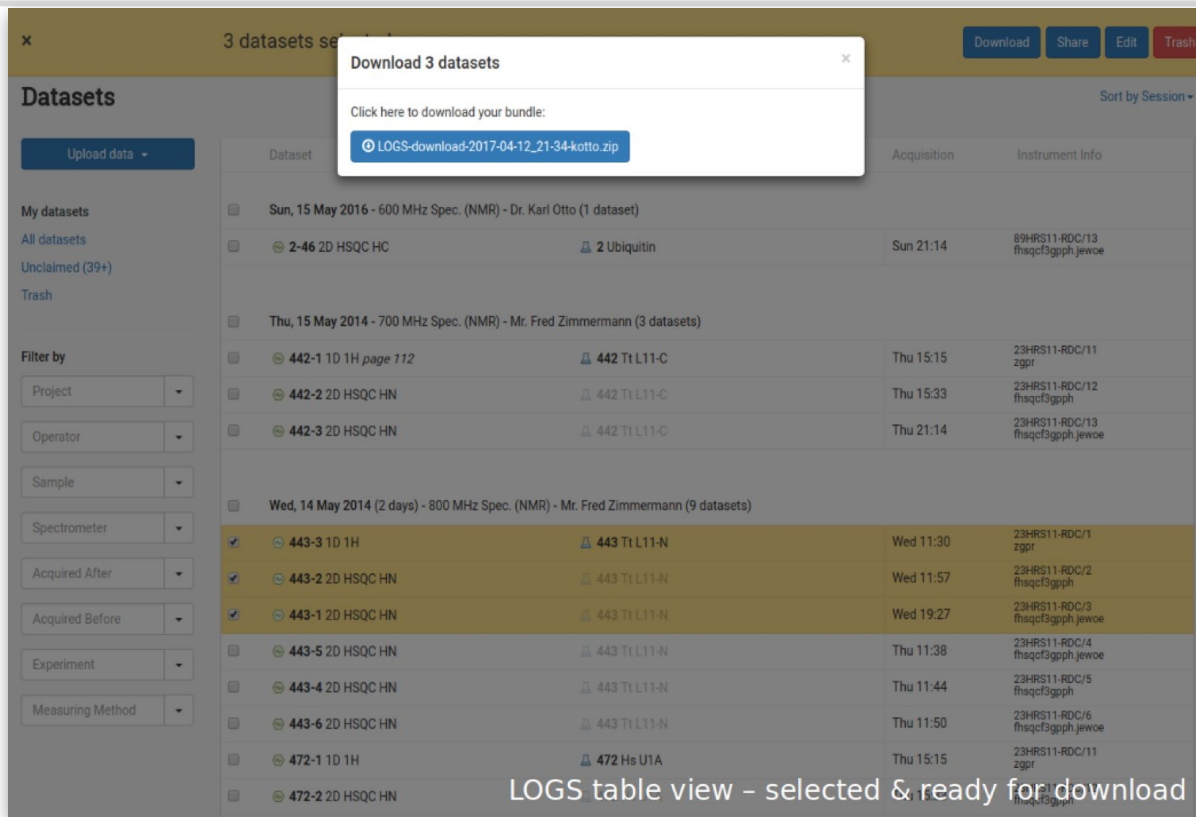
Acquired Before ▾

Experiment ▾

Measuring Method ▾

	Dataset	Sample	Acquisition	Instrument Info
<input type="checkbox"/>	Sun, 15 May 2016 - 600 MHz Spec. (NMR) - Dr. Karl Otto (1 dataset)			
<input type="checkbox"/>	2-46 2D HSQC HC	2 Ubiquitin	Sun 21:14	89HRS11-RDC/13 fhsqc13gpph.jewoe
<input type="checkbox"/>	Thu, 15 May 2014 - 700 MHz Spec. (NMR) - Mr. Fred Zimmermann (3 datasets)			
<input type="checkbox"/>	442-1 1D 1H <i>page 1/2</i>	442 Tt L11-C	Thu 15:15	23HRS11-RDC/11 zgpr
<input type="checkbox"/>	442-2 2D HSQC HN	442 Tt L11-C	Thu 15:33	23HRS11-RDC/12 fhsqc13gpph
<input type="checkbox"/>	442-3 2D HSQC HN	442 Tt L11-C	Thu 21:14	23HRS11-RDC/13 fhsqc13gpph.jewoe
<input type="checkbox"/>	Wed, 14 May 2014 (2 days) - 800 MHz Spec. (NMR) - Mr. Fred Zimmermann (9 datasets)			
<input checked="" type="checkbox"/>	443-3 1D 1H	443 Tt L11-N	Wed 11:30	23HRS11-RDC/1 zgpr
<input checked="" type="checkbox"/>	443-2 2D HSQC HN	443 Tt L11-N	Wed 11:57	23HRS11-RDC/2 fhsqc13gpph
<input checked="" type="checkbox"/>	443-1 2D HSQC HN	443 Tt L11-N	Wed 19:27	23HRS11-RDC/3 fhsqc13gpph.jewoe
<input type="checkbox"/>	443-5 2D HSQC HN	443 Tt L11-N	Thu 11:38	23HRS11-RDC/4 fhsqc13gpph.jewoe
<input type="checkbox"/>	443-4 2D HSQC HN	443 Tt L11-N	Thu 11:44	23HRS11-RDC/5 fhsqc13gpph
<input type="checkbox"/>	443-6 2D HSQC HN	443 Tt L11-N	Thu 11:50	23HRS11-RDC/6 fhsqc13gpph.jewoe
<input type="checkbox"/>	472-1 1D 1H	472 Hs U1A	Thu 15:15	23HRS11-RDC/11 zgpr
<input type="checkbox"/>	472-2 2D HSQC HN	472 Hs U1A	Thu 15:33	23HRS11-RDC/12 fhsqc13gpph
<input type="checkbox"/>	472-3 2D HSQC HN	472 Hs U1A	Thu 21:14	23HRS11-RDC/13 fhsqc13gpph.jewoe

# Get your data easily




The screenshot displays the LOGS web interface. A modal dialog box titled "Download 3 datasets" is open, showing a download link: "LOGS-download-2017-04-12\_21-34-kotto.zip". The background shows a table of datasets with columns for Dataset, Acquisition, and Instrument Info. Three rows are selected, highlighted in yellow.

Dataset	Acquisition	Instrument Info
Sun, 15 May 2016 - 600 MHz Spec. (NMR) - Dr. Karl Otto (1 dataset)		
2-46 2D HSQC HC	Sun 21:14	89HRS11-RDC/13 fhsqc3gpph.jewoe
Thu, 15 May 2014 - 700 MHz Spec. (NMR) - Mr. Fred Zimmermann (3 datasets)		
442-1 1D 1H page 112	Thu 15:15	23HRS11-RDC/11 zgpr
442-2 2D HSQC HN	Thu 15:33	23HRS11-RDC/12 fhsqc3gpph
442-3 2D HSQC HN	Thu 21:14	23HRS11-RDC/13 fhsqc3gpph.jewoe
Wed, 14 May 2014 (2 days) - 800 MHz Spec. (NMR) - Mr. Fred Zimmermann (9 datasets)		
443-3 1D 1H	Wed 11:30	23HRS11-RDC/1 zgpr
443-2 2D HSQC HN	Wed 11:57	23HRS11-RDC/2 fhsqc3gpph
443-1 2D HSQC HN	Wed 19:27	23HRS11-RDC/3 fhsqc3gpph.jewoe
443-5 2D HSQC HN	Thu 11:38	23HRS11-RDC/4 fhsqc3gpph.jewoe
443-4 2D HSQC HN	Thu 11:44	23HRS11-RDC/5 fhsqc3gpph
443-6 2D HSQC HN	Thu 11:50	23HRS11-RDC/6 fhsqc3gpph.jewoe
472-1 1D 1H	Thu 15:15	23HRS11-RDC/11 zgpr
472-2 2D HSQC HN		

LOGS table view – selected & ready for download

# Keep an eye on your experiments

 **LOGS** [Projects](#) [Samples](#) [Datasets](#) [Documents](#) [Search](#) [More](#) ▾

## NMR spectrometer status

Spectrometer	Status/Dataset	Pulse program	Started at	Finished at	Last autoload
Bruker 400	nancy_parker/nmr/or...	zg30	2019-09-19 16:52	<u>2019-09-19 16:54</u>	2019-09-19 16:54
Bruker 600	diego_garcia/nmr/pr...	zgpr	2019-09-19 16:53	<u>2019-09-19 16:55</u>	2019-09-19 16:53
Bruker 700	idle				2019-09-19 16:53
Bruker 800	charles_baker/nmr/or...	cosydfphpr	2019-09-19 16:50	<u>2019-09-19 16:55</u>	2019-09-19 16:53
Bruker 900	external user			2019-09-19 17:42	2019-09-19 16:54

## EPR spectrometer status

Spectrometer	Title	Operator	last modified	Last autoload	
Bruker Elexsys e400	DPPH u 9.44018	karen_cook	2019-09-19 16:52	2019-09-19 16:54	unclaimed
Bruker EMX Nano	p38double_100scans	karen_cook	2019-09-19 16:49	2019-09-19 16:54	unclaimed

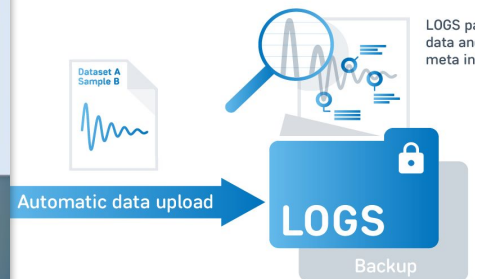
## IconNMR status

Spectrometer	Experiments queued	Length of queue
Bruker 400	16	6 h 58 min 5 s

# IconNMR and automated data management

The screenshot shows the IconNMR software interface. At the top, there is a menu bar with options: File, Run, Holder, View, Find, Parameters, Options, Tools, Help. Below the menu bar is a toolbar with icons for Start, Stop, and Information. The main area is titled "Experiment Table" and contains a table with columns: Holder, Type, Status, Disk, Name, No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, Start Time. The table lists 13 experiments, all with a status of "Available". To the right of the table is a metadata form with fields for project, sample, user, and arbitrary\_other\_field. Below the table is a toolbar with buttons for Submit, Cancel, Edit, Delete, Add, Copy, and Change User. At the bottom, there is a section for "Preceding Experiments" with a table of columns: #, Date, Holder, Name, No., Experiment, Load, ATM, Rotation, Lock, Shim, Acq, Proc, User, Disk, Title/Orig, Remarks. A search bar is located at the bottom left, and a status bar at the bottom right shows "SampleExpress | Busy until: No Jobs! | Day: 00:00 | Night: 00:00 | User: spect".

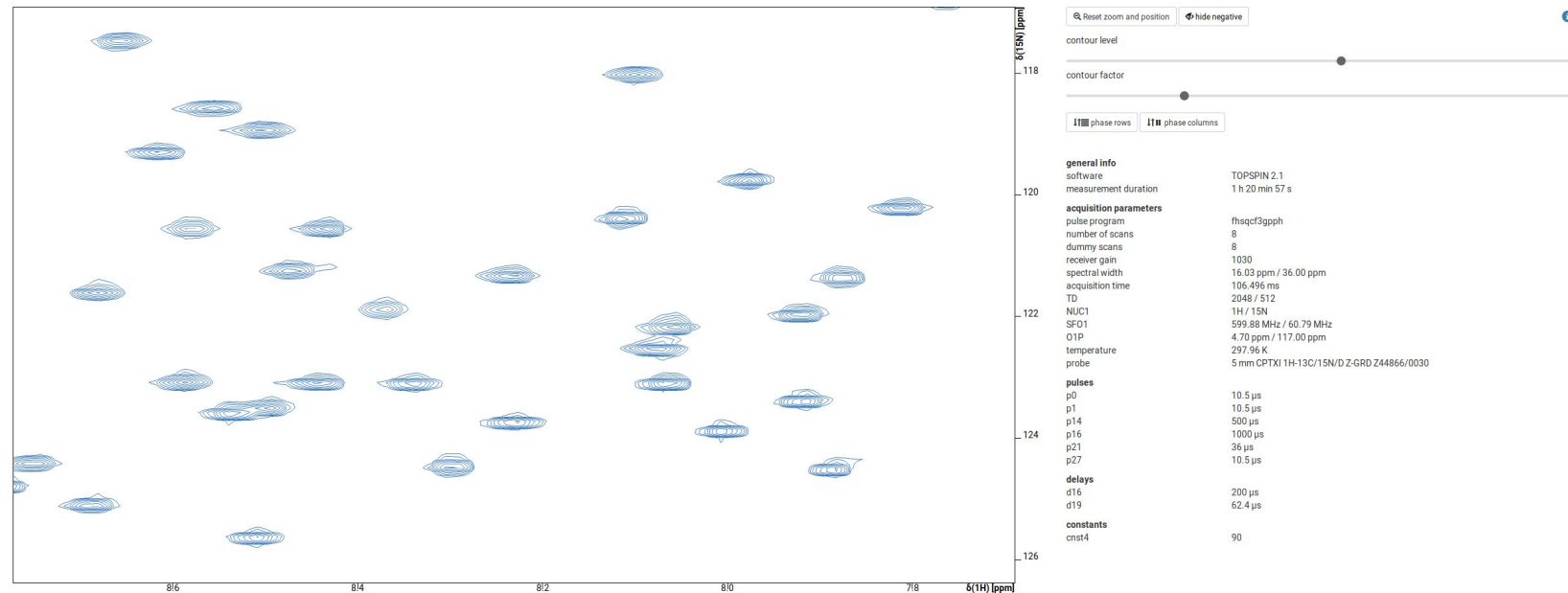
Metadata is automatically transferred from IconNMR



# Process spectra in the browser

Details Documents More data on this sample **View NMR spectrum (Bruker)**

Spectrum FID fft on f2 dimension Bruker Acqus File Bruker Acqus2s File Bruker Pulseprogram

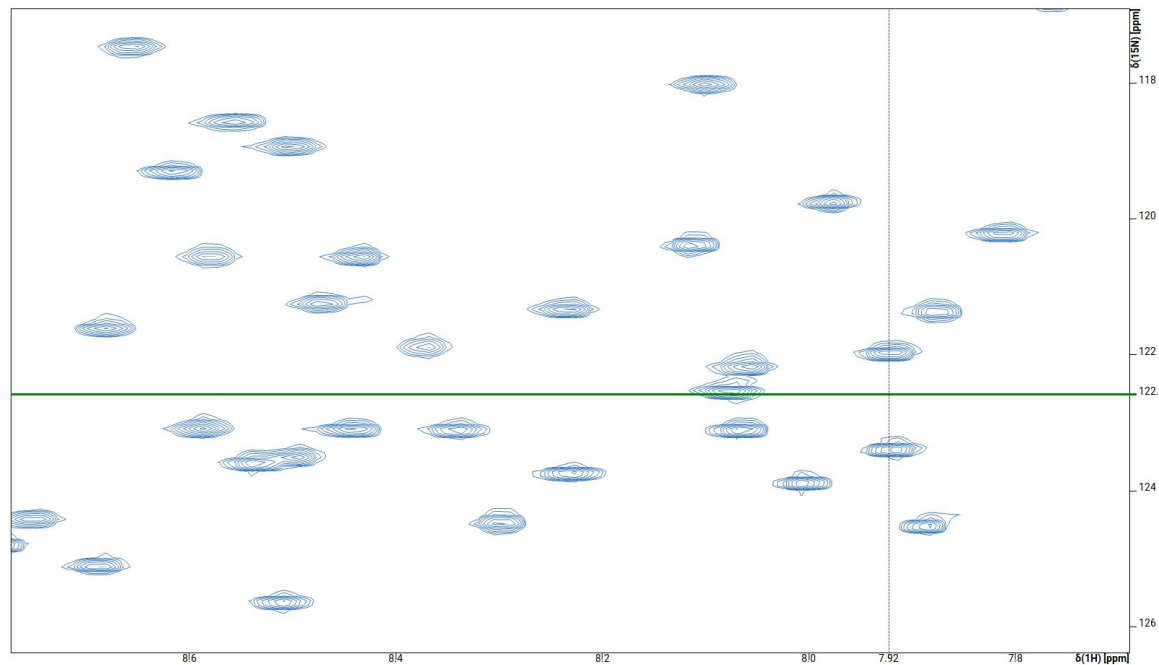




# Phase spectrum in the browser

Details Documents More data on this sample View NMR spectrum (Bruker)

Spectrum FID fft on f2 dimension Bruker Acqus File Bruker Acqu2s File Bruker Pulseprogram



Reset zoom and position hide negative

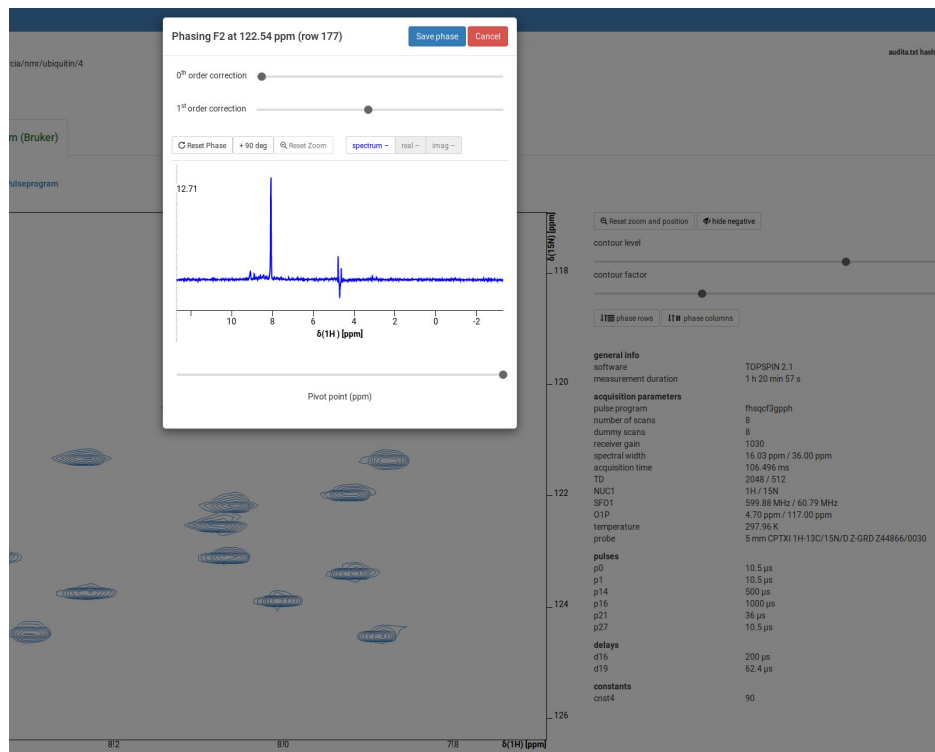
contour level

contour factor

phase rows phase columns

<b>general info</b>	
software	TOPSPIN 2.1
measurement duration	1 h 20 min 57 s
<b>acquisition parameters</b>	
pulse program	fhscqf3gpph
number of scans	8
dummy scans	8
receiver gain	1030
spectral width	16.03 ppm / 36.00 ppm
acquisition time	106.496 ms
TD	2048 / 512
NUC1	1H / 15N
SFO1	599.88 MHz / 60.79 MHz
O1P	4.70 ppm / 117.00 ppm
temperature	297.96 K
probe	5 mm CPTXI 1H-13C/15N/D Z-GRD Z44866/0030
<b>pulses</b>	
p0	10.5 µs
p1	10.5 µs
p14	500 µs
p16	1000 µs
p21	36 µs
p27	10.5 µs
<b>delays</b>	
d16	200 µs
d19	62.4 µs
<b>constants</b>	
cnst4	90

# Phase spectrum in the browser



# Secondary NMR data: 1D spectra annotation

Details Documents **View spectrum**

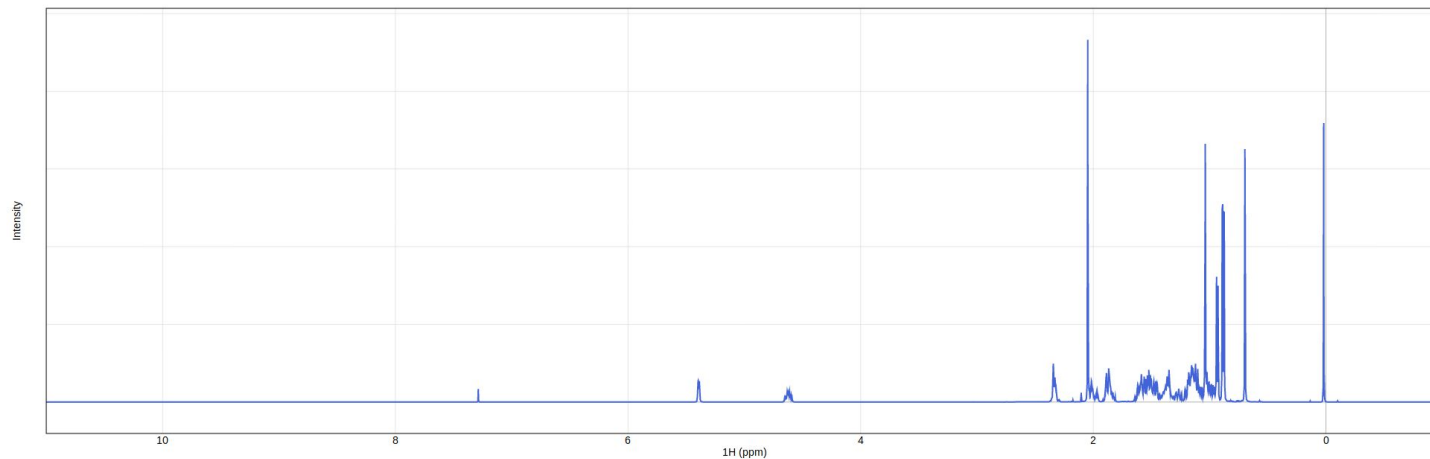
Reset zoom to:  Visible curves  Track  Line  Single  None  Fix axis:  By track  None  Axis ticks:  None  Normalize:  Box zoom:  Annotations:

Export as:

Track 1: proc 1

Dataset name

proc 1  spectrum  fid.re  fid.im



## ▼ Acquisition parameters

Current pulse program	zg30
Number of scans	16
Number of dummy scans	2
Receiver gain	36
Spectral width	12.00 ppm
Spectral width	6002.40 Hz
Acquisition time	5.459 s
Size of fid	65536
Transmitter frequency	500.13 MHz
Transmitter frequency offset	5.00 ppm
Probe temperature	297.16 K
Probe	5 mm PABBO BB-1H/D Z-GRD
	Z8007010077
Observed nucleus	<sup>1</sup> H

## ▼ General information

Software	TOPSPIN2.1.b.10
Measurement duration	2 min 2 s
Dimension	1

# Secondary NMR data: 1D spectra annotation

Details Documents **View spectrum**

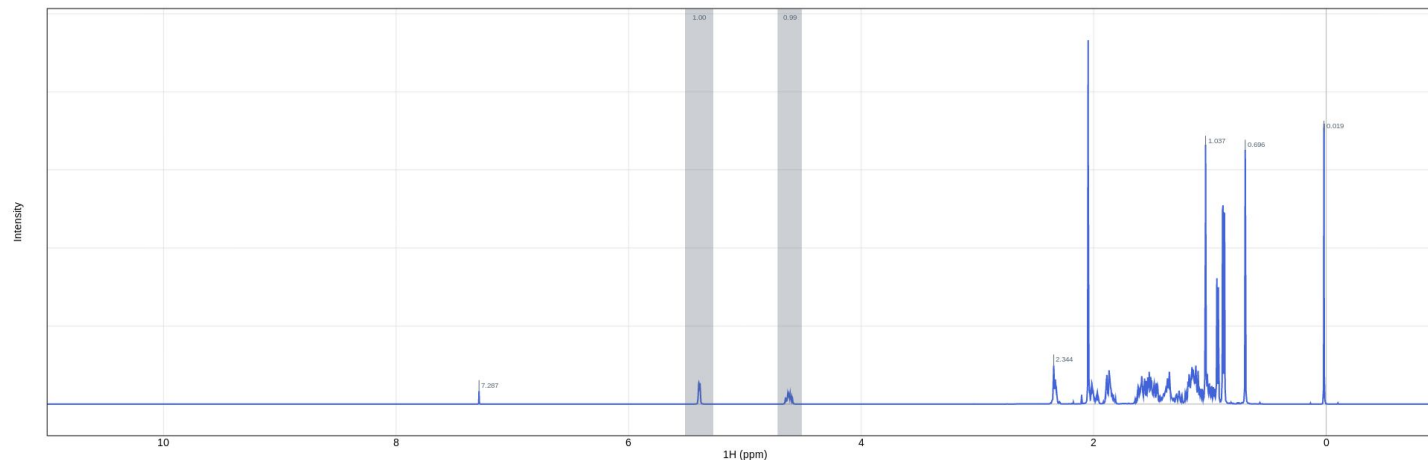
Reset zoom to: Colour by: Show: Plot track: Fix axis: Axis ticks: Normalize: Box zoom: Annotations  
Visible curves Track Line Single None By track None

Export as:  
select

Track 1: proc 1

Dataset name

proc 1  spectrum  fid.re  fid.im



## Acquisition parameters

Current pulse program	zg30
Number of scans	16
Number of dummy scans	2
Receiver gain	36
Spectral width	12.00 ppm
Spectral width	6002.40 Hz
Acquisition time	5.459 s
Size of fid	65536
Transmitter frequency	500.13 MHz
Transmitter frequency offset	5.00 ppm
Probe temperature	297.16 K
Probe	5 mm PABBO BB-1H/D Z-GRD
Observed nucleus	1H

## General information

Software	TOPSPIN2.1.b.10
Measurement duration	2 min 2 s
Dimension	1

# LOGS a tool integrating data formats & meta data

- ✓ Automated retrieving and storing primary digital data
- ✓ Parsing and visualization of the spectra and measuring parameters
- ✓ Additional metadata can manually be added
- ✓ Analysis, annotation and additional (secondary) data can be added
- ✓ Enables the communication and exchange of data between scientist

A **perfect home** for compiled data formats containing multiple data suited for communication between scientist like **NMReData** files

