

# Data station and sharing platform

A data repository for research groups  
and scientific communities



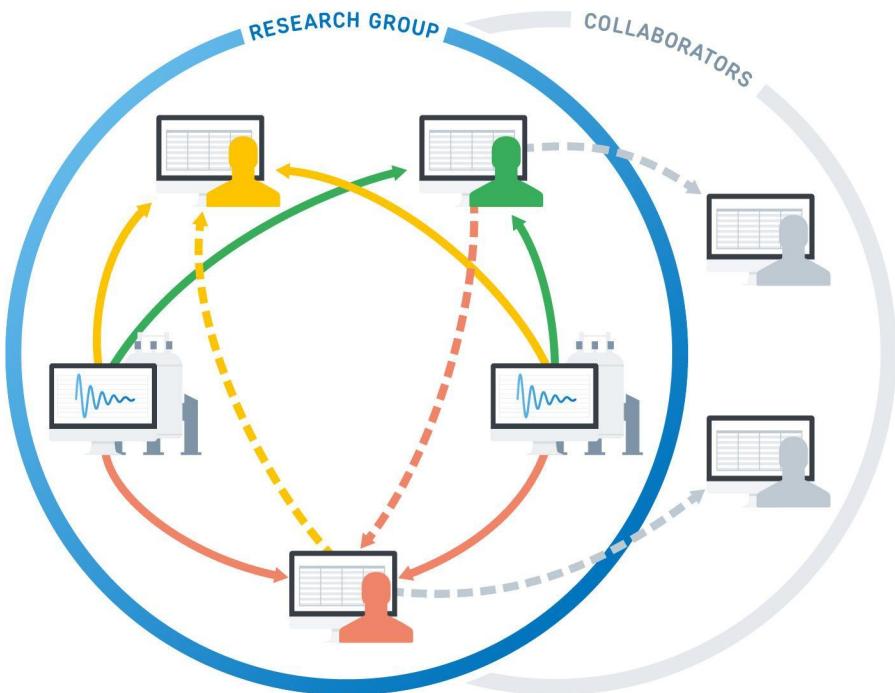
**Dr. Sina Kazemi**  
Developer - Scientific Solutions  
[Sina.Kazemi@signals.company](mailto:Sina.Kazemi@signals.company)  
<http://logs-repository.com>

# Problem with current data management

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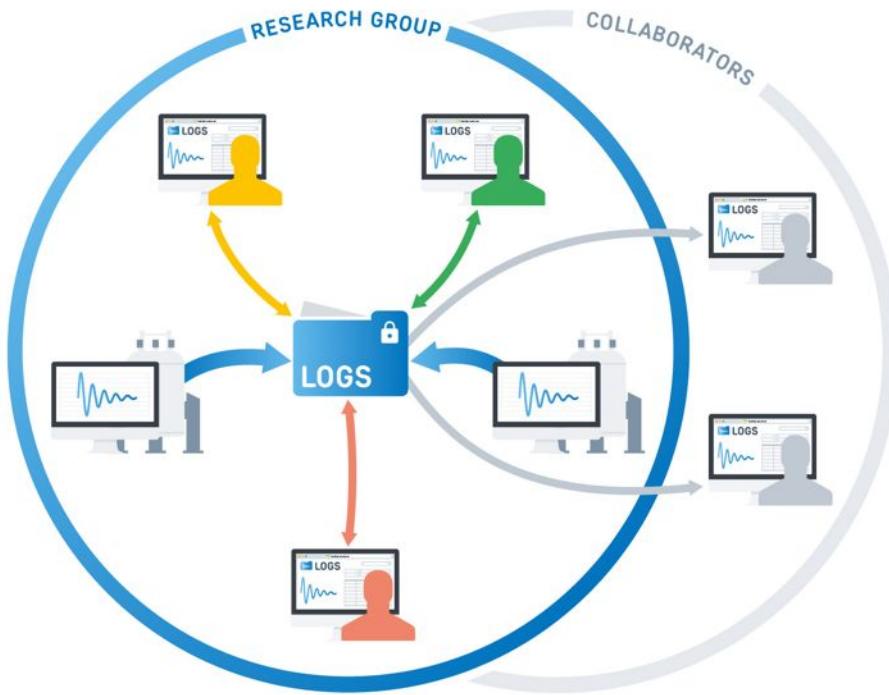
- No findability
- No accessibility
- No retrievability
- No reusability or reproducibility

# 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



**Primary Data  
enters the system automatically**

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

# The data repository for spectroscopists



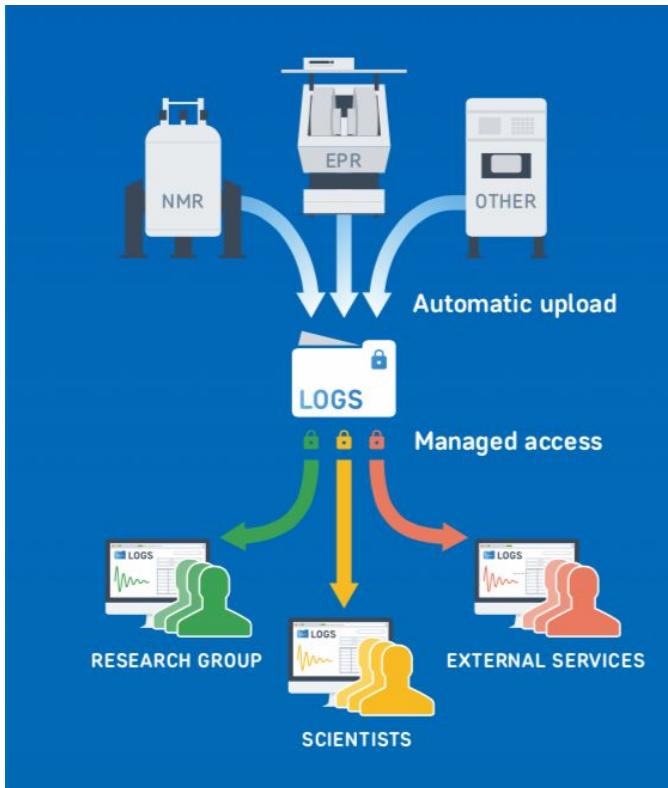
**Primary Data  
enters the system automatically**

- 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

CD (1)

EPR (4)

EM (1)

FT-IR (1)

HPLC (1)

ITC (2)

MPLC (2)

MS (3)

Microscopy (1)

NMR (4)

Raman (1)

TGA (1)

UV/Vis (3)

XRD/XRD-VT (3)

Images

NMReData

- Jasco
  - Bruker, Specman4EPR, Magnetech, fsc2 format
  - EPMA (wip)
  - Bruker Opus
  - Agilent
  - Malvern Analytical, MicroCal
  - Äkta, NGC
  - Bruker (MALDI-TOF, FT-ICR), JEOL (LIFDI MSAxel)
  - Zeiss
  - Bruker, Varian, JEOL (WIP), Magritek (WIP)
  - Acton
  - TA Instruments
  - Jasco, Thermo Scientific, Varian
  - Bruker
  - Formats \*.png, \*.tiff, \*.jpg
- NMReDATA initiative

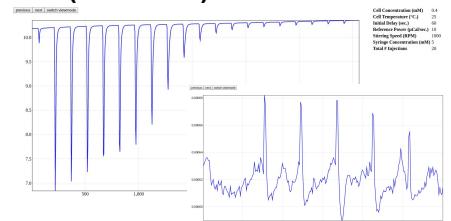


*The list of incorporated dataformats is continuously growing with users requests*

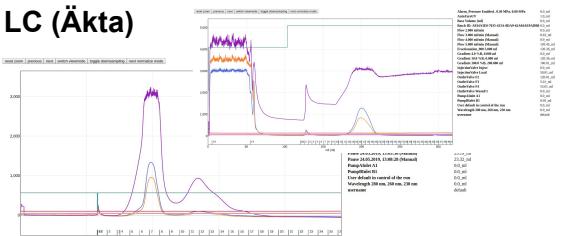
# LOGS as the ultimate data viewer



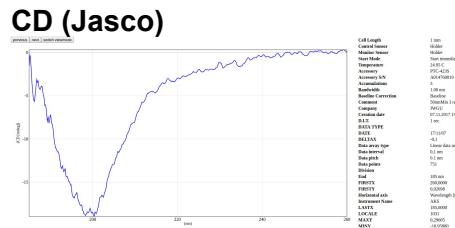
### ITC (MicroCal)



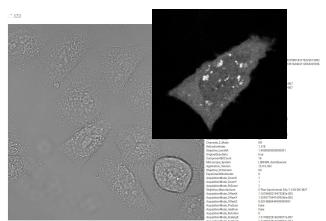
### LC (Äkta)



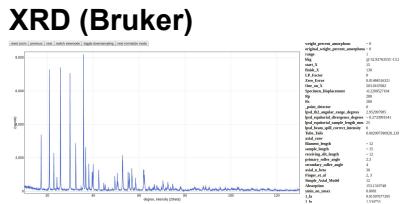
### CD (Jasco)



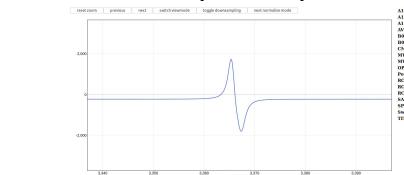
### Microscopy (Zeiss)



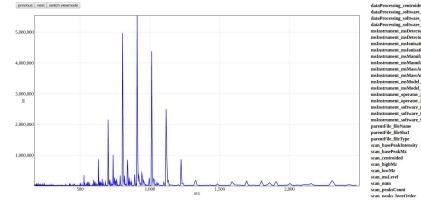
### XRD (Bruker)



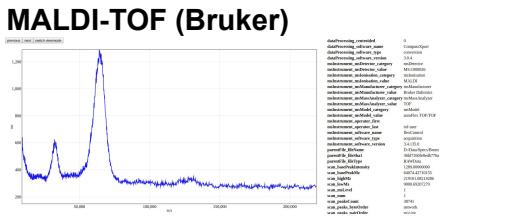
### EPR-CW (Bruker)



### ITC (MicroCal)



### 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)                |                           |             |                                     |
| 2-46 2D HSQC HC   | 2 Ubiquitin suffix        | Sun 21:14   | 89HRS11-RDC/13<br>fhsqcf3gpph.jewoe |
| Wed, 11 May 2016 - 600 MHz Spec. (NMR) - Dr. Karl Otto (1 dataset)                |                           |             |                                     |
| 9-3 2D DARR   | 9 Terephthalic acid       | Wed 18:38   | 89HRS11-Titration/10<br>fhsqcf3gpph |
| Sat, 10 May 2014 (2 days) - 600 MHz Spec. (NMR) - Ms. Anja Schneider (9 datasets) |                           |             |                                     |
| 479-1 1D 1H   | 479 Tt S6                 | Sat 17:44   | 23HRS11/1<br>zgr                    |
| 479-2 2D HSQC HN  | 479 Tt S6                 | Sat 17:46   | 23HRS11/2<br>fhsqcf3gpph            |
| 482-1 2D HSQC HN  | 482 Tt S6 [15N] : AUUGCAC | Sat 17:53   | 23HRS11/3<br>fhsqcf3gpph            |
| 485-1 2D HSQC HN  | 485 Tt S6 [15N] : AUUGCAC | Sat 18:02   | 23HRS11/4<br>fhsqcf3gpph            |
| 480-5 2D HSQC HN  | 480 Tt S6                 | Sat 18:06   | 23HRS11/5<br>fhsqcf3gpph            |
| 480-4 3D HNCACB   | 480 Tt S6                 | Sat 19:04   | 23HRS11/9<br>hncacbgp3d             |
| 480-3 2D HSQC HN  | 480 Tt S6                 | Sat 19:21   | 23HRS11/6<br>fhsqcf3gpph            |

# Filter your datasets

LOGS Projects Samples Datasets Media Search More ▾

Sort by Session ▾

## Datasets

Upload data ▾

My datasets All datasets Unclaimed Trash

Filter by

Project Operator Sample Spectrometer Acquired After Acquired Before

Experiment Reset 2D HSQC HN

Measuring Method Reset NMR

| Dataset  | Sample       | Acquisition | Instrument Info                     |
|--|--------------|-------------|-------------------------------------|
| Thu, 15 May 2014 - 700 MHz Spec. (NMR) - Mr. Fred Zimmermann (2 datasets)          |              |             |                                     |
| 442-2 2D HSQC HN   | 442 Tt L11-C | Thu 15:33   | 23HRS11-RDC/12<br>fhsgcf3gpph       |
| 442-3 2D HSQC HN   | 442 Tt L11-C | Thu 21:14   | 23HRS11-RDC/13<br>fhsgcf3gpph,jewoe |
| Wed, 14 May 2014 (2 days) - 800 MHz Spec. (NMR) - Mr. Fred Zimmermann (7 datasets) |              |             |                                     |
| 443-2 2D HSQC HN   | 443 Tt L11-N | Wed 11:57   | 23HRS11-RDC/2<br>fhsgcf3gpph        |
| 443-1 2D HSQC HN   | 443 Tt L11-N | Wed 19:27   | 23HRS11-RDC/3<br>fhsgcf3gpph,jewoe  |
| 443-5 2D HSQC HN   | 443 Tt L11-N | Thu 11:38   | 23HRS11-RDC/4<br>fhsgcf3gpph,jewoe  |
| 443-4 2D HSQC HN   | 443 Tt L11-N | Thu 11:44   | 23HRS11-RDC/5<br>fhsgcf3gpph        |
| 443-6 2D HSQC HN   | 443 Tt L11-N | Thu 11:50   | 23HRS11-RDC/6<br>fhsgcf3gpph,jewoe  |
| 472-2 2D HSQC HN   | 472 Hs U1A   | Thu 15:33   | 23HRS11-RDC/12<br>fhsgcf3gpph       |
| 472-3 2D HSQC HN   | 472 Hs U1A   | Thu 21:14   | 23HRS11-RDC/13<br>fhsgcf3gpph,jewoe |
| Wed, 14 May 2014 - 900 MHz Spec. (NMR) - Dr. Karl Otto (2 datasets)                |              |             |                                     |
| 468-2 2D HSQC HN   | 468 Gs S4    | Wed 11:57   | 23HRS11-RDC/2<br>fhsgcf3gpph        |
| 468-1 2D HSQC HN   | 468 Gs S4    | Wed 19:27   | 23HRS11-RDC/3<br>fhsgcf3gpph,jewoe  |

# Get your data easily

x      3 datasets selected      Download Share Edit Trash

## Datasets

Sort by Session ▾

|                                     | 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<br>fhsgcf3gpph.jewoe |
| <input type="checkbox"/>            | Thu, 15 May 2014 - 700 MHz Spec. (NMR) - Mr. Fred Zimmermann (3 datasets)          |              |             |                                     |
| <input type="checkbox"/>            | 442-1 1D 1H page 112   | 442 Tt L11-C | Thu 15:15   | 23HRS11-RDC/11<br>zgr               |
| <input type="checkbox"/>            | 442-2 2D HSQC HN   | 442 Tt L11-C | Thu 15:33   | 23HRS11-RDC/12<br>fhsgcf3gpph       |
| <input type="checkbox"/>            | 442-3 2D HSQC HN   | 442 Tt L11-C | Thu 21:14   | 23HRS11-RDC/13<br>fhsgcf3gpph.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<br>zgr                |
| <input checked="" type="checkbox"/> | 443-2 2D HSQC HN   | 443 Tt L11-N | Wed 11:57   | 23HRS11-RDC/2<br>fhsgcf3gpph        |
| <input checked="" type="checkbox"/> | 443-1 2D HSQC HN   | 443 Tt L11-N | Wed 19:27   | 23HRS11-RDC/3<br>fhsgcf3gpph.jewoe  |
| <input type="checkbox"/>            | 443-5 2D HSQC HN   | 443 Tt L11-N | Thu 11:38   | 23HRS11-RDC/4<br>fhsgcf3gpph.jewoe  |
| <input type="checkbox"/>            | 443-4 2D HSQC HN   | 443 Tt L11-N | Thu 11:44   | 23HRS11-RDC/5<br>fhsgcf3gpph        |
| <input type="checkbox"/>            | 443-6 2D HSQC HN   | 443 Tt L11-N | Thu 11:50   | 23HRS11-RDC/6<br>fhsgcf3gpph.jewoe  |
| <input type="checkbox"/>            | 472-1 1D 1H  | 472 Hs U1A   | Thu 15:15   | 23HRS11-RDC/11<br>zgr               |
| <input type="checkbox"/>            | 472-2 2D HSQC HN   | 472 Hs U1A   | Thu 15:33   | 23HRS11-RDC/12<br>fhsgcf3gpph       |
| <input type="checkbox"/>            | 472-3 2D HSQC HN   | 472 Hs U1A   | Thu 21:14   | 23HRS11-RDC/13<br>fhsgcf3gpph.jewoe |

Upload data ▾

My datasets All datasets Unclaimed (39+) Trash

Filter by

- Project
- Operator
- Sample
- Spectrometer
- Acquired After
- Acquired Before
- Experiment
- Measuring Method

# Get your data easily

3 datasets selected

Download 3 datasets

Click here to download your bundle:

LOGS-download-2017-04-12\_21-34-kotto.zip

| Dataset  | Acquisition  | Instrument Info                                  |
|--|--------------|--|
| Sun, 15 May 2016 - 600 MHz Spec. (NMR) - Dr. Karl Otto (1 dataset)                 |              |  |
| 2-46 2D HSQC HC  | 2 Ubiquitin  | Sun 21:14<br>89HRS11-RDC/13<br>fhspcf3gpph.jewoe |
| Thu, 15 May 2014 - 700 MHz Spec. (NMR) - Mr. Fred Zimmermann (3 datasets)          |              |  |
| 442-1 1D 1H page 112   | 442 Tt L11-C | Thu 15:15<br>23HRS11-RDC/11<br>zgpr              |
| 442-2 2D HSQC HN   | 442 Tt L11-C | Thu 15:33<br>23HRS11-RDC/12<br>fhspcf3gpph       |
| 442-3 2D HSQC HN   | 442 Tt L11-C | Thu 21:14<br>23HRS11-RDC/13<br>fhspcf3gpph.jewoe |
| 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<br>23HRS11-RDC/1<br>zgpr               |
| <input checked="" type="checkbox"/> 443-2 2D HSQC HN                               | 443 Tt L11-N | Wed 11:57<br>23HRS11-RDC/2<br>fhspcf3gpph        |
| <input checked="" type="checkbox"/> 443-1 2D HSQC HN                               | 443 Tt L11-N | Wed 19:27<br>23HRS11-RDC/3<br>fhspcf3gpph.jewoe  |
| 443-5 2D HSQC HN   | 443 Tt L11-N | Thu 11:38<br>23HRS11-RDC/4<br>fhspcf3gpph.jewoe  |
| 443-4 2D HSQC HN   | 443 Tt L11-N | Thu 11:44<br>23HRS11-RDC/5<br>fhspcf3gpph        |
| 443-6 2D HSQC HN   | 443 Tt L11-N | Thu 11:50<br>23HRS11-RDC/6<br>fhspcf3gpph.jewoe  |
| 472-1 1D 1H  | 472 Hs U1A   | Thu 15:15<br>23HRS11-RDC/11<br>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 | 2019-09-19 16:54 | 2019-09-19 16:54 |
| Bruker 600   | diego_garcia/nmr/pr...  | zgpr          | 2019-09-19 16:53 | 2019-09-19 16:55 | 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 | 2019-09-19 16:55 | 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 |
| Bruker EMX Nano     | p38double_100scans | karen_cook | 2019-09-19 16:49 | 2019-09-19 16:54 |

### IconNMR status

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

# IconNMR and automated data management

IconNMR: Automation Jun19-2018-1539-spect

File Run Holder View Find Parameters Options Tools Help

Experiment Table

| Holder | Type | Status    | Disk | Name                     | No. | Solvent | Experiment | Pri | Par | Title/Orig | Time | User | Start Time |
|--------|------|-----------|------|--------------------------|-----|---------|------------|-----|-----|------------|------|------|------------|
| ▼ 1    | █ 1  | Available |      | opt/topspin3.5pl7/examda |     |         |            |     |     | spect      |      |      |            |
| ▼ 2    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 3    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 4    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 5    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 6    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 7    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 8    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 9    | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 10   | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 11   | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 12   | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |
| ▼ 13   | █    | Available |      |                          |     |         |            |     |     |            |      |      |            |

Holder Type Status Disk Name No. Solvent Experiment Pri Par Title/Orig Time User Start Time

project: spect Set Start Time

sample:

user:

arbitrary\_other\_field:

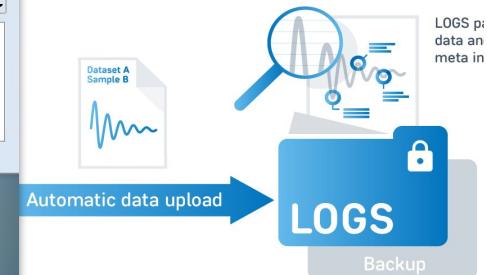
Set Title Set & Copy Title

Submit Cancel Edit Delete Add 1 Copy 1 Preceding Experiments

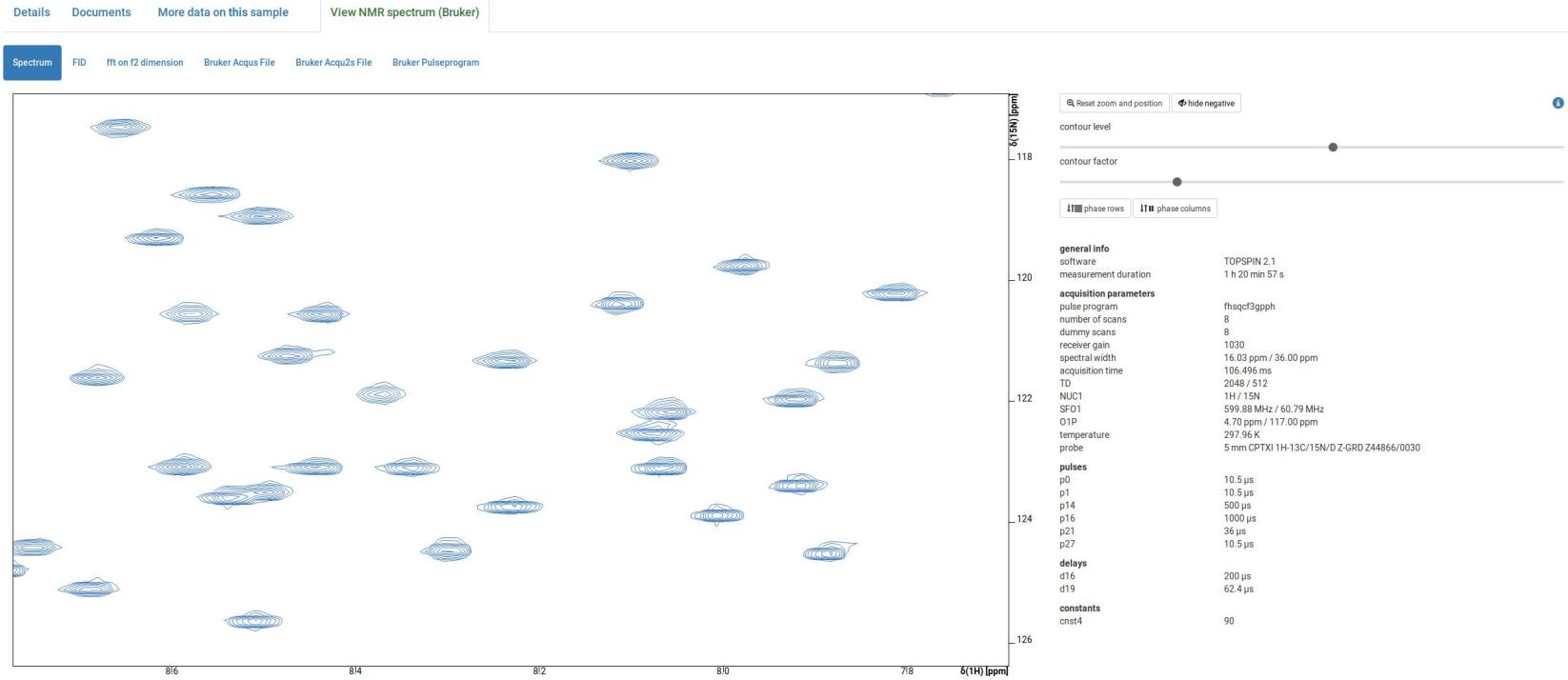
# Date Holder Name No. Experiment Load ATM Rotation Lock Shim Acq Proc User Disk Title/Orig Remarks

Search Preceding SampleXpress Busy until: No Jobs! Day: 00:00 Night: 00:00 User: spect

Metadata is automatically transferred from IconNMR



# Process spectra in the browser



# Phase spectrum in the browser

Details Documents More data on this sample

[View NMR spectrum \(Bruker\)](#)

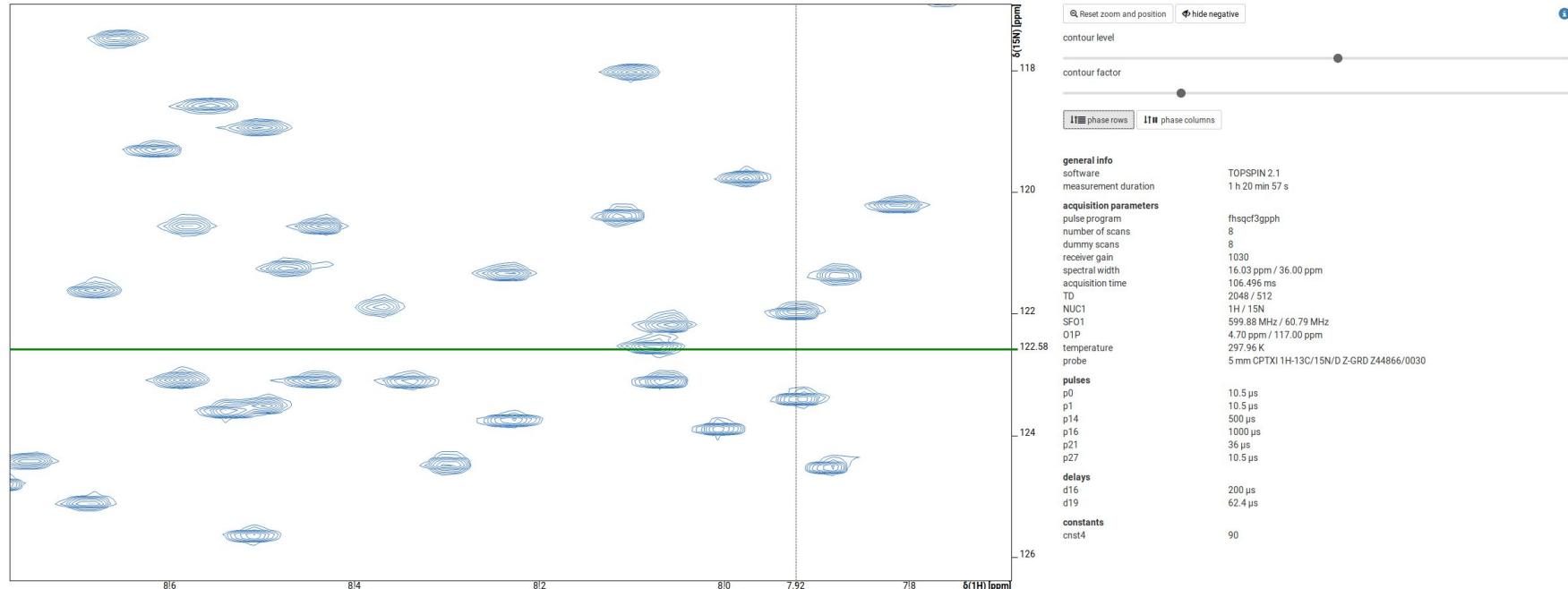
Spectrum

FID fft on f2 dimension

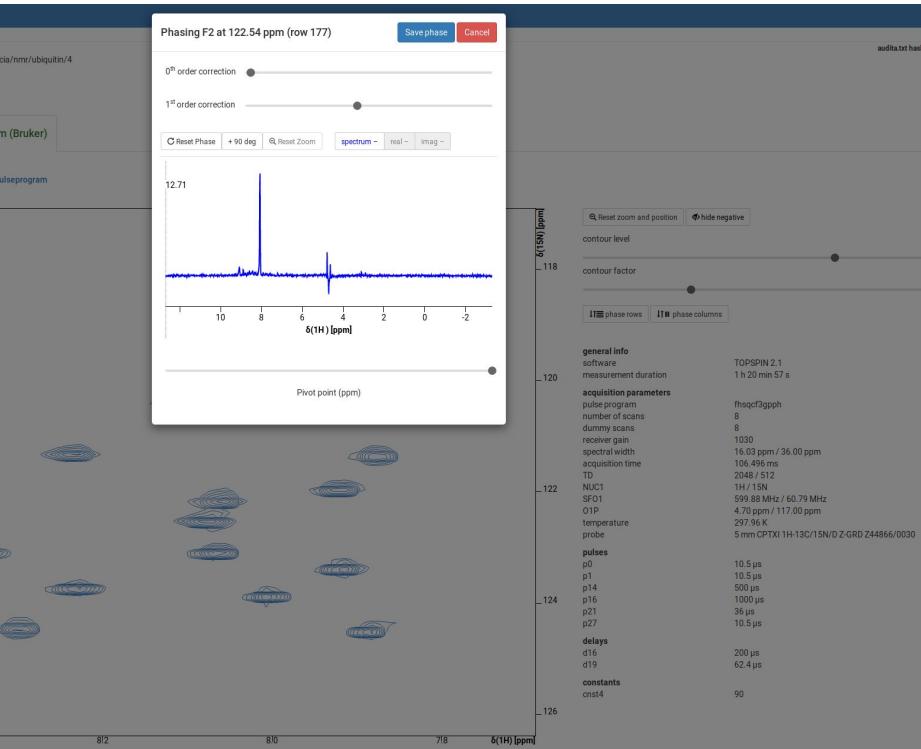
Bruker Acqus File

Bruker Acqus2s File

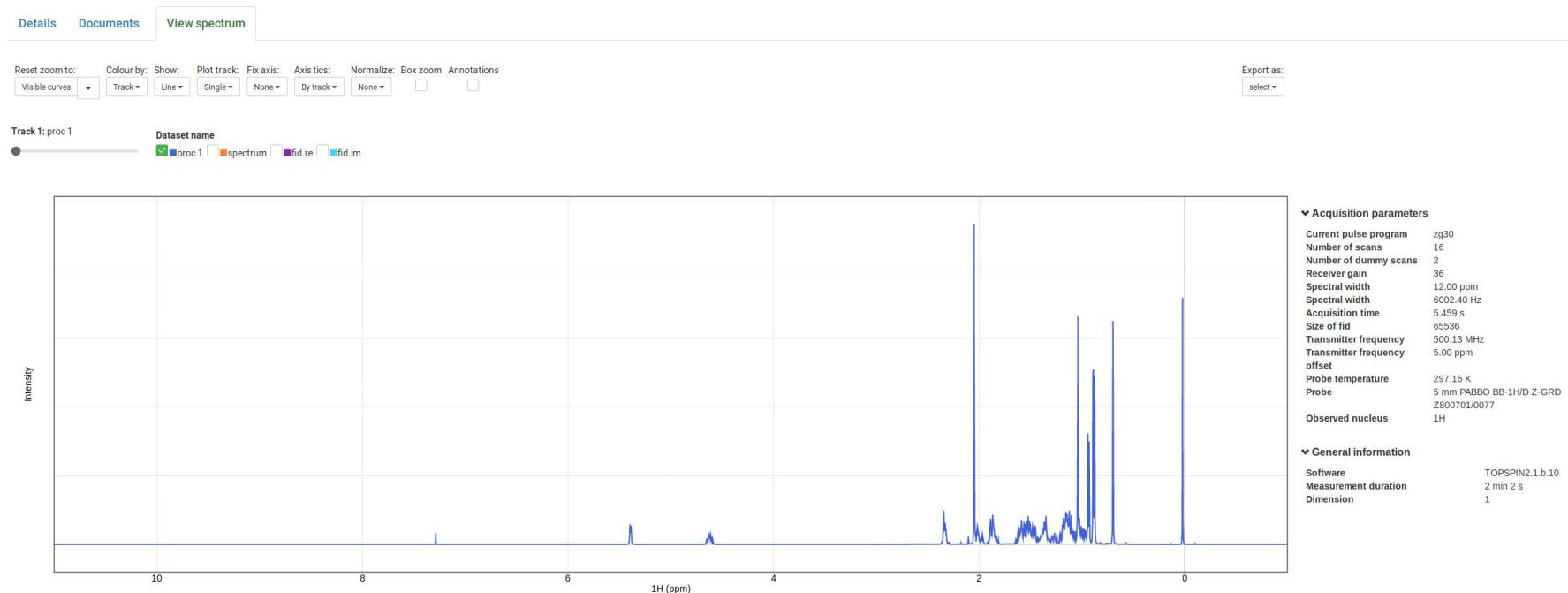
Bruker Pulseprogram



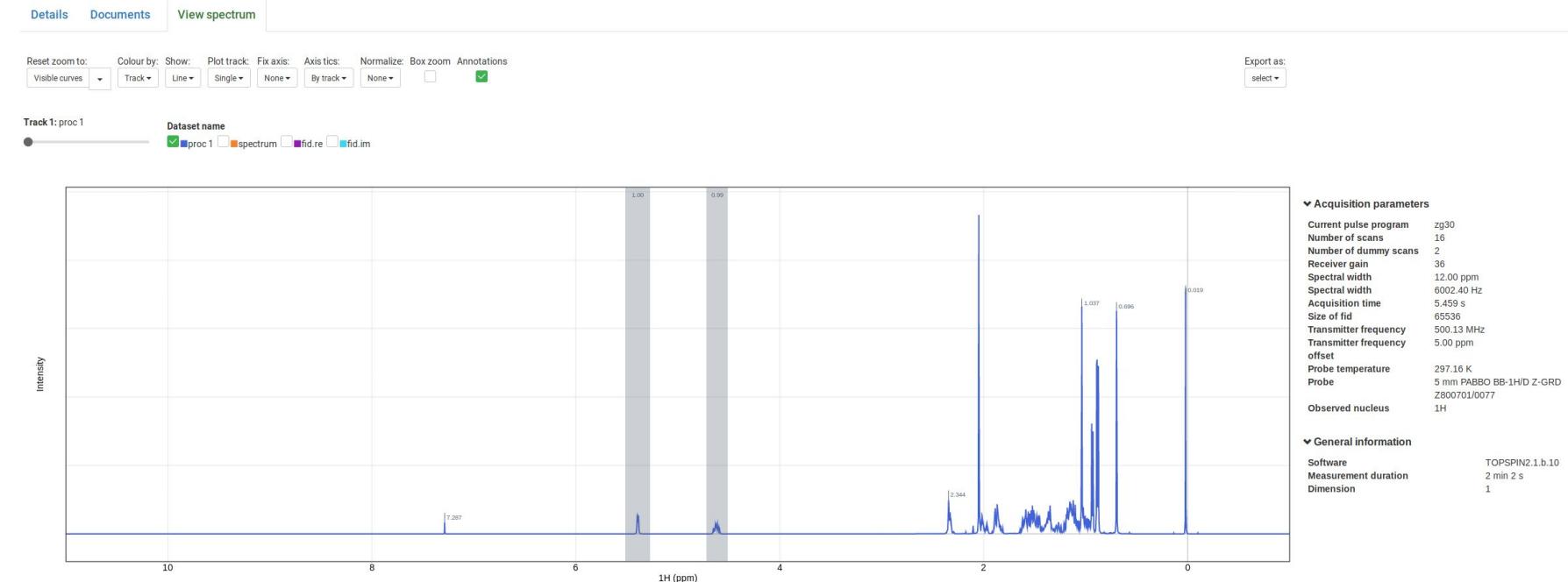
# Phase spectrum in the browser



# Secondary NMR data: 1D spectra annotation



# Secondary NMR data: 1D spectra annotation



# 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

