LOGS

The **SIGNALS** data repository

Data station and sharing platform

A data repository for research groups and scientific communities

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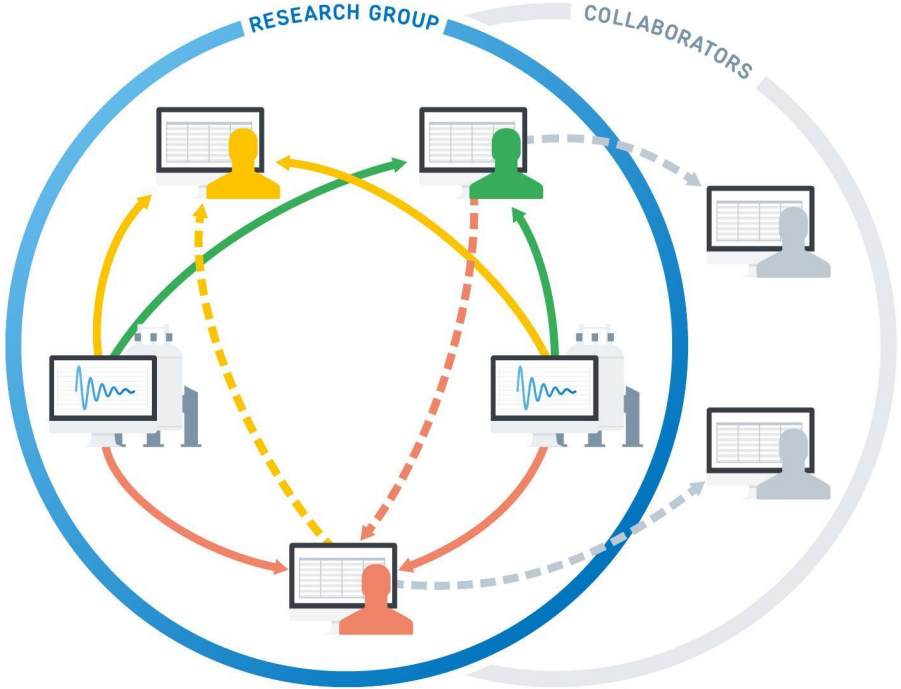
http://logs-repository.com

SIGNALS

Problem with current data management

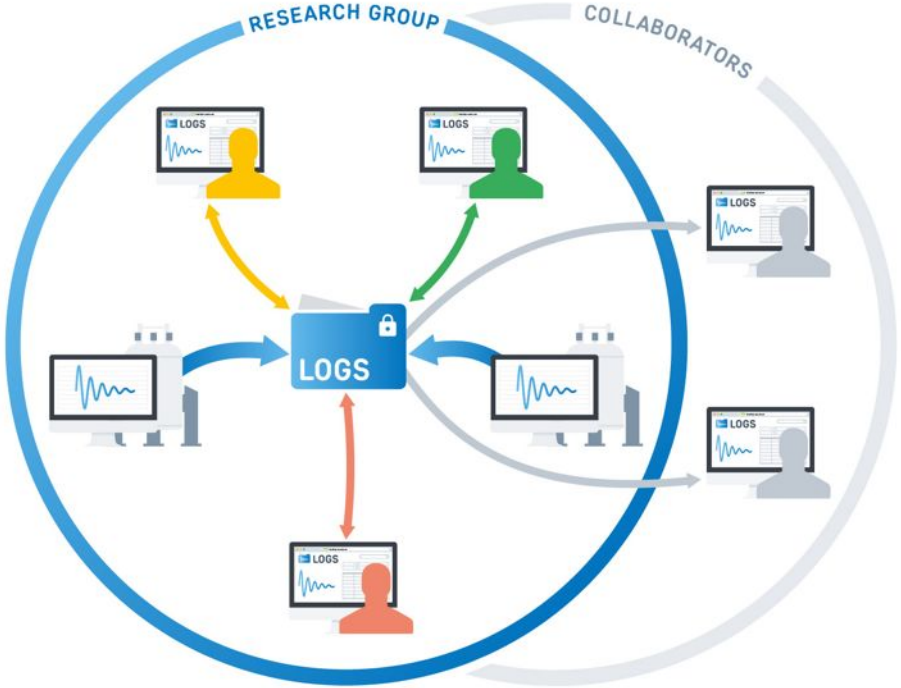
- → No findability
- → No accessibility
- → No retrievability
- → No reusability or reproducibility

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



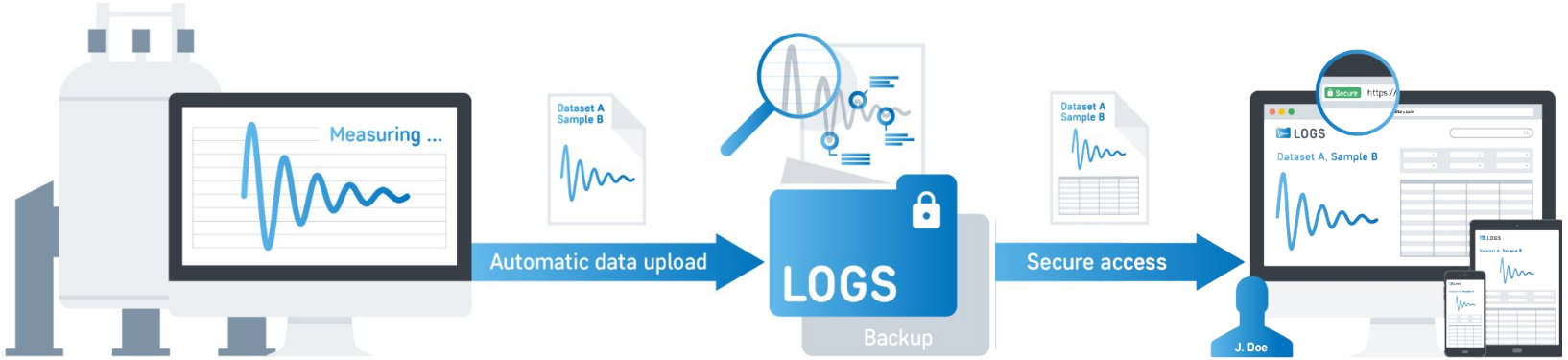
- LOGS checks the instruments periodically and uploads fresh data.
- Every piece of digital data related to do the experiment is saved, ensuring a maximum of automatically retained information.
- Enables and simplifies lab data administration
  - Transportability
  - Back-ups
  - Transparency

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

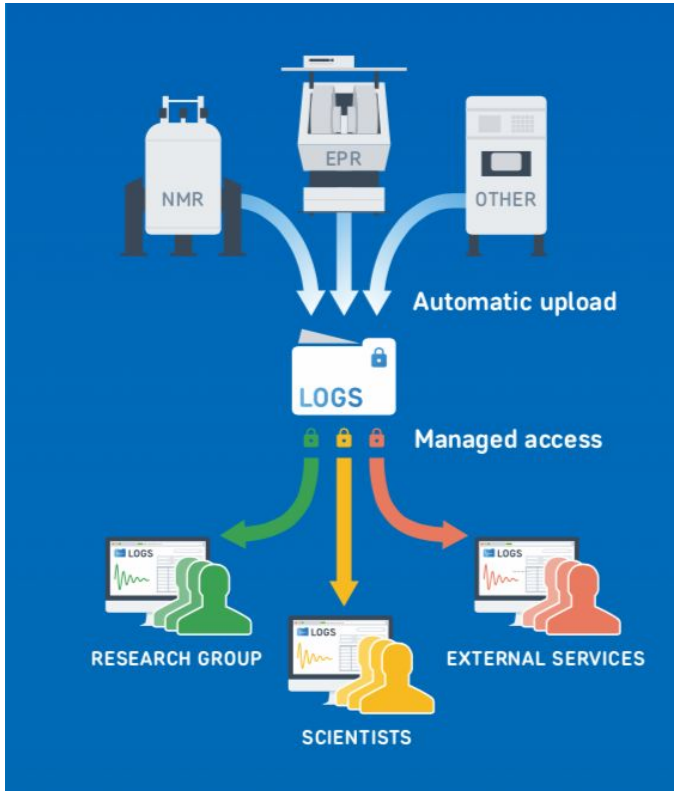
- Data inflow: Primary data automatically uploaded from instrument
- Monitor measurements, in the browser

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

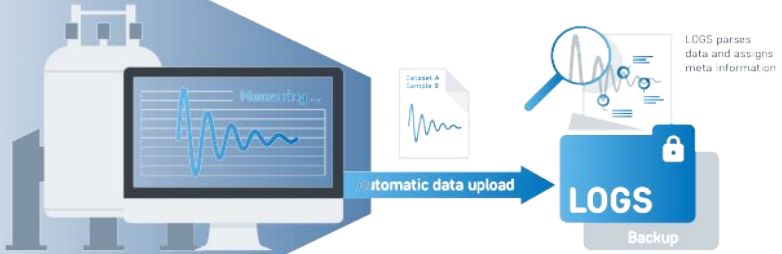


LOGS workflows

- 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

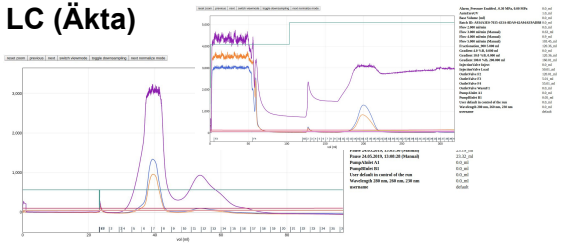
CD (1)	- Jasco
EPR (4)	- Bruker, Specman4EPR, Magnettech, fsc2 format
EM (1)	- EPMA (wip)
FT-IR (1)	- Bruker Opus
HPLC (1)	- Agilent
ITC (2)	- Malvern Analytical, MicroCal
MPLC (2)	- Äkta, NGC
MS (3)	- Bruker (MALDI-TOF, FT-ICR), JEOL (LIFDI MSAxel)
Microscopy (1)	- Zeiss
NMR (4)	- Bruker, Varian, JEOL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



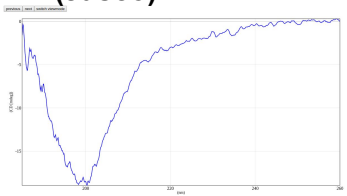
The list of incorporated dataformats is continuously growing with users requests

LOGS as the ultimate data viewer

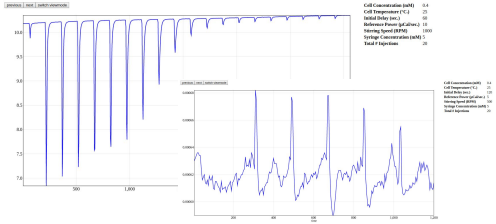
LC (Äkta)



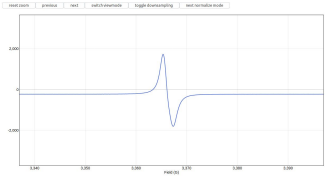
CD (Jasco)



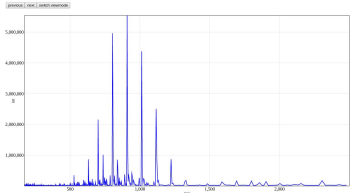
ITC (MicroCal)



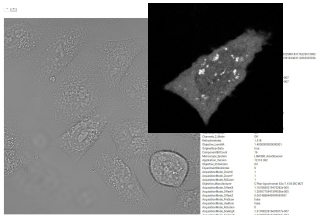
EPR-CW (Bruker)



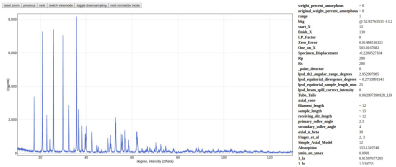
ITC (MicroCal)



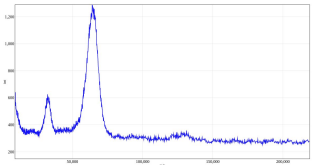
Microscopy (Zeiss)



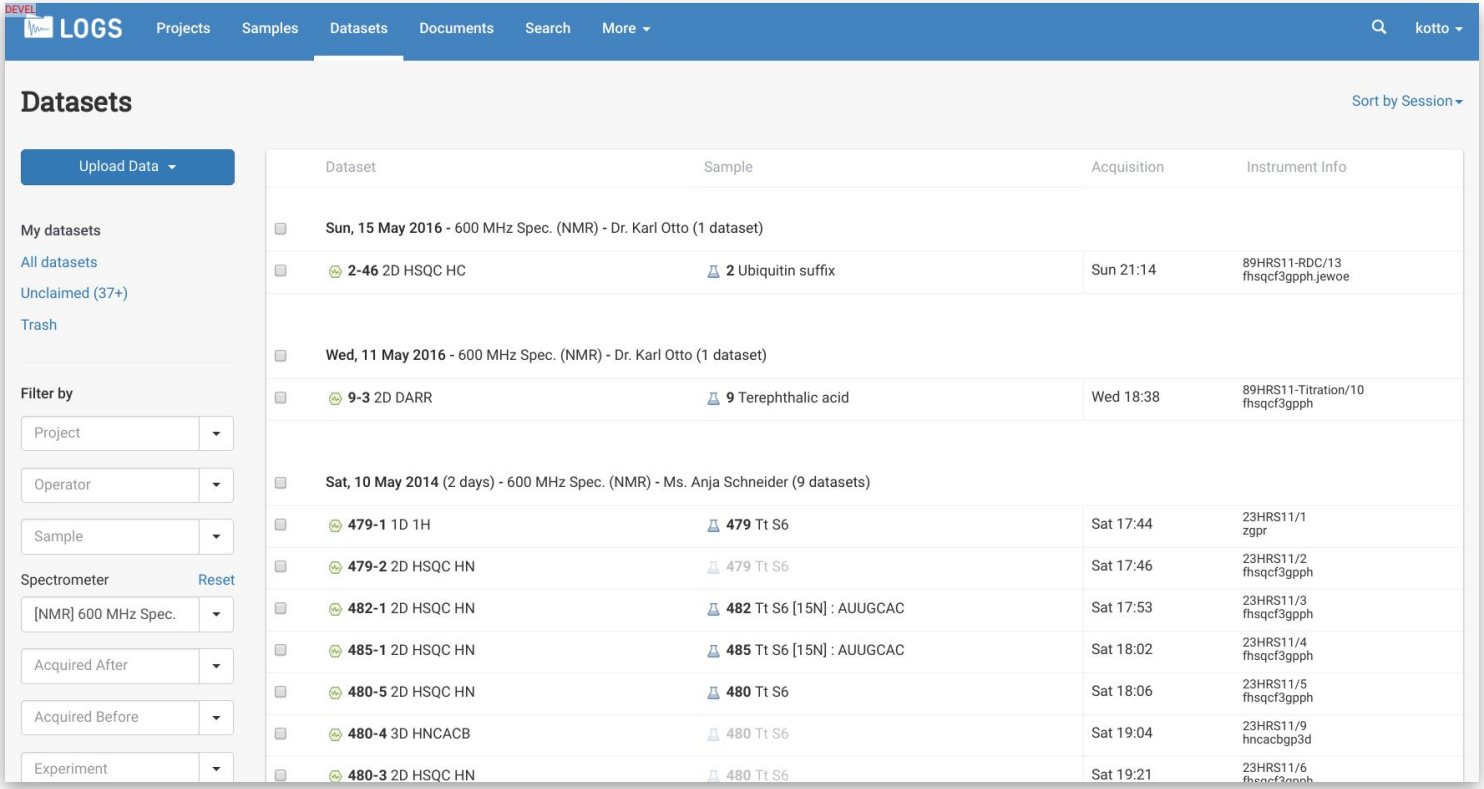
XRD (Bruker)



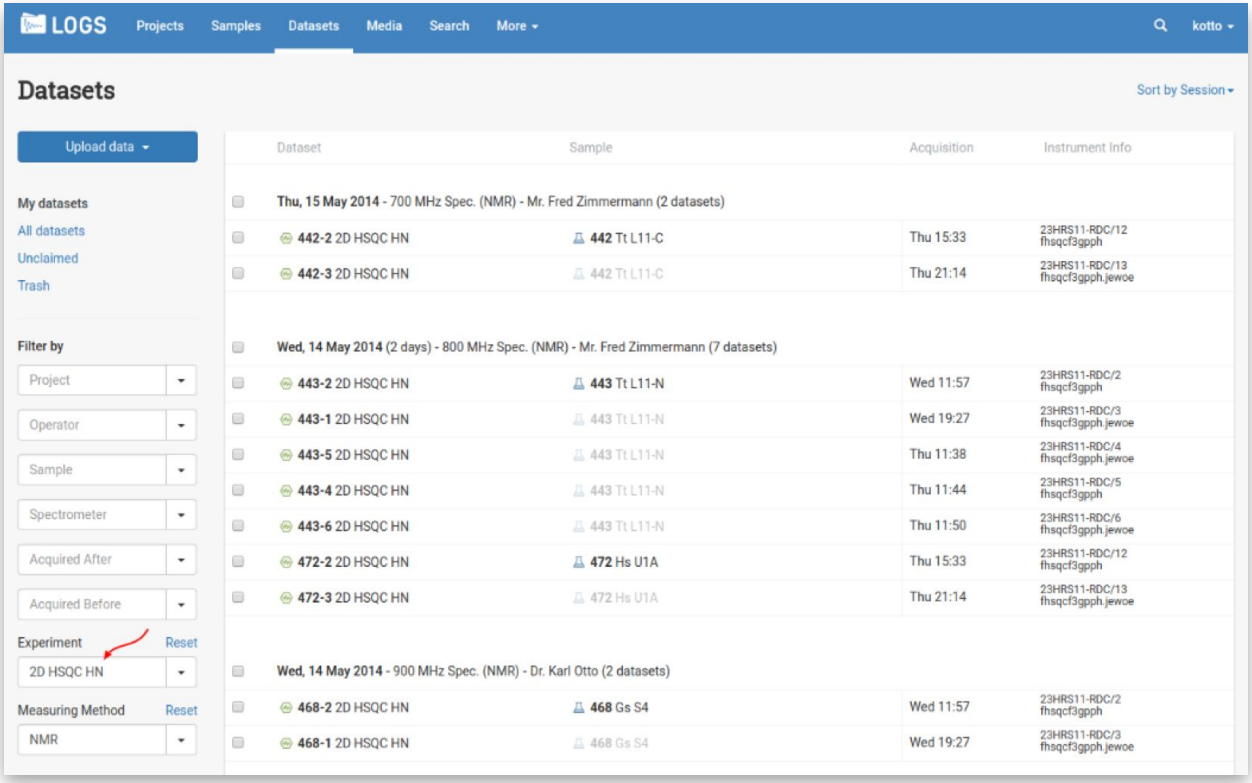
MALDI-TOF (Bruker)



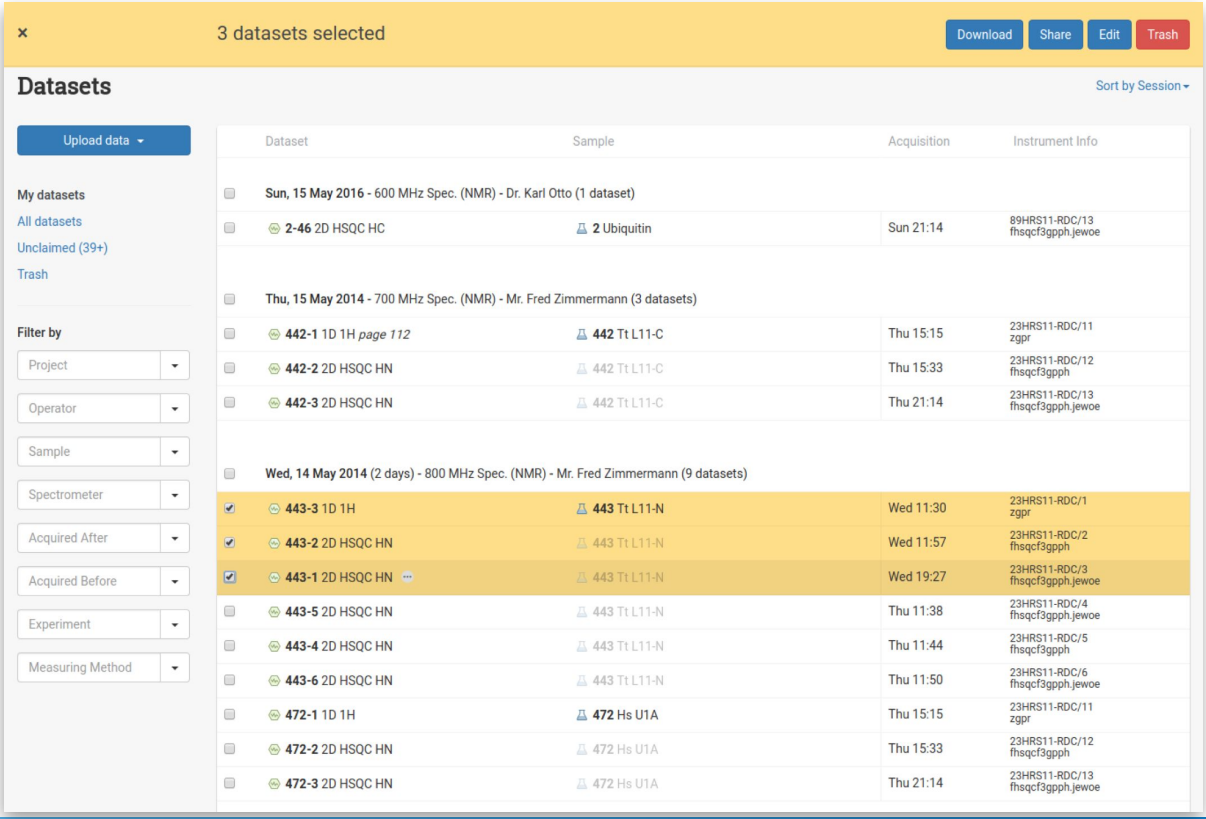
Dataset overview



Filter your datasets



Get your data easily



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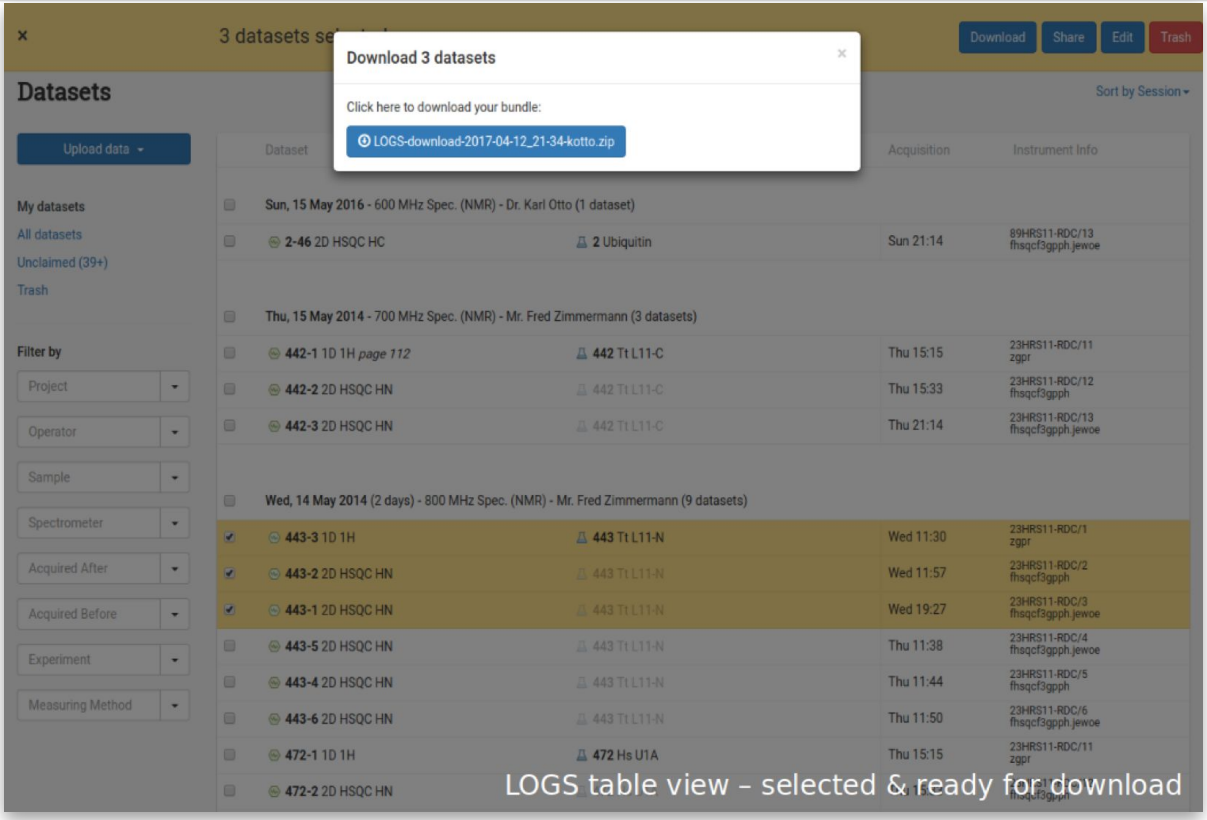
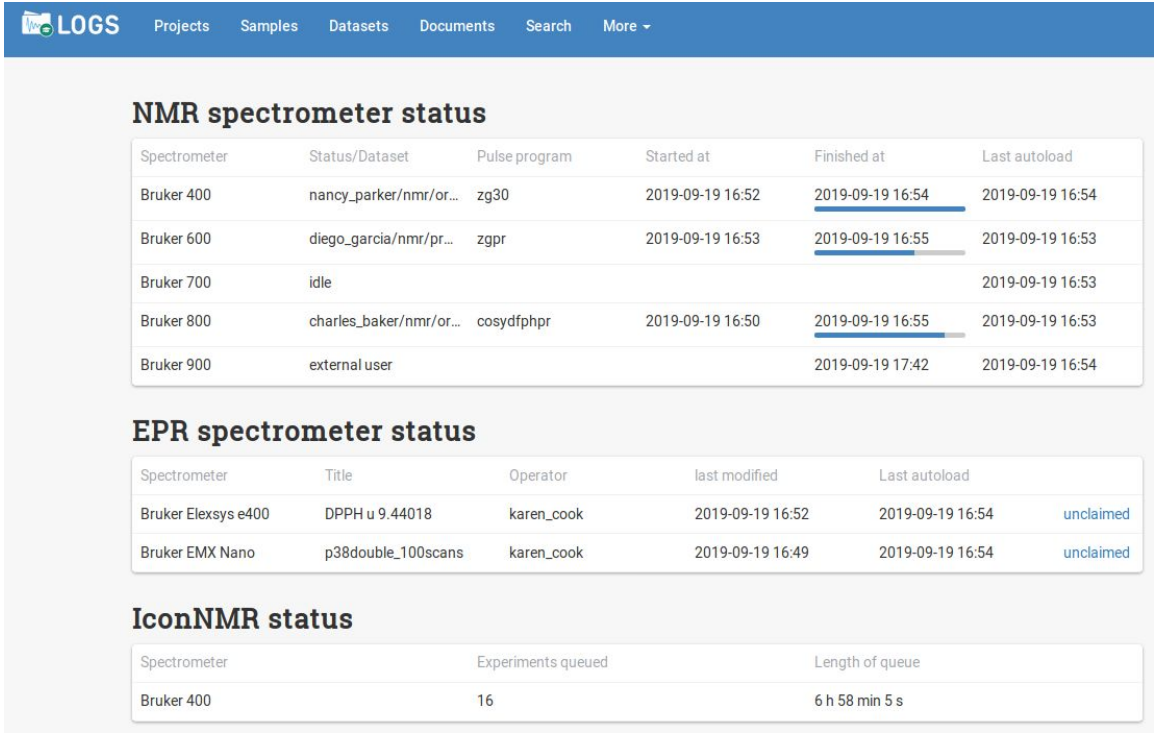
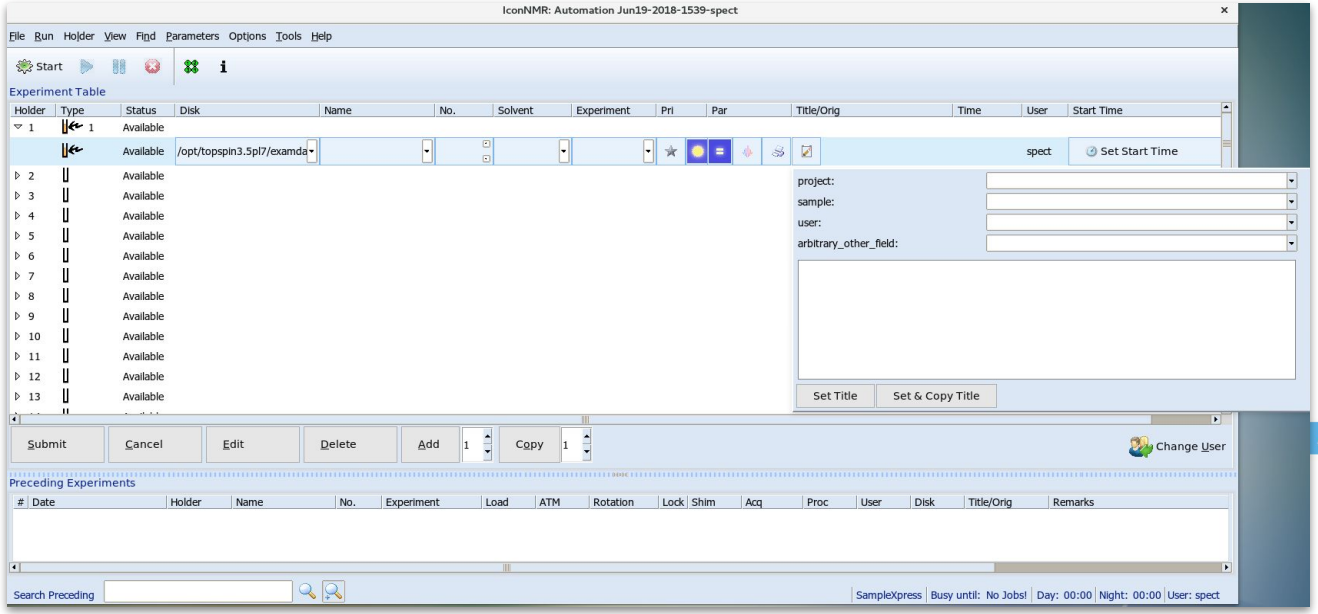


LOGS table view – selected & ready for download

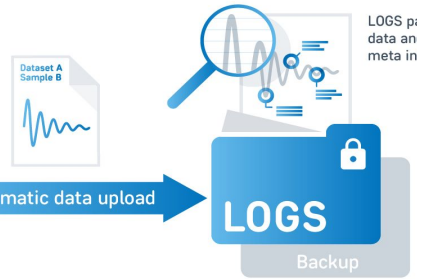
Keep an eye on your experiments



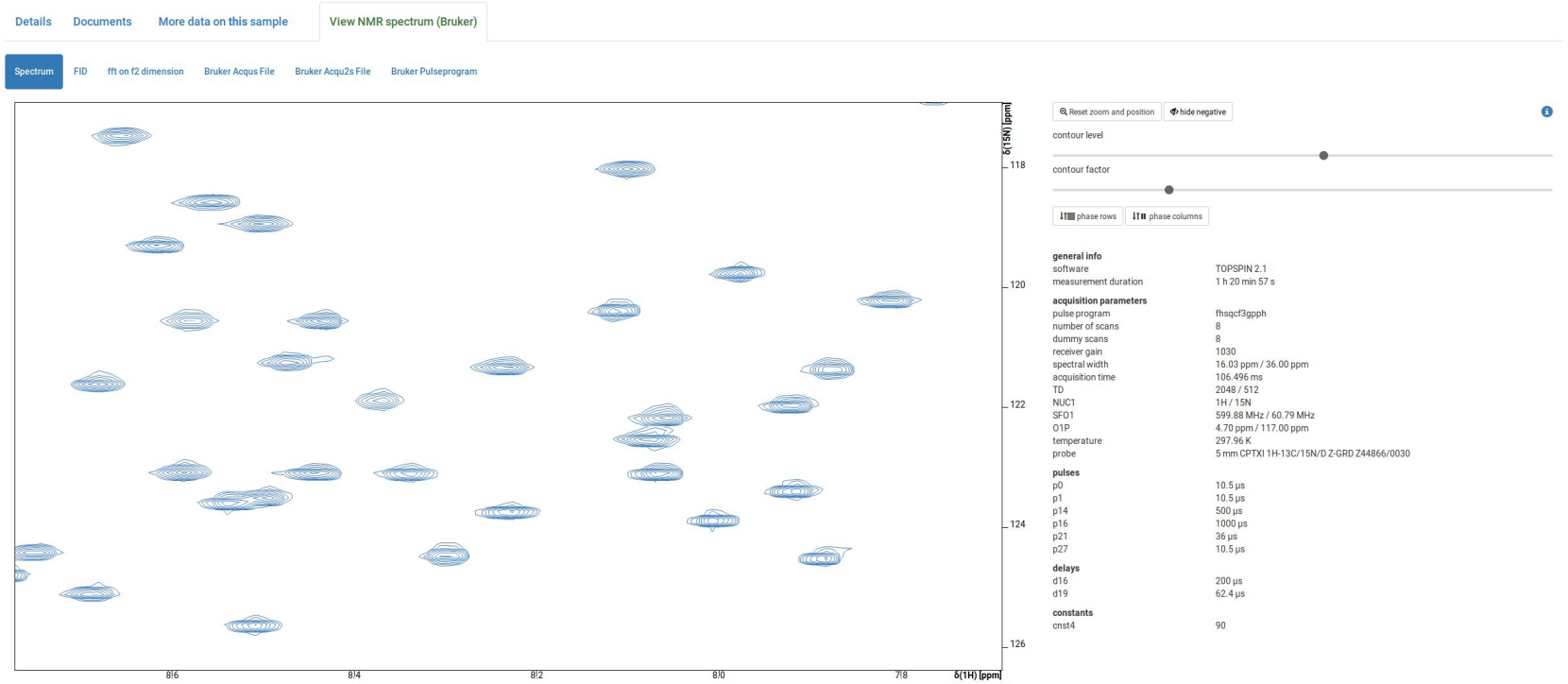
IconNMR and automated data management



Metadata is automatically transferred from IconNMR



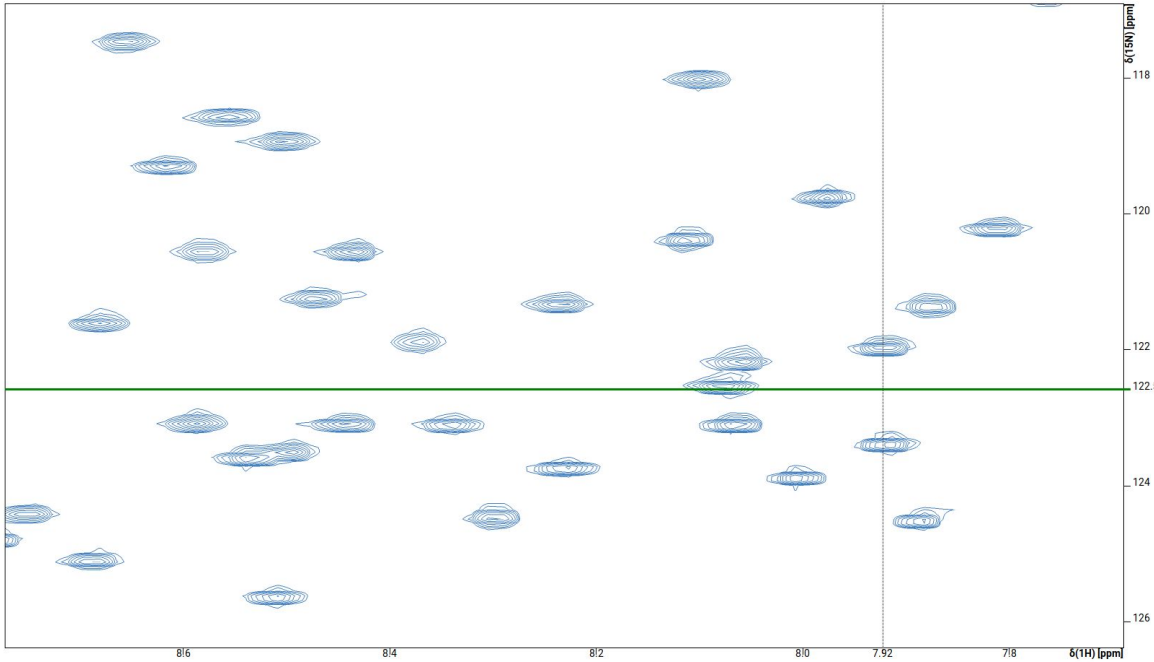
Process spectra in the browser



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 Acqu2s File | Bruker Pulseprogram



Reset zoom and position | hide negative

contour level

contour factor

phase rows | phase columns

general info

software	TOPSPIN 2.1
measurement duration	1 h 20 min 57 s

acquisition parameters

pulse program	fhsqcf3gpph
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

pulses

p0	10.5 µs
p1	10.5 µs
p14	500 µs
p16	1000 µs
p21	36 µs
p27	10.5 µs

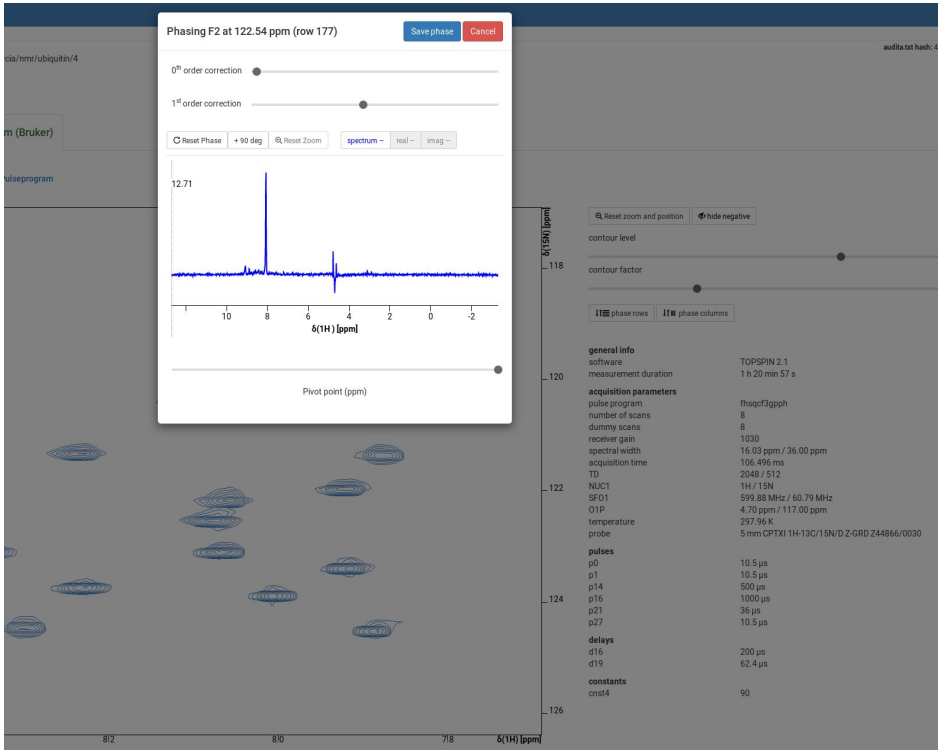
delays

d16	200 µs
d19	62.4 µs

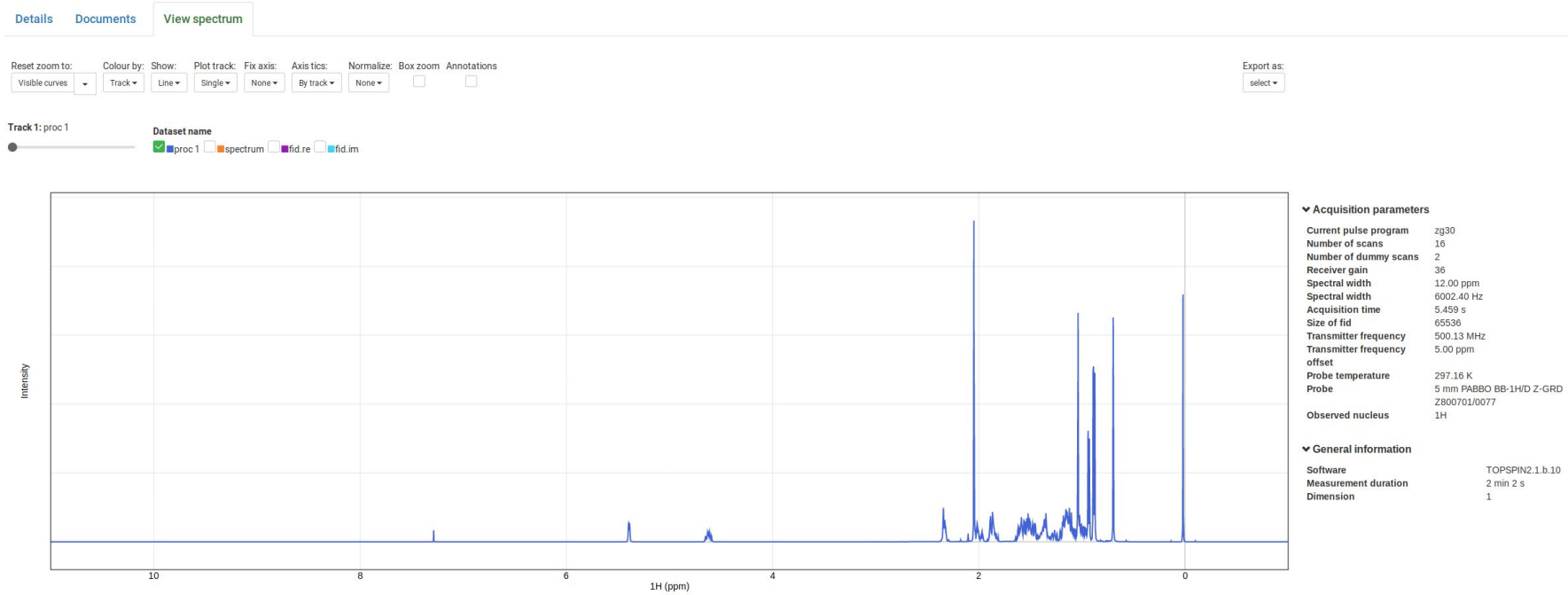
constants

cnst4	90

Phase spectrum in the browser



Secondary NMR data: 1D spectra annotation



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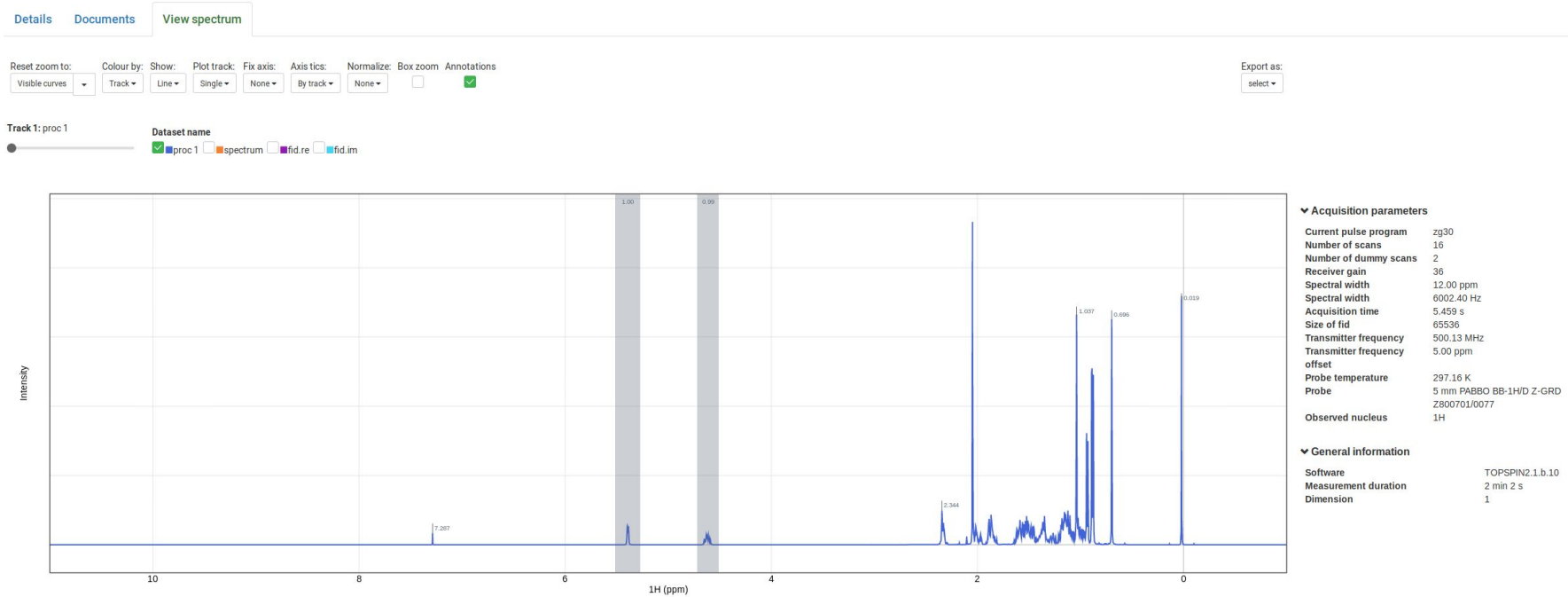

LOGS a tool integrating data formats & meta data

- ✔ 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