LOGS
ELN

Das ELN mit direktem Spektrometeranschluss

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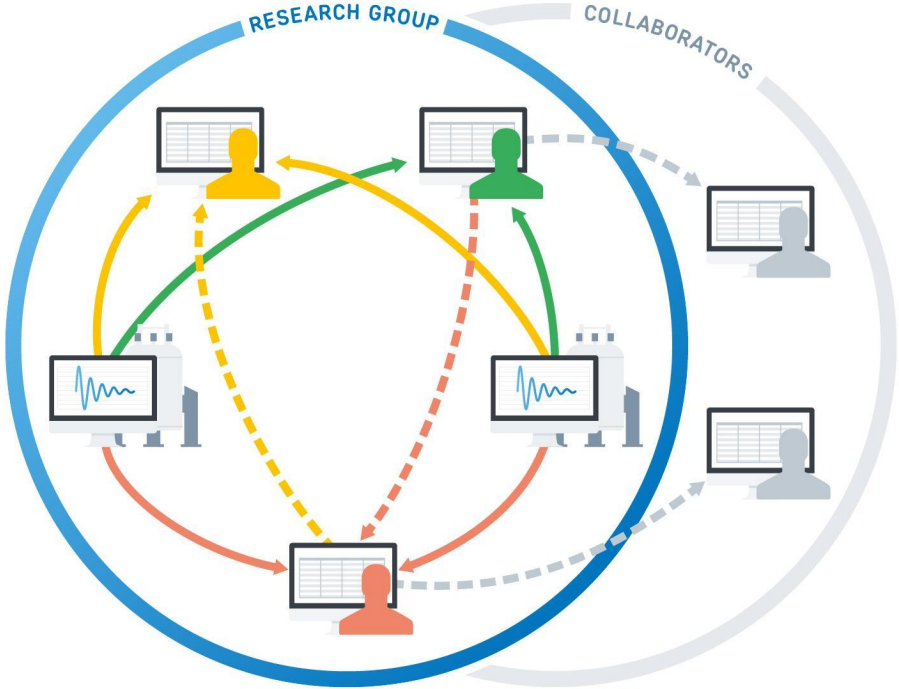
44. Tagung Praktische Probleme der Kernspinresonanz, Berlin-Buch, 22.03.2023

SIGNALS

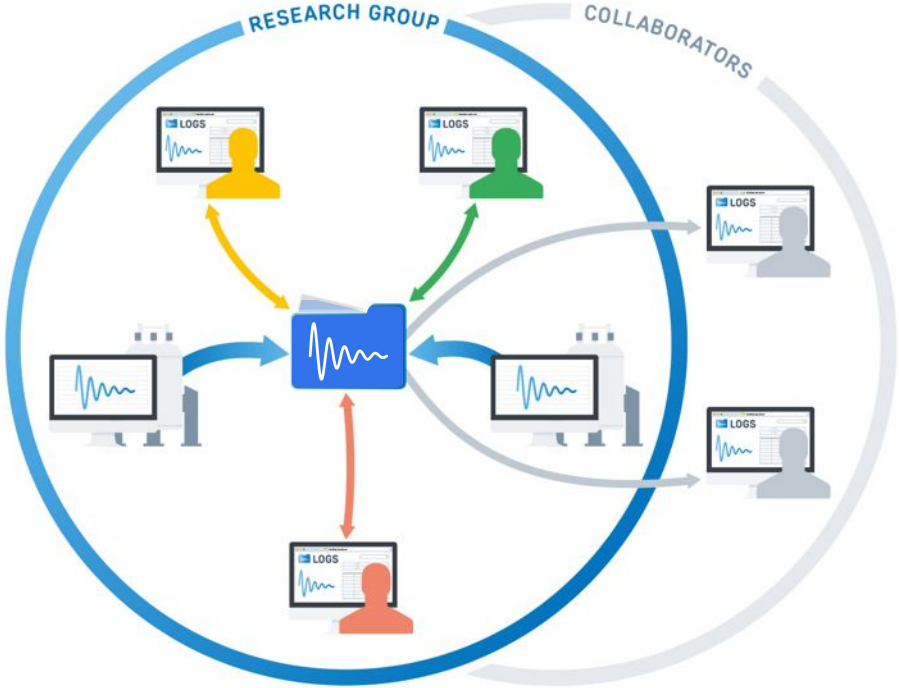
Is storing the data enough?

Problem Source: data pathways are unclear



- **multiple** people, instruments, samples, experiments, ...
- personal data storage
- high fluctuation of lab members
- no recording of contextual information, e.g. experimental parameters

Problem Solution: data is saved in a central hub



- central data storage
- automatic data upload from instruments
- enables and simplifies lab data administration (back-up)
- easy access to data
- parsing datasets, extracts metadata
- **part of lab workflows**

LOGS

LOGS ELN

Electronic Laboratory Notebook

Gather all **written** data

LOGS SDMS

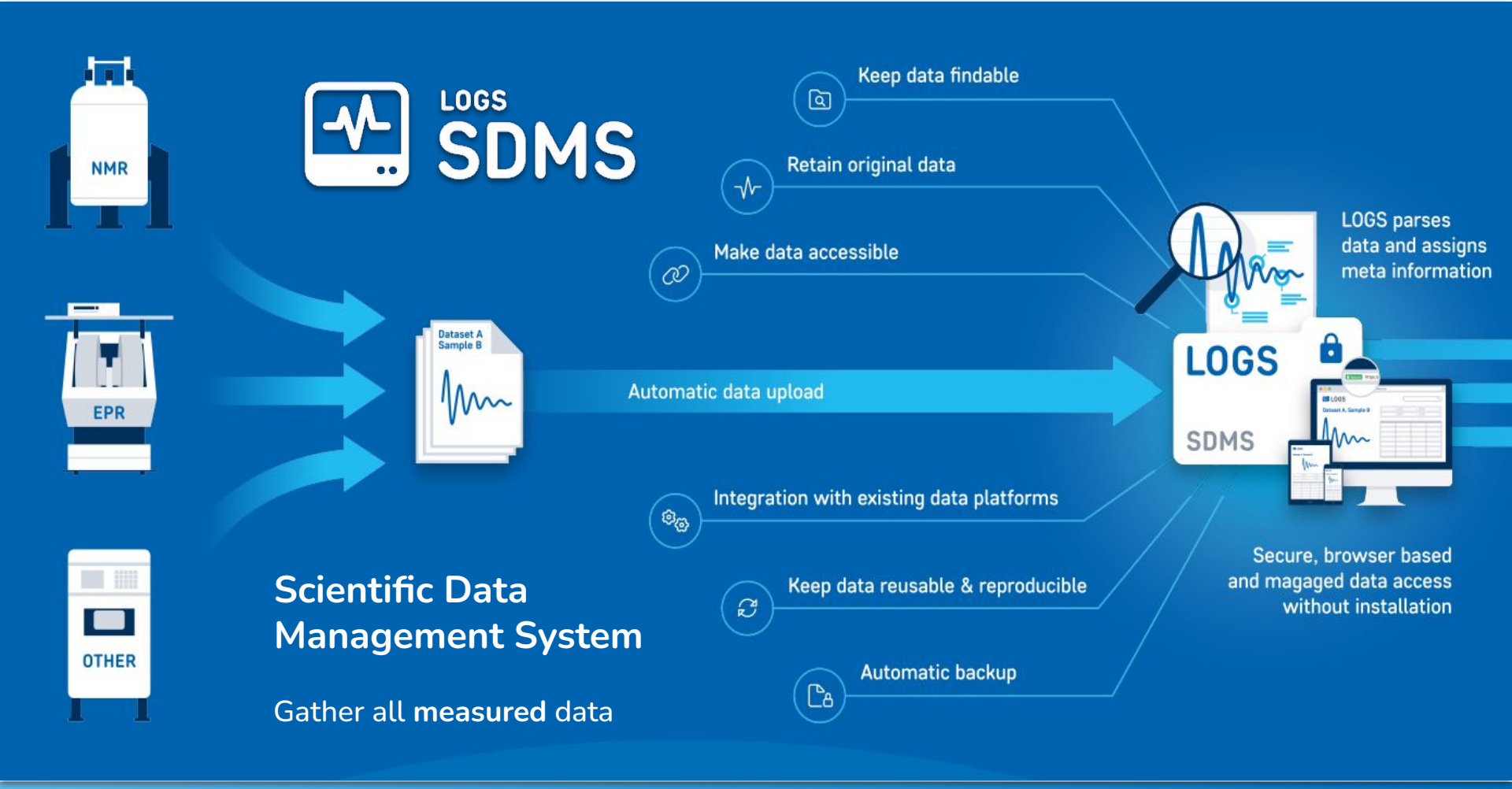
Scientific Data Management System

Gather all **measured** data

LOGS Python

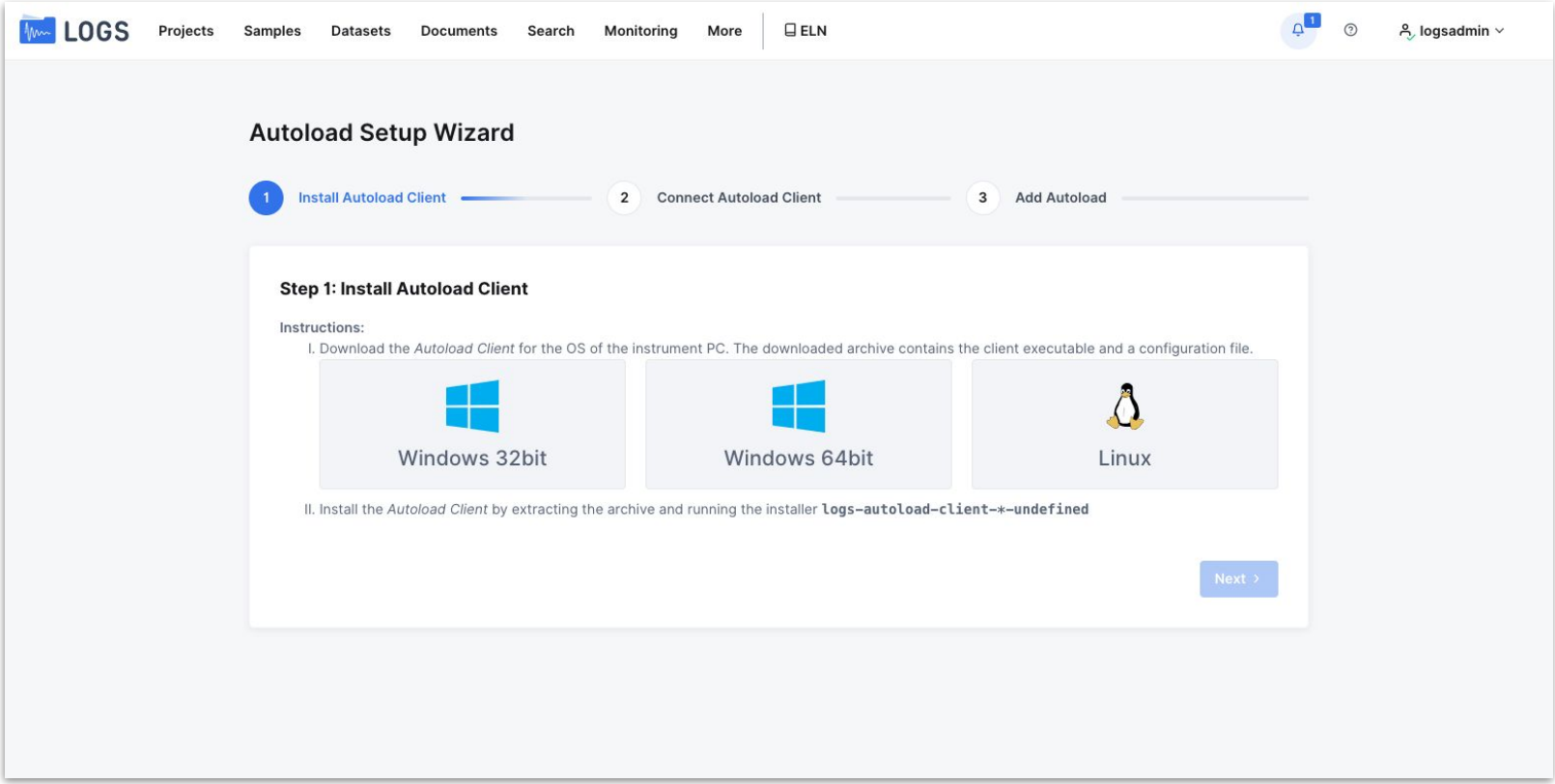
Python LOGS API

LOGS-Py, Scripted interaction with research data and further LOGS content


LOGS
SDMS
NMR
EPR
OTHER
Dataset A
Sample B
Automatic data upload
Keep data findable
Retain original data
Make data accessible
Integration with existing data platforms
Keep data reusable & reproducible
Automatic backup
LOGS parses data and assigns meta information
LOGS
SDMS
Secure, browser based and magaged data access without installation
Scientific Data Management System
Gather all **measured** data

LOGS
SDMS

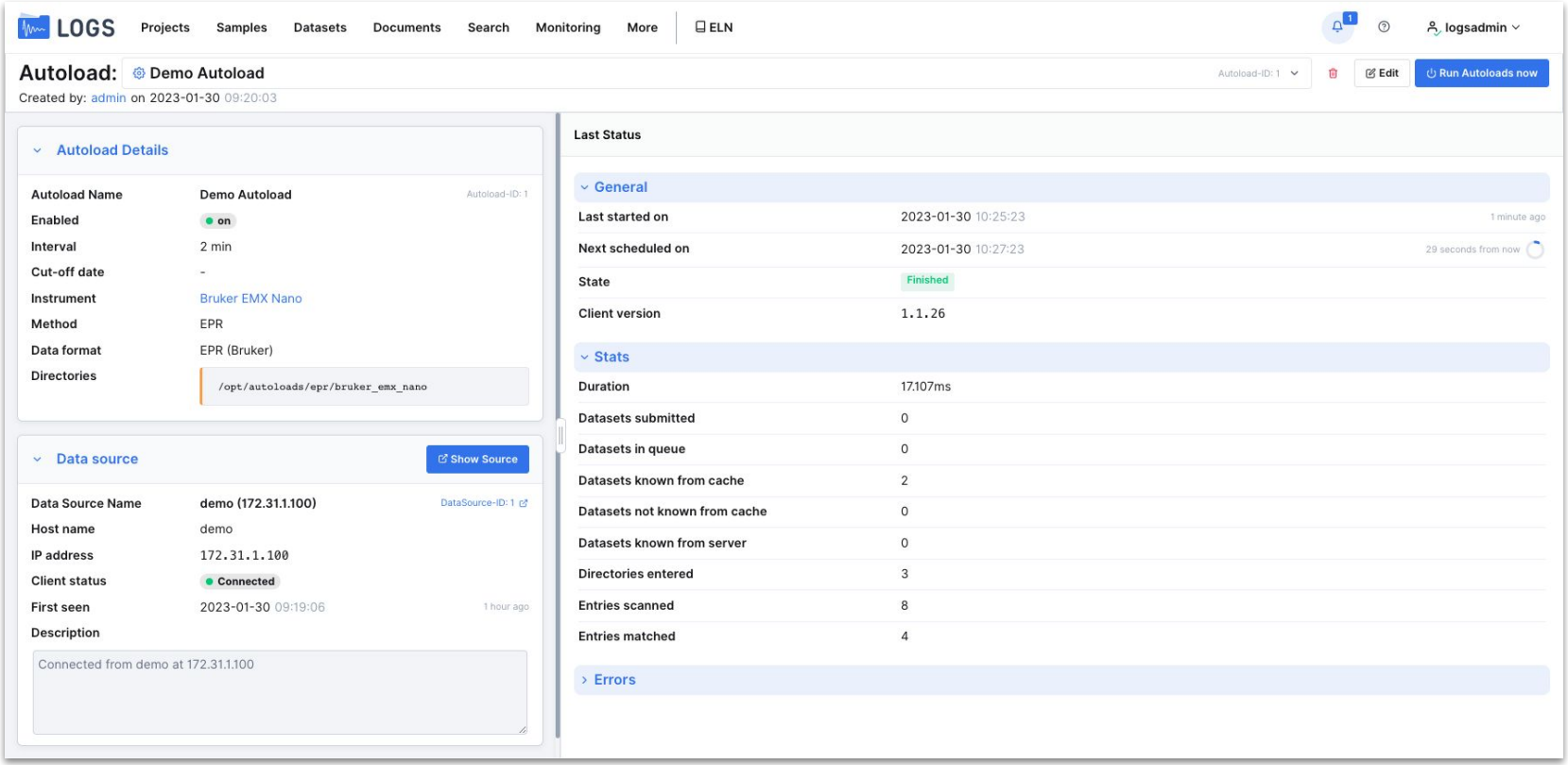
The automated data upload



LOGS SDMS

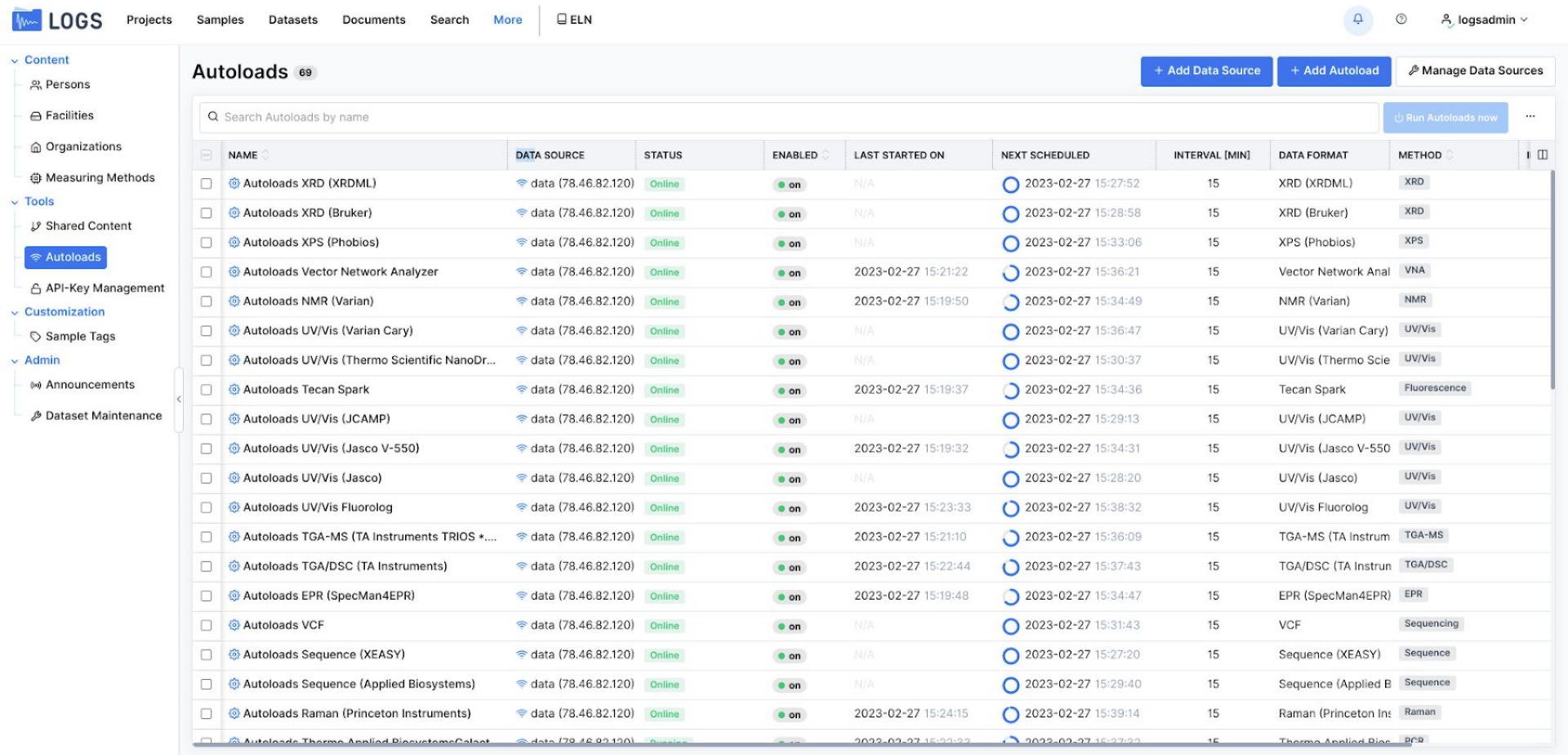
Automatic Upload Configuration

DemoLink



LOGS SDMS

Automatic Upload of your complete Lab



LOGS SDMS

Dataset Table

DEVEL LOGS | Projects | Samples | Datasets | Documents | Search | Monitoring | More | ELN | logsadmin

Datasets 95

Upload dataset

Method
NMR ×

Experiment
Select...

Sample
Select...

Instrument
Select...

Supplementary equipment
Select...

Acquisition date from
mm/dd/yyyy

Acquisition date to
mm/dd/yyyy

Project
Select...

Organization
Select...

Search | 3 datasets selected

METHOD	EXPERIMENT	NAME	SAMPLE	ACQUISITION DATE	PROJECTS	OPERATORS
NMR	BEST-TROSY	P17-800AV/8	#44 P17	2017-12-18 13:06:56	P17	Dr. Mark Price
NMR	HCCCONH	P17-600AV/4	#44 P17	2016-10-06 12:24:29	P17	Dr. Mark Price
NMR	HBCBCGCDC...	P17-800AV/7	#44 P17	2016-09-27 10:01:56	P17	Dr. Mark Price
NMR	HBCBCGCDHD	P17-800AV/6	#44 P17	2016-09-27 08:37:05	P17	Dr. Mark Price
NMR	2D NOESY	P17-600AV/3	#44 P17	2016-08-21 12:45:05	P17	Dr. Mark Price
NMR	2D HSQC HN	P17-600AV/2	#44 P17	2016-08-20 08:00:11	P17	Dr. Mark Price
NMR	1D 1H	P17-600AV/1	#44 P17	2016-08-19 17:21:22	P17	Dr. Mark Price
NMR	2D HSQC HC	P17-800AV/5	#44 P17	2016-08-17 08:13:08	P17	Dr. Mark Price
NMR	2D NOESY	P17-800AV/4	#44 P17	2016-08-15 09:50:11	P17	Dr. Mark Price
NMR	2D TOCSY	P17-800AV/3	#44 P17	2016-08-13 16:43:43	P17	Dr. Mark Price
NMR	2D HSQC HN	P17-800AV/2	#44 P17	2016-08-11 14:33:09	P17	Dr. Mark Price
NMR	1D 1H	P17-800AV/1	#44 P17	2016-08-11 11:58:32	P17	Dr. Mark Price
NMR	1D_1H	organic/1	#47 organic	2015-12-18 15:15:53	-	-

Measured Data in LOGS-SDMS

DemoLink

DEVEL

LOGS | Projects | Samples | Datasets | Documents | Search | Monitoring | More | ELN | logsadmin

Dataset: NCOV_1_248_HN_1200/51 Dataset-ID: 321

Created by: admin on 2021-06-07 11:59:17

Edit | Download

Dataset Details

General

Name	NCOV_1_248_HN_1200/51 Dataset-ID: 321
Dataset Type	Basic Dataset
Method	NMR
Experiment	-
Instrument	Bruker 400
Suppl. Equipment	-
Acquis. Date	2020-10-30 20:15:23 2 years ago
Projects	Privileged User , DEMO "Iron Upgraded"
Organizations	-
Operators	admin
Notes	

NCOV_1-248
pH 6.5 T=298K
25mM TRIS. 450 mM NaCl

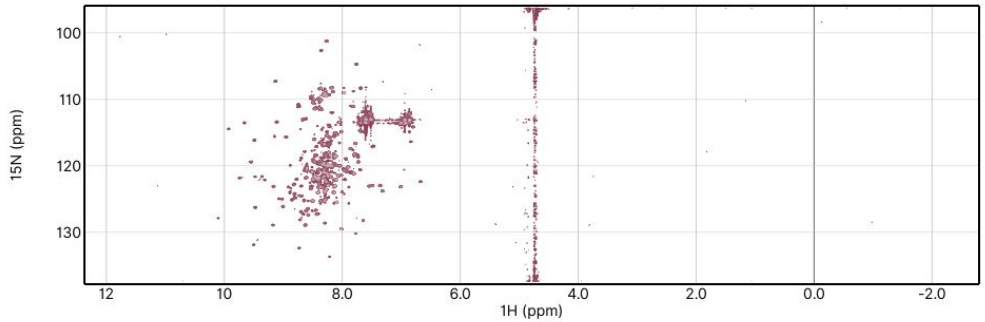
Sample

Edit

Name	LOGS Sample-ID: 48
Sample Type	Basic Sample
Prepared	2021-02-08 Last year
Prepared by	admin

Preview

2D | Tracks: 1



Parameters

Filter

Notes

NCOV_1-248
pH 6.5 T=298K
25mM TRIS. 450 mM NaCl

General info

Software TopSpin 4.0.9

Duration 1 h 15 min 27 s

General acquisition parameters

pulse program b_trosyetf3gpsi.2

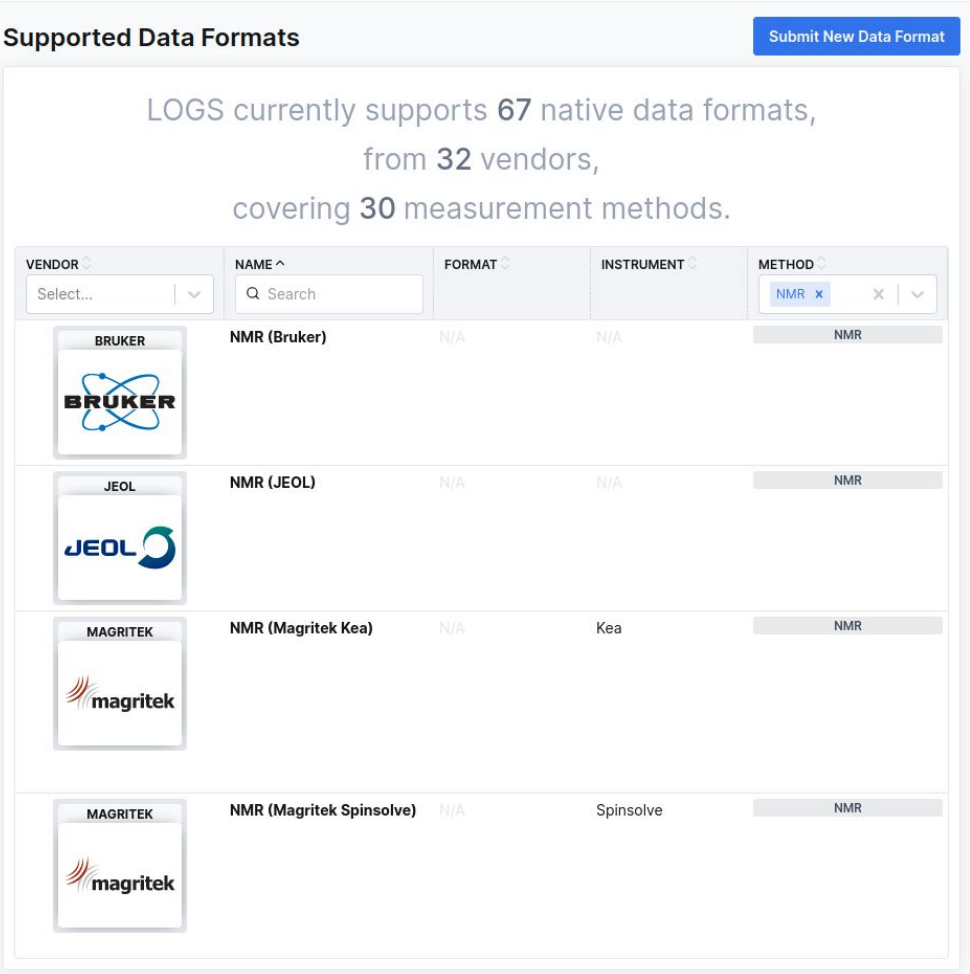
number of scans 16

Files

- NCOV_1_248_HN_1200
  - 51
    - pdata
      - 1
        - 2ii
        - 2ir
        - 2ri
        - 2rr
        - auditp.txt
        - clevels

LOGS SDMS

LOGS supports a growing number of data formats.



LOGS ELN

Electronic Lab Notebook

Scientists

Research groups

External services

Enter all Notes, Protocols, etc.

Link the **written** data to the digital content,
e.g. Datasets, Samples, Persons, Projects, etc.

LOGS ELN — The ELN for Spectroscopy

DemoLink

LOGS | Projects | Samples | Datasets | Documents | Search | Monitoring | More | ELN | logsadmin

A Demo ELN Labbook › Interactions between the … › Jan 30, 2023

Saved! Last saved: 2023-02-06:09:42:45

Manage entry | Previous entries | Save & close

Datasets

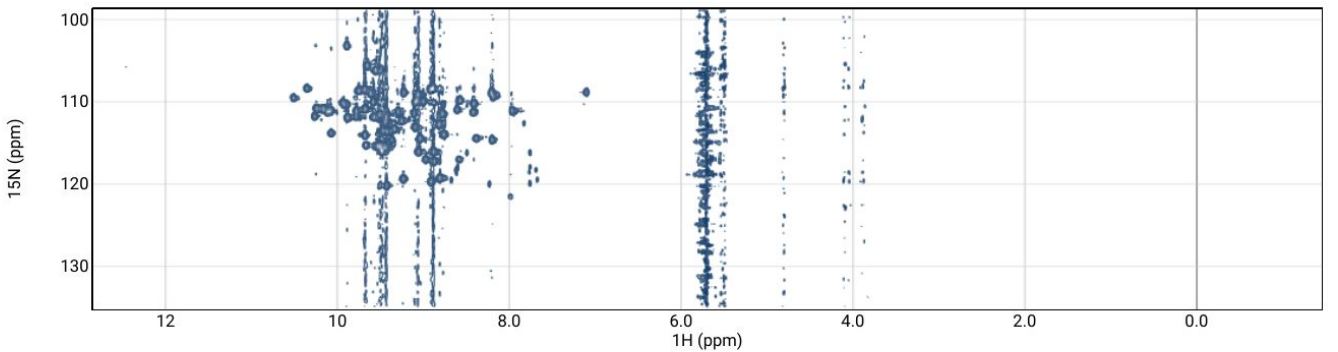
184 Search

ubiquitin/10	NMR 2D H(N...	
2009-12-29	Ubiquitin	
ubiquitin/5	NMR 2D HS...	
2009-12-28	LOGS Demo	
ubiquitin/9	NMR 2D H(N...	
2009-12-28	Ubiquitin	
P17-600AV/4	NMR HCCC...	
2016-10-06	P17	
P17-600AV/2	NMR 2D HS...	
2016-08-20	P17	
P17-600AV/1	NMR 1D_1H	
2016-08-19	P17	
Azol_420uMD2O_HPDINO...	NMR 1D 31P	
2015-05-26	Azol	
Azol_420uMD2O_HPDINO...	NMR 2D NO...	
2015-05-26	Azol	
Azol_420uMD2O_HPDINO...	NMR 2D TO...	
2015-05-24	Azol	

Interactions ELN and SDMS

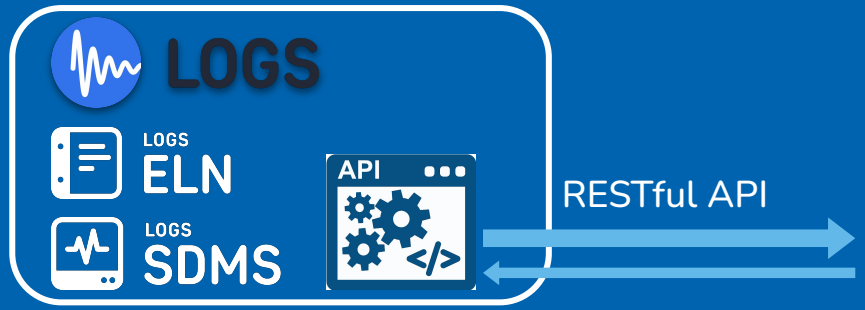
Dataset: ubiquitin/9

Viewer



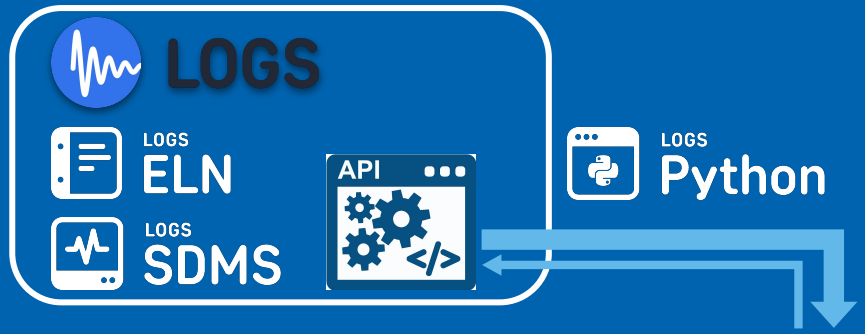
"Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum."

LOGS Python

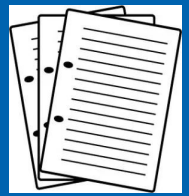


- Extract all your datasets
  - Original files
  - Extracted parameters
  - Extracted tracks
- Metadata and relations (e.g. projects, samples, Persons)
- Communication between 3rd party software
- Extensive data mining

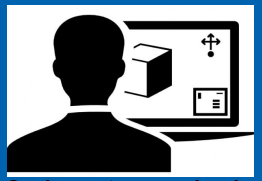
LOGS Python



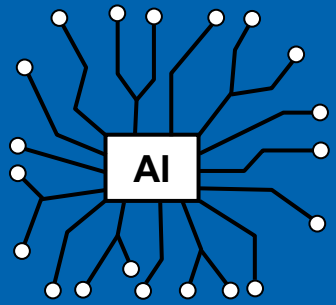
- Use Python native objects
  - no web technology knowledge needed
  - python object system representing your LOGS data
- Integration of exiting analyse tools
- Use vast number available Python modules
- Customize automate your processes



Reports, statistical analysis



3rd party analysis software



LOGS Python

Example code - Get dataset properties

```python
from LOGS.LOGS import LOGS


api_key = "mkYmfo6XlU3rfxPGbx7nPxhLoS8PYDaaaUfF5nlEFAXYAeyHtqGaJ8FOWh3S5ijY"
url = "https://institute.logs-development.com/service"
logs = LOGS(url, api_key)

dataset = logs.dataset(86609)

print("Name:", dataset.name, "Experiment:", dataset.experiment.name)
```

```
> Name: Honey_probe_1353/3 Experiment: HSQC
```

LOGS Python

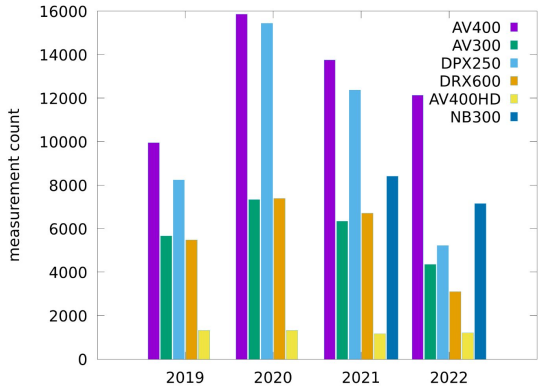
Example code - Loop over datasets

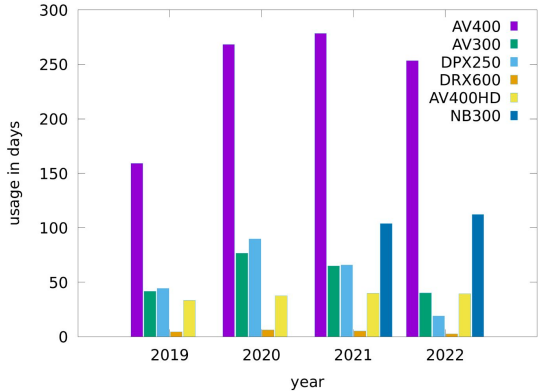
```python
from datetime import datetime
from LOGS.LOGS import LOGS
from LOGS.Entities.DatasetRequestParameter import DatasetRequestParameter


api_key = "mkYmfo6XlU3rfxPGbx7nPxhLoS8PYDaaaUfF5nlEFAXYAeyHtqGaJ8FOWh3S5ijY"
url = "https://institute.logs-development.com/service"

logs = LOGS(url, api_key)

for dataset in logs.datasets(DatasetRequestParameter(experiments=["HSQC"], acquisitionDateFrom=datetime(2022, 1, 1, 0, 0, 0))):
   print("Name:", dataset.name, "  Experiment:", dataset.experiment.name)
```

```
> Name: Honey_probe_1894   Experiment: HSQC
> Name: Honey_probe_9079   Experiment: HSQC
> Name: Honey_probe_5410   Experiment: HSQC
> Name: Honey_probe_3606   Experiment: HSQC
> Name: Honey_probe_2519   Experiment: HSQC
...
```

LOGS Python

Overviews and on production systems





Statistic on effective instrument deployment per year

How many datasets were measured on each instrument

How much time was each instrument busy

Overview of effectiveness of the facility

Find bottleneck in instrumentation

Use detailed information for customer billing

LOGS
Python

Use Case with ELN “Labstep”

LOGS Projects Samples Datasets Documents Search More signals

Dataset: w122111504 Dataset-ID: 50

Created by: Signals, L. on 2022-12-02 09:37:36

Edit Claim Download

Dataset Details

Name	w122111504
Method	EPR
Experiment	-
Instrument	Bruker EPR
Suppl. Equipment	-
Acquis. Date	2022-11-16 10:50:29
Projects	-
Organizations	-
Operators	-
Notes	-

Source information

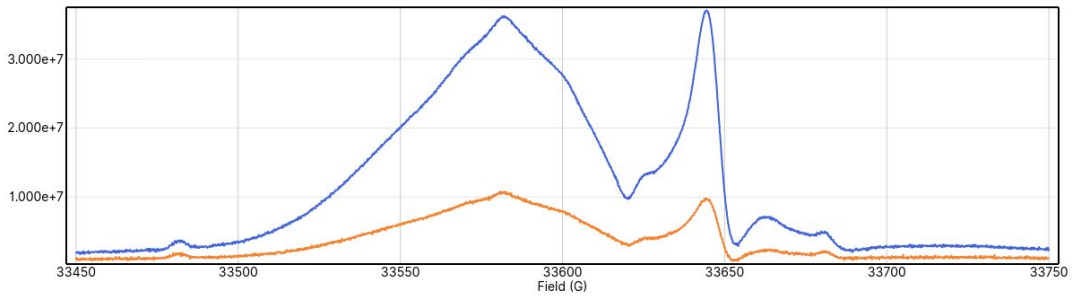
Origin	Manual file upload
Upload date	2022-12-02 09:37:36
File format	EPR (Bruker)
Vendor	Bruker
Path	/w122111504.DSC

Related datasets 30

Sample

Preview

1D Tracks: 1



Parameters

Filter

Title 'w122111504 CCLD pH5ClO FSecho TL39.2 80K 100sc'
Operator xuser
Center field 3.36 T
Sweep width 0.03 T
Number of points 1024
Sweep direction Up
Microwave frequency 94.02 GHz
Microwave band W
PowerAtten 25.0 dB
Power 1.77 µW
Number of averages 100

Files

w122111504.DSC
w122111504.DTA

LOGS Python Use Case with ELN “Labstep”

MPI CEC > EPR Research Group > Experiments

Saved View

Equipment and resources used

Spectrometer	w1
Resonator	flex
cryostat	cryogenic
Sample tube diameter	0.9
standards used	Mn(II) in ZnS

Sample Details

- CCLD

Collection of EPR data

Experiment Details

File name #LOGS_content	Attenuation	Microwave Power	Modulation Amplitude	Receiver Gain	Link
w122111805	35.0	177.1	500	39	logs-ID:79437
w122111601	25.0	1.77	500	39	logs-ID:79318
w122111504	25.0	1.77	-	-	logs-ID:79317
x120111302	15.0	6.33	100	60	logs-ID:70691

Protocols
Inventory
Data
Devices
Signatures
Linked Experiment
Notes
Activity

Thanks for listening