



LOGS  
ELN



## Das ELN mit direktem Spektrometeranschluss

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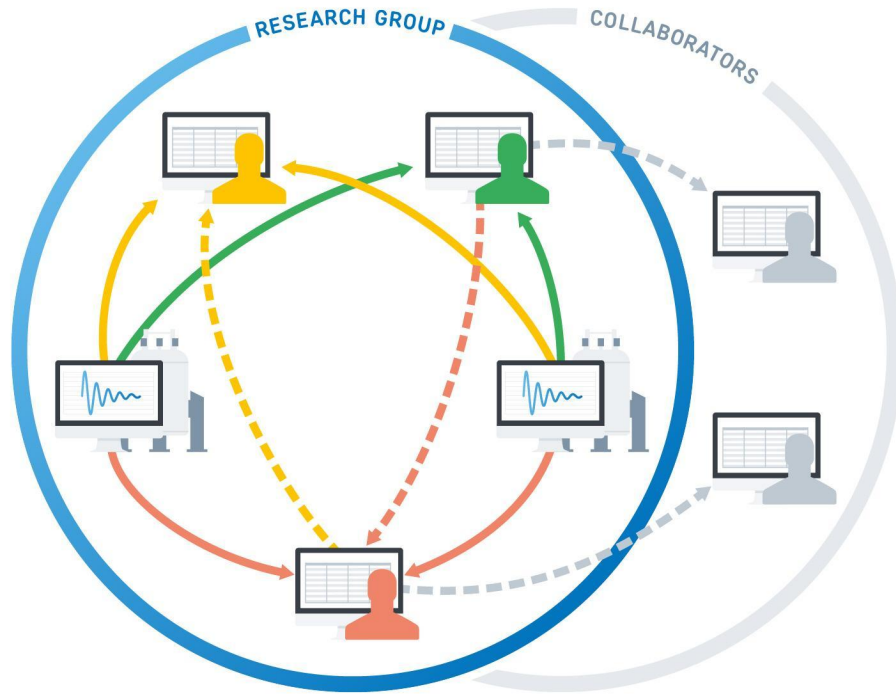
44. Tagung Praktische Probleme der Kernspinresonanz, Berlin-Buch, 22.03.2023

# Is storing the data enough?

Where is your data?

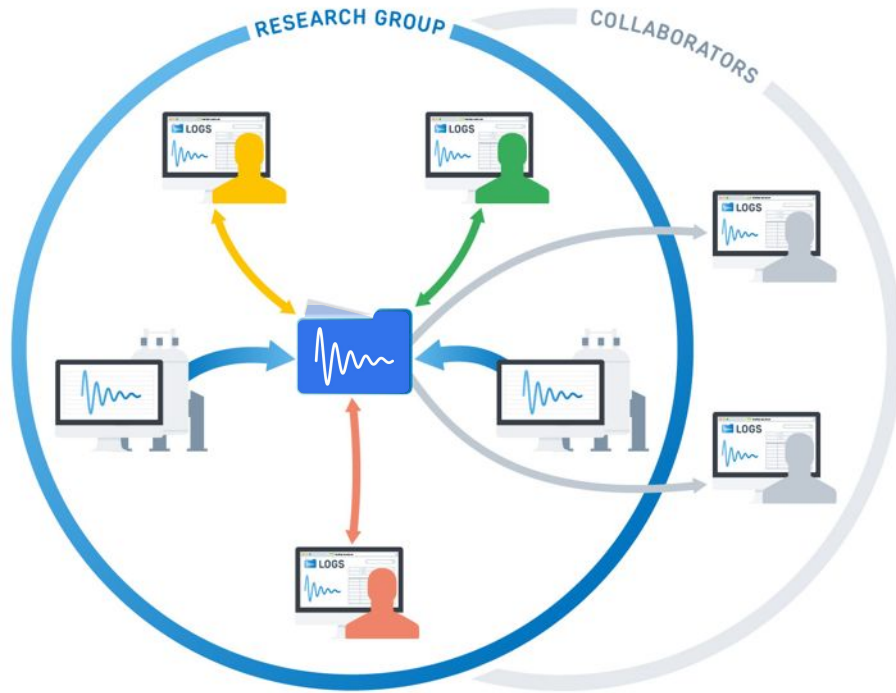


# Problem Source: data pathways are unclear



- **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**



## Electronic Laboratory Notebook

Gather all **written** data



## Scientific Data Management System

Gather all **measured** data



## Python LOGS API

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



LOGS  
SDMS

## Scientific Data Management System

Gather all measured data



Automatic data upload

Keep data findable

Retain original data

Make data accessible

Integration with existing data platforms

Keep data reusable & reproducible

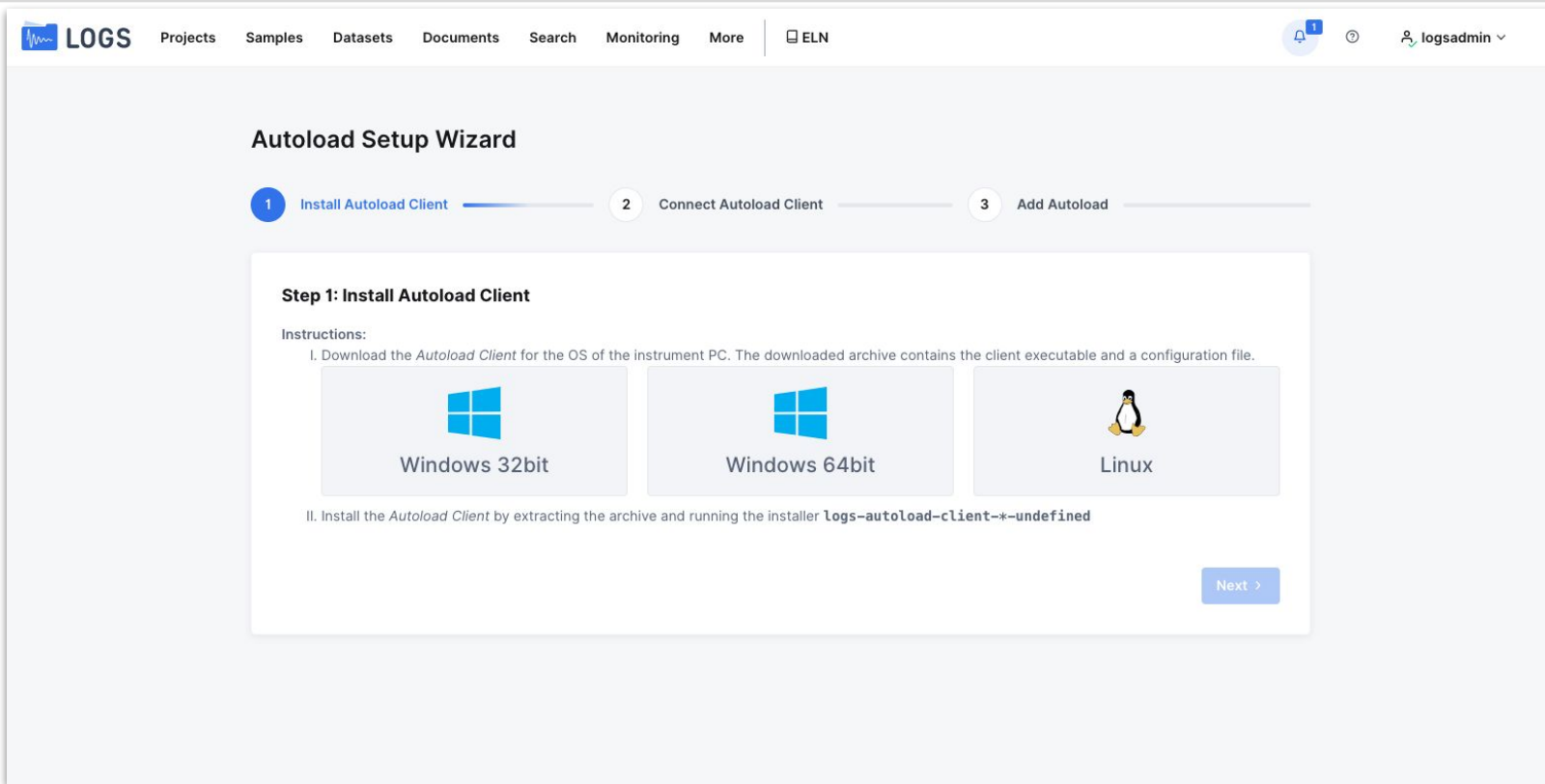
Automatic backup




LOGS parses data and assigns meta information





Secure, browser based and managed data access without installation





The screenshot shows the LOGS web interface with a navigation bar at the top containing 'LOGS', 'Projects', 'Samples', 'Datasets', 'Documents', 'Search', 'Monitoring', 'More', and 'ELN'. On the right side of the navigation bar, there are icons for notifications, a user profile, and the name 'logsadmin'. The main content area is titled 'Autoload Setup Wizard' and features a progress bar with three steps: '1 Install Autoload Client' (active), '2 Connect Autoload Client', and '3 Add Autoload'. Below the progress bar, the 'Step 1: Install Autoload Client' section contains instructions: 'I. Download the Autoload Client for the OS of the instrument PC. The downloaded archive contains the client executable and a configuration file.' This is followed by three selectable options: 'Windows 32bit', 'Windows 64bit', and 'Linux'. Below these options, instruction 'II. Install the Autoload Client by extracting the archive and running the installer `logs-autoload-client-x-undefined`' is provided. A 'Next >' button is located at the bottom right of the instruction box.

 LOGS
Projects
Samples
Datasets
Documents
Search
Monitoring
More
ELN

 1
 logsadmin

**Autoload:** Demo Autoload Autoload-ID: 1

Created by: admin on 2023-01-30 09:20:03 
 Edit
 Run Autoloads now

**Autoload Details**


Autoload Name	Demo Autoload	Autoload-ID: 1
Enabled	<span style="color: green; font-weight: bold;">on</span>	
Interval	2 min	
Cut-off date	-	
Instrument	Bruker EMX Nano	
Method	EPR	
Data format	EPR (Bruker)	
Directories	/opt/autoLoads/epr/bruker_emx_nano	

**Data source** [Show Source](#)

Data Source Name	demo (172.31.1.100)	DataSource-ID: 1
Host name	demo	
IP address	172.31.1.100	
Client status	<span style="color: green; font-weight: bold;">Connected</span>	
First seen	2023-01-30 09:19:06	1 hour ago
Description	Connected from demo at 172.31.1.100	

**Last Status**

**General**


Last started on	2023-01-30 10:25:23	1 minute ago
Next scheduled on	2023-01-30 10:27:23	29 seconds from now 
State	Finished	
Client version	1.1.26	

**Stats**

Duration	17.107ms
Datasets submitted	0
Datasets in queue	0
Datasets known from cache	2
Datasets not known from cache	0
Datasets known from server	0
Directories entered	3
Entries scanned	8
Entries matched	4

**Errors**

LOGS – the SIGNALS Scientific Data Management System





- Content
- Persons
- Facilities
- Organizations
- Measuring Methods
- Tools
  - Shared Content
  - Autoloads
  - API-Key Management
- Customization
  - Sample Tags
- Admin
  - Announcements
  - Dataset Maintenance

## Autoloads 69

[+ Add Data Source](#) [+ Add Autoload](#) [Manage Data Sources](#)

🔍 Search Autoloads by name

[🏠 Run Autoloads now](#) ⋮

<input type="checkbox"/>	NAME	DATA SOURCE	STATUS	ENABLED	LAST STARTED ON	NEXT SCHEDULED	INTERVAL [MIN]	DATA FORMAT	METHOD
<input type="checkbox"/>	Autoloads XRD (XRDML)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:27:52	15	XRD (XRDML)	XRD
<input type="checkbox"/>	Autoloads XRD (Bruker)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:28:58	15	XRD (Bruker)	XRD
<input type="checkbox"/>	Autoloads XPS (Phobios)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:33:06	15	XPS (Phobios)	XPS
<input type="checkbox"/>	Autoloads Vector Network Analyzer	data (78.46.82.120)	Online	on	2023-02-27 15:21:22	2023-02-27 15:36:21	15	Vector Network Anal	VNA
<input type="checkbox"/>	Autoloads NMR (Varian)	data (78.46.82.120)	Online	on	2023-02-27 15:19:50	2023-02-27 15:34:49	15	NMR (Varian)	NMR
<input type="checkbox"/>	Autoloads UV/Vis (Varian Cary)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:36:47	15	UV/Vis (Varian Cary)	UV/Vis
<input type="checkbox"/>	Autoloads UV/Vis (Thermo Scientific NanoDr...)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:30:37	15	UV/Vis (Thermo Scie	UV/Vis
<input type="checkbox"/>	Autoloads Tecan Spark	data (78.46.82.120)	Online	on	2023-02-27 15:19:37	2023-02-27 15:34:36	15	Tecan Spark	Fluorescence
<input type="checkbox"/>	Autoloads UV/Vis (JCAMP)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:29:13	15	UV/Vis (JCAMP)	UV/Vis
<input type="checkbox"/>	Autoloads UV/Vis (Jasco V-550)	data (78.46.82.120)	Online	on	2023-02-27 15:19:32	2023-02-27 15:34:31	15	UV/Vis (Jasco V-550)	UV/Vis
<input type="checkbox"/>	Autoloads UV/Vis (Jasco)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:28:20	15	UV/Vis (Jasco)	UV/Vis
<input type="checkbox"/>	Autoloads UV/Vis Fluorolog	data (78.46.82.120)	Online	on	2023-02-27 15:23:33	2023-02-27 15:38:32	15	UV/Vis Fluorolog	UV/Vis
<input type="checkbox"/>	Autoloads TGA-MS (TA Instruments TRIOS *...)	data (78.46.82.120)	Online	on	2023-02-27 15:21:10	2023-02-27 15:36:09	15	TGA-MS (TA Instrum	TGA-MS
<input type="checkbox"/>	Autoloads TGA/DSC (TA Instruments)	data (78.46.82.120)	Online	on	2023-02-27 15:22:44	2023-02-27 15:37:43	15	TGA/DSC (TA Instrun	TGA/DSC
<input type="checkbox"/>	Autoloads EPR (SpecMan4EPR)	data (78.46.82.120)	Online	on	2023-02-27 15:19:48	2023-02-27 15:34:47	15	EPR (SpecMan4EPR)	EPR
<input type="checkbox"/>	Autoloads VCF	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:31:43	15	VCF	Sequencing
<input type="checkbox"/>	Autoloads Sequence (XEASY)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:27:20	15	Sequence (XEASY)	Sequence
<input type="checkbox"/>	Autoloads Sequence (Applied Biosystems)	data (78.46.82.120)	Online	on	N/A	2023-02-27 15:29:40	15	Sequence (Applied B	Sequence
<input type="checkbox"/>	Autoloads Raman (Princeton Instruments)	data (78.46.82.120)	Online	on	2023-02-27 15:24:15	2023-02-27 15:39:14	15	Raman (Princeton Inc	Raman
<input type="checkbox"/>	Autoloads Thermo Applied Biosystems Calset	data (78.46.82.120)	Online	on	2023-02-27 15:22:22	2023-02-27 15:27:22	15	Thermo Applied Bios	PCR

DEVEL

## Datasets 95

[Upload dataset](#)

**Method**

NMR x ▾

**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... ▾

Q Search 3 datasets selected   ...

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

DEVEL

LOGS Projects Samples Datasets Documents Search Monitoring More ELN

🔔 🔒 👤 logsadmin

Dataset: 📄 NCOV\_1\_248\_HN\_1200/51 Dataset-ID: 321

🗑️ 🔗 Edit 📄 Download

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

## 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

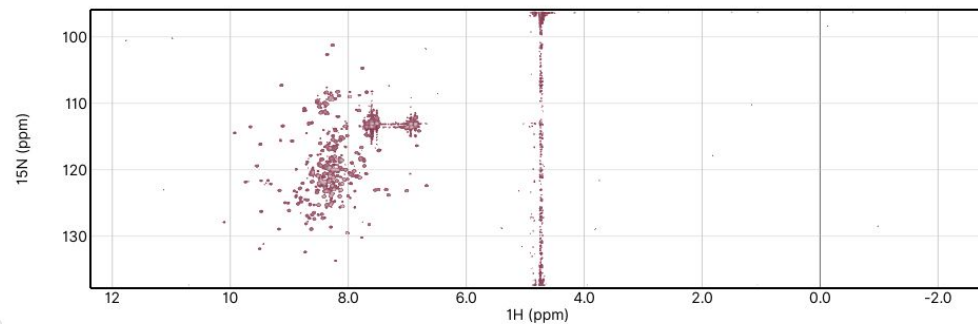
**Sample Type** Basic Sample

**Prepared** 2021-02-08 Last year

**Prepared by** admin

## Preview

2D Tracks: 1



## Parameters

## Files

### 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\_trosyett3gpsi.2  
**number of scans** 16

### NCOV\_1\_248\_HN\_1200

#### 51

#### pdata

##### 1





- 📄 2ii
- 📄 2ir
- 📄 2ri
- 📄 2rr
- 📄 auditp.txt
- 📄 clevels

LOGS supports a growing number of data formats.

## Supported Data Formats

Submit New Data Format

LOGS currently supports **67** native data formats,  
from **32** vendors,  
covering **30** measurement methods.

VENDOR	NAME	FORMAT	INSTRUMENT	METHOD
Select... 	NMR (Bruker)	N/A	N/A	NMR
Select... 	NMR (JEOL)	N/A	N/A	NMR
Select... 	NMR (Magritek Kea)	N/A	Kea	NMR
Select... 	NMR (Magritek Spinsolve)	N/A	Spinsolve	NMR



# Electronic Lab Notebook



Enter all Notes, Protocols, etc.

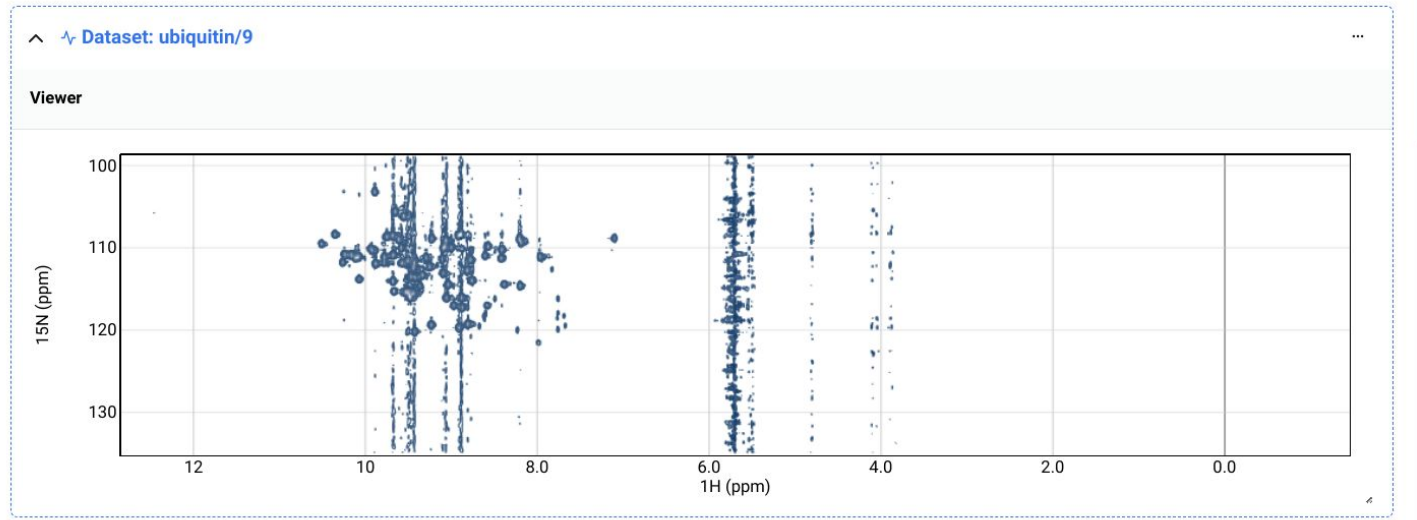
Link the **written** data to the digital content,  
e.g. Datasets, Samples, Persons, Projects, etc.

☰ + ↕+ Datasets 👤 📄+

↶ ↷
B I U     
A ▾
H1 H2 H3 ▾
🔍
☰ ▾
☰ ▾
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α ▾
🕒
☰

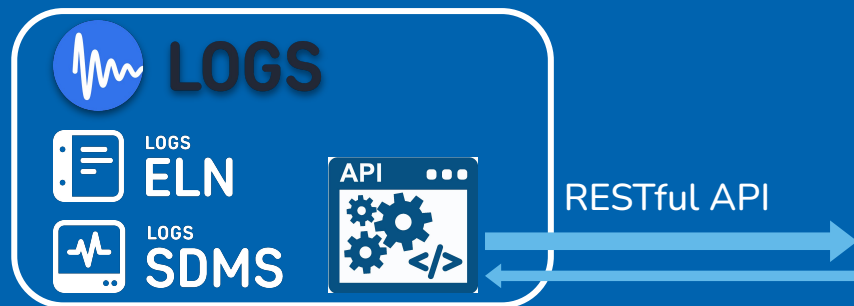
184	Q Search	+	
↕	ubiquitin/10 2009-12-29	NMR 2D H(N... Ubiquitin	>
↕	ubiquitin/5 2009-12-28	NMR 2D HS... LOGS Demo	>
↕	ubiquitin/9 2009-12-28	NMR 2D H(N... Ubiquitin	>
↕	P17-600AV/4 2016-10-06	NMR HCCC... P17	>
↕	P17-600AV/2 2016-08-20	NMR 2D HS... P17	>
↕	P17-600AV/1 2016-08-19	NMR 1D_1H P17	>
↕	Azol_420uMD20_HPDINO... 2015-05-26	NMR 1D 31P Azol	>
↕	Azol_420uMD20_HPDINO... 2015-05-26	NMR 2D NO... Azol	>
↕	Azol_420uMD20_HPDINO... 2015-05-24	NMR 2D TO... Azol	>

## Interactions ELN and SDMS



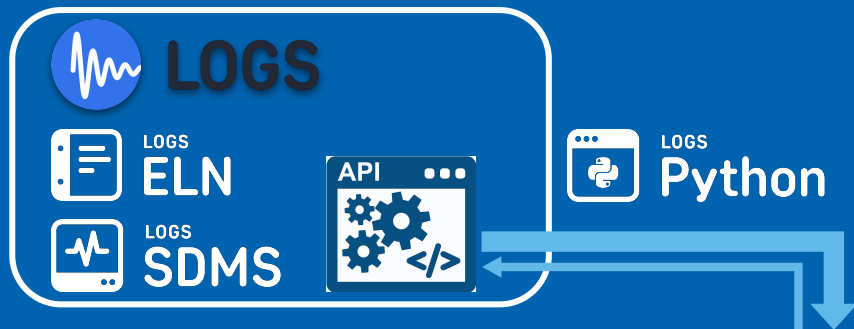
"Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum 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

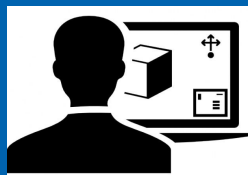
# LOGS Python



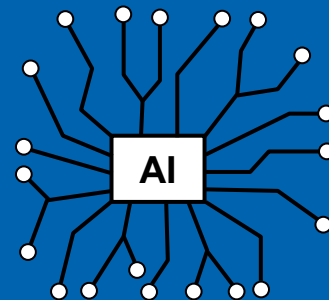
- Use Python native objects
  - no web technology knowledge needed
  - python object system representing your LOGS data
- Integration of existing analysis tools
- Use vast number available Python modules
- Customize automate your processes



Reports, statistical analysis



3rd party analysis software





```
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

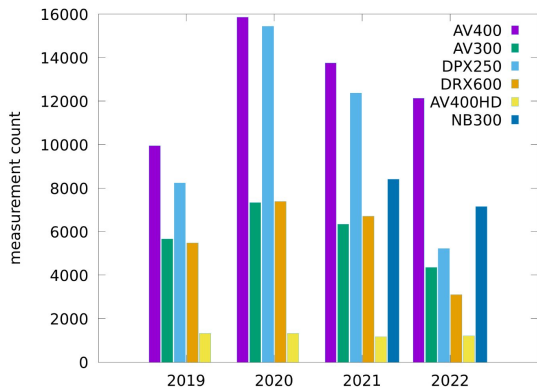
```
from datetime import datetime
from LOGS.LOGS import LOGS
from LOGS.Entities.DatasetRequestParameter import DatasetRequestParameter

api_key = "mkYmfo6XlU3rfxPGbx7nPxhLoS8PYDaaaUfF5nLEFAXYAeyHtgGaJ8FOWh3S5ijY"
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)
```

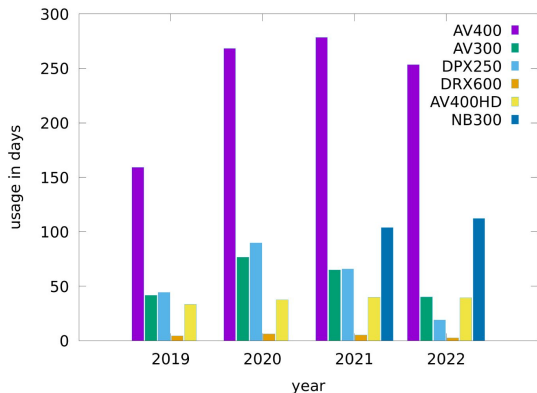
```
> Name: Honey_probe_1894 Experiment: HSQC
> Name: Honey_probe_9079 Experiment: HSQC
> Name: Honey_probe_5410 Experiment: HSQC
> Name: Honey_probe_3606 Experiment: HSQC
> Name: Honey_probe_2519 Experiment: HSQC
...
```



## 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

Dataset: w122111504 Dataset-ID: 50

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

Edit Claim Download

### Dataset Details

Name	w122111504	Dataset-ID: 50
Method	EPR	
Experiment	-	
Instrument	Bruker EPR	
Suppl. Equipment	-	
Acquis. Date	2022-11-16 10:50:29	2 weeks ago
Projects	-	
Organizations	-	
Operators	-	
Notes	-	

### Source information

Origin	Manual file upload	
Upload date	2022-12-02 09:37:36	3 minutes ago
File format	EPR (Bruker)	
Vendor	Bruker	
Path	/w122111504.DSC	

> Related datasets 30

Sample

### Preview

1D Tracks: 1

Parameters

Title	'w122111504 CCLD pH5CIO 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	<a href="#">logs-ID:79437</a>
w122111601	25.0	1.77	500	39	<a href="#">logs-ID:79318</a>
w122111504	25.0	1.77	-	-	<a href="#">logs-ID:79317</a>
x120111302	15.0	6.33	100	60	<a href="#">logs-ID:70691</a>

Protocols  
 Inventory  
 Data  
 Devices  
 Signatures  
 Linked Experiment  
 Notes  
 Activity

**Thanks for listening**