



# Research Data Management – A practical guide

*How to manage scientific data in your daily work*



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# Short Course: Outline

## 1. Introduction – why we need to care about our data?

## 2. Basic principles/tools for research data management

- ✓ Name your data – Conventions and nomenclature
- ✓ Describing your data set – Meta data and ReadMe
- ✓ Structure your data - Folder management
- ✓ Document your scientific /practical work - Electronical lab notes

## 3. Practical „real-life“ example

A portrait of Eric Schmidt, wearing glasses and a dark sweater over a light blue shirt, is positioned on the left side of the image.

**There were 5 exabytes of information  
created between the dawn of civilization  
through 2003, but that much information  
is now created every 2 days.**

**- Eric Schmidt  
Executive Chairman of Google**

**You can have data without information,  
but you cannot have information  
without data.**

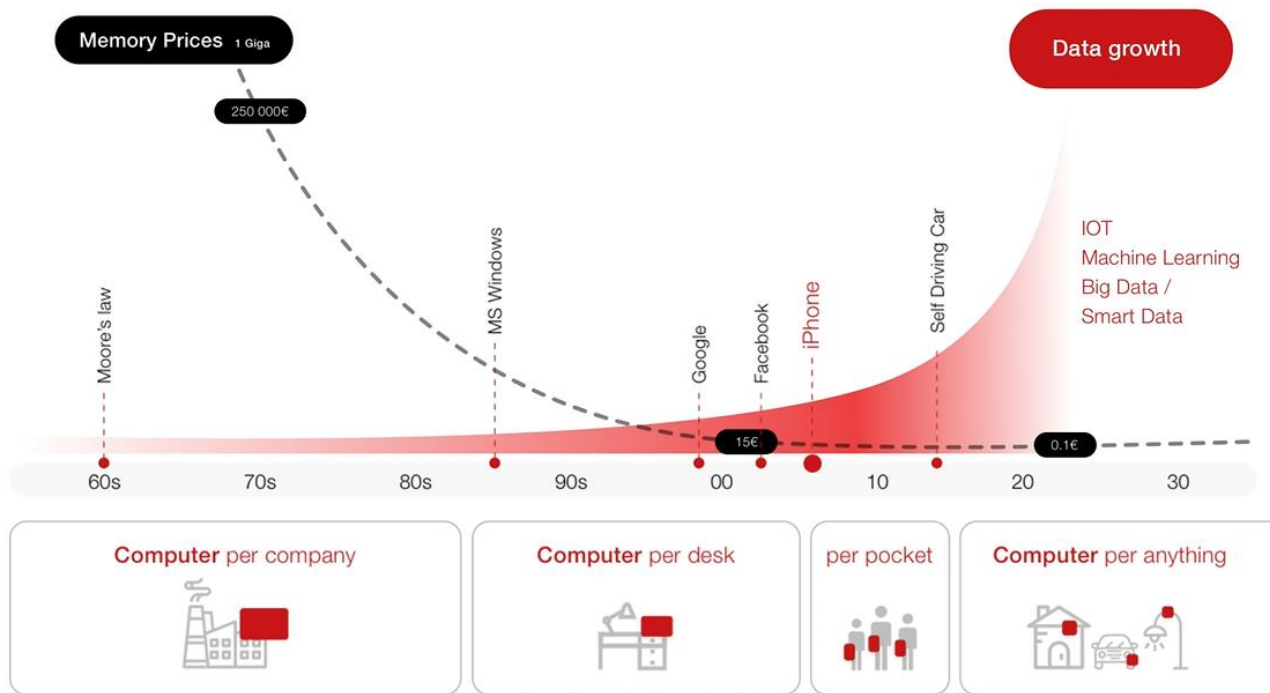
**- Daniel Keys Moran**

**American Computer Programmer and  
Science Fiction Writer**



# 1. Why we need to care about our data?

## Motivation:



# 1. Why we need to care about our data?

## Motivation:

- Data Security





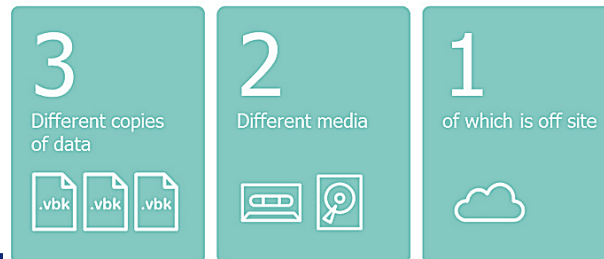
# 1. Why we need to care about our data?

## Motivation:

- **Data Security**

- ✓ Backup (notice: **USB drives are not a backup!**)
- ✓ **3-2-1 Backup rule:**

- **3** copies of data ( 1 x primary copy of raw data, 2 x copies of backup)
- **2** media (copies of data on at least 2 different storage media)
- **1** external backup (original and backups not at the same location)



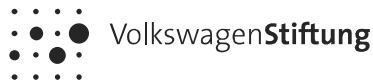
# 1. Why we need to care about our data?

## Motivation:

- **Data Security**
- **Part of “Good Scientific (Research) Practices”**



- Demand of national / international funders
- Institutional rules and policies for handling research data
- Prevention of scientific misconduct: data fabrication, falsification and plagiarism





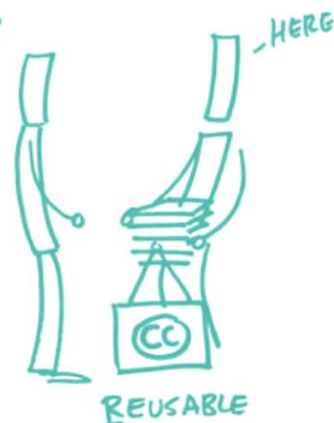
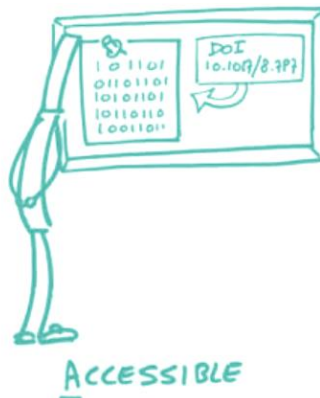
# 1. Why we need to care about our data?

## Motivation:

- Data Security
- Good Scientific (Research) Practice
- FAIR principle

I ... Do I understand the data?

F ... Do I find the data?



A ... Can I access the data?

R ... What I'm allowed to do with the data?

# 1. Why we need to care about our data?

## Motivation:

- **Data Security**
- **Good Scientific (Research) Practice**
- **FAIR principle**



More information about FAIR data: <https://www.go-fair.org/fair-principles/>

## Motivation:

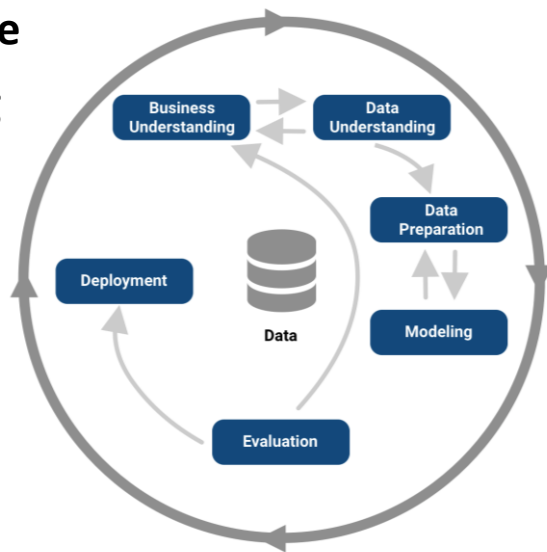
- **Data Security**
- **Good Scientific (Research) Practice**
- **FAIR principle**
- **Data Sharing: [Movie clip](#), open science**



# 1. Why we need to care about our data?

## Motivation:

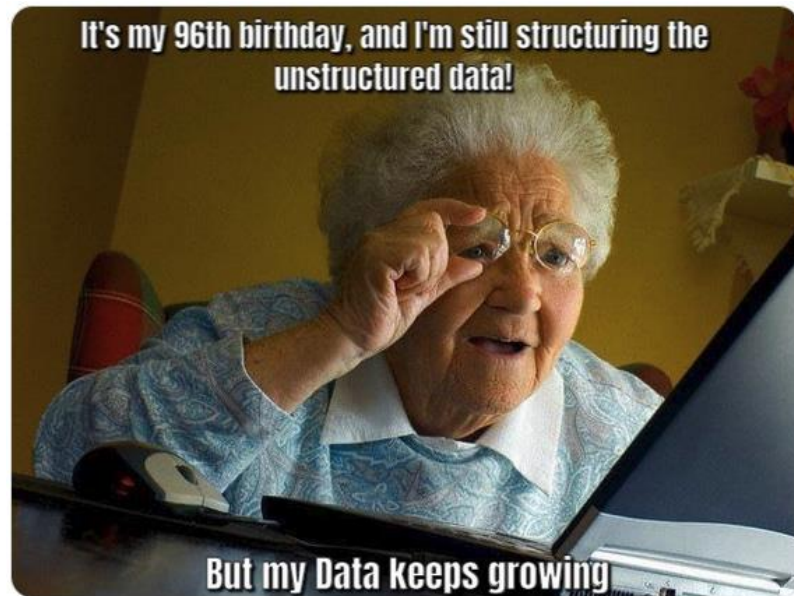
- Data Security
- Good Scientific (Research) Practice
- FAIR principle
- Data Sharing
- Data Science



# 1. Why we need to care about our data?

## Key Points for Data Management:

- Easier to analyze organized, documented data
- Find data more easily
- Don't drown in irrelevant data
- Don't lose data
- Get credit for your data
- Avoid accusations of misconduct

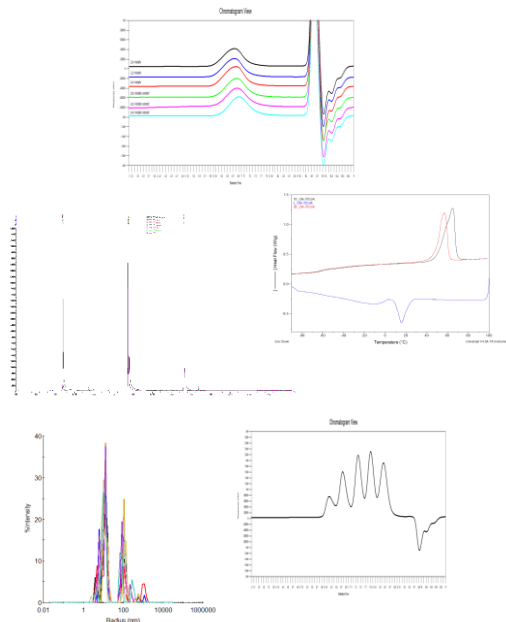


## 2. Basic principles/tools for research data management

Lots of information in your head gets lost over time



You, today



You, in six  
months  
(or anyone  
else)

## 2. Basic principles/tools for research data management

Describe your data!



You, today

And in 6 months!!!





## 2. Basic principles/tools for research data management

Enable integration with other data



DATASET



Data collection

## 2. Basic principles/tools for research data management

Enable long-standing usage of collected data

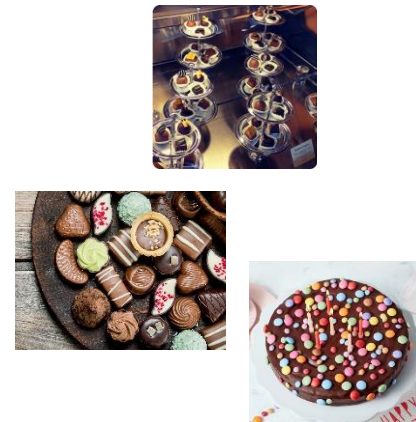


Data collection

Select



Use



Data selection  
for research

## 2. Basic principles/tools for research data management

- ✓ Name your data – Conventions and nomenclature
- ✓ Describing your data set – Meta data and ReadMe
- ✓ Structure your data - Folder management
- ✓ Document your scientific /practical work - Electronical lab notes

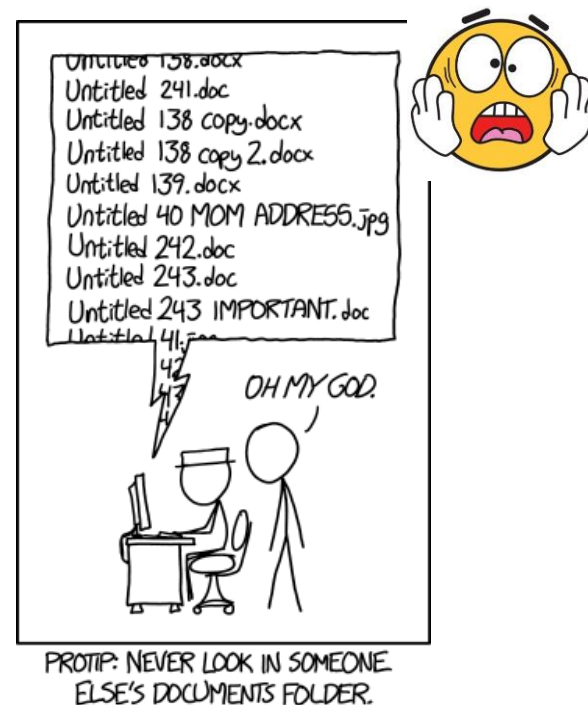
# File Naming

## Do's and Don'ts - Examples



### *Best practices*

- 20240523\_ProjectA\_SEC\_BoyeS\_v1.xlsx
- 20240523\_ProjectA\_MeetingNotes\_BoyeS\_v2.docx
- 20240523\_ManuscriptScience\_BoyeS\_v525.docx
- ...



# File Naming

## Requirements

- Human and machine-readable
- Be consistent
- Use date format ISO 8601: YYYYMMDD
- Include a version number (Creamer et al. 2014)
- Write down naming convention in data management plan



### AVOID:

- Special characters:  
`{ } [ ] < > ( ) * % # ` ; " , : ? ! $ @ ...`
- Space
- Cryptic
- Too long

# File Naming



## Take-Home Tips

- ✓ 1. Think about your files - What related files are you working with?

- You can use different conventions for different file sets
- Do you have established file naming conventions in your discipline or group?

*Example: This convention will apply to all of my AF4 files, from raw data through processed file*

# File Naming



## Take-Home Tips

- ✓ 1. Think about your files
- ✓ 2. Identify metadata (e.g. date, sample, experiment) – What information is needed to easily locate a specific file?

- Descriptive with contextual information
  - Pick three pieces of metadata
- Names should be human readable: understand what's in each one

*Example: For my AF4 measurements, I want to know date, sample ID, and injection number for that sample on that date*



# File Naming



## ✓ Take-Home Tips

- ✓ 1. Think about your files
- ✓ 2. Identify metadata (e.g. date, sample, experiment)
- ✓ 3. Abbreviate or encode metadata - Don't forget to document any codes!

- Standardize the categories and/or replace them with 2- or 3-letter codes

*Example: e.g. 2-letter project abbreviation: project 1 -> P1, project 2 -> P2  
or 3-letter code for technique, SEC, AF4, NMR,...*

# File Naming



## Take-Home Tips

- ✓ 1. Think about your files
- ✓ 2. Identify metadata (e.g. date, sample, experiment)
- ✓ 3. Abbreviate or encode metadata
- ✓ 4. Use versioning - Are you maintaining different versions of the same file?

- Track versions by adding information on the end of file name
  - Use version numbers („v01“ or „v02“)
  - Use version date (YYYYMMDD)

*Example: analysis workflow: \_raw and \_processed*

# File Naming



## Take-Home Tips

- How you want to sort and search
  - Decide which metadata should appear at the beginning
  - Use default order: alphatically, numerically, or chronologically

*Example: AF4 measurement: 5075\_2024-02-16 11-48 - wash 400uL*

- ✓ 5. Think about how you will search for files – **what comes first?**

# File Naming



## Take-Home Tips

- Determine characters for separation of metadata – many computer systems cannot handle space
- Use dashes (file-name.xx) or underscores (file\_name.xx) or capitalize first letter of each word – camel case (FileName.xx)
  - Use default order: alphabetically, numerically, or chronologically
    - Avoid special characters: .,~!@#€\$%&/()=?{ }[ ]`'!

*Example: 20240603\_Presentation\_Course\_FFF2024\_V01.ppt*

- ✓ 6. Deliberately separate metadata elements – avoid spaces or special characters

# File Naming



## Take-Home Tips

- Name conventions should be documented that others in your lab/group can follow this standard
  - Document in a README.txt together with your files
- If the file is moved or shared, users will be able to identify the file from its file name

*Example: My file naming convention is [SA-MPL-EID]\_[YYYYMMDD]\_[###]\_[status].[tif]  
P1\_SEC\_PS30k\_20240423\_2\_raw.txt*

- ✓ 7. Write down your naming conventions – Include a top-level README file on how to navigate the structure

# Describing your data set – Meta data and ReadMe

## Meta data – Enrich your data with meaning!

Meta data helps to understand data

Meta data answers questions:

- ✓ **Who** created the data?
- ✓ **Why** was the data created?
- ✓ **When** was the data created?
- ✓ **How** was the data created?
- ✓ **What** is the content of the data?

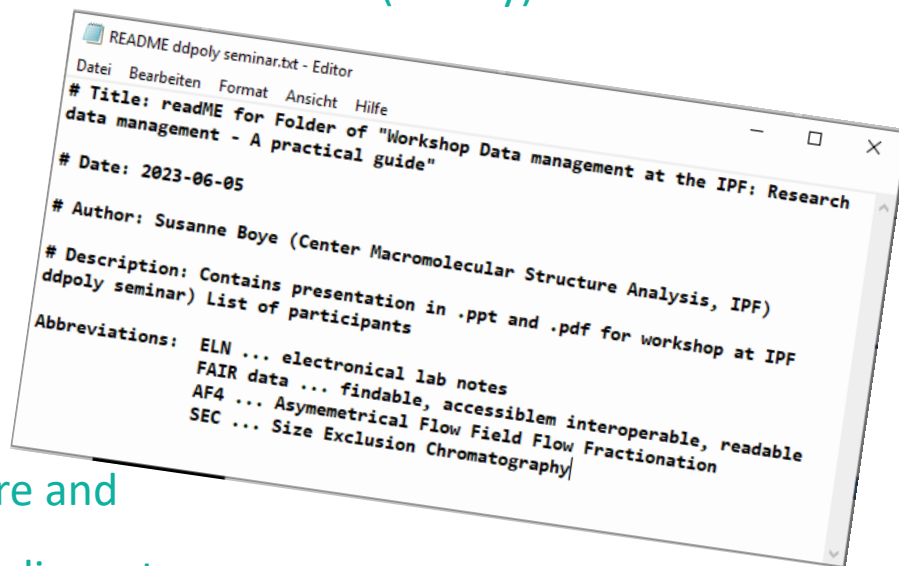
# Describing your data set – Meta data and ReadMe

Easiest way to make data more understandable and reusable:

ReadMe.txt file “Love letter to the Future” – for each folder (ideally)

Content:

- ✓ Title
- ✓ Date
- ✓ Author
- ✓ Description of folder content, structure and organization of files, abbreviations, coding, etc.
- ✓ ... as much information as possible





# Structure your data – Folder Management

## ✓ How to organize your data?

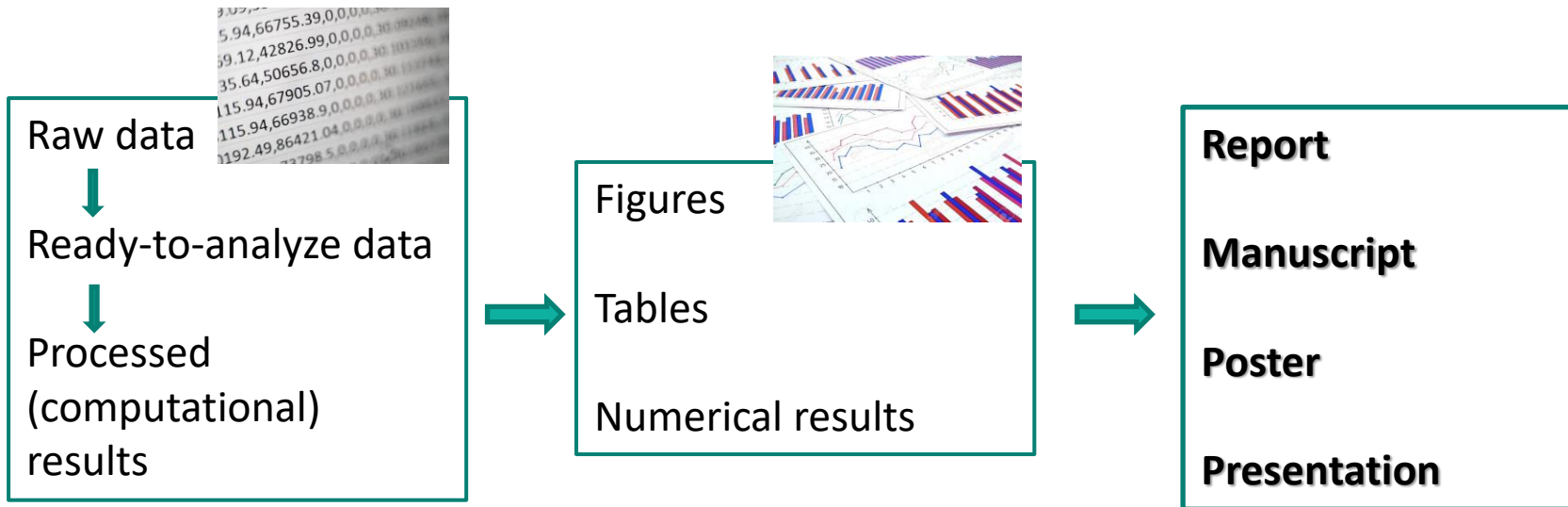
- ✓ Files and data
- ✓ Data growth
- ✓ Change over time
- ✓ Relationships
- ✓ Duplication of data

## DATA CHAOS



# Structure your data – Folder Management

## Data flows



# Structure your data – Folder Management

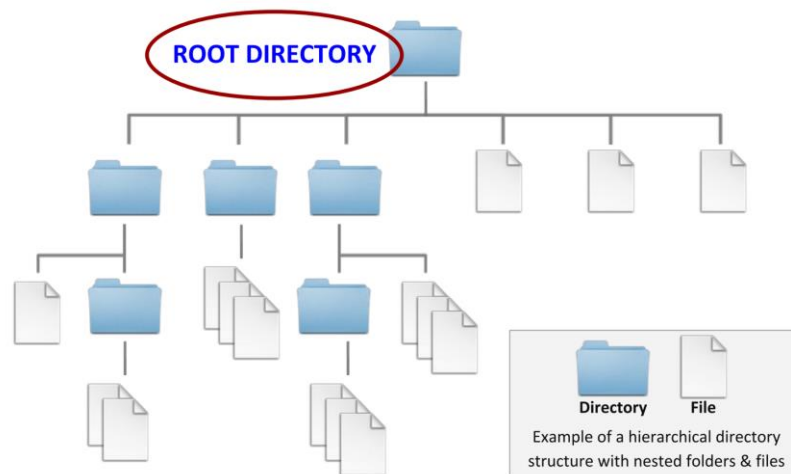
## Data hierarchy

- ✓ One project – one folder
- ✓ Consistent structure for each project



## AVOID:

- ✓ Overlapping categories
- ✓ Too large folders and too deep structures
- ✓ Repetition of information



# Structure your data – Folder Management

## Document your structure

- ✓ Make sure to capture metadata about content of folders and files:

Naming conventions

Who made it, when, where???

- ✓ Create documentation / ReadMe files
- ✓ Establish standardized structures in your group/department

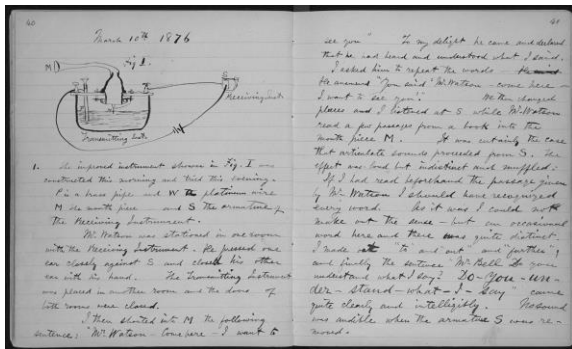
## Take-Home Tips:

- ✓ Dump older files cluttering your working directory
- ✓ Delete unneeded files when the project is finished

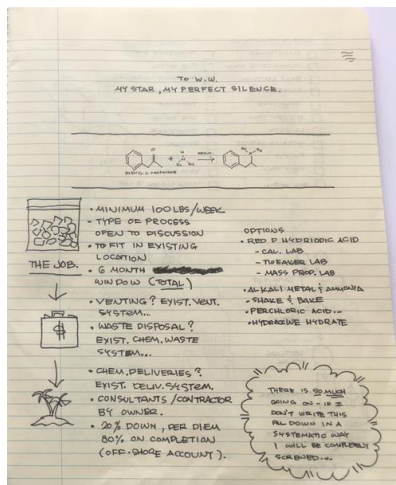


# Document your practical work - Electronical lab notes

## Traditional paper notebooks



Page from a laboratory notebook of Alexander Graham Bell, 1876.



Page from Gale's lab notes "Breaking Bad"



www.eppendorf.com/pipetting

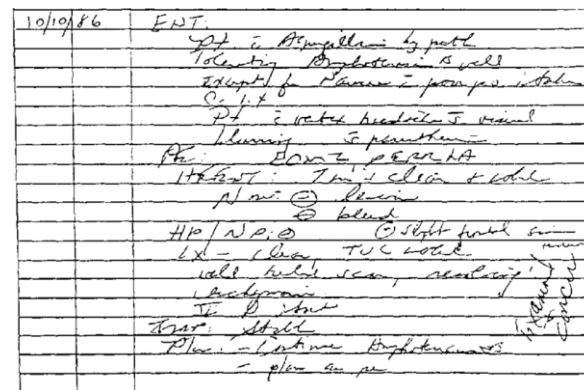
# Document your practical work - Electronical lab notes

## Benefits

- ✓ Helps you to organize yourself and your research.
- ✓ No loose paper on your desk nor any cryptic notes
- ✓ No data loss when researchers move on
- ✓ Simplified summary of your research
- ✓ Documenting helps you to understand old data
- ✓ Easy data sharing
- ✓ Long-term storage and archive



Can you read and understand it?



# Document your practical work - Electronical lab notes

## Digitalization of notes:

- ✓ Is easy to read and to edit – no handwriting
- ✓ Is versioned, changes can be reverted and tracked
- ✓ Is searchable and sortable
- ✓ Use of templates – standardization
- ✓ Links to: resources, other experiments, raw data or analysis workflows
- ✓ Application of APIs - Automated analysis + Data science

**Samples:**

Acronym	Description
FK_AF4_014	Ferrocen-PSome (0.5 mg BCP/ml)
FK_AF4_015	N3-Ferrocen-PSome (0.5 mg BCP/ml)
FK_AF4_016	PSome A (0.5 mg BCP/ml)

Susanne Boye - Apr 18, 2023, 2:31 PM MESZ

**Materials / Device**

Susanne Boye - Jan 11, 2023, 12:49 PM MEZ

Buffer: 1 mM, pH 7.4, + 0.02 % NaN<sub>3</sub>

Channel: LC

Spacer: 490 µm

Membrane: RC (cut-off: 10 kDa)

Pump + AS system: Agilent 1200 series

FFF device: Eclipse Dualtec (Wyatt)

LS detector: DAWN HELEOS-II (Wyatt): λ=660 nm

RI detector: Optilab T-REX (Wyatt): λ=660 nm

Diode array detector: SPD-M20 (Shimadzu), wavelengths:

AUX1 [nm]	AUX2 [nm]	AUX3 [nm]	AUX4 [nm]
254	280	400	500



# Research Data Management

Avoid the scientific data nightmare: [watch the video](#)



### 3. Practical „real-life“ example

## STEPS TO A DATA MANAGEMENT OF A SCIENTIFIC PROJECT



1

#### Data sources

- ✓ Idea/Grant
- ✓ WHO
- ✓ Collaboration partners



2

#### Data collection

- ✓ Experimental Data
- ✓ Discussion
- ✓ Design experiments



3

#### Data preparation

- ✓ Data Cleaning
- ✓ Data Analysis
- ✓ Structure



4

#### Manuscript/Report

- ✓ Figures
- ✓ Writing/Revision
- ✓ Submission/Revision



5

#### Safe & long-term storage

- ✓ Data organization/Read Me Files
- ✓ Supervision
- ✓ Long-term storage, open access

## STEPS TO A DATA MANAGEMENT OF A SCIENTIFIC PROJECT

- **Cloud (IPF Cloud)** → Create one folder for each project. The project should be defined upfront.

Data sources

Data collection

Data preparation

Manuscript/Report

Safe & long-term storage

**Electronic Labbook in combination with  
an inhouse drive or CLOUD service**

- **ELN** <https://www.labarchives.com/> → Create one Notebook for each project. All notebooks should have the same structure.

Data collection

Manuscript/Report

Safe & long-term storage

## STEPS TO AN IDEAL DATA MANAGEMENT OF A SCIENTIFIC PAPER

### CLOUD structure *in progress*

#### Name of Project

- **Read me file** (people involved into the project, nomenclature, status of the project, new ideas...)
- **Electronic Lab Book/protocols** (divided by person involved into the project)
- **Raw data** (organized by chracterization methods, by operator and by positive/negative results)
- **DataAnalysis**
- **Comunication** (Reports, meetings, working plan, emails)
- **Literature**

#### Name of Project-Lab Book

- People involved into the project
- Nomenclature and summary of compounds; Tags
- Meeting Notes; Status of the project
- Experimental Data (can be divided by people involved)

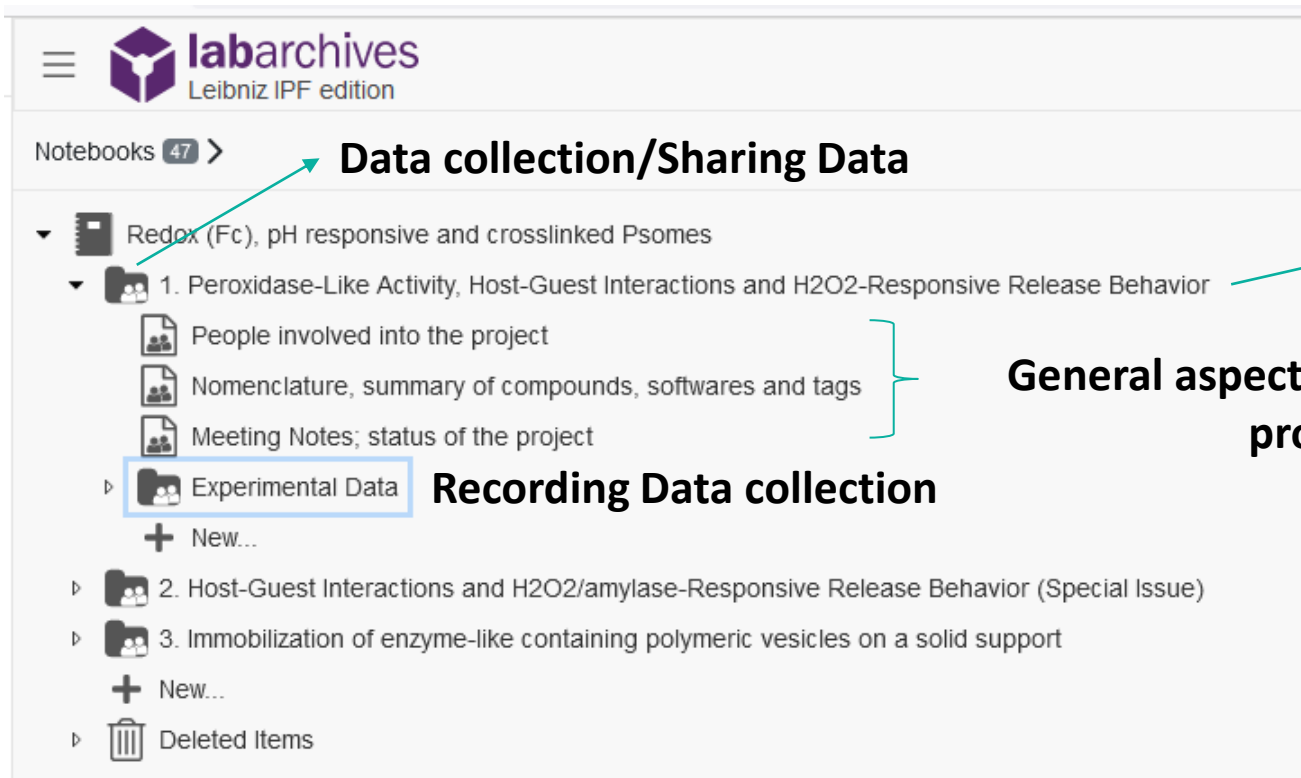
SM 20210510 Fabrication of FcPsomes

SM 20210514 Stability of FcPsomes

SM 20210514 Preparation of FcPsomes for AF4

**When a student finishes:** 1) change the ownership of the notebook, 2) make a PDF file and 3) added it in the ELN folder in the cloud.

## STEPS TO AN IDEAL DATA MANAGEMENT OF A SCIENTIFIC PAPER



The screenshot shows the 'labarchives' interface, specifically the 'Leibniz IPF edition'. The 'Notebooks' section shows 47 items. A project titled 'Redox (Fc), pH responsive and crosslinked Psomes' is expanded, showing a list of sub-items. The 'Experimental Data' folder is highlighted with a blue box. A green arrow points from the 'Data collection/Sharing Data' text to the 'Redox (Fc), pH responsive and crosslinked Psomes' project name. A green bracket groups the sub-items under the project, with an arrow pointing to the 'General aspect to follow up the project' text. A green arrow points from the 'Name of Project' text to the project name. The 'Experimental Data' folder is labeled 'Recording Data collection'.

**Data collection/Sharing Data**

**Name of Project**

**General aspect to follow up the project**

**Recording Data collection**



## STEPS TO AN IDEAL DATA MANAGEMENT OF A SCIENTIFIC PAPER

Workshop > Redox (Fc), pH responsive and crosslinked Psomes\_in progress >

Name		Date modified
Communication		18/04/2023 12:54
Data Analysis_Main Text (Raw Data + Proceed Data + PowerPoint + Pic)		18/04/2023 13:23
Data Analysis_Supporting Information (Raw Data + Proceed Data + PowerPoint + Pic)		18/04/2023 13:24
ELN_Protocols	→ Experimental Description Collection	18/04/2023 13:29
Literature		18/04/2023 13:19
Scientific Data (Organized by characterization methods)	→ Raw Data Collection	18/04/2023 13:20
ReadMe		26/09/2022 12:59

Paper  
preparation



Let's take a look the  
content!

## STEPS TO AN IDEAL DATA MANAGMENT OF A SCIENTIFIC PAPER

CLOUD structure *after acceptance publication*

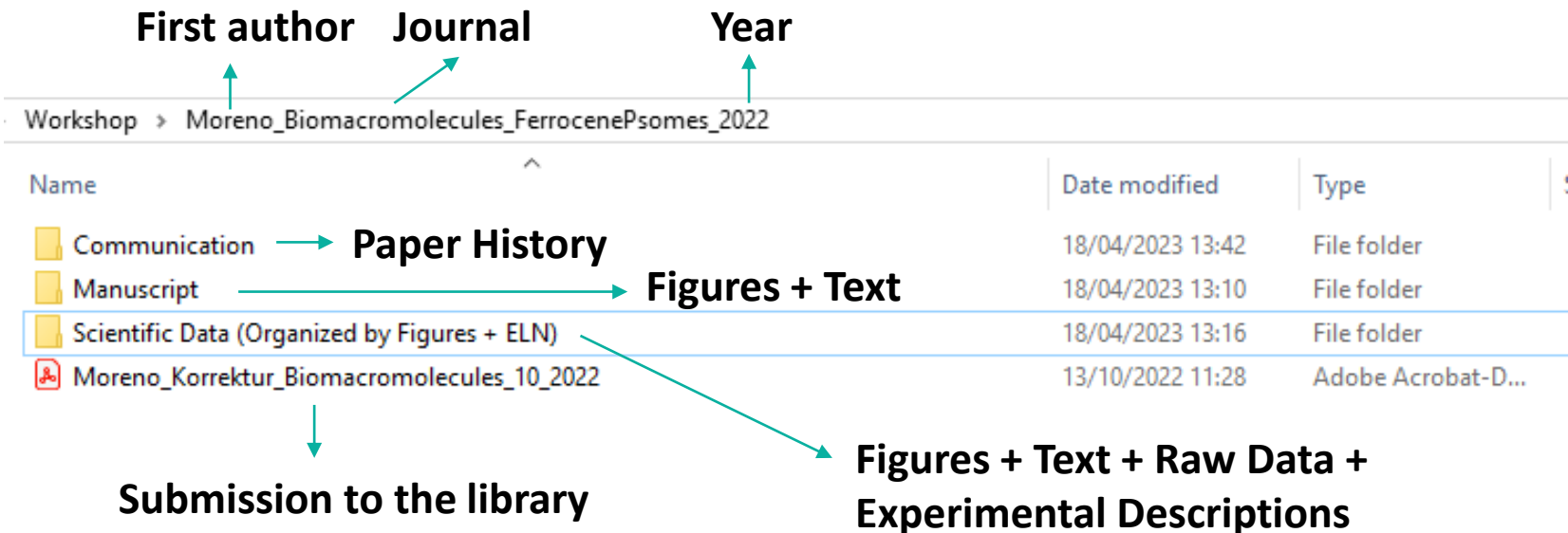
First Author\_Name of Paper/Journal\_Year

- **Communication**
- **Manuscript** (main text and SI, PowerPoint and pics of the last version of Figures, TOC, Readme File)
- **Scientific Data** (Raw data and Processed Data ordered by Figures)
- **Proof of submission to the library**

**The supervisor\* is the responsible to check the last version**



# STEPS TO AN IDEAL DATA MANAGEMENT OF A SCIENTIFIC PAPER



Let's take a look the content!



# Coding and Version Control: git<sup>[5]</sup>

## Distributed version-control for your source code

- Free and open-source software
- Structured source-code management system
- Easy and simple to use for everyday programming
- Reference your compiled code with unique SHA-hash
- Good scientific practice to comment and archive your code!



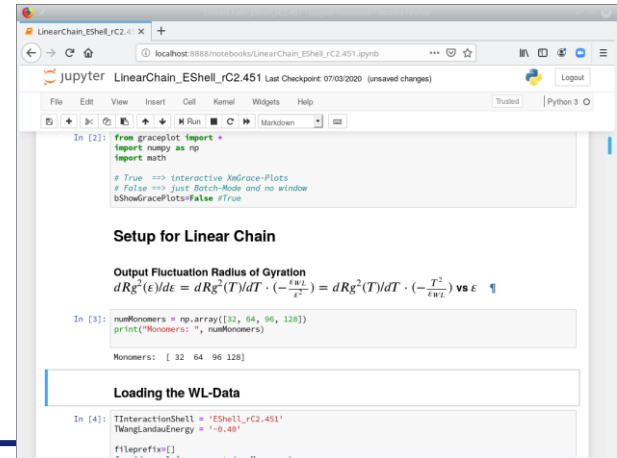
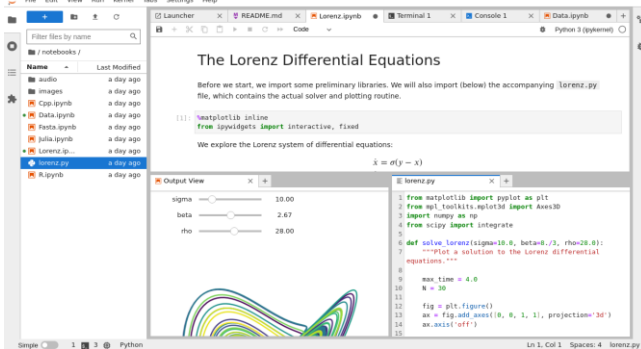
**USE GIT!!!**

# Use IDE: Jupyter and JupyterLab<sup>[6]</sup>

## □ Jupyter: Interactive Computing and Data Processing

- Free and open-source software
- Native Python binding for easy usage (also R)
- Documentation/Latex using Markdown within the source
- Collaboration and exchange of jupyter notebooks

<https://jupyter.org/hub>



# Tools for DMP: DSWizard<sup>[7]</sup> and DMPTool<sup>[8]</sup>

## Data Management Plan (DMP)

- Which data will be produced (type, format)?
- How large will be the data set probably?
- How and where shall the data be stored during and after the project duration? Backups?
- Is it planned to publish the data, and if yes, under which conditions?
- Could legal or ethical problems occur in collecting, analyzing and publishing the data?
- How much does it cost?
- Who is responsible for all the processes of research data management?

## Collaboration Tools and Step-by-Step Survey:



# Connecting data: 5-star-linked-data<sup>[9]</sup>

## Design Pattern for Open Data

1★: data is openly available in some format.

2★: data is available in a structured format, such as Microsoft Excel file format (.xls).

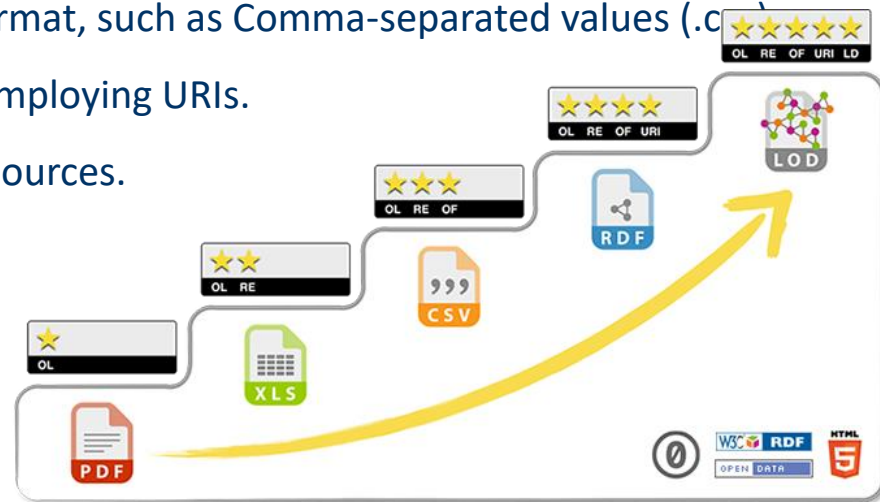
3★: data is available in a non-proprietary structured format, such as Comma-separated values (.csv).

4★: data follows W3C standards, like using RDF and employing URIs.

5★: all on the other, plus links to other Linked Data sources.

**For data publishing use  
public repositories e.g. Zenodo:**

<https://zenodo.org/>

# Connecting data: Example 1

**nature nanotechnology**

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[nature](#) > [nature nanotechnology](#) > [articles](#) > [article](#)

Article | [Open access](#) | Published: 07 August 2023

## Dynamic matrices with DNA-encoded viscoelasticity for cell and organoid culture

[Yu-Hsuan Peng](#), [Syuan-Ku Hsiao](#), [Krishna Gupta](#), [André Ruland](#), [Günter K. Auernhammer](#), [Manfred F. Maitz](#), [Susanne Boye](#), [Johanna Lattner](#), [Claudia Gerri](#), [Alf Honigsmann](#), [Carsten Werner](#) & [Elisha Krieg](#)

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An [Author Correction](#) to this article was published on 31 January 2024

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**Abstract**

[Main](#)

[Material concept](#)

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[DNA sequences encode stress relaxation and he...](#)

[High stability, tunable degradation and biocom...](#)

[DyNAtrix supports development of diverse cells a...](#)

[Conclusions](#)

# Connecting data: Example 1

## Data availability

[Supplementary Information](#) containing materials and methods, supplementary figures, tables, datasets and accession numbers for biological materials are available with this paper. Additional datasets and materials generated during and/or analysed during the current study are available from the corresponding author on reasonable request. The supplementary data and code supporting the findings of this study are openly available on figshare ([https://figshare.com/projects/Dynamic\\_matrices\\_with\\_DNA-encoded\\_viscoelasticity\\_for\\_cell\\_and\\_organoid\\_culture/168281](https://figshare.com/projects/Dynamic_matrices_with_DNA-encoded_viscoelasticity_for_cell_and_organoid_culture/168281)). Source data are provided with this paper.

## Code availability

A Python script for the thermodynamic calculations of CCL interactions is available as Supplementary Code 1 and at figshare (<https://doi.org/10.6084/m9.figshare.23309429>). A Python script for the statistical simulation of the maximum percentage of intramolecular crosslinks as a function of CCL complexity is available as Supplementary Code 2 and at figshare (<https://doi.org/10.6084/m9.figshare.23592636>).

## Source data

### Source Data Fig. 2

Simulation results, rheological data, source data for Fig. 2d and thermodynamic prediction.

### Source Data Fig. 3

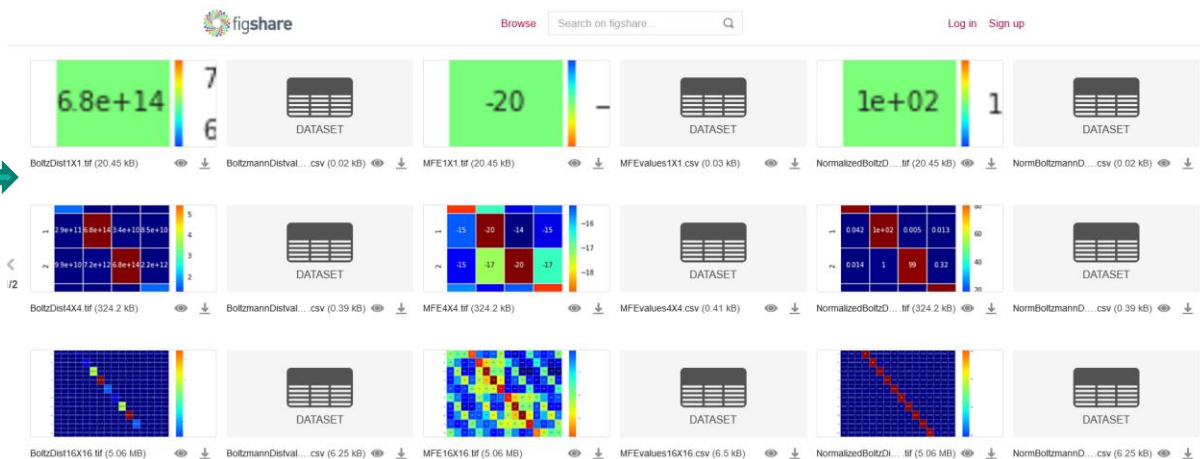
Rheological data.

### Source Data Fig. 4

Rheological data.

### Source Data Fig. 5

RFU value from qPCR, gel volume quantification, statistical source data of cell viabilities and immune response.



[https://static-content.springer.com/.../41565\\_2023\\_1483\\_MOESM12\\_ESM.xlsx](https://static-content.springer.com/.../41565_2023_1483_MOESM12_ESM.xlsx)

MS Excel sheet with numerical data

# Connecting data: Example 2

## scientific data

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[nature](#) > [scientific data](#) > [comment](#) > [article](#)


Comment | [Open access](#) | Published: 15 March 2016

### The FAIR Guiding Principles for scientific data management and stewardship

[Mark D. Wilkinson](#), [Michel Dumontier](#), [Jisbrand Jan Aalbersberg](#), [Gabrielle Appleton](#), [Myles Axton](#), [Arie Baak](#), [Niklas Blomberg](#), [Jan-Willem Boiten](#), [Luiz Bonino da Silva Santos](#), [Philip E. Bourne](#), [Jildau Bouwman](#), [Anthony J. Brookes](#), [Tim Clark](#), [Mercè Crosas](#), [Ingrid Dillo](#), [Olivier Dumon](#), [Scott Edmunds](#), [Chris T. Evelo](#), [Richard Finkers](#), [Alejandra Gonzalez-Beltran](#), [Alasdair J.G. Gray](#), [Paul Groth](#), [Carole Goble](#), [Jeffrey S. Grethe](#), ... [Barend Mons](#)  [+ Show authors](#)

[Scientific Data](#) 3, Article number: 160018 (2016) | [Cite this article](#)

727k Accesses | 5435 Citations | 2221 Altmetric | [Metrics](#)

 An [Addendum](#) to this article was published on 19 March 2019

### Abstract

There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measureable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that focus on the human scholar, the FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals. This Comment is the first formal publication of the FAIR Principles, and includes the rationale behind them, and some exemplar implementations in the community.

## The FAIR principle:

- Findability
- Accessibility
- Interoperability
- Reusability

# Connecting data: Example 2



## Database of Raman and ATR-FTIR spectra of weathered and biofouled polymers

You are here: [MicroPlastiX SpecDB](#)

### Dataset: MicroPlastiX SpecDB

RADAR Metadata	Content	Statistics	Technical Metadata
Alternate identifier:	(URL of the source repository of the project) <a href="https://github.com/robna/MPX_specDB">https://github.com/robna/MPX_specDB</a> (Citable release snap shots of the source repository) <a href="https://doi.org/10.5281/zenodo.8314801">https://doi.org/10.5281/zenodo.8314801</a>		
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**Laureate Robin Lenz**  
**IPF Dresden**

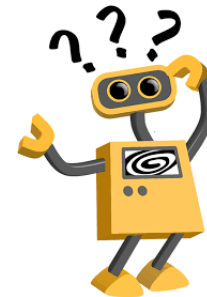




# Thank you for your attention!

## Questions???

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If you have further questions, just contact us:

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