WORKSHOP ON RESEARCH DATA

A. Vieten and J. Steinkamp Johannes Gutenberg University (JGU) Mainz
B. Lindstädt, A. Shutsko & J. Vandendorpe, ZB MED - Information Centre for Life Sciences

Photo by ZB MED

Outline

- Introduction
- Planning
- Data collection: Electronic Lab Notebooks (ELNs)
- Data sharing & publishing
- Data preservation
- Best practice example
- Further offer
- Q&A

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Introduction of the presenters

Team of Experts Research Data at JGU

- **Dr. Anne Vieten** (Department for Research and Technology Transfer) – general RDM aspects, requirements of funders, DMPs, RDMO…)--> University Medicine (UM): only for CRC, RTG, FOR…
  Further projects UM please contact: forschung.um@uni-mainz.de
- **Dr. Jörg Steinkamp** (Data Center – technical RDM aspects, GitLab, data archiving…)
- **Karin Eckert** (University library - Metadata, Gutenberg Open Science,…)
- **Esther Reineke** (University library – good research practise, academic integrity)
- **N.N.** (Mainzed – digital methods in humanities and cultural science …)

forschungsdaten@uni-mainz.de

What are we offering?

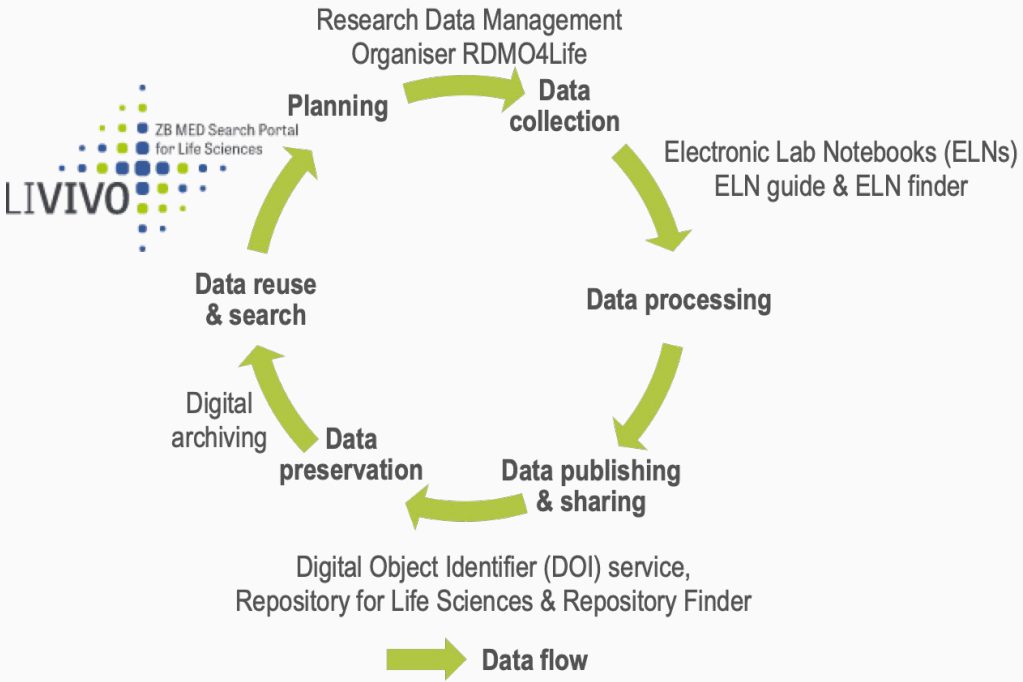
Informational service and assistance:
general RDM aspects, requirements of funders, DMPs incl. RDMO usage, individual RDM-policies, technical RDM aspects, iRODS archive usage, metadata, good scientific practise

Training:
RDM-Introduction, DMPs incl. RDMO, GitLab

Informational events:
Research Data Management Day at JGU, FORSCHUNGSDATEN@RMU both 1 per year

RDM-Infrastructures:
iRODS Archive, Gutenberg Open Science repository, RDMO (DMP-tool), GitLab, Seafile sync and share (cloud storage)

ZB MED - Information Centre for Life Sciences



Website • FAQs • Tutorials

- **INFORMATION:** fostering Open Access and Open Data.
- **KNOWLEDGE:** conducting applied research to improve ZB MED's services, and providing research support in the Life Sciences.
- **LIFE:** German National Library of Medicine, Health, Environment, Nutrition and Agriculture (world's largest library in these fields).

Research Data Management (RDM) team

- **Birte Lindstädt**
  - Background in Economic Geography and Library & Information Science
  - RDM team leader
  - Involved in NFDI4Health and NFDI4Microbiota
- **Aliaksandra Shutsko**
  - Background in Computational Linguistics & Information Science
  - Member of the RDM team
  - Data steward within NFDI4Health
- **Justine Vandendorpe**
  - Background in Organism Biology & Ecology and Computational Evolutionary Biology
  - Member of the RDM team
  - Data steward within NFDI4Microbiota

Research data & Research Data Management (RDM)

A definition of research data

- There is **no consensus** on the definition, the definition varies depending on:
  - Disciplines
  - Research funders [University of Leicester]

- A **definition** of research data:

‘any information that has been collected, observed, generated or created to validate original research findings.’

[University of Leeds]

Examples of research data

- Documents (e.g. text, Word), spreadsheets
- Laboratory notebooks, field notebooks, diaries
- Questionnaires, transcripts, codebooks
- Audiotapes, videotapes
- Protein or genetic sequences
- Spectra
- Test responses
- Slides, artifacts, specimens, samples
- Database contents (e.g., video, audio, text, images)
- Models, algorithms, scripts
- Contents of an app. (e.g., software)
- Methodologies and workflows

Source: NC STATE University Libraries

Examples of research data in medicine

- Data from **basic research** (e.g. sequencing or -omics data)
- **Electronic Medical Records** (EMRs) and **Electronic Health Records** (EHRs)
- **Patient/disease registries** (e.g. ENCePP Resources Database)
- **Health surveys** (e.g. National Cohort Study (NAKO))
- **Clinical** and **health data** (e.g. European Health Information Portal)
- **Clinical trials registries** and **databases** (e.g. German Clinical Trials Register (DRKS))
- **Catalogue for population health data**
- **Thesauri**, **ontologies** and **classifications** and **codes** of diseases or substances (e.g. International Statistical Classification of Diseases and Related Health Problems (ICD))

Research data management

A **definition** of research data management:

> ‘series of steps and methods that aim to make research data usable over the long term’

Steps:

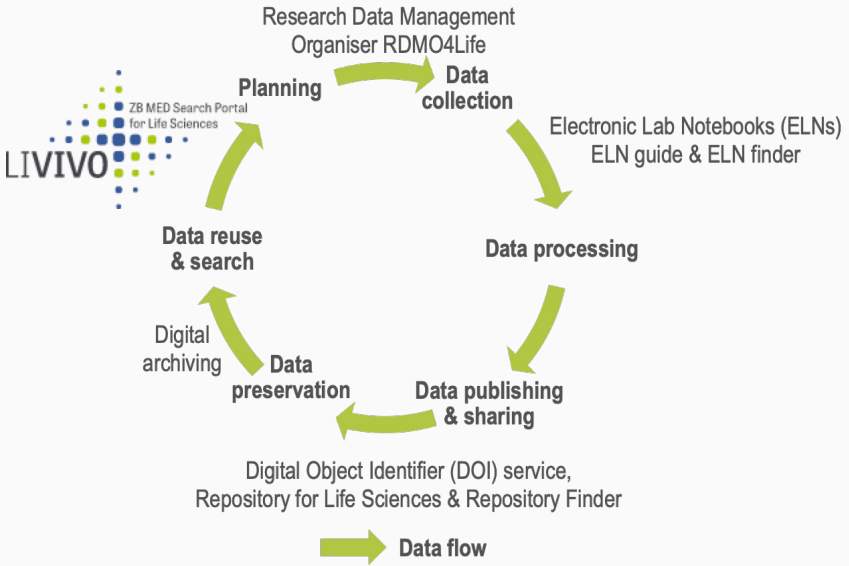
- Planning
- Data collection
- Data processing
- Adding metadata
- Data quality control
- Publishing and safeguarding access to data
- Archiving and ensuring the long-term interpretability of data

Source: ZB MED

ZB MED’s services

PUBLISSO, the ZB MED publication portal for life sciences, offers dedicated services and tools along the research data life cycle:

- RDMO4Life
- ELN guide
- DOI service
- Repository for Life Science
- Digital long-term preservation
- LIVIVO - The Search portal for Life Sciences



Good scientific practice

Defining good scientific practice

Principles, values and standards of behavior and practice that must be achieved and maintained in the delivery of work activities, the provision of care and personal conduct [Academy for Healthcare Science (AHCS)].

Photo by Scott Graham on Unsplash

Examples of good scientific practice

- Core principles: honesty, respect and accountability
- Documenting results
- Safeguarding and storing primary data
- Observing ethical standards

Source: Bosch, 2010, Guidelines for Safeguarding Good Scientific Practice at the Friedrich Schiller University Jena, O'Grady 2021

Photo by frank mckenna on Unsplash

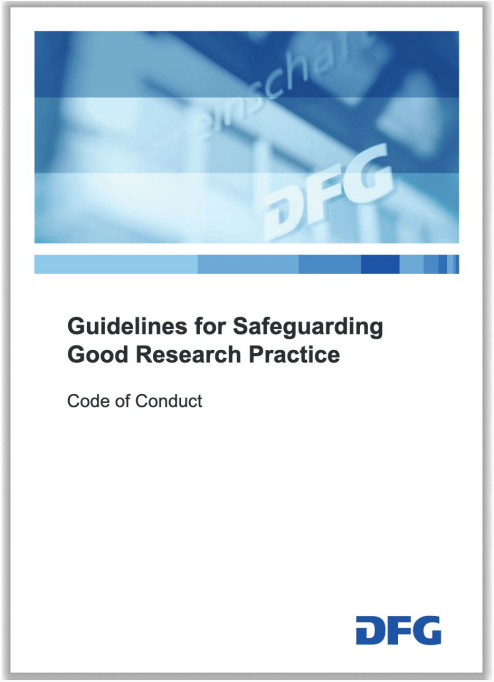
Examples of scientific misconduct

- Giving false information
- Infringement of intellectual property
- Self-plagiarism
- Compromising research activity of others
- Financial conflicts of interest
- Manipulating authorship

Source: Bosch, 2010, Guidelines for Safeguarding Good Scientific Practice at the Friedrich Schiller University Jena, O'Grady 2021

Ways of securing research integrity

- Establishing harmonize codes of good scientific practice such as:
  - DFG's Guidelines for Safeguarding Good Research Practice
  - The European Code of Conduct for Research Integrity
- Regulating procedures for handling allegations of research misconduct.



Source: Bosch, 2010, Guidelines for Safeguarding Good Scientific Practice at the Friedrich Schiller University Jena, O'Grady 2021

Implementation at JGU Mainz

- Will be implemented until summer 2022
- Draft is currently being reviewed by the DFG
- More RDM content than before
- FAIR principles to be fulfilled!

Policies & guidelines

General guidelines

DFG **Guidelines for Safeguarding Good Research Practice**. RDM-relevant guidelines:

- **Guideline 7: quality assurance across phases**
- Guideline 10: legal and ethical frameworks, rights of use
- Guideline 11: methods and standards
- **Guideline 12: documentation**
- **Guideline 13: establishing public access to research results**
- Guideline 14: authorship
- Guideline 15: publication organ
- Guideline 17: archiving

Discipline-specific guidelines

- Guidelines related to personal health data :
  - FAIRDOM's Data Management Checklist
  - Medical informatics initiative (MII)'s set of standardised rules for broad access to and use of primary data from patient care
- Institutional guidelines : ZB MED's Research Data Policy (German only)

Policy at JGU Mainz

https://www.blogs.uni-mainz.de/research-data/files/2020/02/FDM-Leitlinie-f%C3%BCr-die-JGU_.pdf

Leitlinie der Johannes Gutenberg-Universität Mainz zum Umgang mit Forschungsdaten

Die JGU misst dem verantwortungsvollen Umgang mit Forschungsdaten als Grundlage für die wissenschaftliche Integrität und den wissenschaftlichen Fortschritt eine hohe Bedeutung bei. Unter Forschungsdaten sind sämtliche Daten zu verstehen, die im Laufe von Forschungsprozessen entstehen. Der hier verwendete Begriff von Forschungsdaten umfasst daher gleichermaßen Rohdaten, wie auch die aus ihnen abgeleiteten Forschungsergebnisse in Form von Publikationen der Daten und Resultate inklusive der jeweils dazugehörigen Metadaten und Dokumentationen.

Die nachfolgenden Grundsätze dienen der Konsolidierung eines verantwortungsvollen, strukturierten und zeitgemäßen Umgangs mit Forschungsdaten an der JGU.

An der JGU gelten für den Umgang mit Forschungsdaten die folgenden Grundsätze:

Den für ein Forschungsvorhaben verantwortlichen Wissenschaftlerinnen und Wissenschaftlern der JGU obliegt die Verantwortung, ihre Forschungsdaten zu speichern und zu dokumentieren sowie die Daten für eine langfristige Sicherung in dafür geeigneten Einrichtungen, wie z.B. Datenrepositorien vorzubereiten. Dies gilt insbesondere für Rohdaten, die die Grundlage für wissenschaftliche Publikationen waren. Das Management von Forschungsdaten umfasst hierbei alle die Daten betreffenden Prozesse von der Erzeugung, über die Analyse, die Dokumentation, die Publikation, bis zur langfristigen Speicherung bzw. Löschung von Daten. Falls erforderlich, sind die Daten gemäß den geltenden Rechtsvorschriften zum Datenschutz gegen unerlaubten Zugriff zu schützen.

Im Umgang mit Forschungsdaten und in der Forschung sind die Leitlinie zur Sicherung guter wissenschaftlicher Praxis der Deutschen Forschungsgemeinschaft, ethische Grundsätze, urheber- und lizenzrechtliche Regelungen sowie Fachstandards einzuhalten.

Bei dem Beginn neuer, datenproduzierender Forschungsvorhaben ist die Erstellung eines Datenmanagementplans, der alle wesentlichen Aspekte für den Umgang mit Forschungsdaten

Metadata & Metadata standards

Definition of metadata

Metadata = “data about data”

- **Standardised** information
- **Structured** information
- Subset of **documentation**: describes, explains, locates, makes it easier to retrieve, use, manage an information resource
- **Human-** and **machine-readable**

Examples of metadata

- Name
- Topic
- Description of input and output (parameters or format)
- Address/geospatial information
- Licensing information

Importance of metadata

- To make data:
  - **F**indable, **A**ccessible, **I**nteroperable, **R**eusable (**FAIR**)
  - **Understandable**
  - **Citable**
- To facilitate the **long-term archiving** of data
- To make the context for how your data was created, analysed, stored **reproducible**
- To uphold **research integrity**

Types of metadata

Descriptive	***vs.***	**Technical**
e.g. resource identifier, title, author, date of publication, subject, publisher, description		e.g. physical database tables, access permissions, data models, backup rule
Project-specific / dataset-level	***vs.***	**Data-specific**
e.g. project title, description, subject, coverage, creators, publisher, contributors, identifiers		e.g. unique ID, file path, unique project ID, date the file was created
General	***vs.***	**Discipline-specific**
e.g. file name and format, software and hardware used to create the files		e.g. reagent, technical, experimental, analytical, dataset-level

Example of general metadata

Dublin Core Metadata Initiative:

« domain agnostic, basic and widely used metadata standard »
[Cornell University]

- International data **exchange** format
- 22 **elements** – 15 with an **ISO certificate**
- Refinements and encoding schemes for **subject-specification** applications

nr.	Dublin Core element
1	Titel
2	Subject
3	Description
4	Type
5	Source
6	Relation
7	Coverage
8	Creator
9	Publisher
10	Contributor
11	Rights
12	Date
13	Format
14	Identifier
15	Language

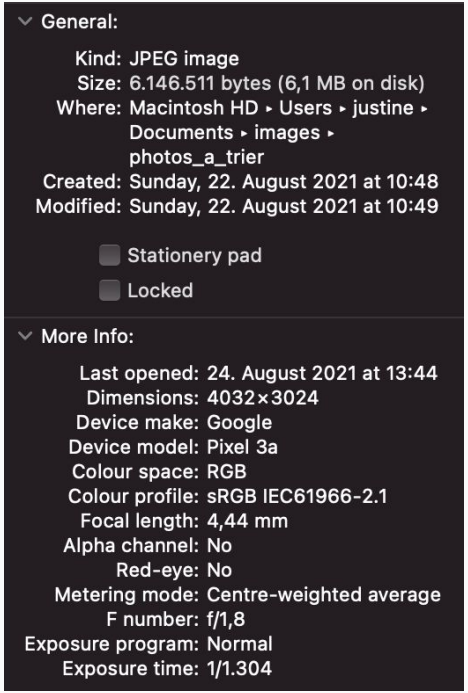
Examples of discipline-specific metadata

Type of metadata	Core information about…
Reagent	Clinical samples, biological or chemical reagents
Technical	Measurements made by the use of research instruments
Experimental	Experimental conditions, the experimental protocol, and the equipment used to generate the data
Analytical	Data analysis methods
Dataset-level	Objectives of the research project, participating investigators, recent publications, and funding sources

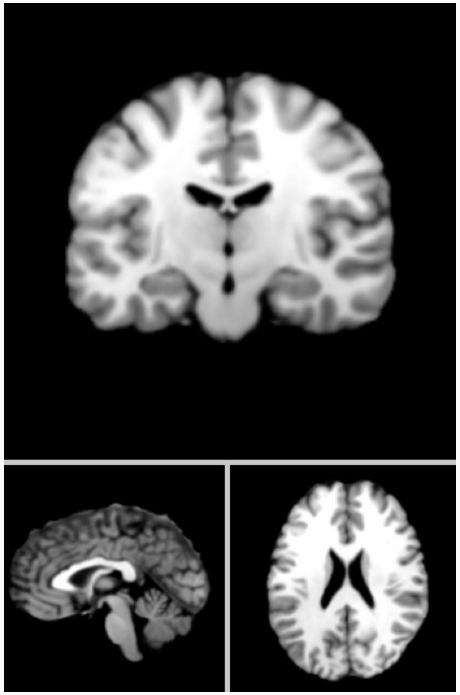
Source: Harvard University

Technical metadata

- **Automatically generated** by software associated to research instruments (e.g. metadata generated by cameras in images files)
- Metadata acquisition can be partly configured in the **software settings**
- Metadata **export** must sometimes be initiated deliberately



Technical metadata



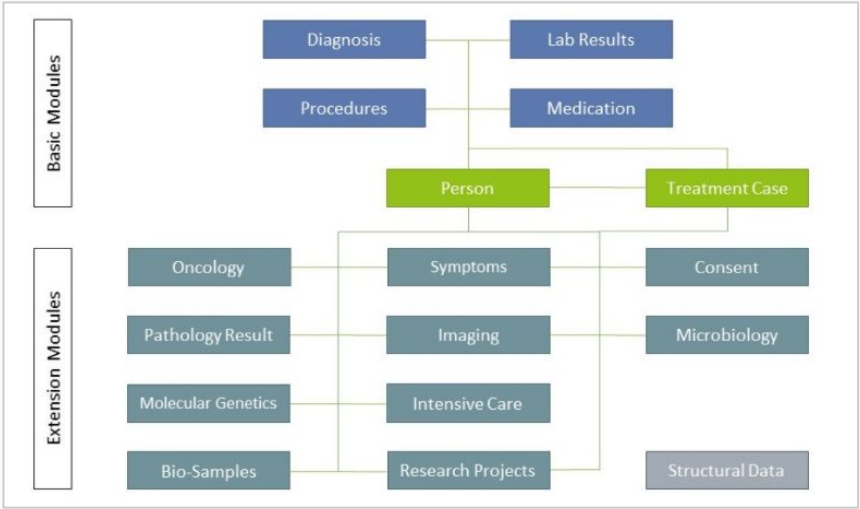
Metadata element	Metadata value
Scanner model	Siemens 3T Prisma
Head coil	24-channels
Sequence	T1-weighted MPRAGE
TR	2300 ms
TE	2.98 ms
Flip angle	9°
Voxel size	1 x 1 x 1 mm^3
FOV	256 x 256 mm^2
Number of slices	176
Slice thickness	1 mm

Examples of metadata standards in the life sciences

- **To report:**
  - Clinical data: SNOMED CT
  - Diseases and health conditions: ICD
  - Data derived by relevant methods in biosciences: MIBBI
- **To index** journal articles and books in the life sciences: MeSH
- **To exchange:**
  - Clinical and translational research data: CDISC - ODM-XML
  - Healthcare information electronically: HL7 FHIR
- **Formats:**
  - For neutron, x-ray, and muon science: NeXus
  - For storing microscopy information: OME-XML

Recommendations on using metadata standards in the life sciences

The German medical informatics initiative (MII)'s recommendations for the joint use of standardised metadata on data availability, analysis options and collaboration options.



[Core data set of the MII]

FAIR data principles

FAIR data principles

- **Definition:** a concise and measurable set of principles that may act as a guideline for those wishing to enhance the reusability of their data holdings [Wilkinson et al. 2016]:
  - **F**indability
  - **A**ccessibility
  - **I**nteroperability
  - **R**eusability

- **Aims** [Wilkinson et al. 2016]**:**
  - Improving the **infrastructure** supporting the reuse of scholarly data
  - Enhancing the ability of **machines** to automatically find and use data
  - Supporting the reuse of data by **individuals**

- **Example of FAIR health data**

To be Findable

- (Meta)data are assigned a globally unique and **persistent identifier**
- Data are described with rich **metadata**
- Metadata clearly and explicitly include the **identifier** of the data it describes
- (Meta)data are registered or indexed in a **searchable resource**

[Wilkinson et al. 2016]

To be Accessible

- (Meta)data are retrievable by their identifier using a **standardized communications protocol** (e.g., http(s))
- The protocol is **open**, **free**, and **universally implementable**
- The protocol allows for an **authentication** and **authorization procedure**, where necessary
- **Metadata** are accessible, even when the data are no longer available

[Wilkinson et al. 2016, GO FAIR]

FAIR ≠ FOIR (O = Open)

To be Interoperable

Interoperability: ‘each computer system at least has knowledge of the other system’s data exchange formats’

- (Meta)data use a formal, accessible, shared, and broadly applicable **language for knowledge representation** (e.g., controlled vocabularies/ontologies/thesauri, a good data model)
- (Meta)data use **vocabularies** that follow FAIR principles (e.g., using FAIR Data Point)
- (Meta)data include **qualified references** to other (meta)data (e.g., specifying if one datasets builds on another one, properly citing all datasets)

[Wilkinson et al. 2016, GO FAIR]

To be Reusable

- Meta(data) are richly described with a plurality of accurate and relevant **attributes** (i.e. metadata that richly describes the context under which the data was generated such as the experimental protocols, the species used)
- (Meta)data are released with a clear and accessible **data usage license**
- (Meta)data are associated with detailed **provenance**

[Wilkinson et al. 2016, GO FAIR]

Outline

- Introduction
- **Planning**
- Data collection: Electronic Lab Notebooks (ELNs)
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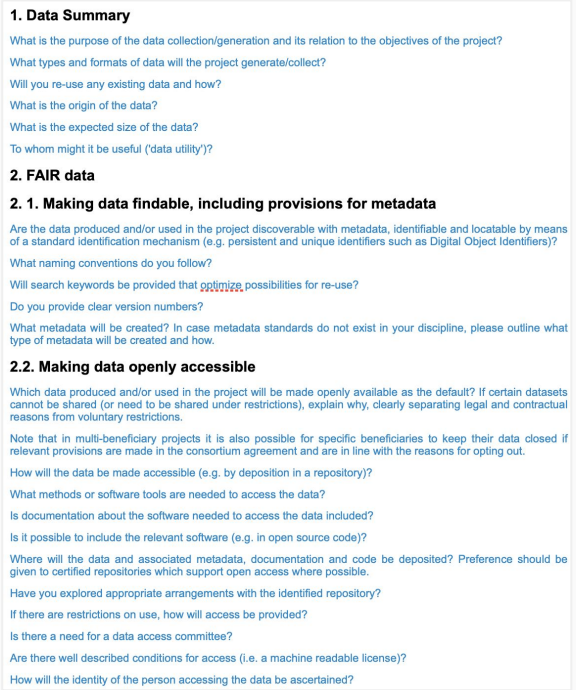
Data Management Plans (DMPs)

A definition of DMPs

Formal and **living document** to **describe** the **data**, their **generation** and **processing** during the project, as well as how the **data** and **research results** will be **archived** afterwards to remain **available**, **usable** and **comprehensible**.



1. Data Summary

What is the purpose of the data collection/generation and its relation to the objectives of the project?

What types and formats of data will the project generate/collect?

Will you re-use any existing data and how?

What is the origin of the data?

What is the expected size of the data?

To whom might it be useful ('data utility')?

2. FAIR data

2. 1. Making data findable, including provisions for metadata

Are the data produced and/or used in the project discoverable with metadata, identifiable and locatable by means of a standard identification mechanism (e.g. persistent and unique identifiers such as Digital Object Identifiers)?

What naming conventions do you follow?

Will search keywords be provided that optimize possibilities for re-use?

Do you provide clear version numbers?

What metadata will be created? In case metadata standards do not exist in your discipline, please outline what type of metadata will be created and how.

2.2. Making data openly accessible

Which data produced and/or used in the project will be made openly available as the default? If certain datasets cannot be shared (or need to be shared under restrictions), explain why, clearly separating legal and contractual reasons from voluntary restrictions.

Note that in multi-beneficiary projects it is also possible for specific beneficiaries to keep their data closed if relevant provisions are made in the consortium agreement and are in line with the reasons for opting out.

How will the data be made accessible (e.g. by deposition in a repository)?

What methods or software tools are needed to access the data?

Is documentation about the software needed to access the data included?

Is it possible to include the relevant software (e.g. in open source code)?

Where will the data and associated metadata, documentation and code be deposited? Preference should be given to certified repositories which support open access where possible.

Have you explored appropriate arrangements with the identified repository?

If there are restrictions on use, how will access be provided?

Is there a need for a data access committee?

Are there well described conditions for access (i.e. a machine readable license)?

How will the identity of the person accessing the data be ascertained?

[European Commission]

Examples of DMPs from the University of Minnesota

- **Roles** and **responsibilities** of project/institutional staff in the **management/retention** of data
- **Types** of data to be collected and shared
- Metadata **documentation**
- Data **preparation** for transformations/sharing/preservation and **format** of the final dataset
- Data **sharing** (prevention or agreement) and data **confidentiality**
- Method of data **access** (e.g. repository, archiving)
- **Expected schedule** for data access
- Data **secondary use** and associated **limitations**

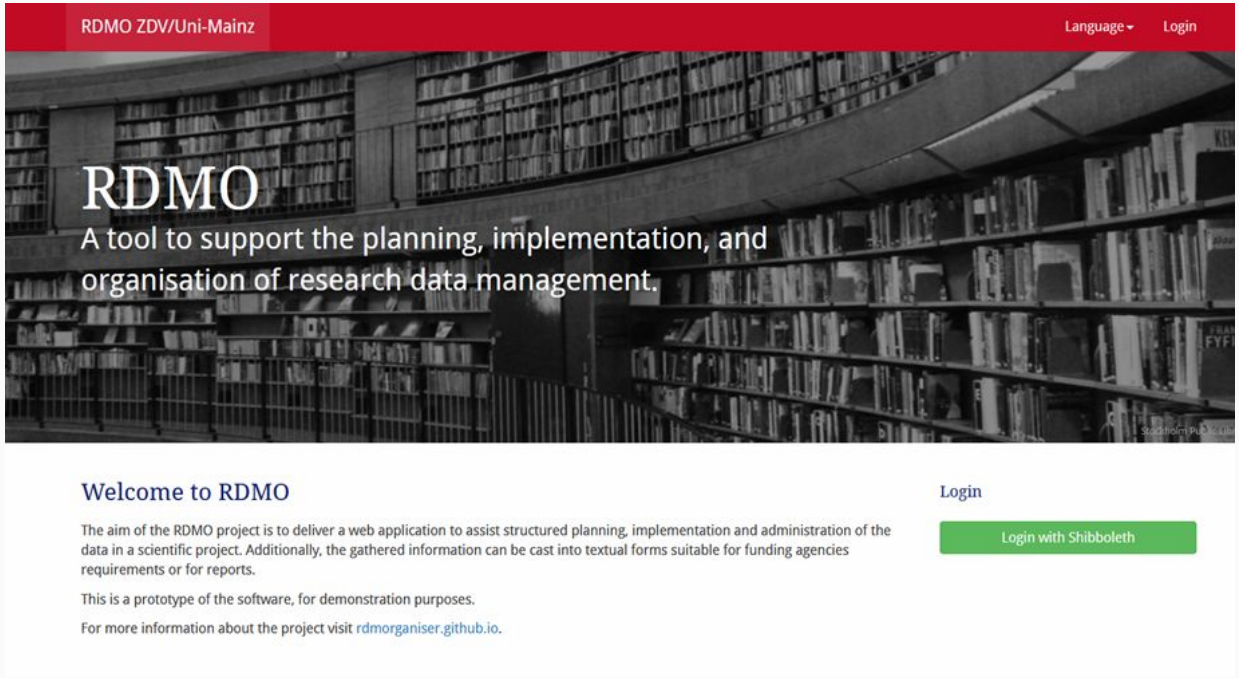
Importance of DMPs

- Giving the project's team an overview about the **data**, their **storage** and **usage**

  → Easing **coordination** and **common handling** of research data
- Supporting **research integrity**
- Prevent **data loss** and **security holes**
- Facilitating **data reuse**
- **Saving** yourself **time** in the future
- Increasing **data citation**
- **Requirement** from funding organizations (sometimes)

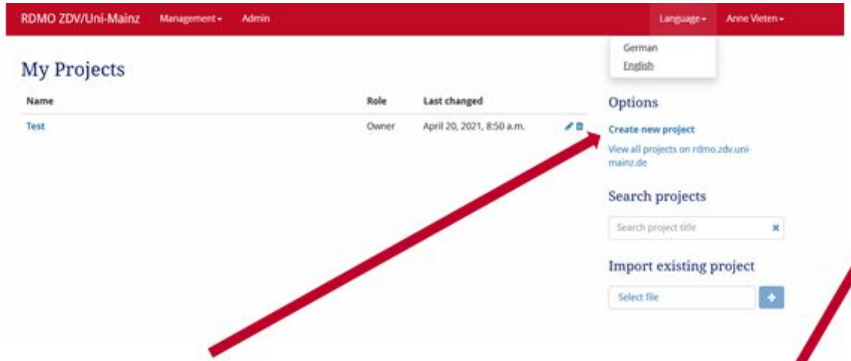
Software tool to set up DMPs

Research Data Management Organiser (RDMO) at JGU Mainz

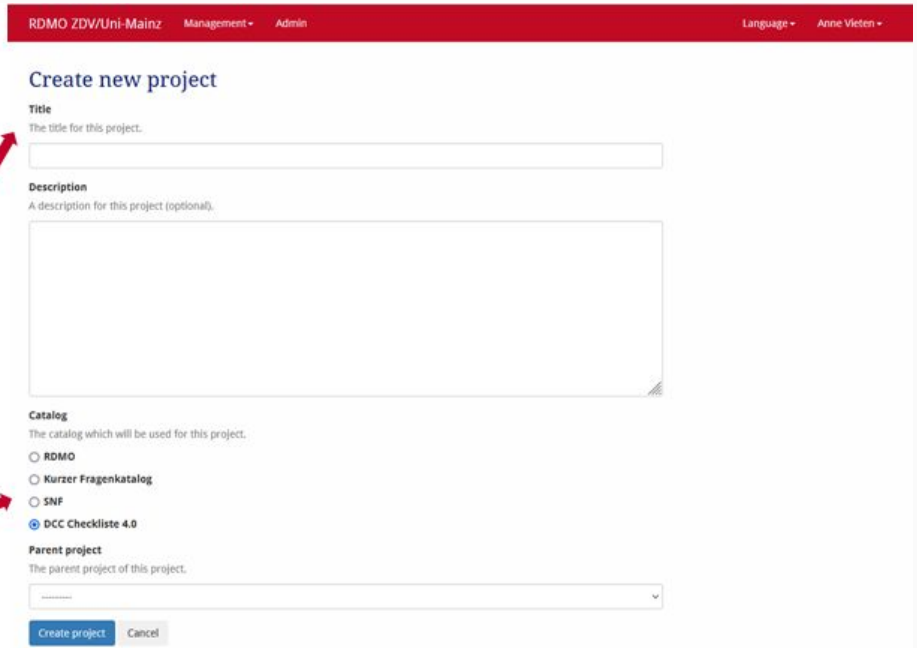


https://rdmo.zdv.uni-mainz.de

Research Data Management Organiser (RDMO) at JGU Mainz



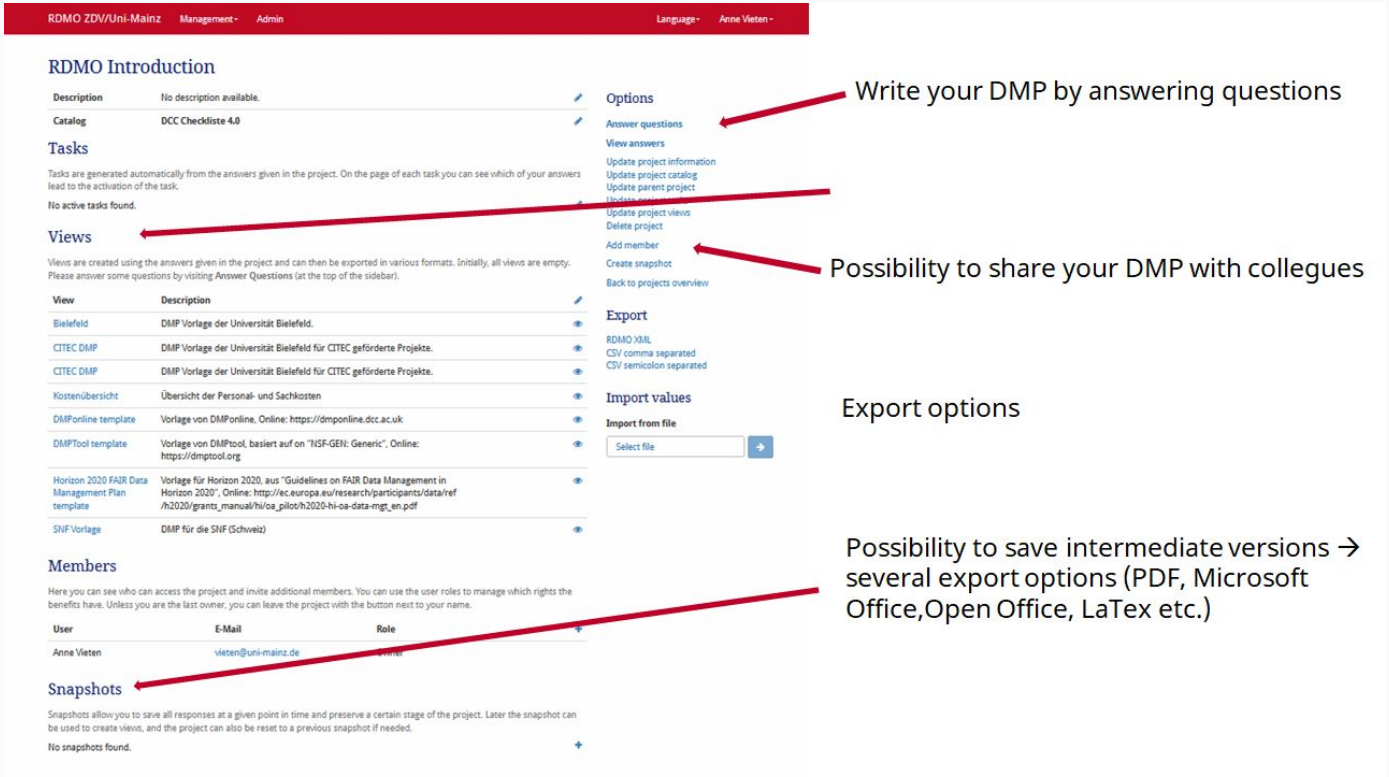
Choose „Create new Project“



Title and describe your project

Choose a catalog and create the project

Research Data Management Organiser (RDMO) at JGU Mainz



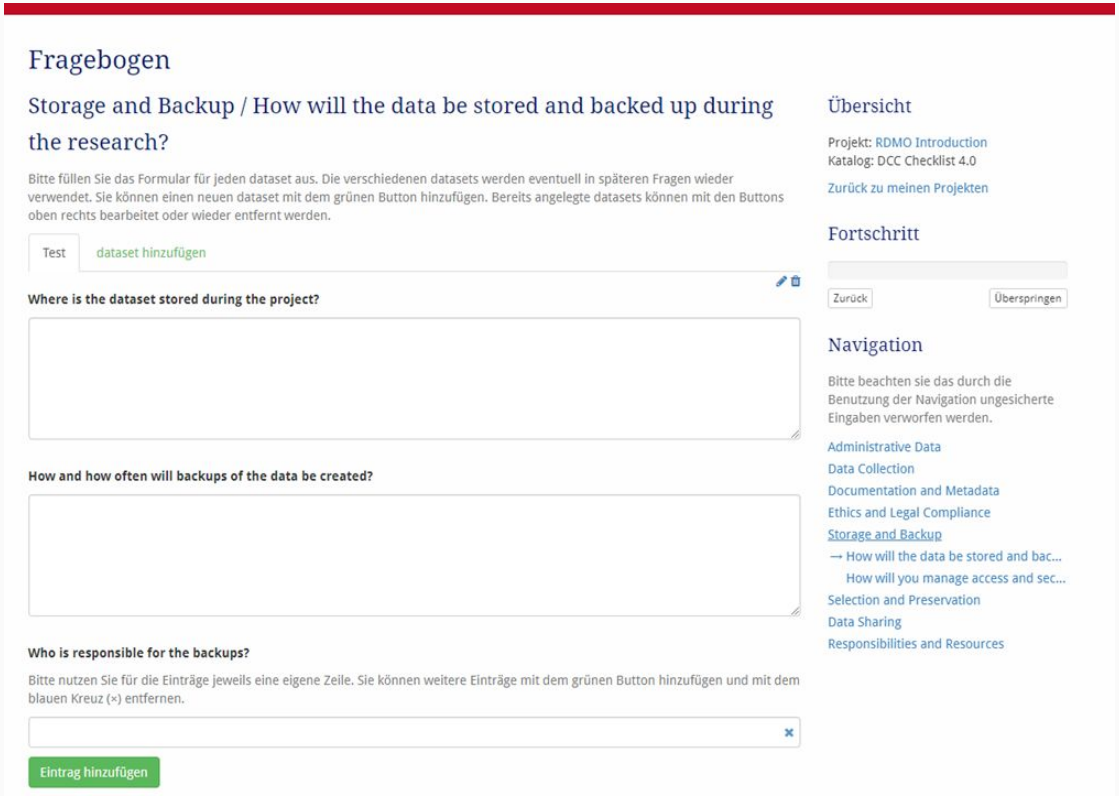
Write your DMP by answering questions

Possibility to share your DMP with collegues

Export options

Possibility to save intermediate versions → several export options (PDF, Microsoft Office,Open Office, LaTex etc.)

Research Data Management Organiser (RDMO) at JGU Mainz



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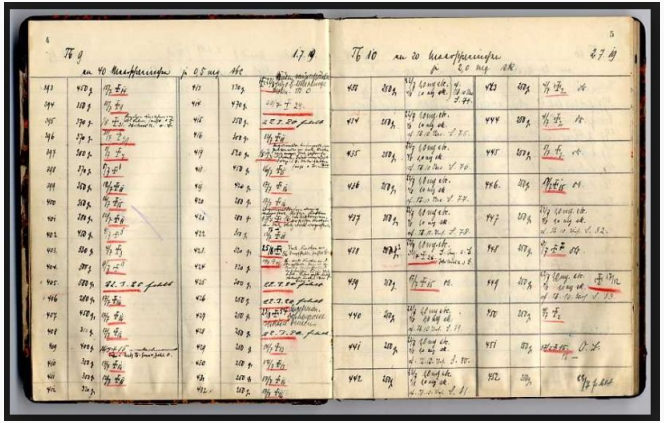
A definition of ELNs

- **Software**
- **Documentation** of experiments and research data
- Replacement of the **paper format** in the context of the digital transformation
- Examples of **features**: protocol templates, collaboration tools, support for electronic signatures and the ability to manage the lab inventory



Übersicht Methoden

Anzahl der Datensätze: 15

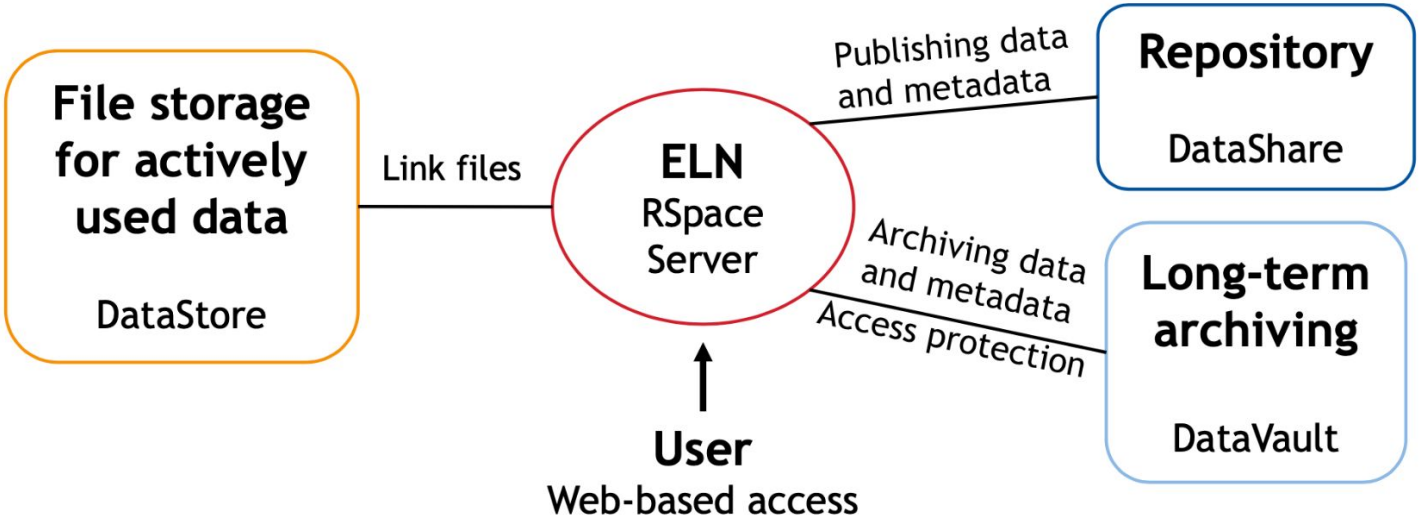
MethID	Methodenname	Methodenart	Schritte	Status	Benutzt
9	LA1: Isolierung von Soja und Pflanzen-DNA	allgemeingültig	29	freigegeben	Ja
10	LA2: Nachweis von Soja- u. Pfl.-DNA per rt PCR	allgemeingültig	9	freigegeben	Nein
11	LA3: GVO-Nachweis bei Soja	allgemeingültig	4	freigegeben	Ja
12	LE1: Colony PCR und ALF Sequenzierung	allgemeingültig	11	freigegeben	Ja
13	LE2: In vitro Transkription	allgemeingültig	6	freigegeben	Ja
14	LE3: Immunoblot	allgemeingültig	16	freigegeben	Ja
15	LE4: SDS-Page	allgemeingültig	4	freigegeben	Ja
1	MS1: Agarose-Gelelektrophorese	allgemeingültig	8	in Bearbeitung	Nein
2	MS2: Restriktionsverdau	allgemeingültig	3	freigegeben	Ja
8	MS3: Ligation	allgemeingültig	8	freigegeben	Ja

Neue Methode 1 von 2

Benefits of using an ELN

- Boosting **efficiency** of everyday task thanks to, for instance:
  - Protocol templates
  - Search features
  - Access to the ELN anywhere, anytime
- Increased **verifiability** and **traceability** of research findings, preventing:
  - Media discontinuities between handwritten and digital entries
  - Information loss due to illegibility
- Networked **digital research environment**
  - Seamless interfaces to other programs, such as Application Programming Interfaces (APIs)
  - Im- and export functions
  - Direct links to research data repositories, data services and publishing platforms

The ELN communicates in a networked research environment



Caption: Integration of the ELN RSpace into the research data management infrastructure of the University of Edinburgh (based on Macdonald and Macneil 2015)

Based on: Krause, E.: Elektronische Laborbücher im Forschungsdatenmanagement – Eine neue Aufgabe für Bibliotheken?, ABI Technik 2016; 36(2): 78–87

Types of Electronic Lab Notebooks

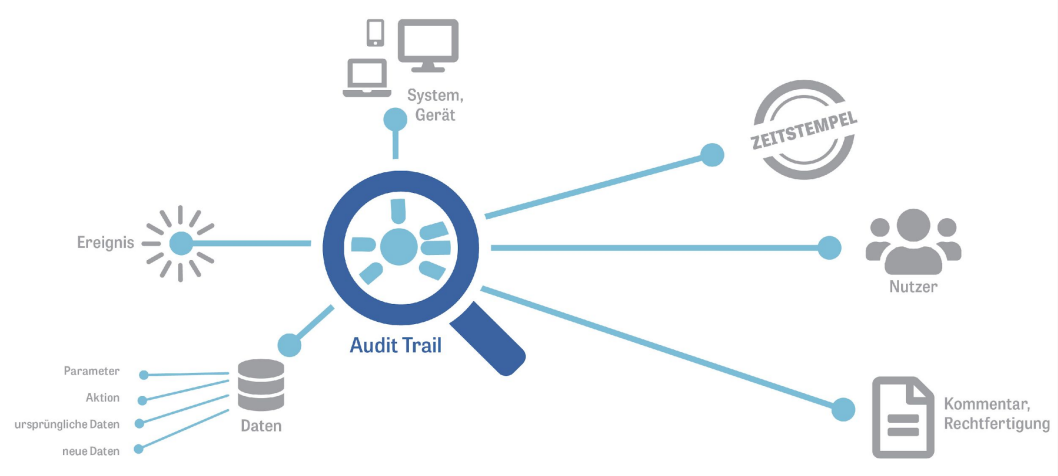
Basic systems	Specialized systems	High end systems
• Text entries • Attachments • Annotation • Search function • Sharing via the cloud	+	+
	• Subject-specific functions • Templates • Freehand drawing • Basic inventory management • Task assignment • Rights management • Extensions/API • Audit trail	• Laboratory Information Management System (LIMS) • Inventory management • Workflows • Link to lab equipment • Analysis • Data mining
e.g. Evernote	e.g. Labfolder	e.g. Limsophy LIMS

The FAIR data principles and using an ELN

- **Findable**
  - Assignment of persistent identifiers (e.g. DOI)
  - Extensive search functions of ELNs (e.g. database, full-text and conditional searches)
  - Support for the assignment of metadata / tags (e.g. extraction from documents)
- **Accessible**
  - Starting point for institutional research data management (e.g. connection to repositories or archives)
  - Storage of data in fixed, accessible locations (e.g. not on researchers' USB sticks / portable hard drives)
- **Interoperable**
  - Use / connection of controlled vocabularies in metadata
  - Export to standard formats
- **Reusable**
  - Description of data (e.g. facilitated metadata capture)
  - Audit trail
  - Documentation of data generation (e.g. logging methods) and of devices used (e.g. devices provide their output directly to the ELN)

Using an ELN and good scientific practices

- Audit trail
- Version control
- Authentication functions
- No deletion of data possible
- Searchability of entries
- “Freezing” of work statuses
- Marking of entries



Audit Trail, inspired by [Johner, C. (2016): „Was sollte ein Audit-Trail enthalten?“]

Electronic Lab Notebook (ELN) guide

ELN guide

- **Content:** criteria for choosing an ELN
- **Target audience:**
  - Information infrastructures
  - Researchers
- **Languages:**
  - German
  - English

ZB MED service

Electronic Lab Notebook (ELN) finder & filter

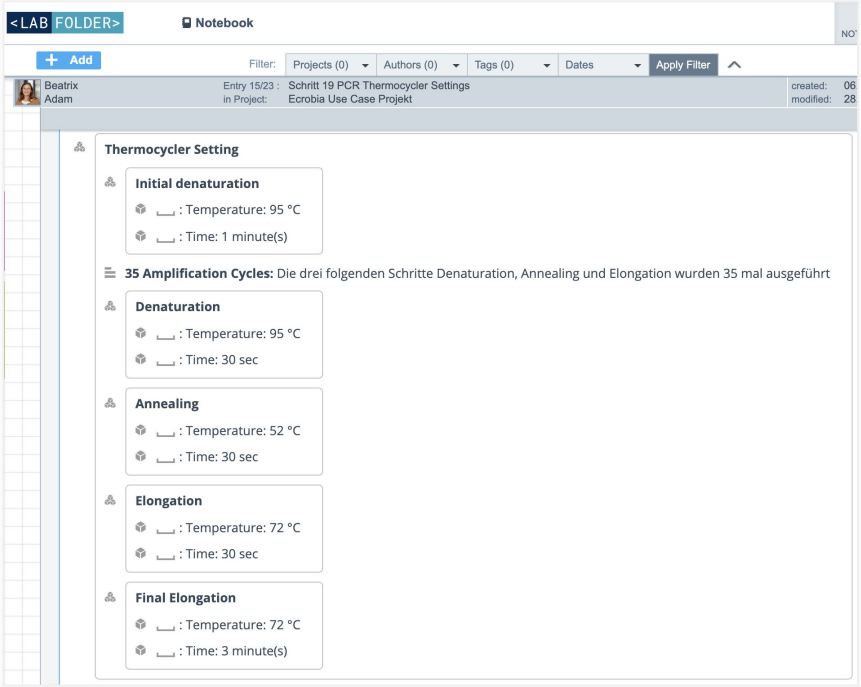
- **ELN finder:** interactive tool for **filtering** ELNs based on different criteria (under development in collaboration between ZB MED and TU Darmstadt (library)).
- **ELN filter** (in German only): step towards the ELN finder.

Name	Land	Referenzen	Preismodell (akademische Nutzung)	Weitere Informationen
↗ *Arx-span*	USA	Unbekannt	Unbekannt	Unbekannt
↗ *Bench-ling*	USA	Unbekannt	↗ *Kostenlose akademische Version* für Per-sonen, Labore und Lehre mit eingeschränktem Funktionsumfang	Unbekannt

ZB MED service

Examples of ELNs in molecular biology

- eLABJournal
- LabCollector
- Labfolder
- LabWare ELN
- Limsophy LIMS
- OpenBIS



Labfolder

Outline

- Introduction
- Planning
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- **Data sharing & publishing**
- Data preservation
- Best practice example
- Further offer
- Q&A

Referencing research data

Digital Object Identifier (DOI)

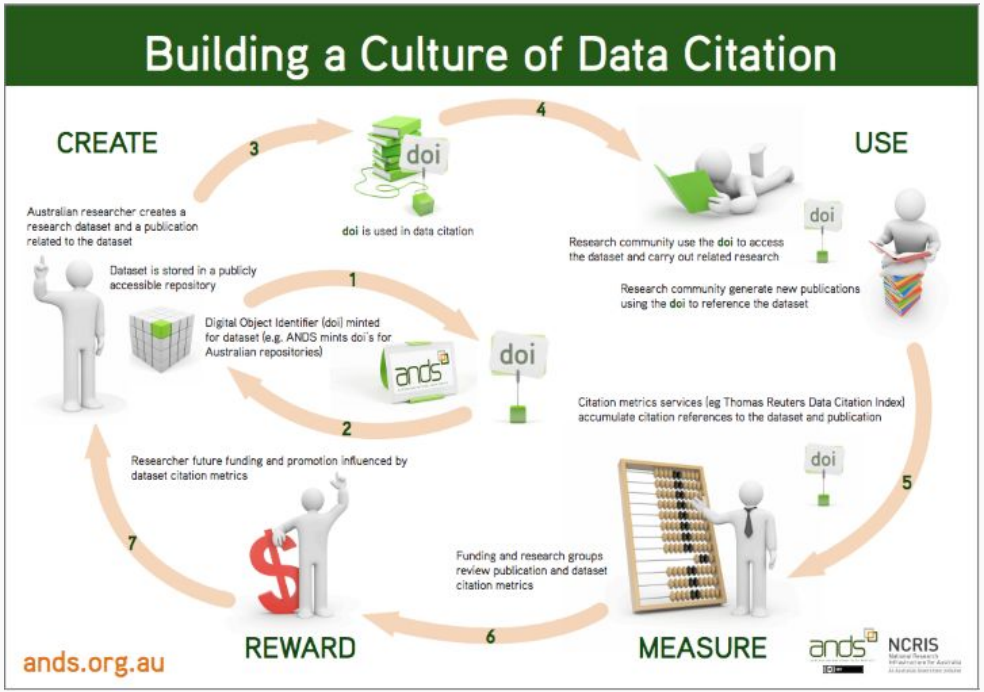
DOI: ‘system for providing persistent and actionable identification and resolution to resource objects in a digital environment’ [Carpenter 2012]

[TIB]

Benefits:

- Providing a **reference** to the object itself (i.e. the reference is still valid even if the URL changes).
- Making research data **accessible** and **citable** over the long term.

Building a culture of data citation



[ands]

DOI service of UB Mainz

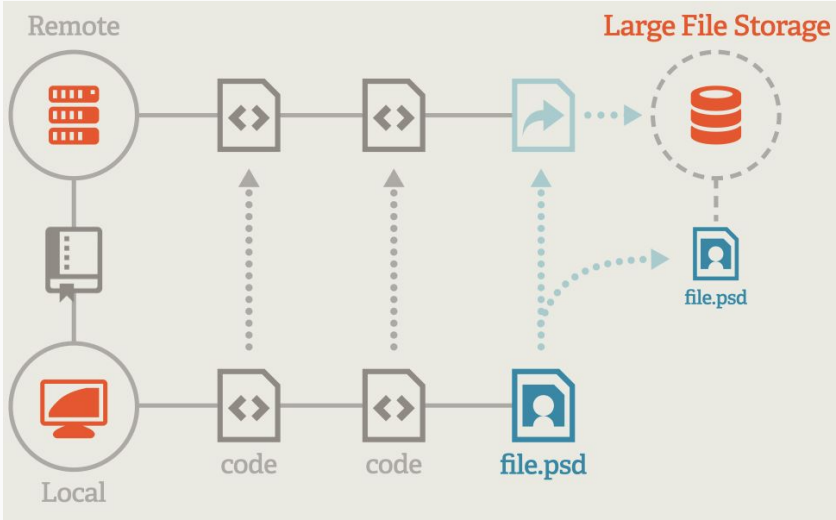
DOI for articles and textual datasets* published in Gutenberg Open Science repository

*soon

Sharing research data: collaboration tools

General purpose collaboration tools

- **SharePoint**: web-based platform that integrate with Microsoft Office.
- **Git-based tools:**
  - **GitHub** providing hosting for software development and version control.
  - **GitLab** providing wiki, issue-tracking and a deployment platform.
  - **git-annex** ang **Git Large File Storage** providing file managing/versioning systems without checking the file contents into git.



Git Large File Storage

Local services of JGU Mainz

Seafile RLP:

- Sync and Share (Cloud service)
- 100 GB per JGU scientist
- Enables data exchange
- Collaborative Work on documents
- via Only Office

https://seafile.rlp.net

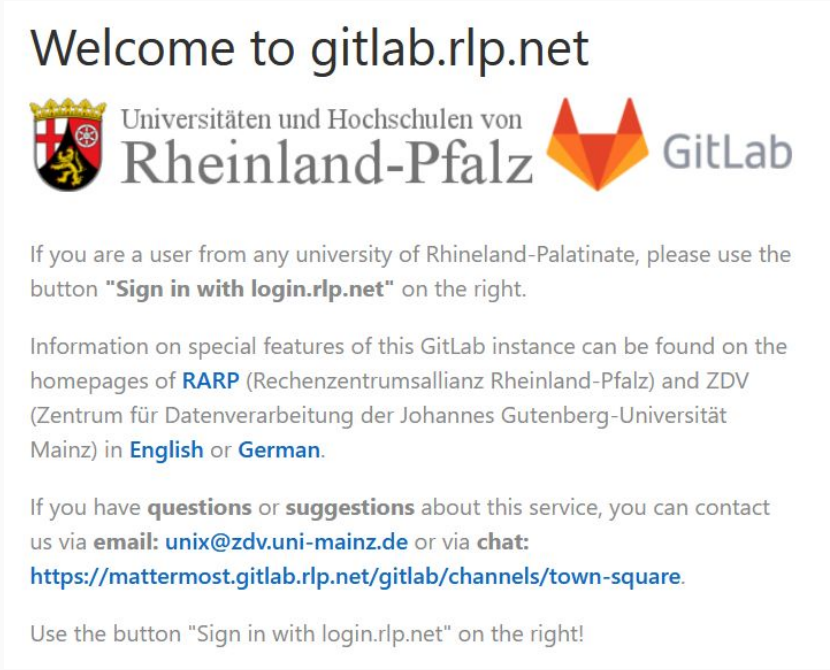
Local services of JGU Mainz

Versioning tool GitLab:

- code, text, vector graphics
- saves and documents changes to files and their source code
- Braching
- Issue tracking
- …

Additional feature; Mattermost for easy and quick communication

https://gitlab.rlp.net



Publishing research data

Data repositories

Research data can be published as an **independent information object** in a data repository AND:

- As a data supplement in an **enhanced publication**
- Documented in a **data paper** published in a data journal

Data repositories include:

- **Interdisciplinary repositories** such as Figshare and Zenodo
- **Institutional repositories**: see example in the next slides
- **Discipline-specific repositories**: see examples in the next slides

Local repositories

- Institutional Open Access repository
- Pre and post prints, PhD thesis
- Textual research data*
- Searchable by meta data
- Self archiving
- DOI

*soon
https://openscience.ub.uni-mainz.de/?locale=en

Examples of discipline-specific repositories

GenBank: 'an annotated collection of all publicly available DNA sequences'

- **Submission tools**:
  - Web-based submission tools (BankIt, Submission Portal)
  - Submission preparation tools (tbl2asn, Genome Workbench)
- **Submission types**:
  - mRNA or genomic sequence data
  - Complete Microbial Genomes
  - Whole Genome Shotgun (WGS) Sequences
  - …

Sample GenBank Record

This page presents an annotated sample GenBank record (accession number **U49845**) in its *GenBank Flat File* format. You can see the corresponding live record for U49845, and see examples of other records that show a range of biological features.

```
LOCUS       SCU49845     5028 bp    DNA             PLN       21-JUN-1999
DEFINITION  Saccharomyces cerevisiae TCP1-beta gene, partial cds, and Axl2p
            (AXL2) and Rev7p (REV7) genes, complete cds.
ACCESSION   U49845
VERSION     U49845.1  GI:1293613
KEYWORDS    .
SOURCE      Saccharomyces cerevisiae (baker's yeast)
  ORGANISM  Saccharomyces cerevisiae
            Eukaryota; Fungi; Ascomycota; Saccharomycotina; Saccharomycetes;
            Saccharomycetales; Saccharomycetaceae; Saccharomyces.
REFERENCE   1  (bases 1 to 5028)
  AUTHORS   Torpey,L.E., Gibbs,P.E., Nelson,J. and Lawrence,C.W.
  TITLE     Cloning and sequence of REV7, a gene whose function is required for
            DNA damage-induced mutagenesis in Saccharomyces cerevisiae
  JOURNAL   Yeast 10 (11), 1503-1509 (1994)
  PUBMED    7871890
REFERENCE   2  (bases 1 to 5028)
  AUTHORS   Roemer,T., Madden,K., Chang,J. and Snyder,M.
  TITLE     Selection of axial growth sites in yeast requires Axl2p, a novel
            plasma membrane glycoprotein
  JOURNAL   Genes Dev. 10 (7), 777-793 (1996)
  PUBMED    8846915
REFERENCE   3  (bases 1 to 5028)
  AUTHORS   Roemer,T.
  TITLE     Direct Submission
  JOURNAL   Submitted (22-FEB-1996) Terry Roemer, Biology, Yale University, New
            Haven, CT, USA
FEATURES             Location/Qualifiers
     source          1..5028
                     /organism="Saccharomyces cerevisiae"
                     /db_xref="taxon:4932"
                     /chromosome="IX"
                     /map="9"
     CDS             <1..206
                     /codon_start=3
                     /product="TCP1-beta"
                     /protein_id="AAA98665.1"
                     /db_xref="GI:1293614"
                     /translation="SSIYNGISTSGLDLNNGTIADMRQLGIVESYKLKRAVVSSASEA
```

Annotated sample GenBank record for a *Saccharomyces cerevisiae* gene

Examples of discipline-specific repositories

ZB MED's Repository for Life Sciences

- Permanent publishing and archiving of data from the life sciences:
  - **Raw research data** = singular research data
  - **Enhanced publication** = research data linked to a full text
- **Requirements:**
  - Licensing of the data in the sense of **Open Data** to give the possibility of subsequent use
  - Providing a detailed **description** to ensure that the published research data can be clearly interpreted and reused in the future
  - Giving **essential information** (e.g. title, author(s), format)
- **Information for authors and institutions**

Examples of repository finders

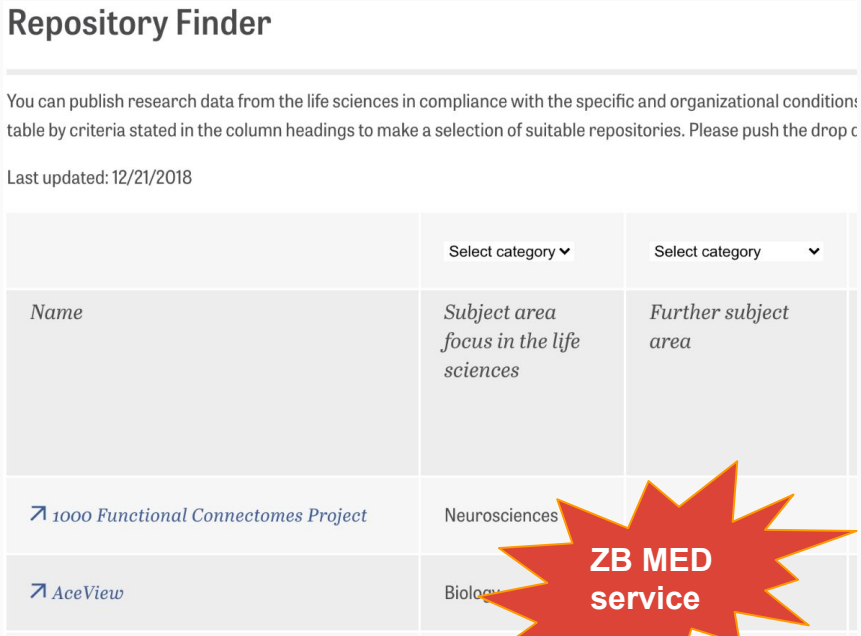
DataCite's **re**gistry of **re**search data **re**positories (**re3data**): global **registry** of research data **repositories**:

- from **different academic disciplines**
- that enable permanent **storage** of and **access** to data sets

Examples of repository finders

Repository Finder: ZB MED's curated selection of repositories from re3data

- **Target audience**: researchers who would like to publish their research data
- **Criteria:**
  - **Subject:** Life Sciences
  - **Data access:** open
  - **Data upload:** open (registration at most)



Privacy issues

What are the challenges?

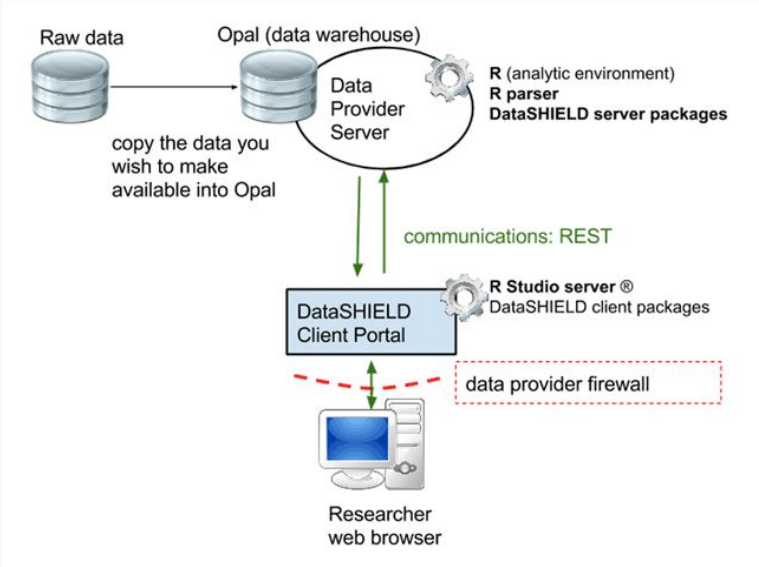
- Obtaining (broad) **informed consent** from participants
  - to respect their right to **health data privacy**
  - because **NOT sharing** clinical trial data comes with drawbacks (e.g. duplication of trials, bias in the body of evidence, slowing scientific progress)
- Properly **pseudo-/anonymising** data
- Finding **alternative approaches** to data pseudo-/anonymisation, which do not satisfy the General Data Protection Regulation (GDPR) [Rocher *et al.* 2019]

Where can solutions be found?

- **Informed consent**: template text for patient consent forms
- **Pseudo-/anonymisation** tools
  - Amnesia
  - Data privacy tool
- Alternative to pseudo-/anonymisation - **distributed approach**: personal data remain in their original location, and data owners enable analytical tasks to visit data sources and execute the task, leading to data being (re)used [Beyan *et al.* 2020]
  - Personal Health Train (PHT) Approach [Beyan *et al.* 2020]
  - DataSHIELD [Wilson *et al.* 2017]

Example of infrastructure for distributed data analysis

DataSHIELD: ‘distributed approach that allows the analysis of sensitive individual- level data from one study, and the co- analysis of such data from several studies simultaneously without physically pooling them or disclosing any data’ [Wilson *et al.* 2017].



An example infrastructure for single site DataSHIELD.

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Storage

What is storage?

Difference between backup, archive and publication

	Backup	Archive	Publication
Access	Possibility of co-working solutions	For the data producer only	Access to *others*
Reuse	• To keep data still being worked on safe • To restore the original only	Partial reuse	Possibility of *reuse*
Persistence	~ 1 year	~ 10 years	Depends on the publishing institution
Versions	Usually several data versions	Final version, static records	Final version
Formats	Working formats	Preservation formats	Depends on the publishing institution
Location	Often stored locally	Stored at official institutions	

Source: Cozatl *et al.* 2021

Which formats and media should be used?

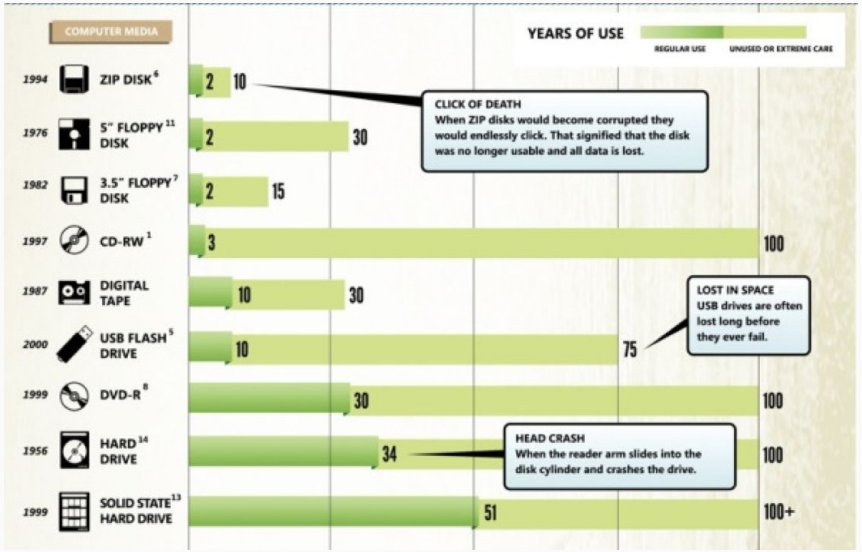
Format recommendation

Save files in the original software format and in an additional recommended file format, i.e. a format that is:

- **Open** (>< proprietary)
- **Machine-readable**
- **Well-documented**
- In **widespread use**

(e.g. CSV, XML, TXT, PDF/A)

Media: the lifespan of storage data



Source: [Crashplan]

Benefits of long-term preservation

To researchers

- To make data:
  - Findable, Accessible, Interoperable, Reusable (FAIR)
  - Readable
- Requirement from funding organizations (sometimes)

To societal challenges

- Reproducibility
- Integrity & validity
- Financial implications
- Global responses (e.g. CoViD-19)
- Reduce animal testing
- Cultural & political heritage
- Economic benefits

Source: Venkataraman 2021, Rathmann *et al.* 2021

What are valuable data and what are not?

Five steps to decide what data to keep:

1. Identify **reuse purposes** that the data could fulfil
2. Identify data that must be kept considering **funder requirements** and **legal** or **policy compliance risks**
3. Identify data that should be kept as it may have **long-term value**
4. Weigh up the **costs**
5. Complete the **data appraisal**, including how to prepare the data for deposit or the justification for not keeping them

Source: DCC, Rathmann *et al.* 2021

IRODs Archive JGU

iRODS Archive JGU

- Long term archive
- 2 copies at different locations (tape and SSD/HDD)
- Encrypted storage
- granual access control (permissions)
- basic metadata
- command line Linux tool and WebUI*
- 10+ years
- publication possibility
- Works like virtual file system

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- ➔ Q&A

National Research Data Infrastructure (NFDI)

The National Research Data Infrastructure (NFDI)

https://www.youtube.com/watch?v=uJ01g9m8uE4&t=78s&ab_channel=DFGbewegt

Natural & Life-Science related NFDI consortia

Natural & Life-Science related NFDI consortia

- Chemistry Consortium in the NFDI (NFDI4Chem)
- German Human Genome-Phenome Archive (GHGA)
- NFDI Consortium Earth System Science (NFDI4Earth)
- NFDI Consortium of Plant Research (DataPLANT)
- NFDI for Biodiversity, Ecology & Environmental Data (NFDI4Biodiversity)
- NFDI for Catalysis-Related Sciences (NFDI4Cat)
- NFDI for Microbiota Research (NFDI4Microbiota)
- NFDI for Personal Health Data (NFDI4Health)

Involvement of JGU Mainz in NFDI consortia

JGU is Co-Applicant in:

- NFDI4Chem
- PUNCH4NFDI
- NFDIxCS (3rd round)

JGU is Participant in:

- NFDI4Culture
- NFDI4Health
- TEXT+
- NFDI4Objects (3rd round)
- NFDI4Memory (3rd round)

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Further offer: content

- **Topics:** same as today, but covered in more details
  - Topics covered by **ZB MED**:
    - Discipline-specific content, e.g. ELNs, metadata
    - Best practice examples, such as NFDI4Health and NFDI4Microbiota
  - Topics covered by **JGU Mainz**:
    - Local services and infrastructure
    - Role within NFDI4Chem
- **Target audience:** subject specific, e.g. for (bio-)medical researchers working in the lab, researchers running clinical trials/studies

Further offer: format

- **6-hour** workshop, spread over two or four days
- **Interactive activities**, such as:
  - Polls
  - Exercises
  - Discussions
- **Cost of ZB MED:** ~ 900 Euro (preparation, conducting, follow-up)

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- ➔ **Q&A**

Q&A

Photo by Jon Tyson on Unsplash

Thank you!

For further information we are at your disposal

ZB MED – Information Centre for Life Sciences
Gleueler Straße 60
50931 Köln

forschungsdaten@zbmed.de
www.zbmed.de

Johannes Gutenberg University Mainz
Saarstr. 21
55122 Mainz

forschungsdaten@uni-mainz.de
https://www.forschungsdaten.uni-mainz.de/