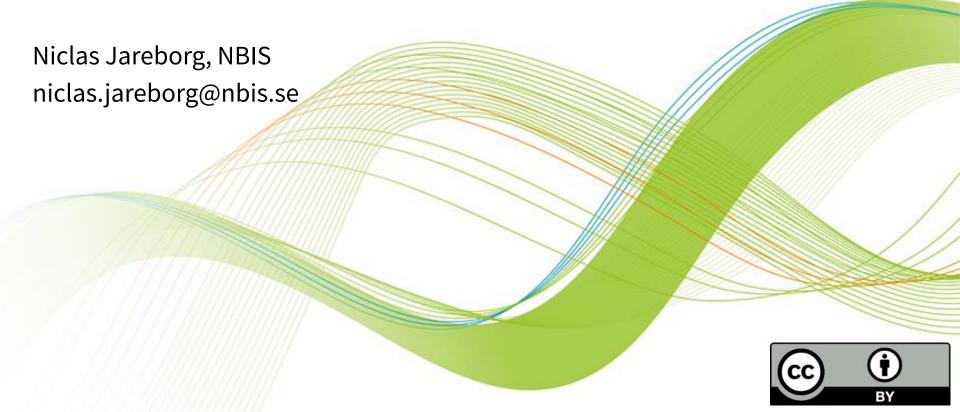




Managing your data







How do you know how an old result was generated?



The Research Data Life Cycle

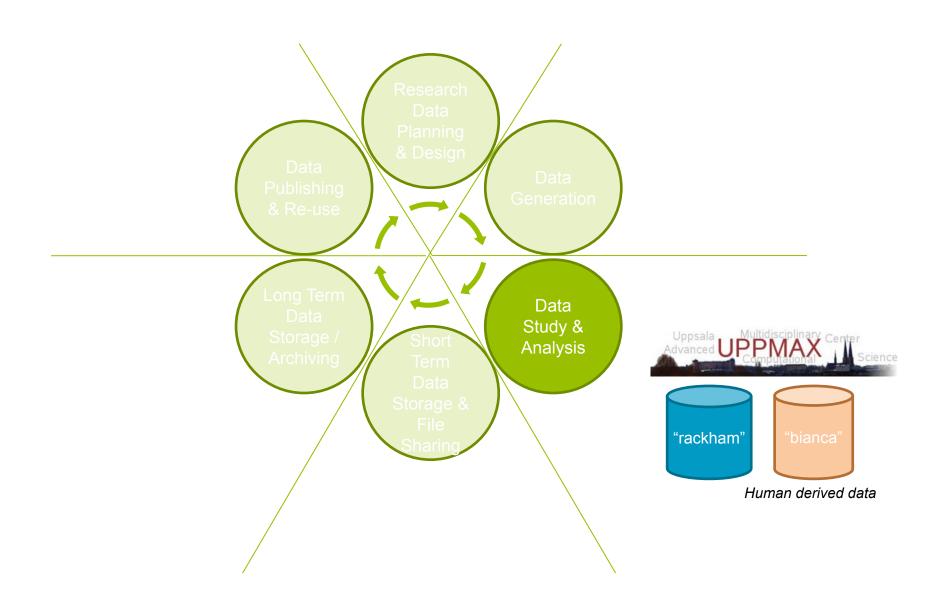






Study & Analysis







Structuring data for analysis



- Guiding principle
 - "Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why."
- Research reality
 - "Everything you do, you will have to do over and over again"
 - Murphy's law





My rule of thumb: every analysis you do on a dataset will have to be redone 10–15 times before publication. Plan accordingly. #Rstats





Structuring data for analysis



Poor organizational choices lead to significantly slower research progress

"Your primary collaborator is yourself six months from now, and your past self doesn't answer e-mails."



First step - Organization

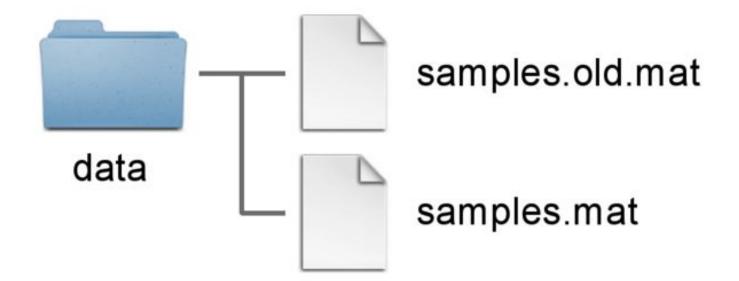






Now what?

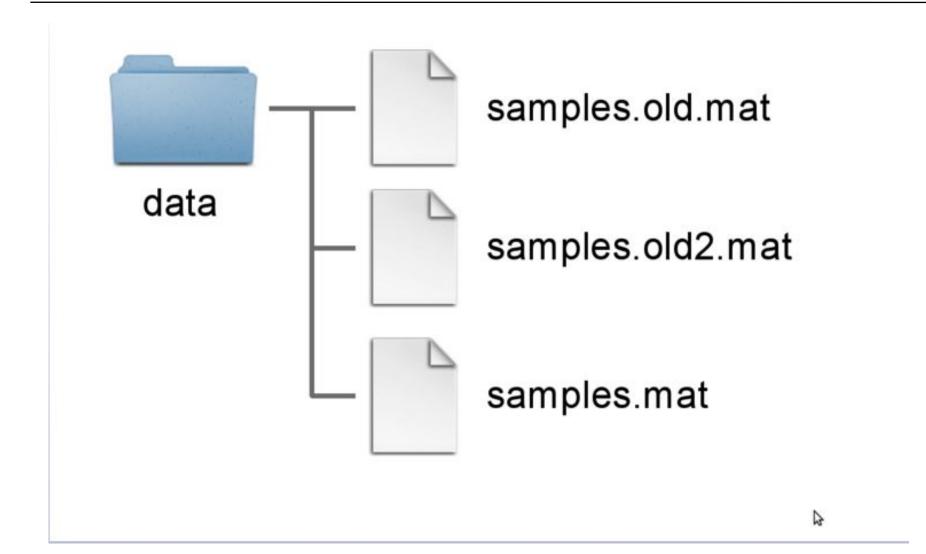






I guess this is alright

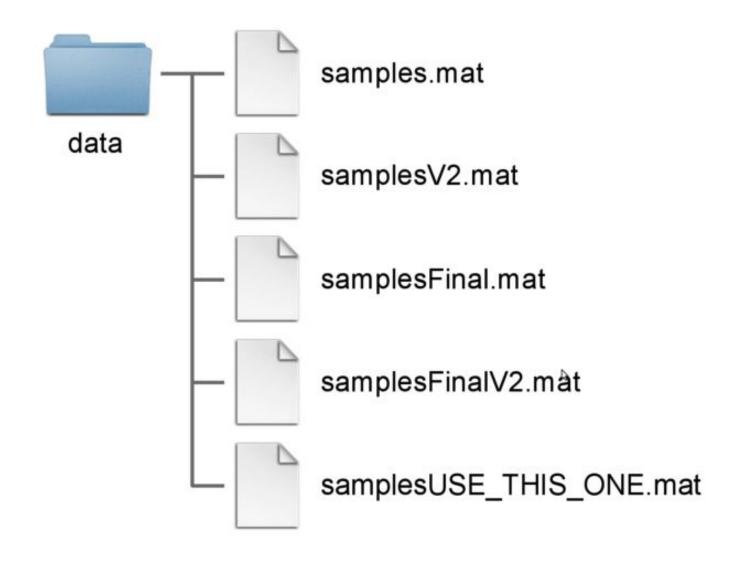






Which one is the most recent?

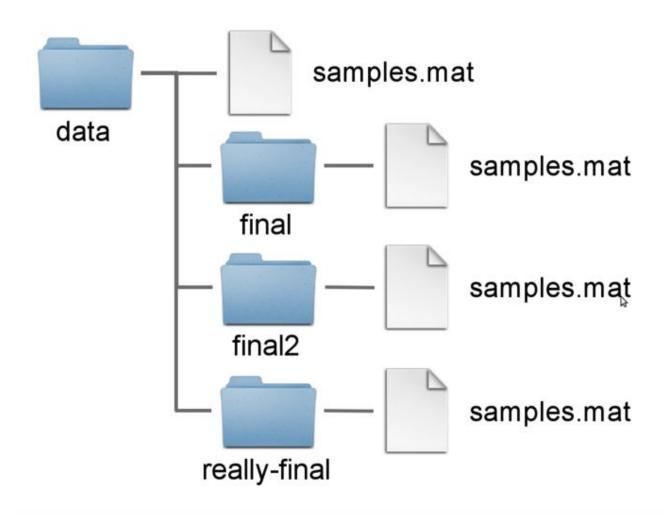






Another (bad) common approach SciLifeLab

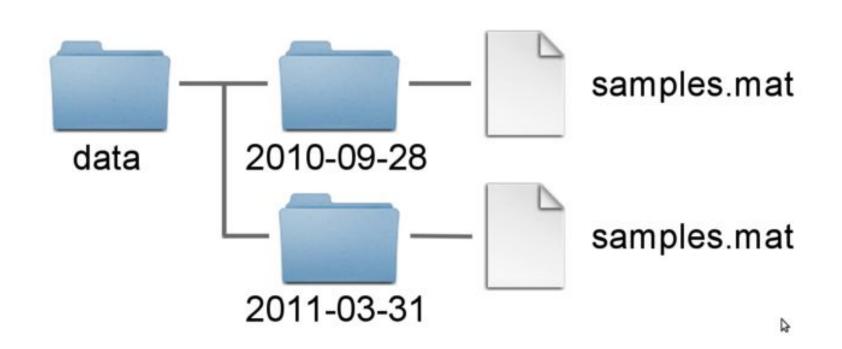






A possible solution







Suggested best practices



- There is a folder for the raw data, which do not get altered, or intermixed with data that is the result of manual or programmatic manipulation. I.e., derived data is kept separate from raw data, and raw data are not duplicated.
- Code is kept separate from data.
- Use a version control system (at least for code) e.g. git
- There is a **scratch directory for experimentation**. Everything in the scratch directory can be deleted at any time without negative impact.
- There should be a **README in every directory**, describing the purpose of the directory and its contents.
- Use file naming schemes that makes it easy to find files and understand what they are (for humans and machines)
- Use **non-proprietary formats** .csv rather than .xlsx
- Etc...



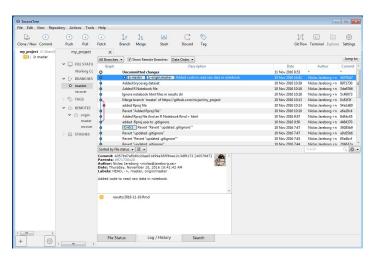
Version control



- What is it?
 - A system that keeps records of your changes
 - Allows for collaborative development
 - Allows you to know who made what changes and when
 - Allows you to revert any changes and go back to a previous state
- Several systems available
 - git, RCS, CVS, SVN, Perforce, Mercurial, Bazaar
 - git
 - Command line & GUIs
 - Remote repository hosting
 - GitHub, Bitbucket, etc









Suggested best practices



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- Etc...



File naming



- Three principles
 - Machine readable
 - Human readable
 - 3. Plays well with default ordering

NO

myabstract.docx
Joe's Filenames Use Spaces and Punctuation.xlsx
figure 1.png
fig 2.png
JW7d^(2sl@deletethisandyourcareerisoverWx2*.txt

YES

2014-06-08_abstract-for-sla.docx joes-filenames-are-getting-better.xlsx fig01_scatterplot-talk-length-vs-interest.png fig02_histogram-talk-attendance.png 1986-01-28_raw-data-from-challenger-o-rings.txt



Suggested best practices



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- Etc...



Non-proprietary formats



- A text-based format is more future-safe, than a proprietary binary format by a commercial vendor
- Markdown is a nice way of getting nice output from text.
 - Simple & readable formating
 - Can be converted to lots of different outputs
 - HTML, pdf, MS Word, slides etc
- Never, never, never use Excel for scientific analysis!
 - Script your analysis bash, python, R, ...





Tabular data / Spreadsheets



DO

- Keep your raw data raw; calculations and analyses should be done in a copy of the file
- Put variables in columns and observations in rows
- Give each column a descriptive heading that does not include spaces, numbers, or special characters
- Differentiate between zero and null values
- Validate your data
- Keep a separate txt file with a title and a legend describing your dataset, and outlining any steps you take to tidy your data
- Use a version control system and back up your files
- Export each data file in an open non-proprietary format such as CSV or TAB, with a name that appropriately reflects the content of that file
- Check your data thoroughly. Your data should receive the same care as your publications

DO NOT

- Put more than 1 piece of information in a cell
- Use colour coding, embedded charts, comments or tables – your spreadsheet is not a lab book
- Include special (i.e. non alphanumeric) characters within the spreadsheet, including commas
- Use merged or blank cells
- Create multiple worksheets within a spreadsheet

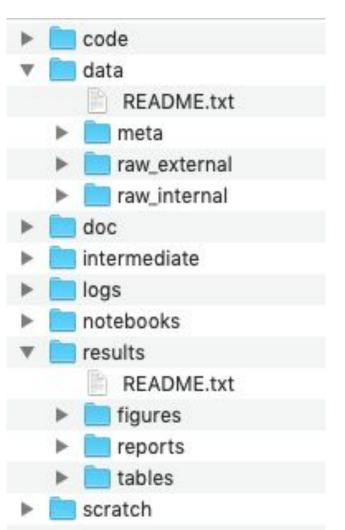
F10000





Directory structure for a sample project





all code needed to go from input files to final results raw and primary data, essentially all input files, **never** edit!

documentation for the study

output files from different analysis steps, can be deleted

logs from the different analysis steps

output from workflows and analyses

temporary files that can be safely deleted or lost



Metadata



- "Data about the data"
 - From what was the data generated?
 - How do the samples differ?
 - What where the experimental conditions?
 - Etc

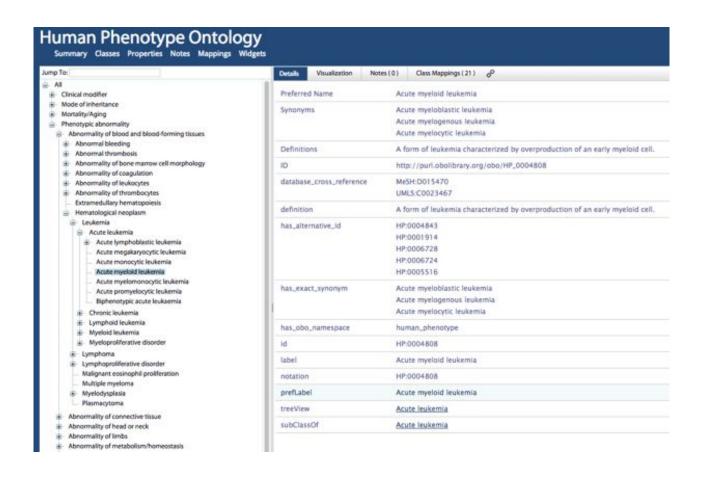
SampleID	Species	Strain	Treatment	Dose	Organ	etc
A9876	rat	Balb/c	Paracetamol	10 mg	liver	
A6543	brown rat	Bagg Albino	•	0	liver	



Metadata standards



- Controlled vocabularies / taxonomies / Ontologies
 - Agreed terms for different phenomena





Metadata standards



HOW STANDARDS PROLIFERATE: (SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)

SITUATION: THERE ARE 14 COMPETING STANDARDS.



500N:

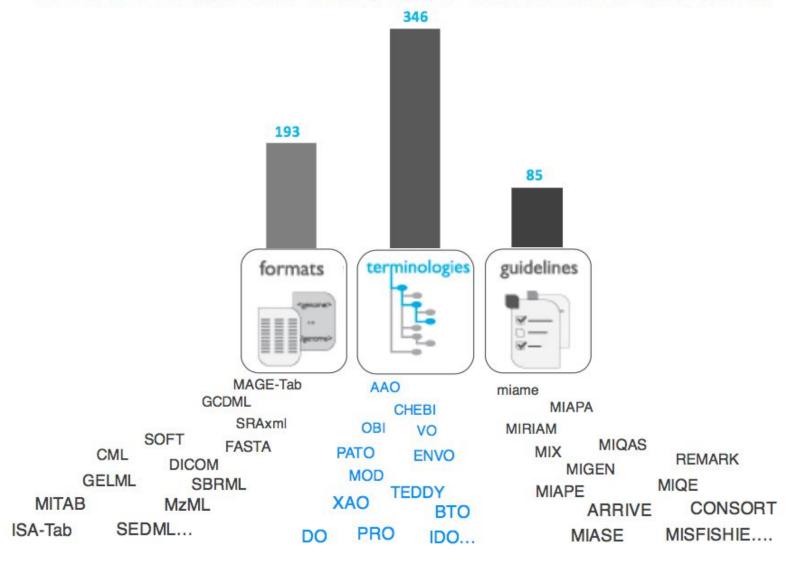
SITUATION: THERE ARE 15 COMPETING STANDARDS.



Life science standards



In the life sciences there are >600 content standards

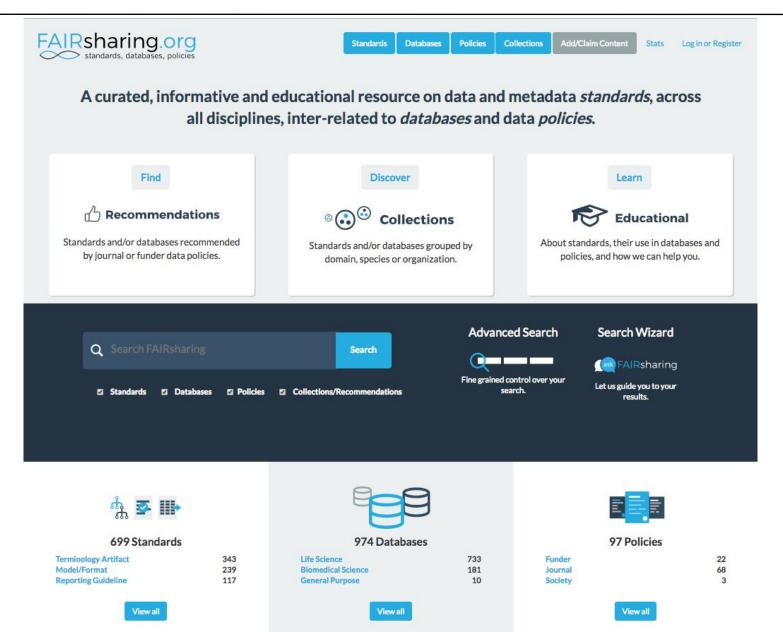




FAIRsharing.org







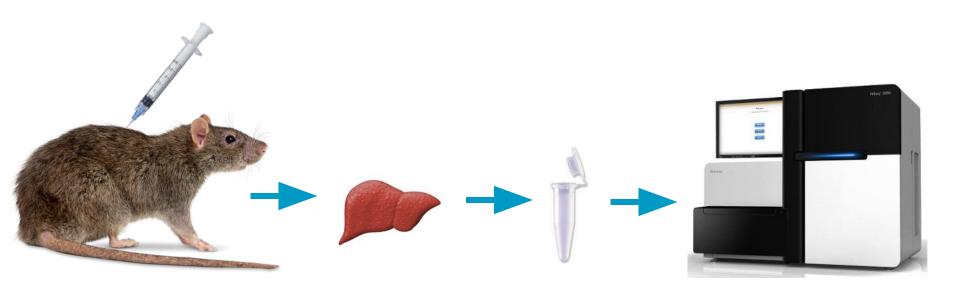


Metadata



SampleID	Species NCBI:txid	! SciName	Strain MGI_ID	name	Compound ChEBI_ID	name	Dose mg
A9876	10116	Rattus norvegicus	MGI:2161072	BALB/c	CHEBI: 46195	paracetamol	10
A6543	10116	Rattus norvegicus	MGI:2161072	BALB/c	null	null	null

. . .

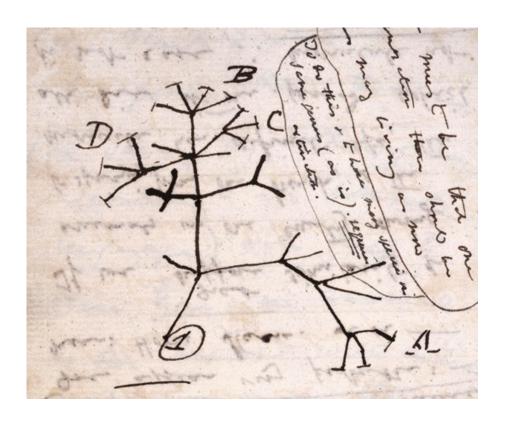




Lab notebooks



- Why?
 - You have to understand what you have done
 - Others should be able to reproduce what you have done





Lab notes – useful practices



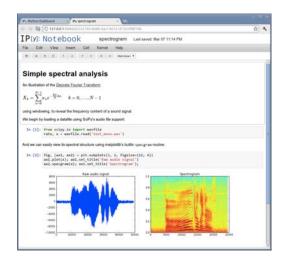
- Put in separate directory (e.g. results, documentation)
- Dated entries
- Entries relatively verbose
- Link to data and code (including versions)
 - Point to commands run and results generated
- Embedded images or tables showing results of analysis done
- Observations, Conclusions, and *ideas* for future work
- Also document analysis that doesn't work, so that it can be understood why
 you choose a particular way of doing the analysis in the end

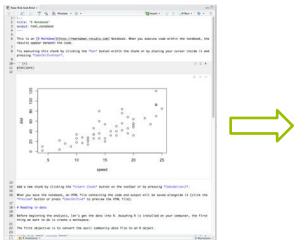


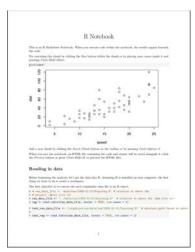
Where to take down notes



- Paper Notebook
- Word processor program / Text files
- Electronic Lab Notebooks Systems
- Computational Notebooks
 - e.g. <u>jupyther</u>, <u>R Notebooks</u> in RStudio
 - Plain text work well with version control (Markdown)
 - Embed and execute code
 - Convert to other output formats
 - html, pdf, word



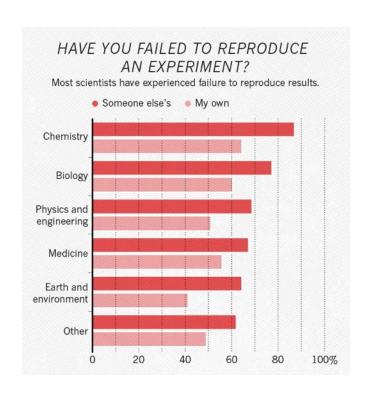


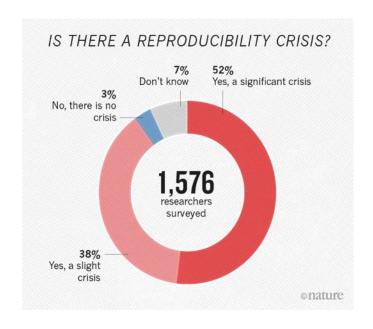




A reproducibility crisis







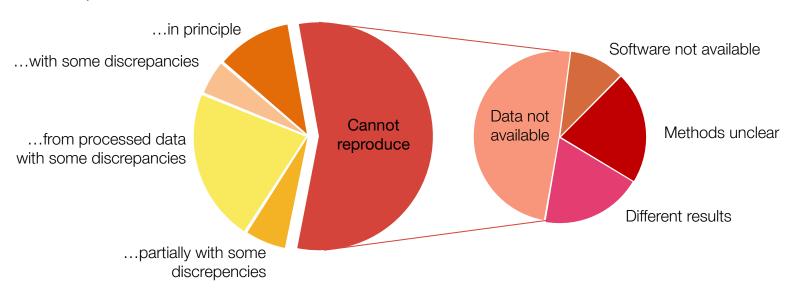


A reproducibility crisis



Reproduction of data analyses in 18 articles on microarray-based gene expression profiling published in Nature Genetics in 2005–2006:

Can reproduce...



Summary of the efforts to replicate the published analyses.

Adopted from: loannidis et al. Repeatability of published microarray gene expression analyses.

Nature Genetics 41 (2009) doi:10.1038/ng.295

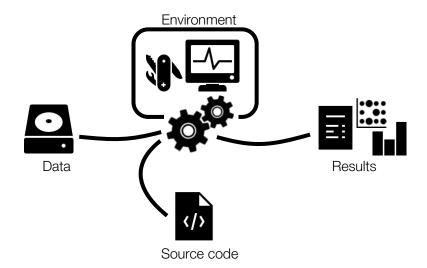


What do we mean by reproducible research?



		Dat	ta
		Same	Different
Code	Same	Reproducible	Replicable
_Code	Different	Robust	Generalizable

All parts of a bioinformatics analysis have to be reproducible:





Reproducible Research tutorials

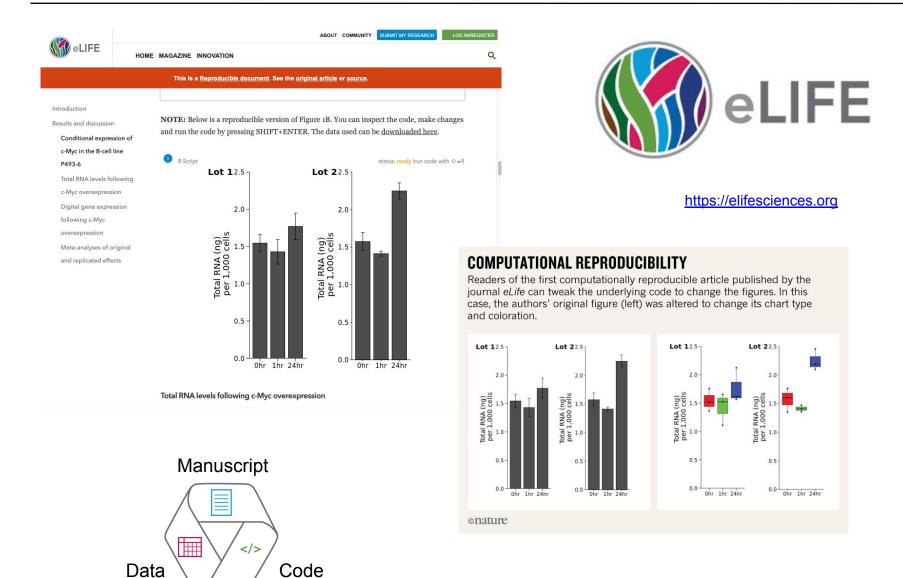


↑ NBIS Reproducible research course Environment management	
Search docs Set up and manage the project environment	
Welcome	
About Start here!	
The course	
Version control Schedule Version control Track and backup your project history Move from separate scripts to a con	
Travelinfo	
Feedback Snaken	nake
Tutorials	
Introduction to the tutorials Reports	lotebooks
Introduction to the tutorials Connect code, output and text in fancy reports Document your exploration to the tutorials	
The case study R Markdown	or
The case study Setup R Markdown from R Studio	.CI
For Mac / Linux users	
For Windows users Containerization	
Make your project self-contained and distributable	
Conda Snakemake docker	
Snakemake	
Git	
Jupyter Reproducible Interactive	
R Markdown Do it all! Workflow environment notebooks	
Docker	
Take down	
Cloud services developers lave.	



Reproducible publications

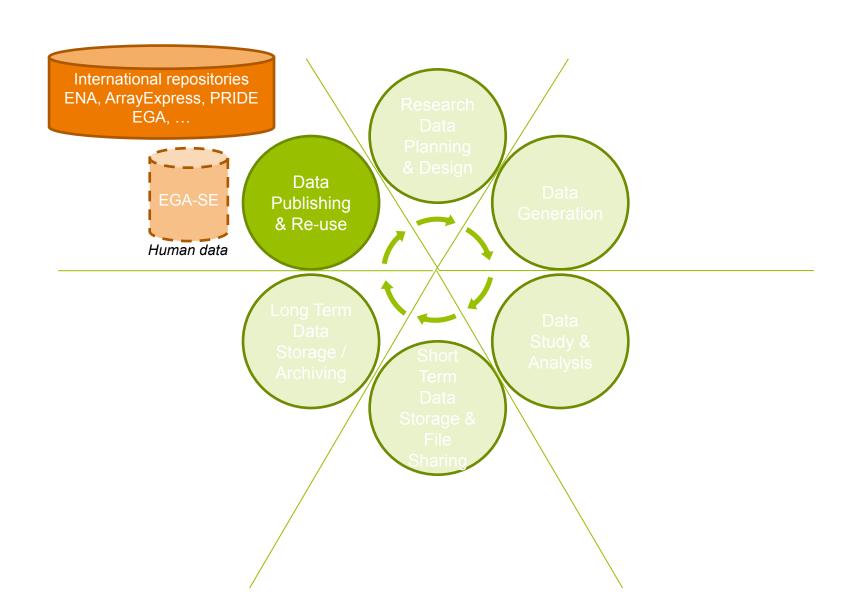






Data Publishing & Re-use









Why should you make research data available for others?



Open Access



The practice of providing **on-line access** to scientific information that
is **free of charge** to the end-user
and that is **re-usable**.





Open Access



- Democracy and transparency
 - Publicly funded research data should be accessible to all
 - Published results and conclusions should be possible to check by others
- Research
 - Enables others to combine data, address new questions, and develop new analytical methods
 - Reduce duplication and waste
- Innovation and utilization outside research
 - Public authorities, companies, and private persons outside research can make use of the data
- Citation
 - Citation of data will be a merit for the researcher that produced it





Open Access to research data



- Strong international movement towards Open Access (OA)
- European Commission recommended the member states to establish national guidelines for OA
 - Swedish Research Council (VR) submitted proposal to the government Jan 2015
- Research bill 2017–2020 28 Nov 2016
 - "The aim of the government is that all scientific publications that are the result of publicly funded research should be openly accessible as soon as they are published. Likewise, research data underlying scientific publications should be openly accessible at the time of publication." [my translation]
- 2018 VR assigned by the government to coordinate national efforts to implement open access to research data









Research Ethics



- Is it ethical to do bad/careless science?
 - Wasting resources
 - ... or even resulting in dangerous medical practices
 - Contribute to the current research credibility crisis
 - harming the profession
 - harming the public trust
- But!
 - Careless science -> longer CV





What is needed for others to be able to re-use your data?



Data Management Snafu







FAIR



- To be useful for others data should be
 - FAIR Findable, Accessible, Interoperable, and Reusable
 ... for both Machines and Humans

Wilkinson, Mark et al. "The FAIR Guiding Principles for scientific data management and stewardship". Scientific Data 3, Article number: 160018 (2016) http://dx.doi.org/10.1038/sdata.2016.18



Box 2 | The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
- A1.1 the protocol is open, free, and universally implementable
- A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- 12. (meta)data use vocabularies that follow FAIR principles
- 13. (meta)data include qualified references to other (meta)data

To be Reusable:

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
- R1.1. (meta)data are released with a clear and accessible data usage license
- R1.2. (meta)data are associated with detailed provenance
- R1.3. (meta)data meet domain-relevant community standards

DOI: 10.1038/sdata.2016.18





SciLifeLab G20 HANGZHOU SUMMIT

'We support appropriate efforts to promote open science and facilitate appropriate access to publicly funded research results on findable, accessible, interoperable and reusable (FAIR)'

HANGZHOU, CHINA 4-5 SEPTE





FAIR



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- R1.3. (meta)data meet domain-relevant community standards



Findable



- Long-term storage
 - Data should not disappear



- Persistent identifiers
 - Possibility to refer to a dataset over long periods of time
 - Unique
 - e.g. DOIs (Digital Object Identifiers)



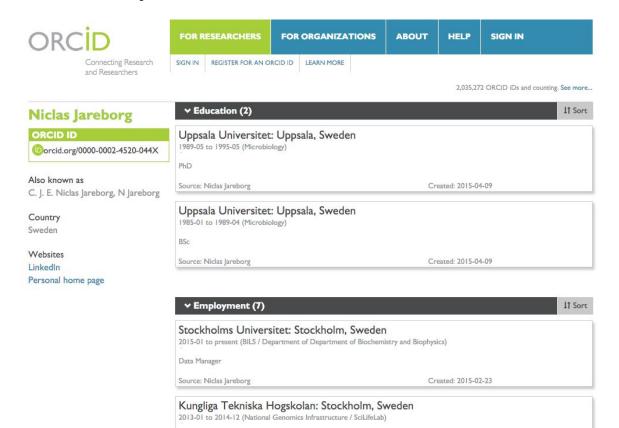
- Discoverability
 - Expose dataset metadata through search functionalities



Persistent identifier for yourself



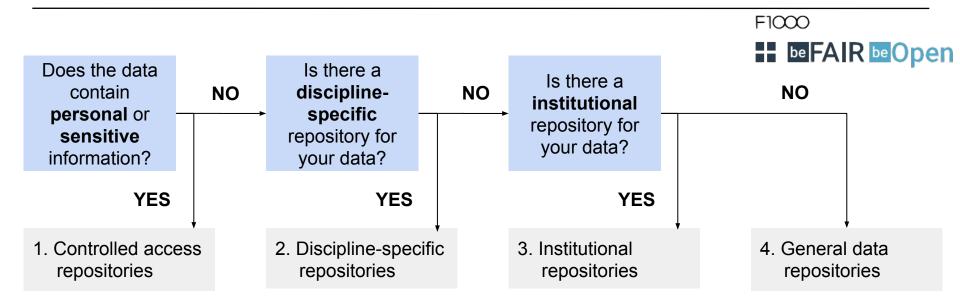
- ORCID is an open, non-profit, community-driven effort to create and maintain a registry of unique researcher identifiers and a transparent method of linking research activities and outputs to these identifiers.
- http://orcid.org
- Persistent identifier for you as a researcher





Repositories































Etc...



Accessible



International public repositories

























dbSNP Short Genetic Variations



- Best way to make data FAIR
- Domain-specific metadata standards

Strive towards uploading data to its final destination already at the beginning of a project

Study & Analysis



Recommended repositories



ELIXIR Deposition Database list

Deposition Database	Data type	International collaboration framework ¹
ArrayExpress	Functional genomics data. Stores data from high-throughput functional genomics experiments.	
BioModels	Computational models of biological processes.	
BioSamples	BioSamples stores and supplies descriptions and metadata about biological samples used in research and development by academia and industry.	NCBI BioSamples database
BioStudies	Descriptions of biological studies, links to data from these studies in other databases, as well as data that do not fit in the structured archives.	
EGA	Personally identifiable genetic and phenotypic data resulting from biomedical research projects.	European Bioinformatics Institute and the Centre for Genomic Regulation
EMDB	The Electron Microscopy Data Bank is a public repository for electron microscopy density maps of macromolecular complexes and subcellular structures.	
ENA	Nucleotide sequence information, covering raw sequencing data, contextual data, sequence assembly information and functional and taxonomic annotation.	International Nucleotide Sequence Database Collaboration
EVA	The European Variation Archive covers genetic variation data from all species.	dbSNP and dbVAR
IntAct	IntAct provides a freely available, open source database system and analysis tools for molecular interaction data.	The International Molecular Exchange Consortium
MetaboLights	Metabolite structures and their reference spectra as well as their biological roles, locations and concentrations, and experimental data from metabolic experiments.	
PDBe	Biological macromolecular structures.	wwPDB
PRIDE	Mass spectrometry-based proteomics data, including peptide and protein expression information (identifications and quantification values) and the supporting mass spectra evidence.	The ProteomeXchange Consortium



Scientific Data Recommended Data Repositories

Biological sciences 1

Nucleic acid sequence 🧷

Sequence information should be deposited following the MIxS guidelines.

Simple genetic polymorphisms or structural variations should be submitted to dbSNP or dbVar (please note that these repositories cannot accept sensitive data derived from human subjects); the NCBI Trace Archive may be used for capillary electrophoresis data, while SRA accepts NGS data only.

DNA DataBank of Japan (DDBJ)	view FAIRsharing entry		
European Nucleotide Archive (ENA)	view FAIRsharing entry		
GenBank	view FAIRsharing entry		
dbSNP	view FAIRsharing entry		
European Variation Archive (EVA)	view FAIRsharing entry		
dbVar	view FAIRsharing entry		
Database of Genomic Variants Archive (DGVa)	view FAIRsharing entry		
EBI Metagenomics	view FAIRsharing entry		
NCBI Trace Archive	view FAIRsharing entry		
NCBI Sequence Read Archive (SRA)	view FAIRsharing entry		
NCBI Assembly			

Protein sequence 1

UniProtKB view FAIRsharing entry

Molecular & supramolecular structure 🧷

These repositories accept structural data for small molecules (COD); peptides and proteins (all); and larger assemblies (EMDB).

Small molecule crystallographic data should be uploaded to Dryad or figshare before manuscript submission, and should include a .cif file, a structural figure with probability ellipsoids, and structure factors for each structure. Both the structure factors and the structural output must have been checked using the IUCR's CheckCIF routine, and a copy of the output must be included at submission, together with a justification for any alerts reported.

Protein Circular Dichroism Data Bank (PCDDB) view FAIRsharing entry

https://www.elixir-europe.org/platforms/data/elixir-deposition-databases

https://www.nature.com/sdata/policies/repositories#life



"Long-tail data" repositories



- Research data that doesn't fit in structured data repositories
- Data publication persistent identifiers
- Metadata submission not tailored to Life Science
 - Affects discoverability
 - (Less) FAIR
- Sensitive data a potential issue
 - Figshare https://figshare.com/
 - scilifelab.figshare.com coming soon!
 - EUDAT http://eudat.eu/
 - Data Dryad http://datadryad.org/
 - Zenodo http://www.zenodo.org/

←more generi

more specific >



SampleID

Species

Interoperable & Re-useable *Metadata*



Standards

Repositories have recommended standards

Strain

Controlled vocabularies / Ontologies



Dose

Dampield	NCBI: txid	SciName	MGI_ID	name	ChEBI_ID	name	mg
A9876	10116	Rattus norvegicus	MGI:2161072	BALB/c	CHEBI: 46195	paracetamol	10
A6543	10116	Rattus norvegicus	MGI:2161072	BALB/c	null	null	null
						Rarent .	

Compound



Interoperable & Re-useable *Metadata*



- Standards
 - Controlled vocabularies / Ontologies
 - Agreed terms for different phenomena

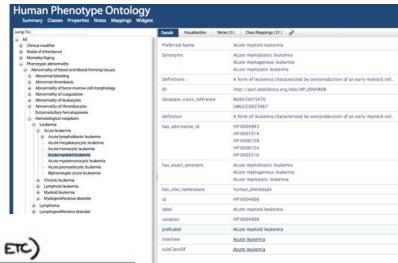
HOW STANDARDS PROLIFERATE: (SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)

SITUATION: THERE ARE 14 COMPETING STANDARDS.





STANDARDS.

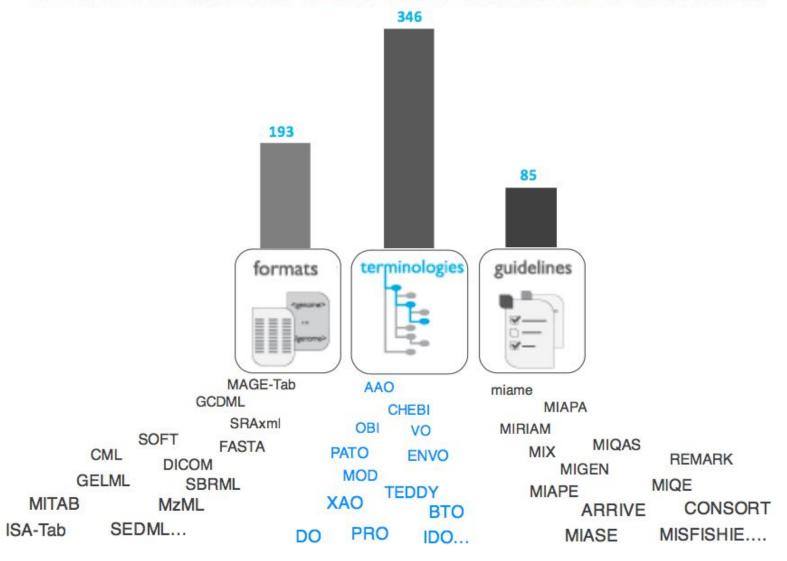




FAIRsharing.org



In the life sciences there are >600 content standards

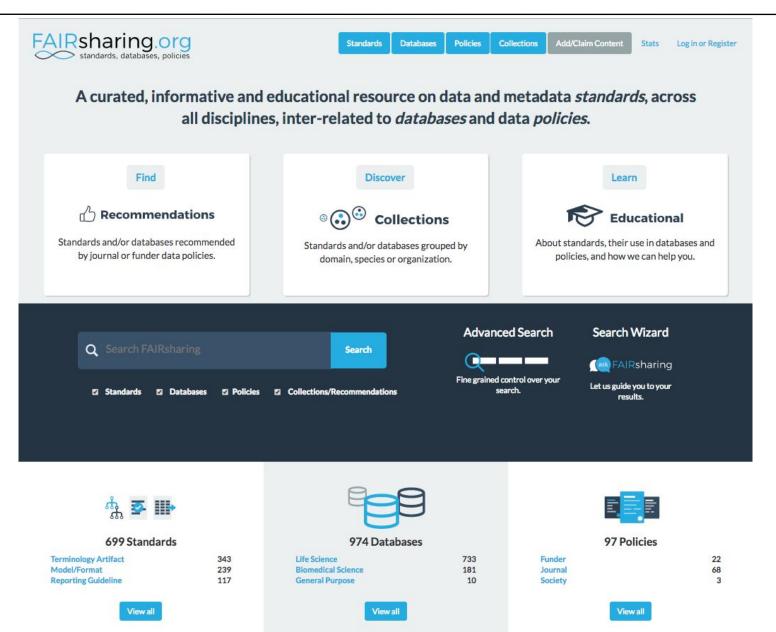




FAIRsharing.org









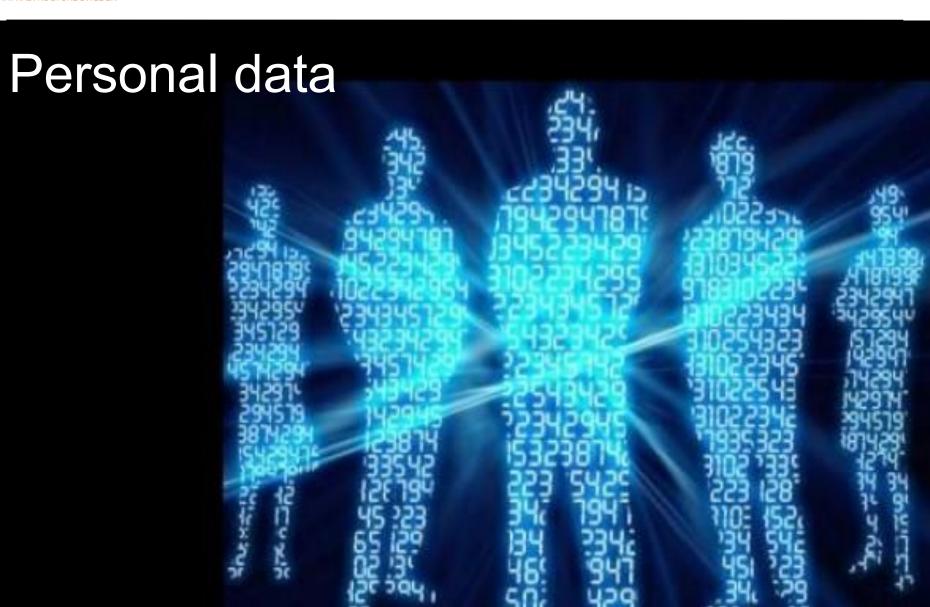


Can you share all types of data publicly?

If not, what would be the reasons?









Personal data - Legislation







GDPR



- All kinds of information that is directly or indirectly referable to a natural person who is alive constitute personal data
- To process personal data:
 - All processing of personal data must fulfil the fundamental principles defined in the Regulation, among them are:
 - Decide a purpose and stick to it
 - Identify the legal basis for data processing before it starts
- Have you defined the purpose and legal basis for handling personal data in your project?



GDPR – Sensitive data



- Special categories (Sensitive data)
 - _____ racial or ethnic origin, [...] genetic data, [...], data concerning health ... Art. 9 (1)
 - Processing is prohibited unless...
 - explicit consent is given Art. 9 (2)a
 - processing is necessary for scientific research in accordance with Article 89(1) based on Union or Member State law which shall be proportionate to the aim pursued, respect the essence of the right to data protection and provide for suitable and specific measures to safeguard the fundamental rights and the interests of the data subject. Art. 9 (2)j
 - Member State specific conditions and limitations possible for processing of health & genetic data Art. 9 (4)
 - Sweden
 - Consent?
 - Public interest → Ethical review necessary (often includes consent)



GDPR - Help



A Data Protection Officer (dataskyddssombud)

https://insidan.liu.se/dataskyddsforordningen/anmalan-

av-personuppgiftsbehandling?l=sv

- The natural person that is responsible for ensuring that the organization/company adheres to the GDPR
- Educate
- Audit
- Contact point between organization and Data Protection Agency

GU LU https://personuppgifter.blogg.lu.se https://medarbetarportalen.gu.se/projekt-process/aktu ella-projekt/dataskyddsforordning SU ΚI https://www.su.se/medarbetare/organisation-styrning/j uridik/personuppgifter/dataskyddsf%C3%B6rordninge https://ki.se/medarbetare/gdpr-pa-karolinska-institutet **KTH** UmU https://intra.kth.se/anstallning/anstallningsvillkor/att-va ra-statligt-an/behandling-av-person/dataskyddsforordn https://www.aurora.umu.se/regler-och-riktlinjer/juridik/ ingen-gdpr-1.800623 personuppgifter/ UU LiU https://mp.uu.se/web/info/stod/dataskyddsforordninge

n



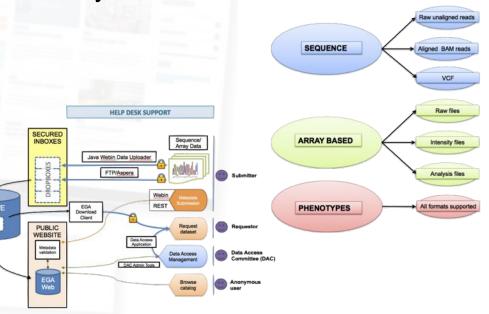
What about publishing sensitive data? Scil



"As open as possible, as closed as necessary"

EGA – European Genome-phenome Archive

- EUROPEAN GENOME-PHENOME ARCHIVE
- Repository that promotes the distribution and sharing of genetic and phenotypic data consented for specific approved uses but not fully open, public distribution.
- All types of sequence and genotype experiments, including case-control, population, and family studies.
- Data Access Agreement
 - Defined by the data owner
- Data Access Committee DAC
 - Decided by the data owner





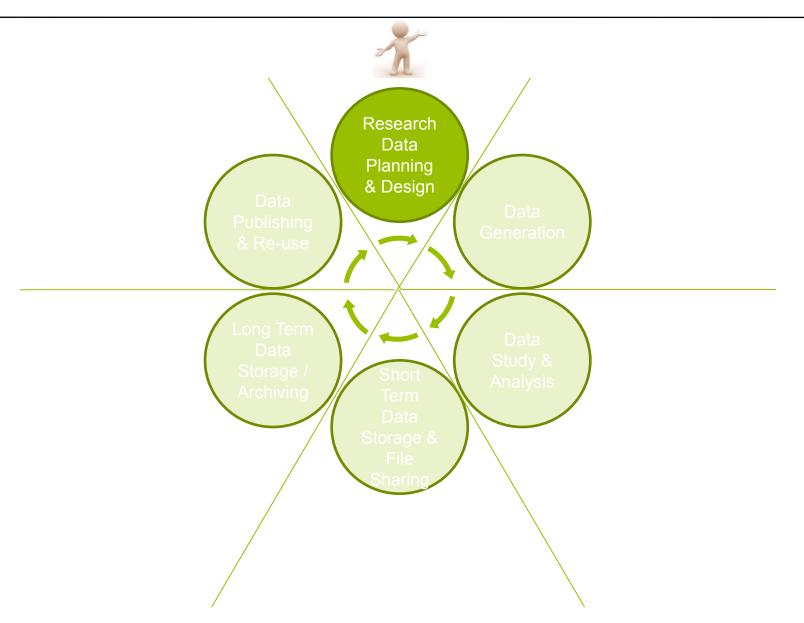


When should you start planning for how to manage you data?



Planning & Design







Data Management Plans



Will become a standard part of the research funding application process

- Data collection data types and volumes, analysis code
- Data organization folder and file structure, and naming
- Data documentation data and analysis, metadata standards
- **Data storage** storage/backup/protection & time lines
- **Data policies** conditions/licences for using data & legal/ethical issues
- Data sharing When and How will What data (and code) be shared
- **Roles and responsibilities** who's responsible for what & is competence available
- Budget People & Hardware/Software



By 2019, all who receive grants from us must have a data management plan

As from spring 2019, if you are awarded a grant from the Swedish Research Council you must have a plan for how the research data generated within your project shall be managed.

You must not send in your data management plan to us when you apply for a grant, but your administrating organisation will be responsible for ensuring that a data management plan is in place when you start your project or corresponding, and that the plan is maintained.



Data Management Plans







EDITORIAL · 13 MARCH 2018

Everyone needs a data-management plan

They sound dull, but data-management plans are essential, and funders must explain why.

By 2019, all who receive grants from us must have a data management plan

As from spring 2019, if you are awarded a grant from the Swedish Research Council you must have a plan for how the research data generated within your project shall be managed.

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National guidelines



- VR & SUHF (Association of Swedish Higher Education Institutions)
 - Work in progress
- Central parts of a data management plan
 - Based on Science Europe's "Core Requirements for Data Management Plans"
 - Description of data reuse of existing data and/or production of new data
 - Documentation and data quality
 - 3. Storage and backup
 - 4. Legal and ethical aspects
 - 5. Accessibility and long-term storage
 - 6. Responsibility and resources



Planning ahead



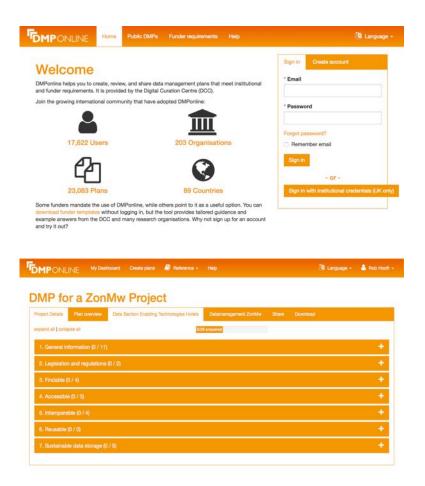
Consider structuring metadata in the format needed by the repository already at planning stage



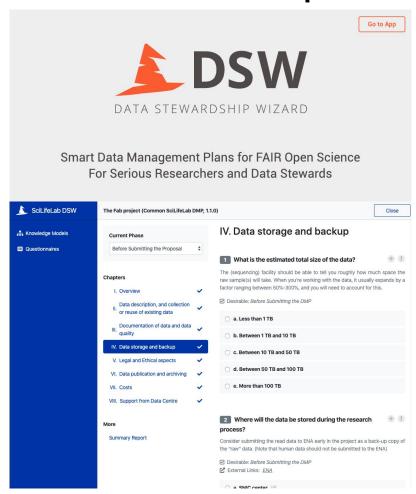
DMP tools



DMPonline



ELIXIR Data Stewardship Wizard



https://ds-wizard.org/

https://dsw.scilifelab.se



NBIS Data Management support



- Project planning
 - Metadata
 - File formats
 - Licensing
 - Data Management Plans
- Data analysis
- Data publication and submission
 - Support submissions to public repositories
 - Metadata
 - DOIs to dataset (if needed)



Take home messages



- Consider doing a Data Management Plan for your project
 - How do you ensure that your research output is FAIR?
- Plan for submitting "raw data" to public repositories as early as possible
- Organize project metadata from the start
 - In ways that makes it easy to submit to public repositories
 - Use available standards
- Pick a thought-through file and folder structure organization for your computational analyses
- Strive for reproducibility
 - Data & Code
- Be aware that there are legal aspects to processing human data
- Ask for help if you need it!



Source Acknowledgements



- Research Data Management, EUDAT -http://hdl.handle.net/11304/79db27e2-c12a-11e5-9bb4-2b0aad496318
- Noble WS (2009) <u>A Quick Guide to Organizing Computational Biology Projects. PLoS Comput Biol 5(7): e1000424. doi:10.1371/journal.pcbi.1000424</u>
- Reproducible research
 - Reproducible Science Curriculum <u>https://github.com/Reproducible-Science-Curriculum/rr-init</u>
 - Leif Väremo & Rasmus Ågren
 - https://bitbucket.org/scilifelab-lts/reproducible research example/src
 - https://nbis-reproducible-research.readthedocs.io/en/latest/
- GDPR
 - Datainspektionen –
 https://www.datainspektionen.se/lagar--regler/dataskyddsforordningen/
- ... and probably others I have forgotten