

# School on Synchrotron Light Sources and their Applications



## Open Science and FAIR data

25<sup>th</sup> January, 2023

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Role: ESRF Data Policy manager and PaNOSC coordinator



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852

# Outline of Talk

This talk will address the topic of Open Science and FAIR Data for scientists doing research in order to answer the following questions:

- **Open Science and FAIR Data**

What is this ?

Why do this ?

What to do ?

What to expect ?

What to try ?

What to learn ?



## Andy Götz

1. Joined **ESRF** in **1988**, worked on **accelerator controls**, **beamline controls**, **data management**, **manager**
2. Managed the software team who developed the software for the ESRF upgrade **ESRF-EBS**
3. Coordinated the EU H2020 **PaNOSC** project (<https://panosc.eu>) on making **FAIR data reality** for Photon and Neutron sources in Europe (**2018 – 2022**)
4. Participating in the **Photon and Neutron** efforts for **FAIR data** (**2002 – now**)
5. Member of the **IUCr Commission on Data** (**2015 – now**)



**Kilobytes**  
to  
**Petabytes**  
in  
**40 years**



# Definition of Science by the Science Council

Science is the pursuit and application of knowledge and understanding of the natural and social world following a systematic methodology.

Scientific methodology includes the following:

- Objective observation: Measurement (not necessarily using mathematics as a tool)
- Evidence
- Experimentation: for testing hypotheses
- Induction: rules or conclusions drawn from facts or examples
- Repetition
- Critical analysis
- Verification and validation: critical exposure to scrutiny, peer review and assessment

**Science is Evidence based  
The Evidence is the Data**

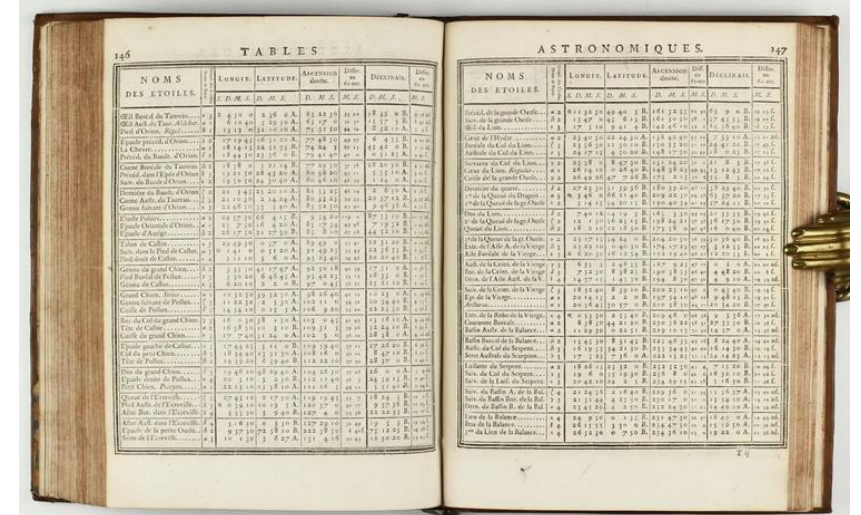
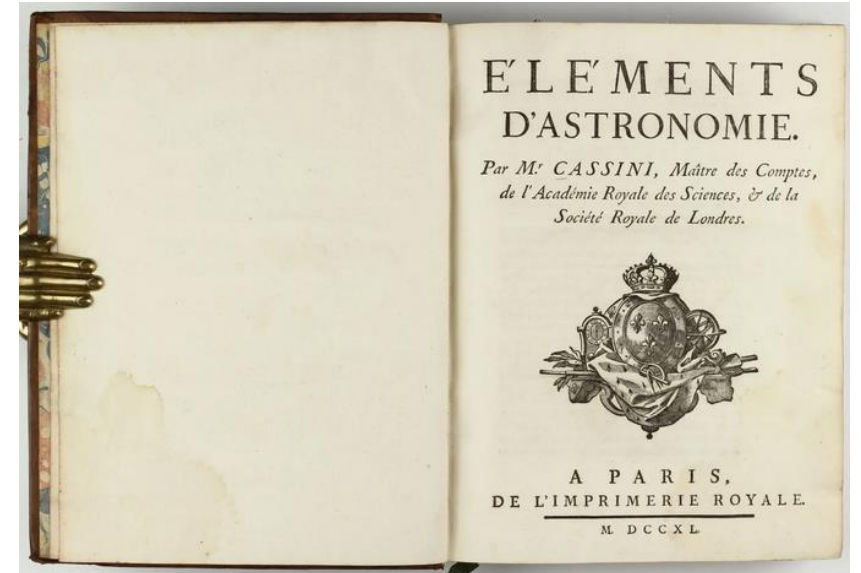
<https://sciencecouncil.org/about-science/our-definition-of-science/>





# Evolution of publishing data

- In the beginning data were published as tables in the Annals of the journals ...



# Digital technology makes publishing data easier

- Today they are published via databases and digital media ...

European Southern Observatory

ESO — Reaching New Heights in Astronomy

Public Science User Portal Intranet Contact Site Map Search Go!

Science Users Information > Science Archive Facility 18 Jan 2024

## Science Archive Facility

### Welcome to the ESO Science Archive Facility

The ESO Science Archive Facility contains data from ESO telescopes at La Silla Paranal Observatory, including the APEX submillimeter telescope on Llano de Chajnantor. All raw data from the La Silla Paranal Observatory are stored together with the corresponding calibrations, as well as selected products both contributed by the **community** or generated at **ESO**. In addition, the raw UKIDSS/WFCAM data obtained at the UK Infrared Telescope facility in Hawaii are available.

The Principal Investigators of successful proposals for time on ESO telescopes have exclusive access to their scientific data for the duration of a proprietary period, normally of one year, after which the data becomes available to the community at large. Please read the **ESO Data Access Policy** statement for more information, along with the **relevant FAQs**.

Browsing the archive does not require authentication. Please **acknowledge the use of archive data** in any publication.

There are three main ways to access the archive, varying for content and presentation/interface: the usual Raw Data query form, the innovative Science Portal to browse and access the processed data, and the novel Programmatic and Tools access which permits direct database access to both raw and processed data, and to the ambient condition measurements, also in a scriptable and VO manner. Other query forms are available in the table at the bottom of this page.

Raw Data

Science Portal  
Processed Data

Catalogue Facility  
Catalogue Data

Programmatic  
Raw, Processed, Catalogue, and Ambient Data

Community Forum  
Share ideas, ask questions, send feedback

<http://archive.eso.org/cms.html>

ARS  
Astronomers' Action Society

ISC

# Example of federated data search portal

<https://data.panosc.eu/search/?q=lung>

The screenshot displays the panosc search portal interface. At the top left is the panosc logo. A search bar contains the query 'lung', and a magnifying glass icon is followed by the text '18 documents found'. On the left side, there is a sidebar with several filter categories: Facility (set to 'all'), Technique (a dropdown menu), Chemical Formula (an empty input field), Incident Wavelength (with 'min', 'max', and 'nm' dropdowns), Incident Photon Energy (with 'min', 'max', and 'eV' dropdowns), Temperature (with 'min', 'max', and 'K' dropdowns), and Pressure (with 'min', 'max', and 'Pa' dropdowns). The main content area shows three search results, each with a relevance score in a pink bar on the right:

- 10.15151/ESRF-ES-436648953** (0.900): **Insight into effects of COVID-19 on human heart and lung tissue at sub-cellular level**. COVID-19 affects multiple vital organs and leads to drastic changes in tissue architecture not only in the lung but also in the heart. The understanding of these alterations is currently very limited and no high resolution 3D data is available. We propose to investigate dama...  
Released by **ESRF** on May 7th 2024
- 10.16907/7eb141d3-11f1-47a6-9d0e-76f8832ed1b2** (0.900): **Micrometer-resolution X-ray tomographic imaging of a complete intact post mortem juvenile rat lung**. In the associate article to these data sets, we present an X-ray tomographic imaging method that is well suited for pulmonary disease studies in animal models, to resolve the full pathway from gas intake to gas exchange. Current state-of-the-art synchrotron-based...  
Released by **PSI** on January 1st 2020
- 10.5291/ILL-DATA.9-13-653** (0.900): **Structural changes to the air-water interface following cholesterol oxidation in mixed lung lipid monolayers**. The presence of lung surfactant at the air-water interface of the lung is vital to prevent death from respiratory failure. Ozone, a pollutant in ambient air, is known to damage some components of lung surfactant and is linked with death from respiratory failure but the...  
Released by **ILL** on September 26th 2021

The bottom result is partially visible:

- 10.15151/ESRF-ES-782797417** (0.876): **Revealing modifications of asbestos after prolonged stay in the lungs**. The knowledge of the carcinogenetic and cytotoxic mechanisms of asbestos in living organism is still uncomplete, also due to a lacking characterization of the asbestos modifications during its prolonged stay in the biological tissue. To gain new knowledge on the structura...  
Released by **ESRF** on April 19th 2025

**SCARS**  
Science Clusters' Action  
Research & Society

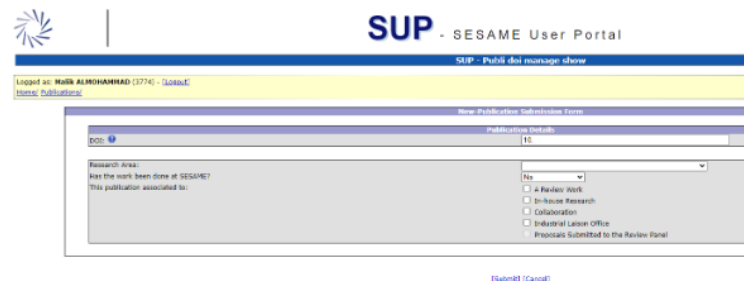




# Synchrotron facilities now propose data repositories

## Example of SESAME – thanks to Malik AlMohammad + Salman Matalgah

SESAME Data Portal



Cite Data DOIs

Dataset List 21 Logbook Shipping Samples Proposal

For users that want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the documentation for proceeding: <https://confluence.esrf.fr/display/SCKB/Globus>

Filter by samples x

	Date	Sample	Dataset	Definition	Files	Size	Processed	Download
	16:46 13 Oct 2023		Se_EXAFS_Tatiana-20231013T091917		20	6.8 MB		Download
	08:36 13 Oct 2023		Zn_EXAFS_Tatiana-20231013T071125		4	708.2 KB		Download
	07:10 13 Oct 2023		Zn_EXAFS_Tatiana-20231013T070328		3	114.0 KB		Download
	06:42 13 Oct 2023		Zn_EXAFS_Tatiana-20231012T203557		20	6.8 MB		Download
	20:30 12 Oct 2023		Zn_EXAFS_Tatiana-20231012T202949		3	10.7 KB		Download
	19:15 12 Oct 2023		Cd_EXAFS_Tatiana-20231012T115316		20	5.9 MB		Download
	11:18 12 Oct 2023		Cd_EXAFS_Tatiana-20231012T031730		20	5.9 MB		Download
	01:24 12 Oct 2023		Cd_EXAFS_Tatiana-20231011T180059		20	5.9 MB		Download
	15:52 11 Oct 2023		Cd_EXAFS_Tatiana-20231011T145436		5	1010.8 KB		Download
	14:53 11 Oct 2023		Cd_EXAFS_Tatiana-20231011T145207		3	40.6 KB		Download
	14:51 11 Oct 2023		Cd_EXAFS_Tatiana-20231011T145036		3	22.9 KB		Download

Simple LDAP

1 SESAME staff or long term visitors, please sign in with Your Sup Account

Session expired

Username

Password

Sign in

[or sign in as anonymous](#)

Don't have an account yet? [Register now](#)

[I need further assistance](#)

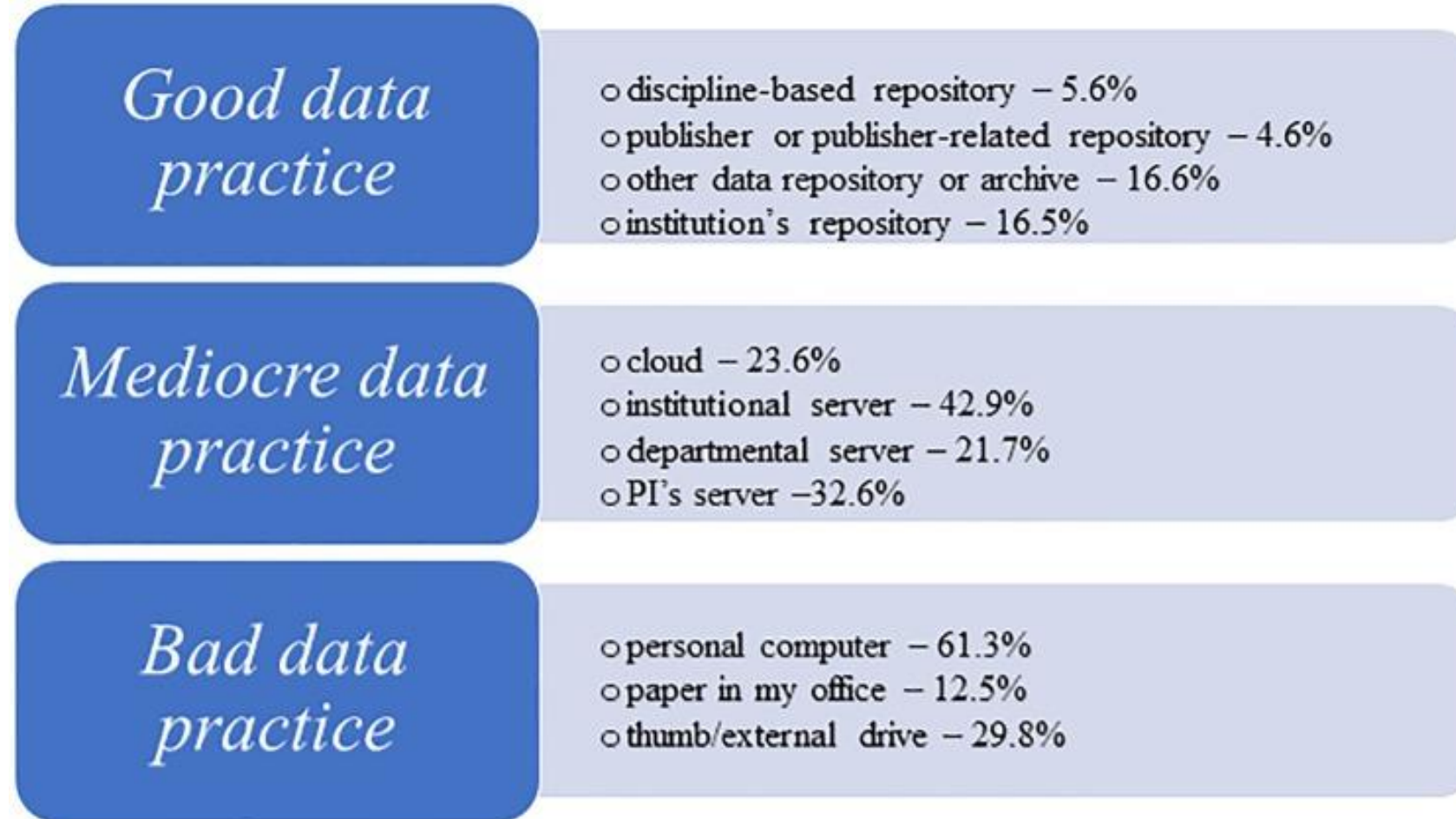
### Important note

In order to login to the Data Portal of the SESAME or browse embargoed data you need to be declared a member of a proposal on the SESAME User Portal. Once this is done your account will be activated 45 days before the first experiment starts. If you need access earlier please contact the [SESAME User Office](#). Anonymous login to browse open data is always possible.

During and according to the General Data Protection Regulation, all SESAME Data portal users who did not consent to the [User Portal Privacy Statement](#) have had their account deactivated. Please contact the [User Office](#) if you wish to reactivate it.



# Adoption of good data practices are still poor



# State of Open Data 2023

## Support is not making its way to those who need it

Almost three-quarters of respondents have never received support with planning, managing or sharing research data.

With the global increase in policies and mandates to share data openly, who researchers are approaching for support becomes a pertinent question.

If respondents stated that they were aware of the concept of a data management plan, they were then asked if they have access to support from specialist data managers and we saw over 50% of our respondents state that they do have access to specialist research data managers in their research setting, but who else has been providing support?

Almost three quarters of respondents **had never received support** with planning, managing or sharing research data. When respondents were asked if they had ever received support with managing or making their data openly available, only 23% said they had. Of that 23%, 61% received support from informal internal sources such as colleagues or supervisors. Two other sources of support ranked highly with our respondents; their institutional libraries (31%) and their research office/in-house institutional expertise (26%).

Do you have access to support from specialist data managers?



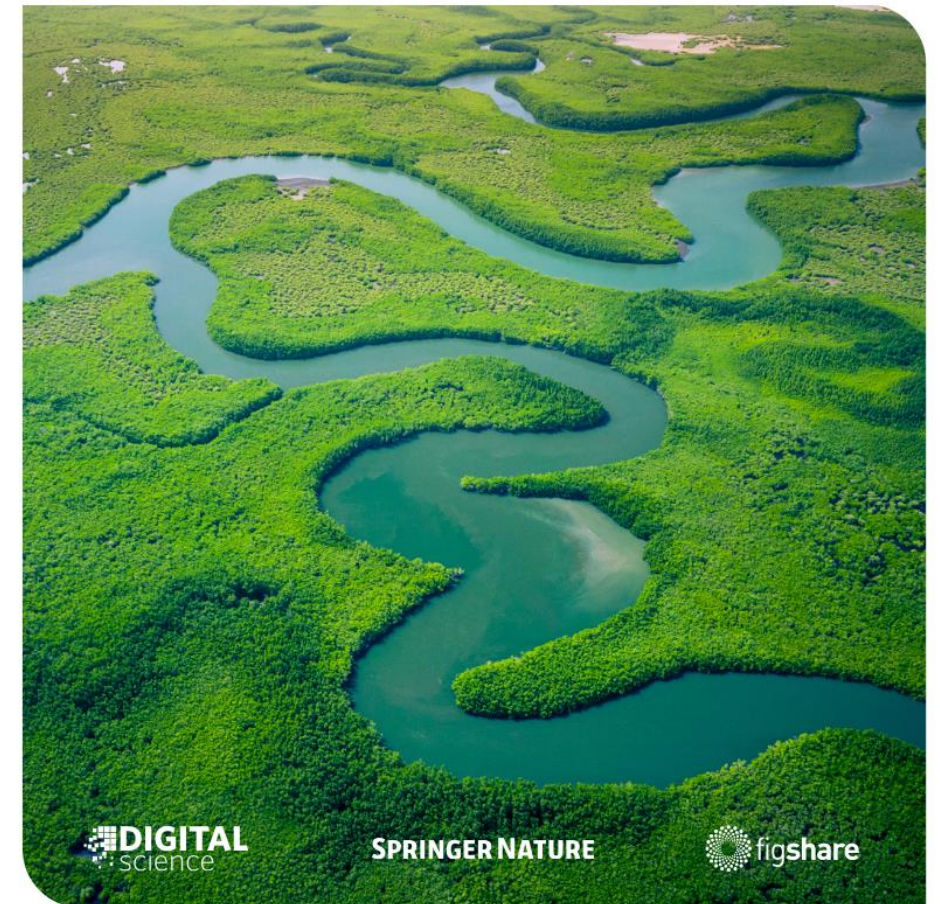
Graph showing the responses to the question 'Do you have access to support from specialist data managers?' This question was only asked if respondents stated that they were aware of the concept of a data management plan. This graph shows the number of respondents for each answer.

<https://www.digital-science.com/state-of-open-data/>

# The State of Open Data 2023

The longest-running longitudinal survey and analysis on open data.

With opening remarks from Springer Nature's CPO, Harsh Jegadeesan, and Digital Science's CEO, Daniel Hook. Authors Mark Hahnel, Graham Smith, Niki Scaplehorn, Henning Schoenenberger and Laura Day.





# AlphaFold demonstrates the power of Open Data + AI

The screenshot shows the top navigation bar of the RCSB PDB website with links for Deposit, Search, Visualize, Analyze, Download, Learn, About, Documentation, Careers, and COVID-19. It also includes 'MyPDB' and 'Contact us' buttons. Below the navigation is the PDB logo and statistics: 214,458 Structures from the PDB and 1,068,577 Computed Structure Models (CSM). A search bar is present with a dropdown for '3D Structures' and a search input field. Below the search bar are logos for PDB-101, PDB, EMDDataResource, NAKB, wwPDB Foundation, and PDB-Dev. A teal banner reads 'Access Computed Structure Models (CSMs) of all available n...'. On the left is a dark blue sidebar with navigation options: Welcome, Deposit, Search, Visualize, Analyze, Download, and Learn. The main content area features a paragraph about RCSB PDB's role in science and education, followed by two bullet points: 'Experimentally-determined 3D structures from the Protein Data Bank (PDB) archive' and 'Computed Structure Models (CSM) from AlphaFold DB and ModelArchive'. Below this is a sub-header 'These data can be explored in context of external annotations providing a structural view of biology.' and a promotional banner for 'Explore NEW Features' and 'PDB-101 Training Resources'.

RCSB PDB Deposit Search Visualize Analyze Download Learn About Documentation Careers COVID-19 MyPDB Contact us

RCSB PDB PROTEIN DATA BANK 214,458 Structures from the PDB 1,068,577 Computed Structure Models (CSM)

3D Structures Enter search term(s), Entry ID(s), or sequence Include CSM

Advanced Search | Browse An

PDB-101 PDB EMDDataResource NAKB wwPDB Foundation PDB-Dev

Access Computed Structure Models (CSMs) of all available n

Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

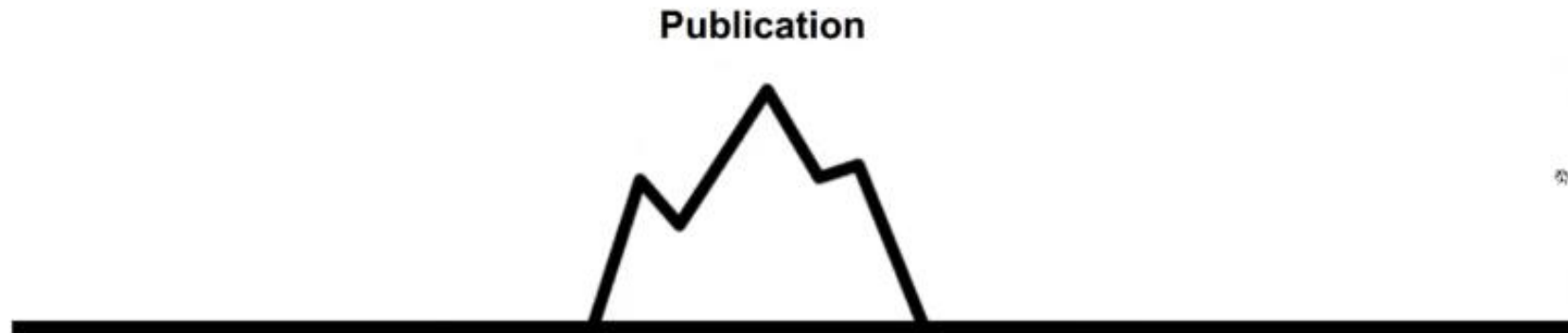
- Experimentally-determined 3D structures from the **Protein Data Bank (PDB)** archive
- Computed Structure Models (CSM)** from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.

Explore NEW Features PDB-101 Training Resources

“AlphaFold is the singular and momentous advance in life science that demonstrates the power of AI. Determining the 3D structure of a protein used to take many months or years, it now takes seconds. AlphaFold has already accelerated and enabled massive discoveries, including cracking the structure of the nuclear pore complex. And with this new addition of structures illuminating nearly the entire protein universe, we can expect more biological mysteries to be solved each day.”

# Science produces Publications

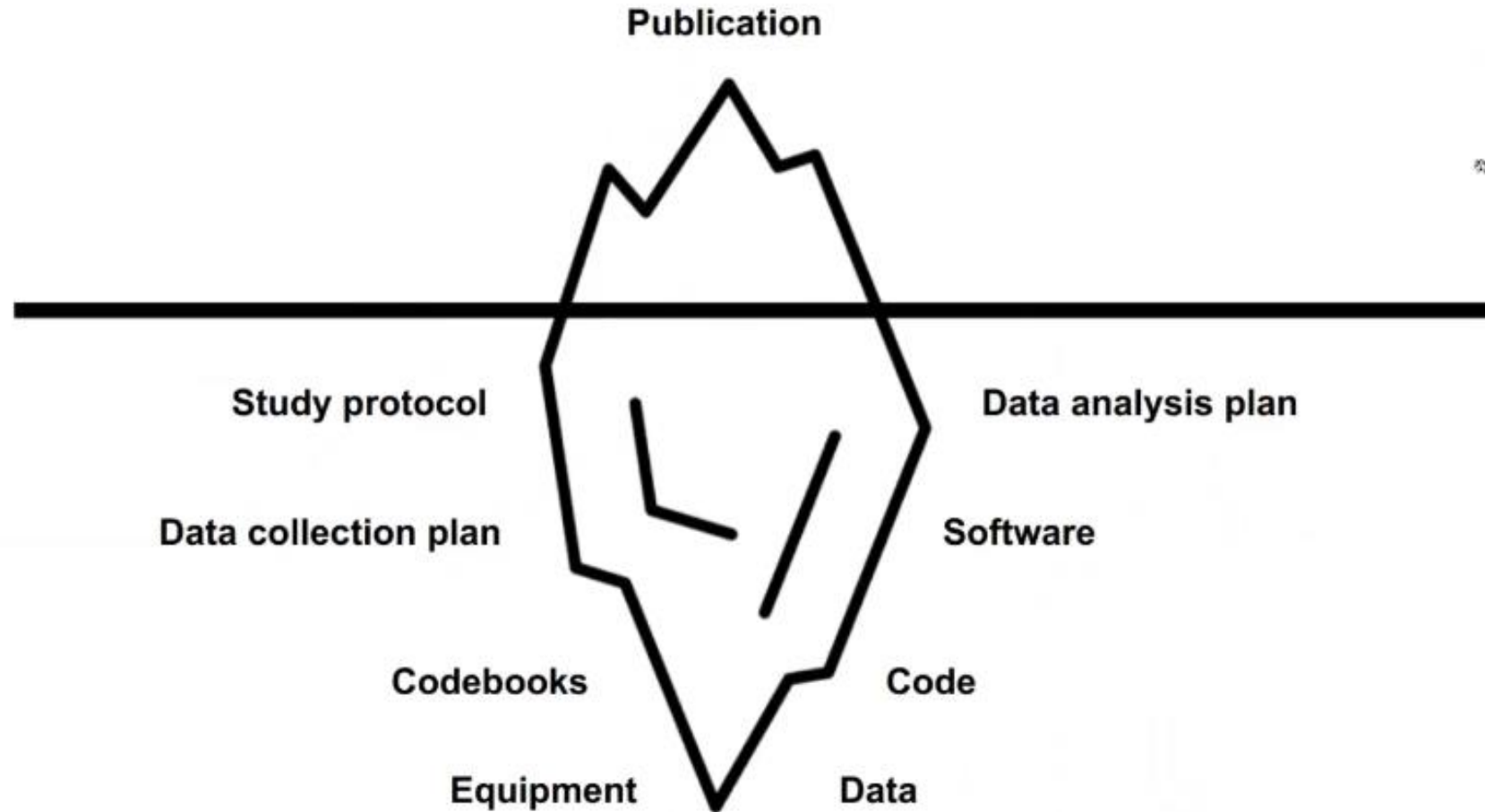


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852





# Science produces much more than Publications



# Open Science



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Reproducibility and Replicability

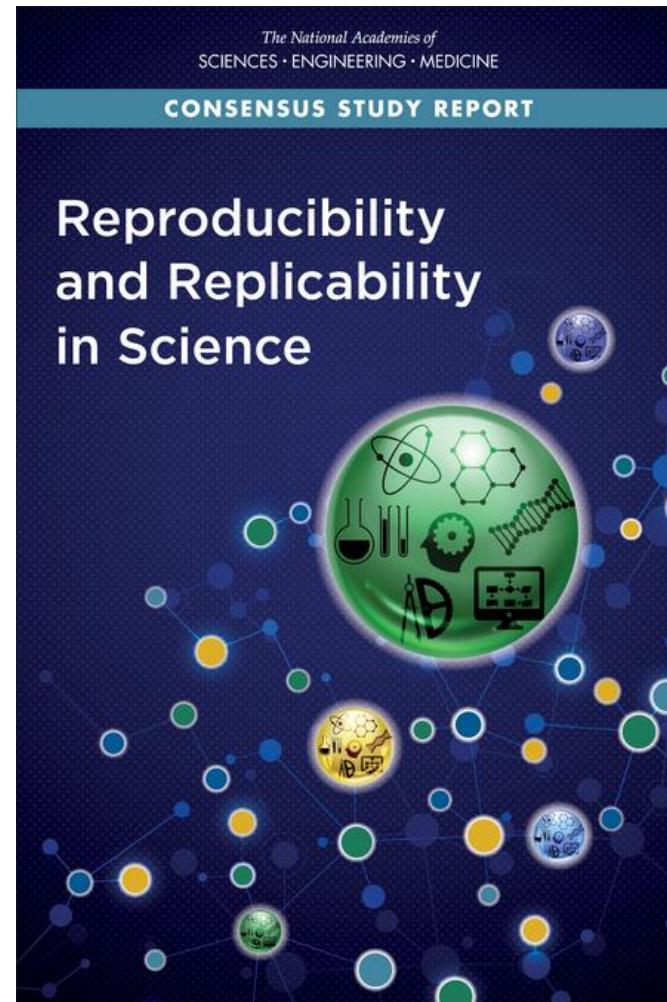
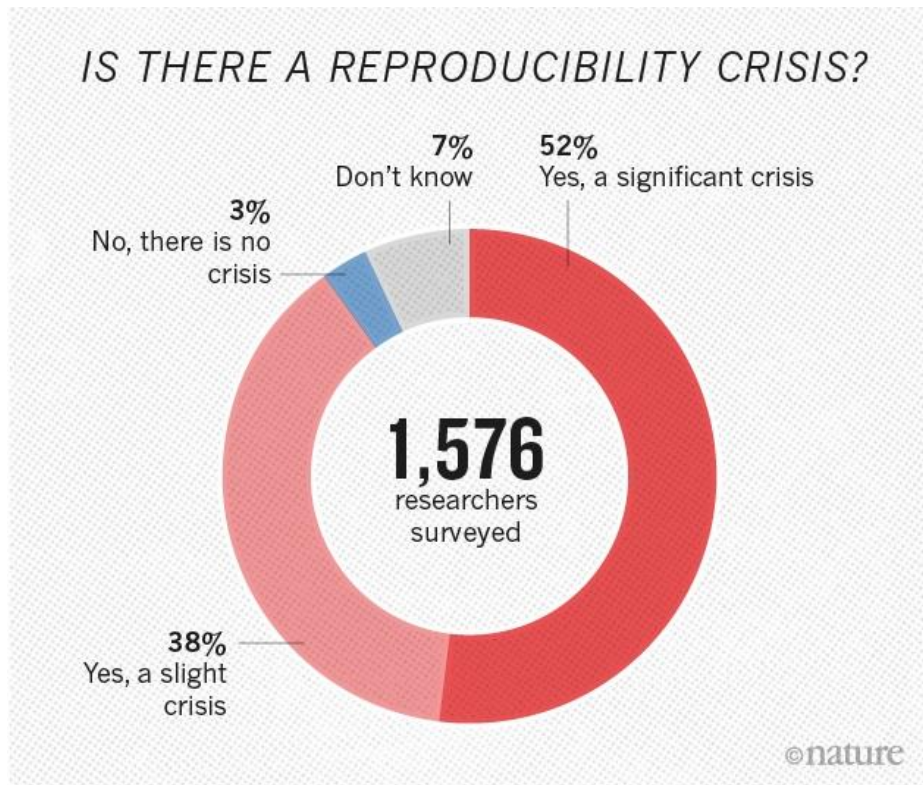
Published: 25 May 2016

## 1,500 scientists lift the lid on reproducibility

Monya Baker

*Nature* 533, 452–454 (2016) | [Cite this article](#)

5320 Accesses | 1225 Citations | 3871 Altmetric | [Metrics](#)



Further reading:

- [Replication crisis – Wikipedia](#)
- <https://phys.org/news/2017-03-science-crisis.html>

Research and innovation programme under grant agreement No. 823852

# What is Open Science?

- ✓ Open Science is: *“to make the primary outputs of publicly funded research results – publications and the research data – publicly accessible in digital format with no or minimal restriction”*

<https://www.oecd.org/sti/inno/open-science.htm>

“Work, Finish, Publish” → “Work, Finish, Publish, Release”

Michael Faraday 1791-1867

Open Science





# ChatGPT: What is Open Science?



what is open science



Open science is an umbrella term that encompasses a variety of practices and principles aimed at making scientific research more transparent, accessible, and reproducible. This includes making research data, methods, and findings openly available to the public, as well as promoting collaboration and openness in the scientific process. The goal of open science is to increase the efficiency and effectiveness of scientific research, and to ensure that the knowledge generated by the scientific enterprise is widely accessible and can be used to benefit society. Open science practices can include open data sharing, open access publishing, preregistration of study designs, and the use of open-source software.



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Open Science Gateway  
for Research & Society

pariwise

<https://chat.openai.com/chat>

# Pillars of Open Science

## 1. Open Access

- publications should be freely accessible either as Gold (journal) or Green (preprint) access

## 2. Open Data

- data should be FAIR and freely accessible under a licence which allows re-use without restriction

## 3. Open Source Software

- source code should be made available on a publicly accessible repository under an Open Source licence

## 4. Open Hardware

- hardware designs should be accessible, like software, under an Open Source licence

## 5. Open Educational Resources

- educational resources (videos, e-training courses etc.) should be made available to all

## 6. Citizen Science

- citizens who follow the scientific method should be encouraged and facilitated and engage with scientists



# Open Access publications – Green vs. Gold

## GREEN

- Articles are free to read after an embargo period
- Bioscientifica automatically make the final published version, also known as the version of record, free
- Authors may deposit a version of their accepted manuscript in an online repository after this time
- There is no cost to authors.

## GOLD

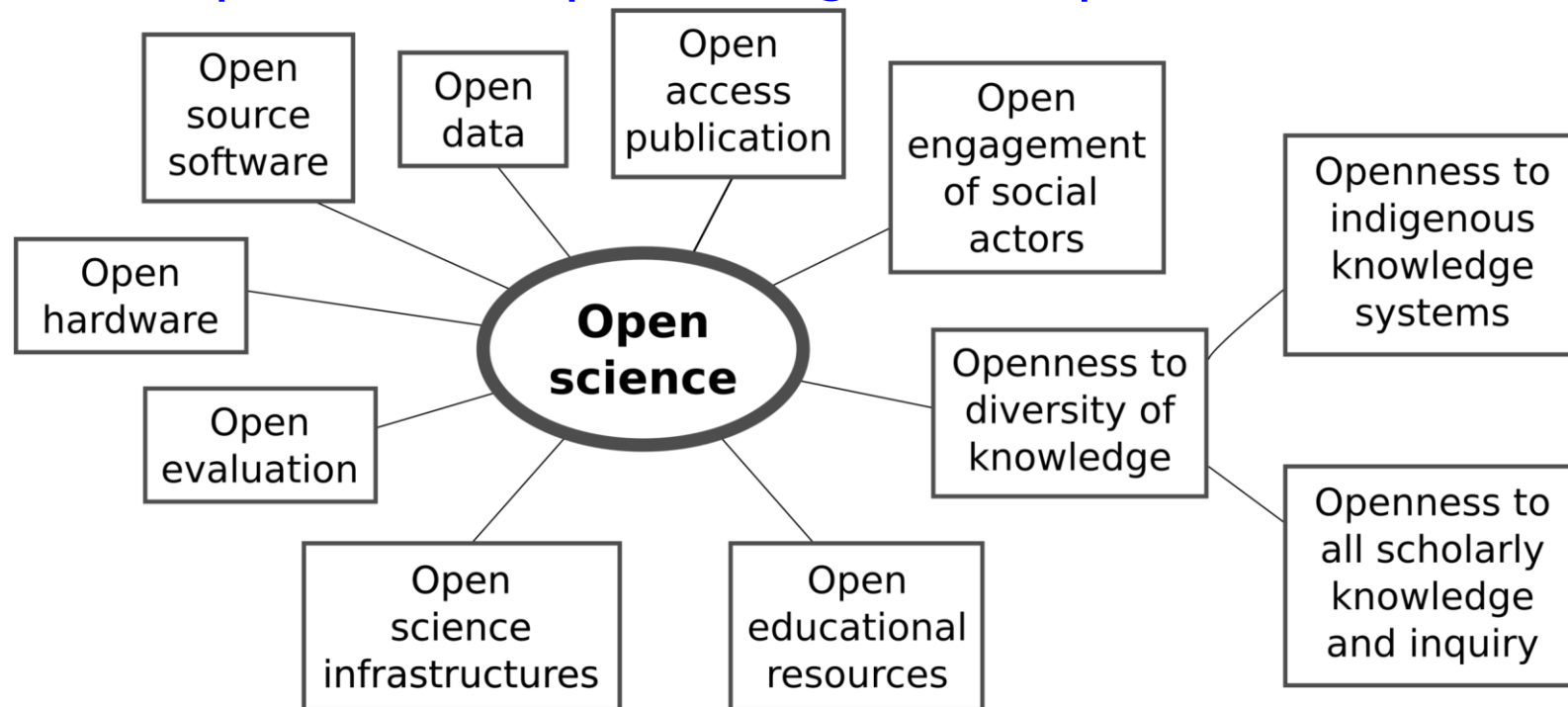
- Authors (or their funders or institutions) pay an Article Publication Charge (APC) upon acceptance
- The final published version is free immediately
- Bioscientifica deposits the article in PubMed Central
- Authors retain copyright and a range of licenses are available
- Journal could be fully open access (eg. *EDM Case Reports*) or hybrid (eg. *European Journal of Endocrinology*).

<https://www.bioscientifica.com/authors/preparing-papers/publishing-open-access/>



# Open Science - origin

“Open Science can be seen as a continuation of, rather than a revolution in, practices begun in the 17th century with the advent of the academic journal, when the societal demand for access to scientific knowledge reached a point at which it became necessary for groups of scientists to share resources with each other” - [https://en.wikipedia.org/wiki/Open\\_science](https://en.wikipedia.org/wiki/Open_science)







## ANNEX VI Recommendation on Open Science

*This Recommendation outlines a common definition, shared values, principles and standards for open science at the international level and proposes a set of actions conducive to a fair and equitable operationalization of open science for all at the individual, institutional, national, regional and international levels.*

<https://unesdoc.unesco.org/ark:/48223/pf0000380399>

*Updated recommendations on the following:*

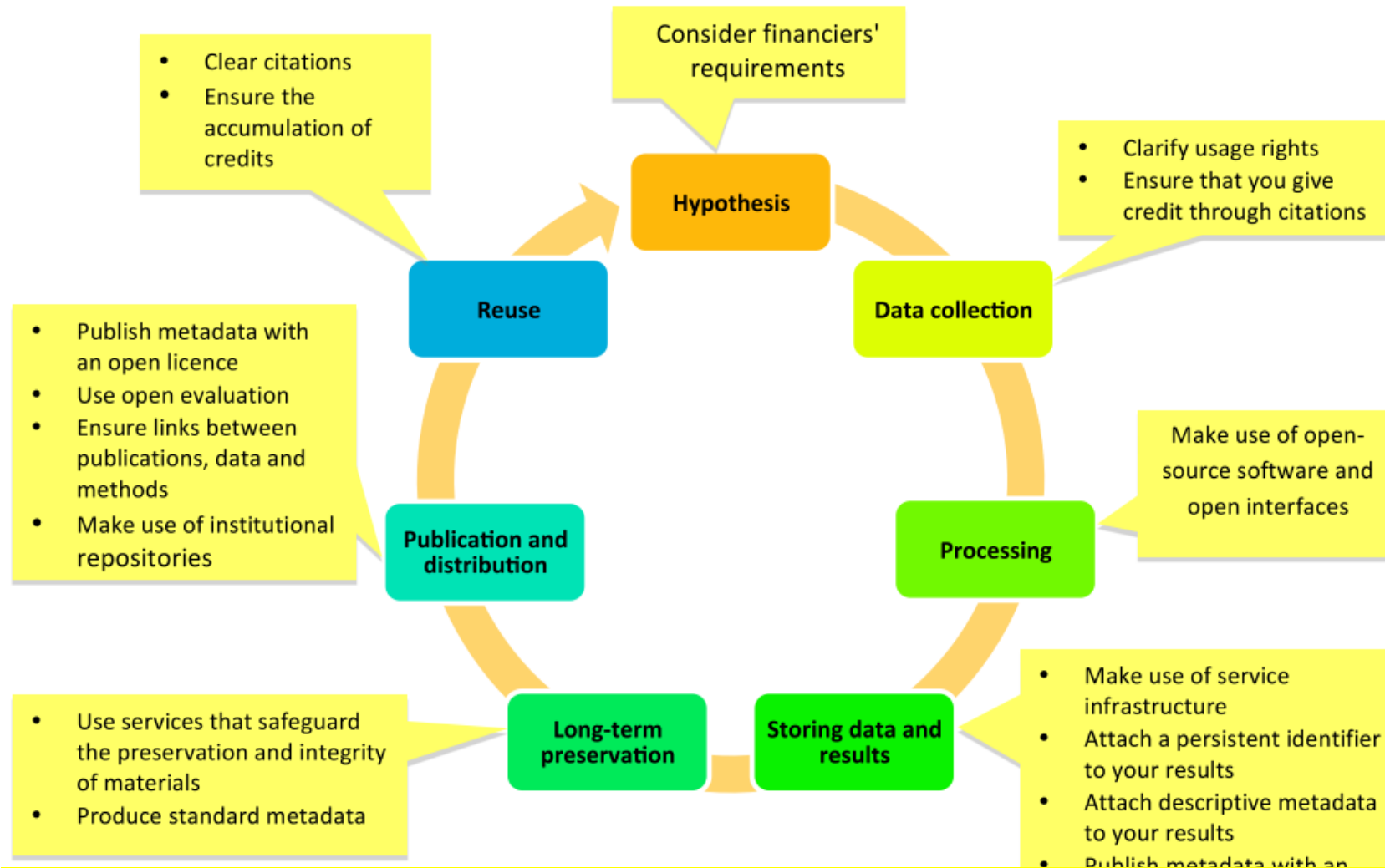
1. Scientific publications
2. Open research data
3. Open educational resources
4. Open source software and source code
5. Open hardware
6. Scientific knowledge
7. Open science infrastructures
8. Open engagement of societal actors
9. Open dialogue with other knowledge systems
10. Public + Private sector



# Open Science



# Open Science is about extending the principles of openness to the whole research cycle (FOSTER)

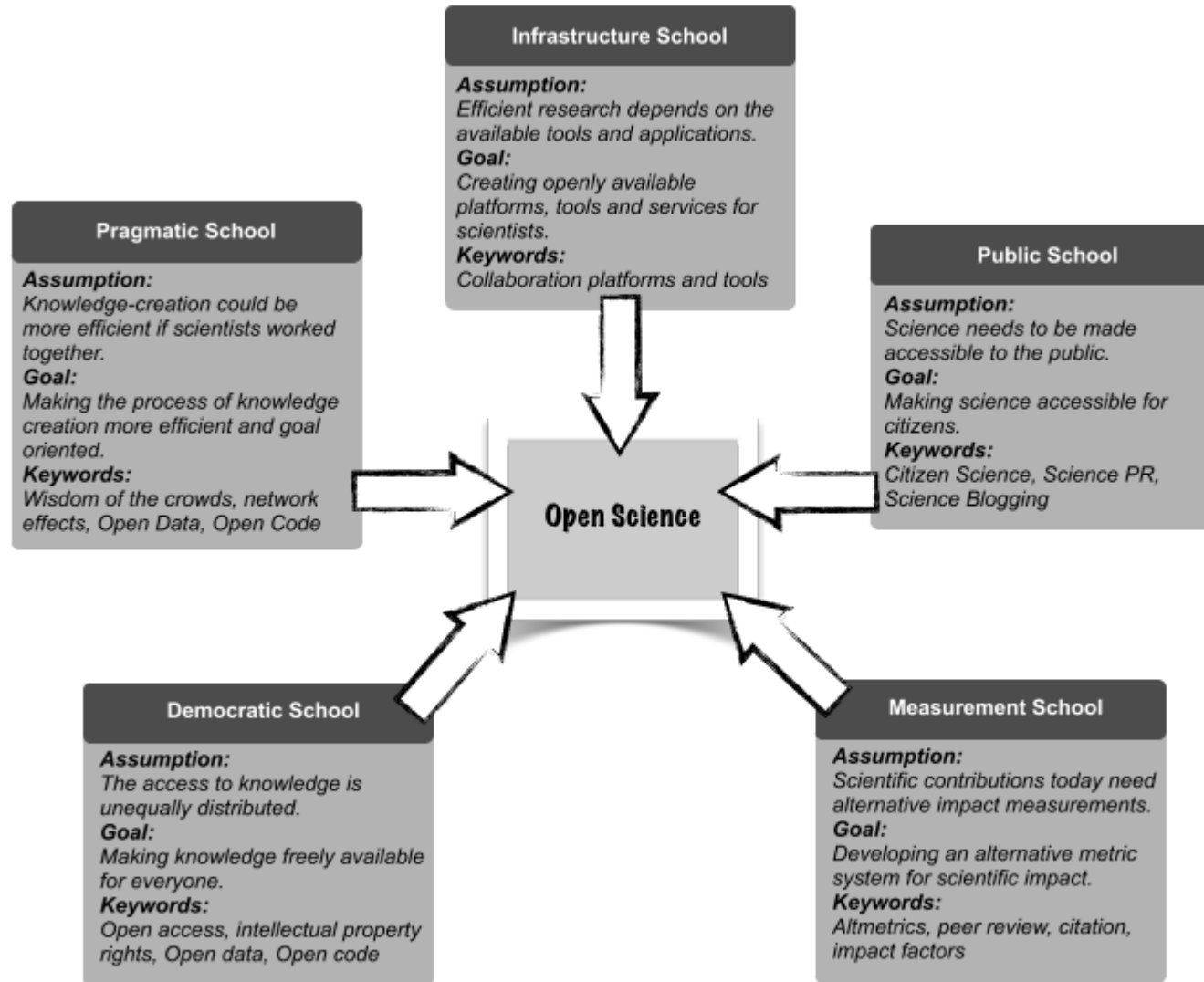


This project has received funding from the European Union Horizon 2020 research and innovation programme under grant agreement No 101019719.

<https://www.fosteropenscience.eu/content/what-open-science-introduction>



# Five schools of Thought for Open Science



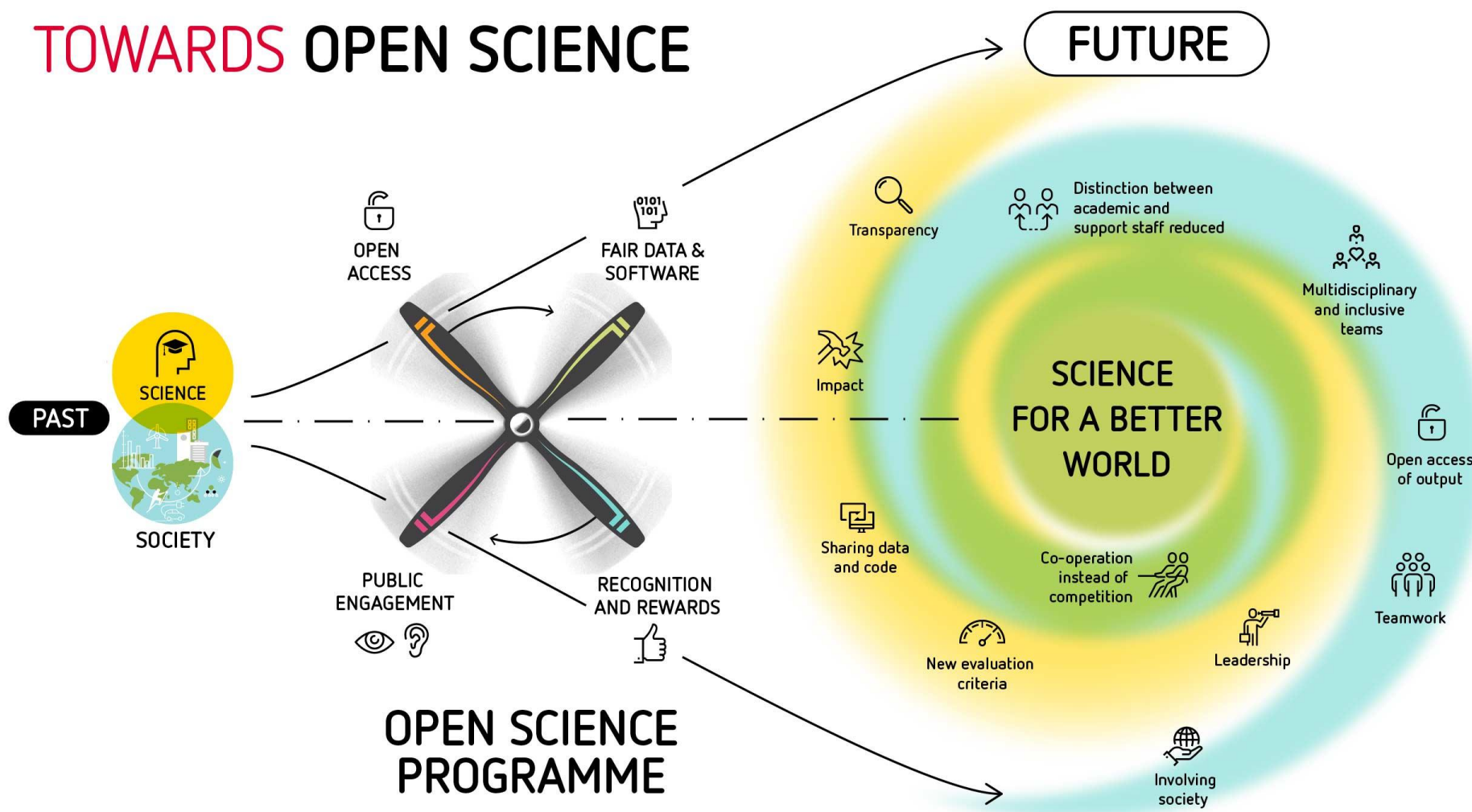
# Impact of open science on the future



www.uu.nl/openscience

## TOWARDS OPEN SCIENCE

FUTURE



This project

<https://narratives.insidehighered.com/four-pillars-of-open-science/assets/rALfdOrDqh/uugraphic-2-2560x1597.jpeg>

OSCARs  
Open Science Clusters' Action  
Research & Society

NOSC





# European Open Science Cloud

The Vienna Declaration on the European Open Science Cloud

Vienna, 23 November 2018

We, Ministers  
European

1. Recall the  
Brussels on 1

2. Recall

**EU funded 22 EOSC Projects in H2020 +  
a further 19 EOSC Projects in Horizon Europe**

Declaration" signed in

Europe. Confirm that  
Member

its nature  
to build trust and

ion of cloud  
the world,

<https://eosc.eu/horizon-europe-projects/>

# African Open Science Platform



<https://aosp.org.za>



[About us](#)

[Partnerships](#)

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The Africa Open Science Platform (AOSP) was established in 2017 with an aim to position African scientists at the cutting edge of data intensive science by stimulating interactivity and creating opportunity through the development of efficiencies of scale, building critical mass through shared capacities, and amplifying impact through a commonality of purpose and voice.





# CERN publishes Open Science policy

<https://openscience.cern/>

CERN Accelerating science Sign in Directory

OpenScience at CERN OPEN SCIENCE POLICIES OPEN SCIENCE ELEMENTS HISTORY NEWS ABOUT SEARCH

## Welcome to the CERN Open Science portal

At CERN, we believe that the practice of open science is key to delivering on our organizational mission: to perform world-class research in fundamental physics at the forefront of human knowledge; provide a unique range of particle accelerator facilities that enable this research, educate the next generation of scientists; and unite people from all over the world to push the frontiers of science and technology, for the benefit of all.

### CERN publishes comprehensive Open Science Policy

CERN's core values include making research open and accessible for everyone. A new policy now brings together existing open science initiatives to

### CERN Council acknowledges new Open Science Policy

At its 209th session, the CERN Council acknowledged the introduction of CERN's new Open Science Policy. The delegates of CERN's 23 member states appreciated the Organization's efforts toward

### SCOAP3 reaches 50'000 articles milestone

The [Sponsoring Consortium for Open Access Publishing in Particle Physics \(SCOAP<sup>3</sup>\)](#)—the world's largest disciplinary open access initiative—has reached the milestone of over 50'000 research articles

2022-05-10

## CERN Council adopted an Open Science Policy on 2022-09-29

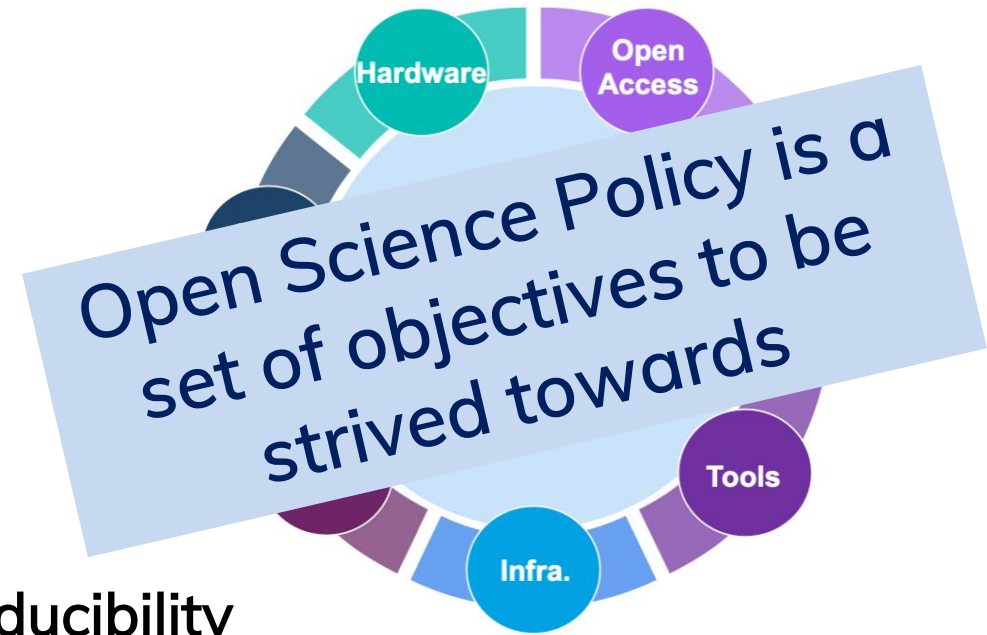


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# CERN Open Science policy

1. Open access to publications
2. Open data
3. Open source software
4. Open hardware
5. Research integrity, reuse and reproducibility
6. Infrastructure provision for open science
7. Research assessment and evaluation
8. Education, training and outreach
9. Citizen Science



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# EMBL Open Science Policy

→ EMBL adopted an Open Science Policy for EMBL staff in December 2021 and is implementing it since January 2022.

→ Two main aspects:

1. Public availability of research outputs
2. Research assessment and fair attribution of credit

**1. ORCID**

**2. DORA**

## Open science at EMBL: a transparent way of working

EMBL announces the release of its new Open Science Policy, contributing to positive culture change across the life sciences



EMBL Open Science Policy. Credit: Holly Joynes/EMBL



This project has received

<https://www.embl.org/documents/wp-content/uploads/2021/12/ip71-open-science-and-open-access-policy.pdf>

under grant agreement No. 823852



BRIEFING ROOM

## OSTP Issues Guidance to Make Federally Funded Research Freely Available Without Delay

AUGUST 25, 2022 • PRESS RELEASES

THE WHITE HOUSE

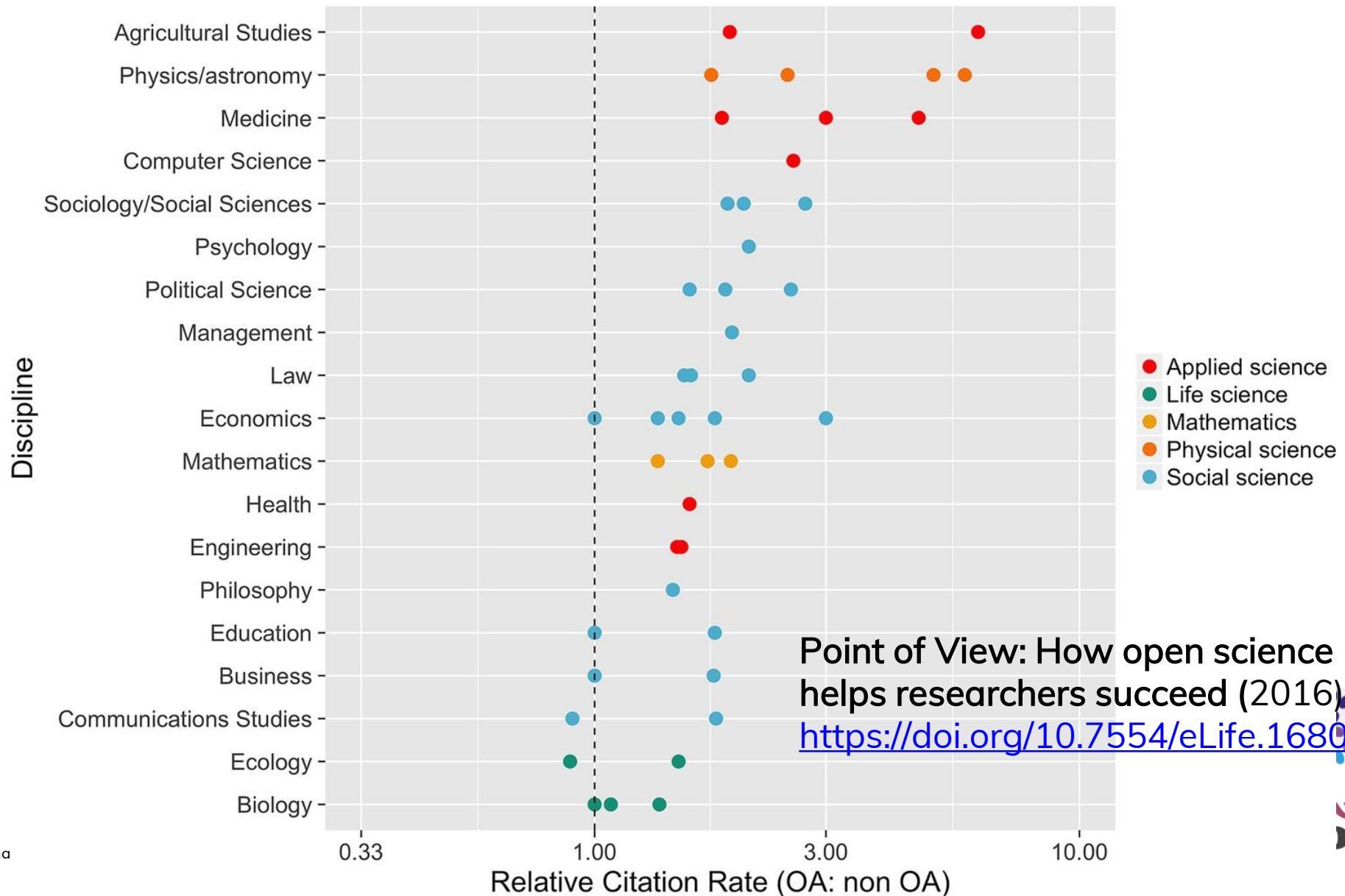
- 1. Update their public access policies as soon as possible, and no later than December 31st, 2025, to make publications and their supporting data resulting from federally funded research publicly accessible without an embargo on their free and public release;*
- 2. Establish transparent procedures that ensure scientific and research integrity is maintained in public access policies; and,*
- 3. Coordinate with OSTP to ensure equitable delivery of federally funded research results and data.*



This project has r

<https://www.whitehouse.gov/wp-content/uploads/2022/08/08-2022-OSTP-Public-Access-Memo.pdf>

# Open access leads to more citations



This project has



# Open science is beneficial for scientists

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

Article | [Open Access](#) | [Published: 04 November 2021](#)

## Imaging intact human organs with local resolution of cellular structures using hierarchical phase-contrast tomography

[C. L. Walsh](#) , [P. Tafforeau](#) , [W. L. Wagner](#), [D. J. Jafree](#), [A. Bellier](#), [C. Werlein](#), [M. P. Kühnel](#), [E. Boller](#), [S. Walker-Samuel](#), [J. L. Robertus](#), [D. A. Long](#), [J. Jacob](#), [S. Marussi](#), [E. Brown](#), [N. Holroyd](#), [D. D. Jonigk](#) , [M. Ackermann](#)  & [P. D. Lee](#) 

[Nature Methods](#) **18**, 1532–1541 (2021) | [Cite this article](#)

**82k** Accesses | **25** Citations | **2147** Altmetric | [Metrics](#)

This article is in the 99<sup>th</sup> percentile (ranked 192<sup>nd</sup>) of the 436,034 tracked articles of a similar age in all journals and the 98<sup>th</sup> percentile (ranked 2<sup>nd</sup>) of the 79 tracked articles of a similar age in *Nature Methods*

*“If you don't want to share data why become a scientist?”*  
*Claire Walsh (UCL)*



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agree



The graphic features the PaNOSC logo at the top left, which includes the text 'photos and neutron open science cloud'. Below the logo is a circular portrait of Claire Walsh. To the right of the portrait, the text reads 'Interview with Claire Walsh (UCL - ESRF) on the Human Organ Atlas'. At the bottom, there is a blue banner with the text 'PaNOSC has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852'. This banner also contains the logos for the European Union, ESRF (The European Synchrotron), and UCL.

## Welcome to the Human Organ Atlas

The Human Organ Atlas uses... to span a previously possible range of human anatomy, the

Historically, other structures with sub-micron accuracy, while clinical CT and MRI scans can image down to just below a millimetre. HiP-CT bridges these scales, from 20 micron voxels, and locally down to microns.

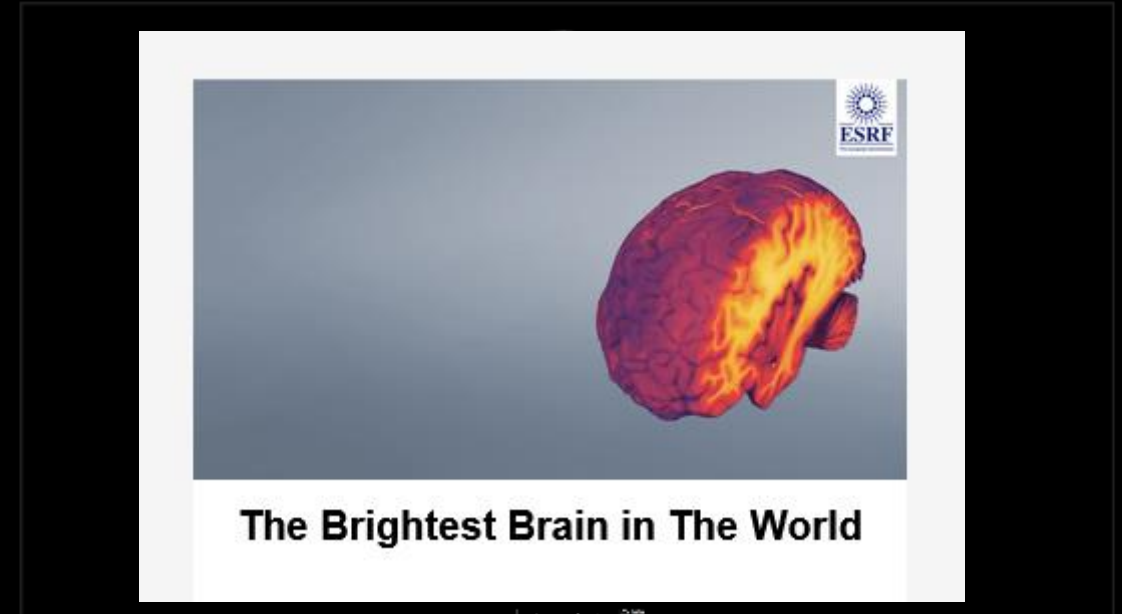
We hope... enabled by the ESRF-EBS, will act as a reference to provide new insights into... To stay up to date, follow [@HiP-CT](#)

**Medical + Citizen science**

### Funding

This project has been made possible by funding from:

- The [European Synchrotron Radiation Facility \(ESRF\)](#) — funding proposal MD-1252
- The [Chan Zuckerberg Initiative](#), a donor-advised fund of the Silicon Valley Community Foundation
- The [German Registry of COVID-19 Autopsies \(DeRegCOVID\)](#), supported by the German Federal Ministry of Health
- The Royal Academy of Engineering, UK
- The UK Medical Research Council



**The Brightest Brain in The World**

HiP-CT imaging and 3D reconstruction of a [complete brain](#) from the body donor LADAF-2020-31. More videos can be viewed on the [HiP-CT YouTube channel](#).

### Collaborators

- [UCL](#), London, England: **Peter D Lee, Claire Walsh, Simon Walker-Samuel, Rebecca Shipley, Sebastian Marussi, Joseph Jacob, David Long, Daniyal Jafree, Ryo Torii, Charlotte Hagen**
- [ESRF](#), Grenoble, France: **Paul Tafforeau, Elodie Boller**
- Medizinische Hochschule Hannover, Germany: **Danny D Jonigk, Christopher Werlein, Mark Kuehnel**
- Universitätsmedizin der Johannes Gutenberg-Universität Mainz, Germany: **M Ackermann**
- University Hospital of Heidelberg, Germany: **Willi Wagner**
- Grenoble Alpes University, Department of Anatomy, French National Center for Scientific Research: **A Bellier**

# Open science vs. science

*Most of these assumptions are not new, as the tradition of openness itself is at the roots of science, but the current developments of information and communication technologies have transformed the scientific practices to a level that requires a different approach to research (FOSTER)*

<https://www.fosteropenscience.eu/content/what-open-science-introduction>

**Q: "What is the difference between Open Science and 'science'?"**

*A: Open Science refers to doing traditional science with more transparency involved at various stages, for example by openly sharing code and data. Many researchers do this already, but don't call it Open Science.*

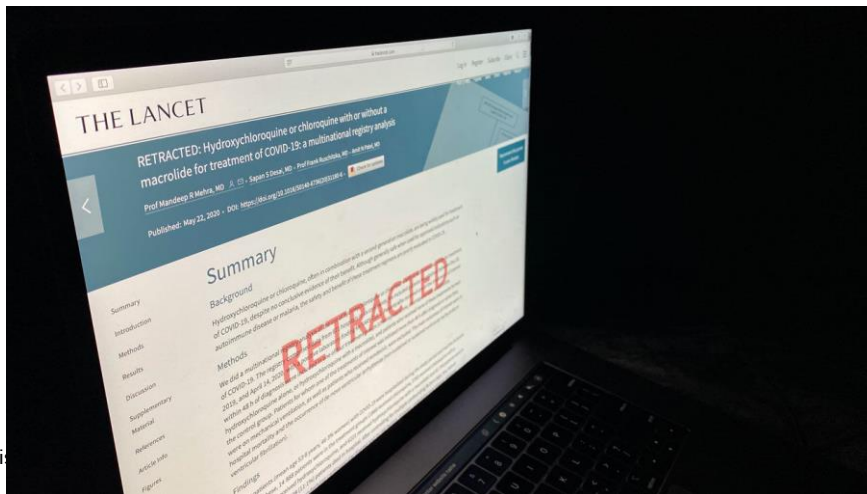
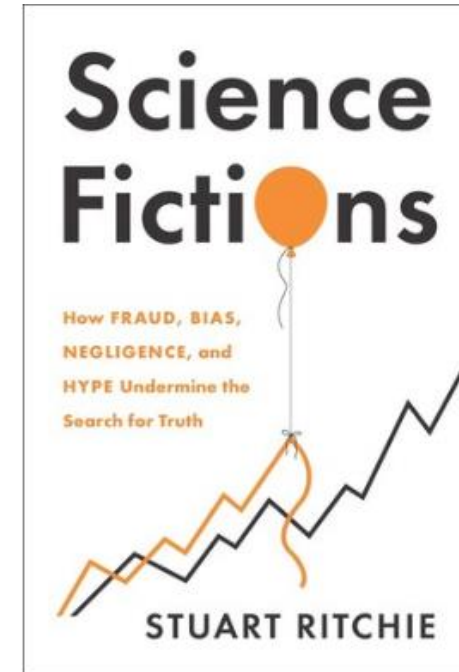




# European Conduct of Scientific Integrity

## Open Science improves integrity, scientific method

- Recommend to follow the EU Code of Integrity
  - <https://allea.org/code-of-conduct/>
- To **AVOID** having your papers **RETRACTED**
  - <https://retractionwatch.com/>



Our list of retracted or withdrawn COVID-19 papers is up to over 375. There are more than 46,000 retractions in The Retraction Watch Database — which is now part of Crossref. The Retraction Watch Hijacked Journal Checker now contains well over 200 titles. And have you seen our leaderboard of authors with the most retractions lately — or our list of top 10 most highly cited retracted papers? Or The Retraction Watch Mass Resignations List?

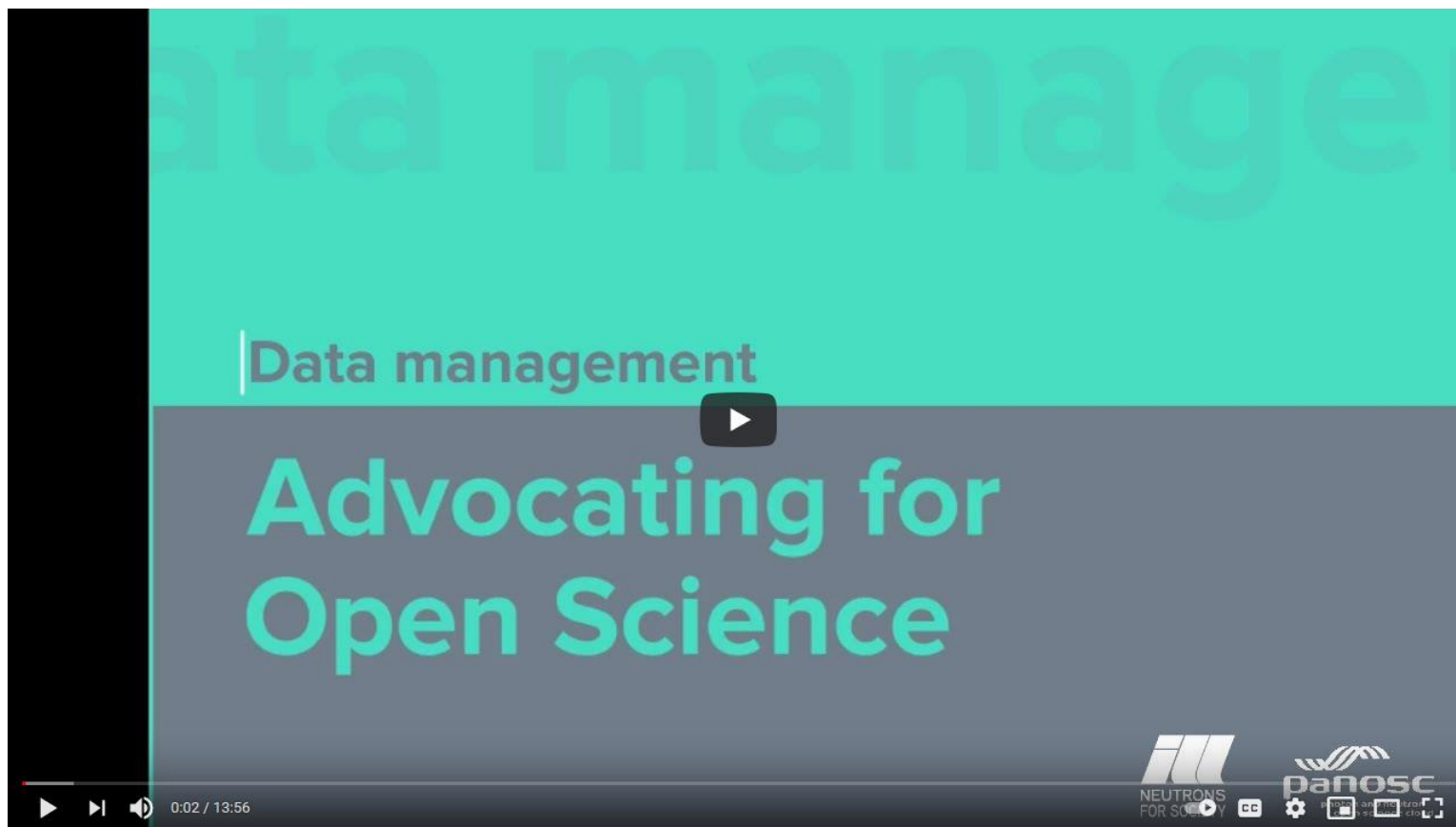


This

ovatio

# Open Science Ambassador

Watch this interview of Petr Čermák, a strong advocate of open on the advantages of Open Science for neutrons and science in general



<https://youtu.be/QKAc1y6HZNk>



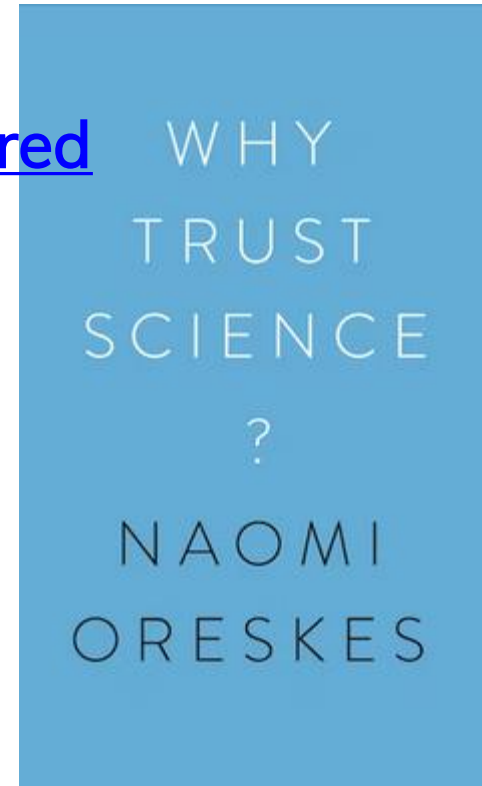
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Further reading – Open Science

Many resources are available on Open Science, here are some used for this talk

- [Phys.org](https://phys.org)
  - [Five questions about open science answered](#)
  - [Data sharing can offer help in science's reproducibility crisis](#)
- UNESCO
  - Recommendation on Open Science
- EU
  - [Progress on Open Science](#)



# FAIR Data



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852

# The publication that started the FAIR movement

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

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

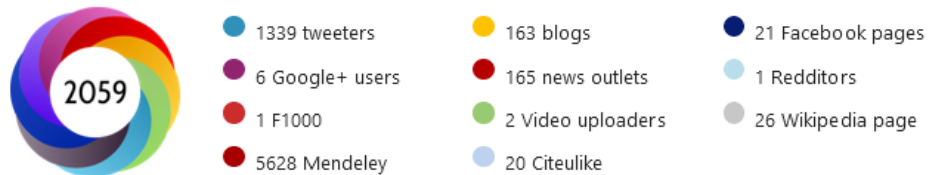
[Mark D. Wilkinson](#), [Michel Dumontier](#), [IJsbrand Jan Aalbersberg](#), [Gabrielle Appleton](#), [Myles Axton](#), [Arie Baak](#), [Niklas Blomberg](#), [Jan-Willem Boiten](#), [Luiz Bonino da Silva Santos](#), [Philip E. Bourne](#), [Jildau Bouwman](#), [Anthony J. Brookes](#), [Tim Clark](#), [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

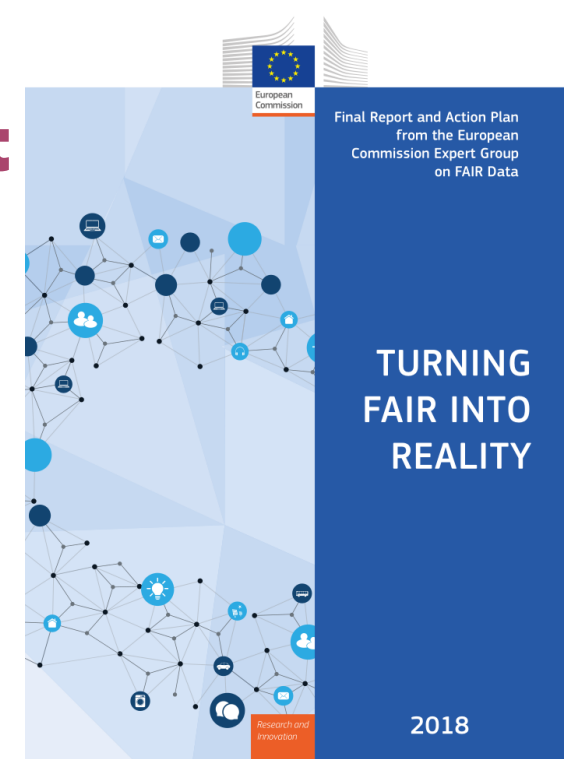
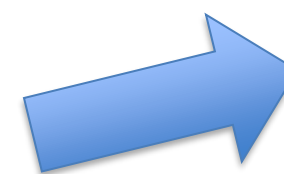
[Scientific Data](#) **3**, Article number: 160018 (2016) | [Cite this article](#)

**523k** Accesses | **5193** Citations | **2059** Altmetric | [Metrics](#)

### Online attention



This article is in the 99<sup>th</sup> percentile (ranked 41<sup>st</sup>) of the 299,830 tracked articles of a similar age in all journals and the 99<sup>th</sup> percentile (ranked 1<sup>st</sup>) of the 23 tracked articles of a similar age in *Scientific Data*



<https://data.europa.eu/doi/10.2777/1524>

<https://www.go-fair.org/>  
**GO FAIR**



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Data availability – the wrong + right way



Data availability

Data available on reasonable request to the authors.



Open Research

## Data Availability Statement

The data that support the findings of this study are openly available in Zenodo at <https://doi.org/10.5281/zenodo.6993871> , reference number 6993871.



# Open Research Europe recommendations for data

My Submissions

Article Guidelines

Article Guidelines (New Versions)

Open Data, Software and Code Guidelines

Open Data and Accessible Source Materials Guidelines (HSS)

Prepublication Checks

Article Processing Charges

Finding Article Reviewers

## What is required when submitting an article

1. [Your dataset\(s\) must be deposited in an appropriate data repository.](#)
2. [Your dataset\(s\) must have a license applied which allows reuse by others \(CC0 or CC-BY\).](#)
3. [Your dataset\(s\) must have a persistent identifier \(e.g. a DOI\), allocated by a data repository.](#)
4. [You must provide a data availability statement as a section at the end of your article, including elements 1-3.](#)
5. [You must include a data citation and add a reference to data to your reference list.](#)
6. [Your dataset\(s\) should not contain any sensitive information, for example in relation to human research participants.](#)
7. [You should share any related software and code.](#)
8. [Your dataset\(s\) must be useful and reusable by others, adhere to any relevant data sharing standards in your discipline and align with the FAIR Data Principles.](#)
9. [Your dataset\(s\) should link back to your article, if possible.](#)

<https://open-research-europe.ec.europa.eu/for-authors/data-guidelines/>



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# FAIR Principles

<https://www.go-fair.org/fair-principles/>

## Findable

- > F1: (Meta) data are assigned globally unique and persistent identifiers
- > F2: Data are described with rich metadata
- > F3: Metadata clearly and explicitly include the identifier of the data they describe
- > F4: (Meta)data are registered or indexed in a searchable resource

## Accessible

- > A1: (Meta)data are retrievable by their identifier using a standardised communication protocol
- > A1.1: The protocol is open, free and universally implementable
- > A1.2: The protocol allows for an authentication and authorisation where necessary
- > A2: Metadata should be accessible even when the data is no longer available

## Interoperable

- > I1: (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation
- > I2: (Meta)data use vocabularies that follow the FAIR principles
- > I3: (Meta)data include qualified references to other (meta)data

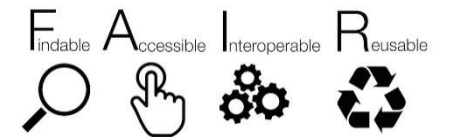
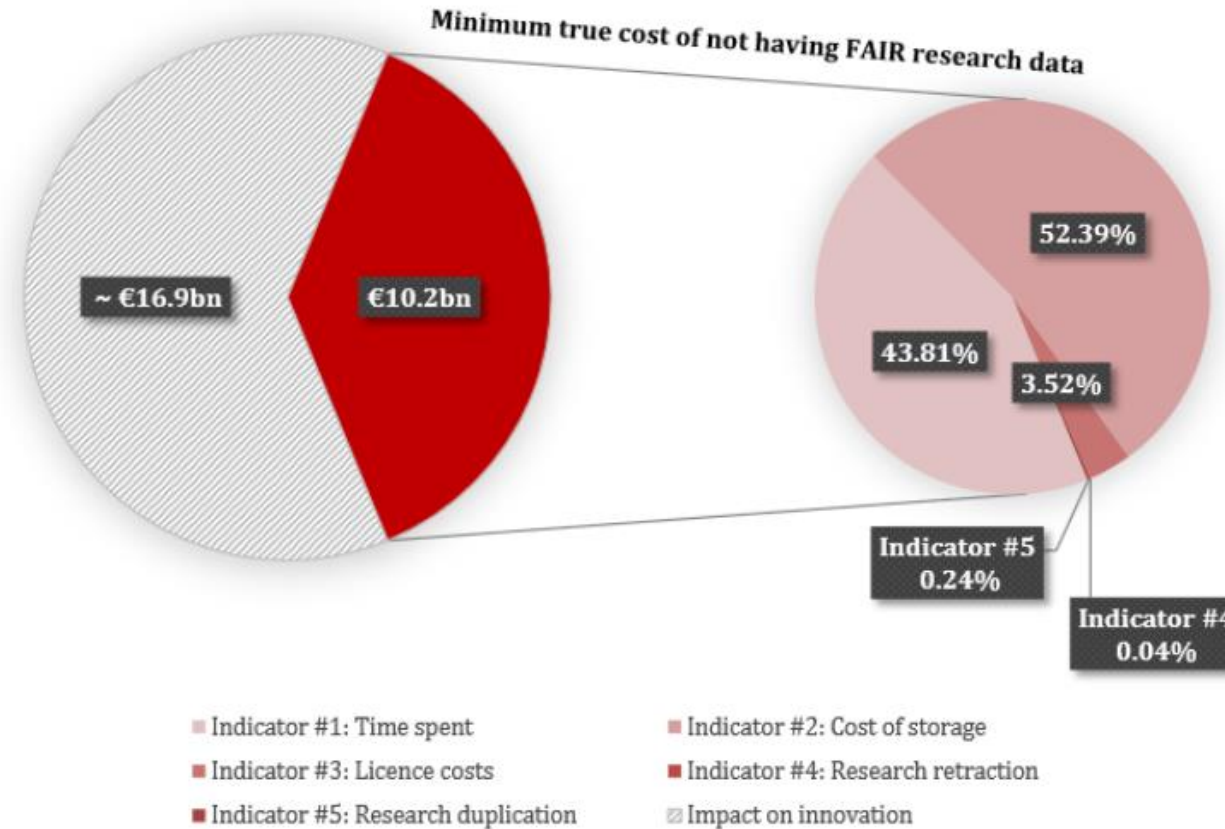
## Reusable

- > 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



# The cost of not having FAIR data = estimated €10.2bn / year

Likely cost of not having FAIR research data



“Cost-benefit analysis for FAIR research data “ (<https://op.europa.eu/s/pevt>)

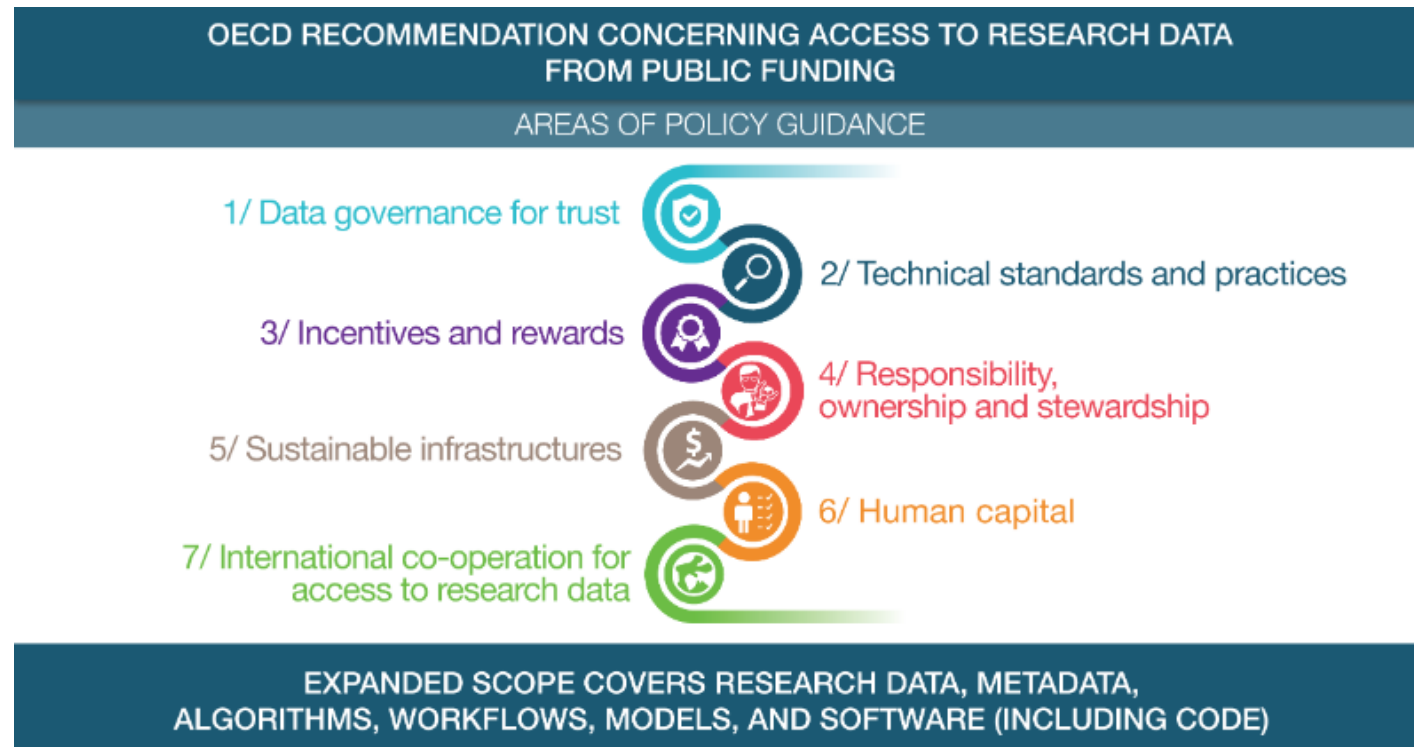


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Open data for publicly funded research

- The OECD recommendation in 2006 had a big impact on data policies
- The recommendation was updated in 2021  
(<https://www.oecd.org/sti/recommendation-access-to-research-data-from-public-funding.htm> )





# Data policies

1. Check the research-data requirements of your funding agency and field of research.

A Data policy defines the rules of access and usage to the data produced. Research Institutes like the EIROforum ones all have data policies in place now.

- You are required to accept the data policy when requesting access
- Data is not considered as property but has a usage licence
- Data are under **embargo** (varying from 1 yr, 3 yr, 5 yr) for use by the original creators for a limited amount of time **before being made open**.



# Research Facilities Data Policies

- ESA – open data policy for most data (since 2010)
- ILL – open data policy (since 2012)
- ESRF – open data policy (since 2015)
- EMBL – open access policy (since 2015)
- ESO – open data policy (updated in 2016)
- EuXFEL – open data policy (since 2017)
- EUROfusion – proposal for open data policy (in progress since 2018)
- CERN – open data policy for LHC (since 2020)
- CERIC-ERIC – open data policy (since 2021)
- SESAME – open data policy (since 2023)
- PSI, SOLEIL, ELETTRA, HZB, MAXIV, ...



# ESRF Data Policy

<https://www.esrf.fr/datapolicy>



EUROPEAN SYNCHROTRON RADIATION FACILITY

30 2015

## *The ESRF Data Policy*

The ESRF aims to implement a Data Policy in 2016.

The main elements of this policy are:

- Data ownership
- Data access
- Data archiving
- Open access

This policy follows largely the recommendations of the PaN-data Europe Strategic Working Group laying out a common framework for scientific data management at photon and neutron facilities (Deliverable D2.1, PaN-data Europe, co-funded by the European Commission under the 7th Framework Programme)

**Updated to be FAIR  
compliant in 2023**



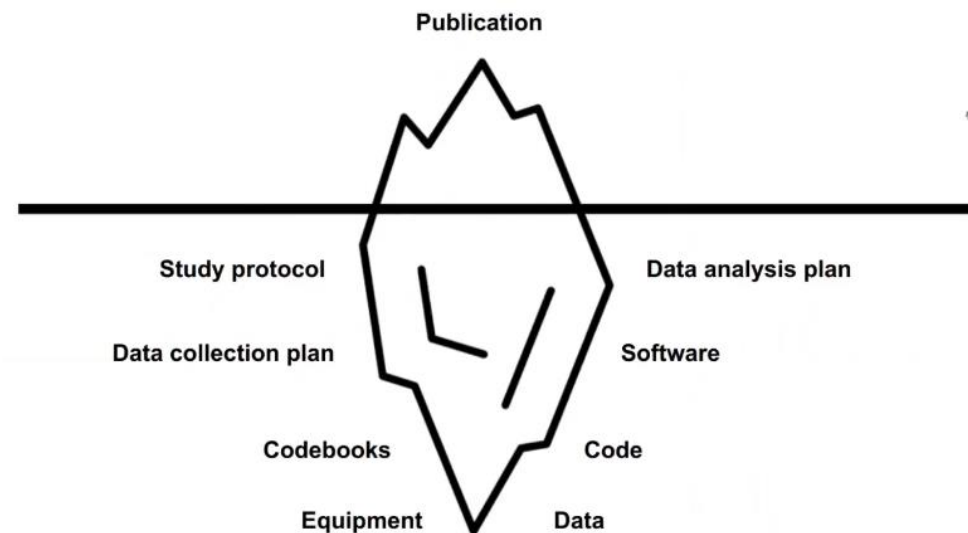
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Data and research outputs

## 3. List the various types of data and research outputs that you expect to produce.

- Output from your research is everything you produced to come up with your findings including :
  - Raw data
  - Metadata
  - Processed data
  - Analysis workflows
  - Logbooks
  - Software
  - Etc.



# Metadata and Why it is important

8. Provide metadata that allows others to understand, cite and reuse your data files.

*Documentation or information about a data set.*

<https://data.research.cornell.edu/content/writing-metadata>

- **Metadata is all additional data you need to understand your data**
- Examples range from file name, time, to experiment condition, energy, sample name, sample parameters, ...
- Use the standard vocabularies defined for your domain e.g. [Nexus](#), [FITS](#), ...





# Metadata vocabularies

Many standard vocabularies exist for processed data. There are fewer vocabularies for raw data but they do exist. Check the existing standards for your domain.

- Don't invent a new vocabulary until you are sure none exists
- Databases of standard vocabularies:
  - <https://fairsharing.org/> - FAIRsharing as a community approach to standards, repositories and policies
  - <https://www.dcc.ac.uk/guidance/standards/metadata/list> - list of Metadata standards



# Metadata – Take away messages

Metadata have a tendency to get treated as 2<sup>nd</sup> class data.

Whatever you do **TAKE YOUR METADATA SERIOUSLY!**

The quality of your data depends on it!

- **RECORD** them DIGITALLY
- **STORE** them with your DATA
- **FOLLOW** the STANDARD(s)
- **ENSURE** others can **UNDERSTAND** your (meta)data



# Example vocabulary – Nexus for photon and neutron sources

## NeXus

NeXus is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.

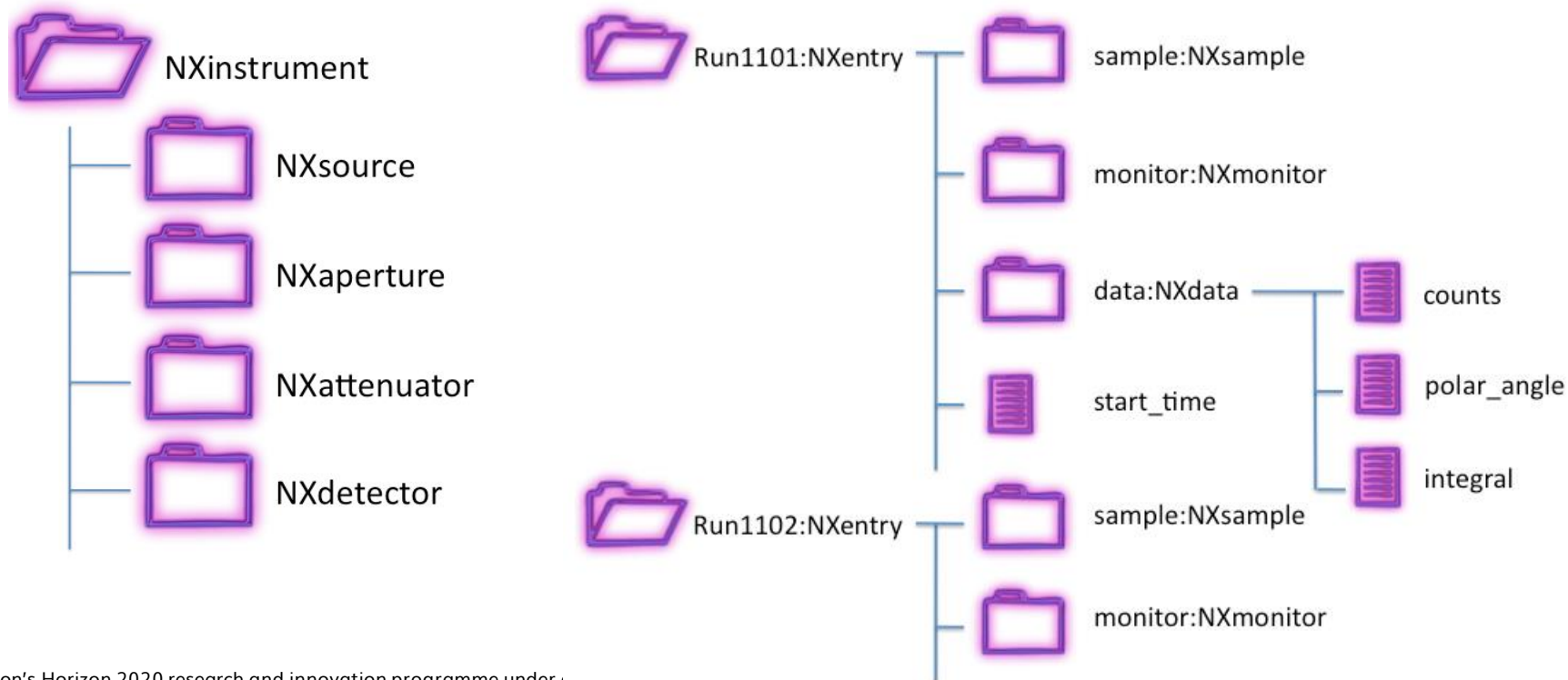
Home

GitHub Organisation

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<https://www.nexusformat.org/>

Nexus provides a standard vocabulary for:



# Example vocabulary – Nexus for photon and neutron sources

## Example of structure of data file from ESRF:

Name	Description	Type	Shape	Link
lima.h5		NXroot		
entry_0000	"Lima 2D de..."	NXentry		
end_time	"2020-09-08..."	string	scalar	
instrument		NXinstrument		
mpx_cdte_22_eh1		NXdetector		
acquisition		NXcollection		
data	3D data	uint16	100 × 516 × 516	
detector_information		NXcollection		
header		NXcollection		
image_operation		NXcollection		
plot		NXdata		
data	3D data	uint16	100 × 516 × 516 Soft	
measurement		NXcollection		
data	3D data	uint16	100 × 516 × 516 Soft	
start_time	"2020-09-08..."	string	scalar	
title	"Lima 2D de..."	string	scalar	

## NeXus

NeXus is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.

[Home](#)

[GitHub Organisation](#)

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# Data formats

5. Define appropriate data file formats (see <https://fairsharing.org/> for formats).
7. Check what data format and structure the chosen archive might request.

Data formats refer to how the bytes in a file are interpreted. Not the data vocabularies. Data formats must be readable over the long term (for archiving). Data formats must be efficient

- Example data formats:
  - CSV (Comma Separated Values)
  - TIFF for images
  - HDF5 as container
- **USE** the **STANDARD**(s) for your **community**

Further reading: [ETD Guidance Brief File Formats](#)





# E-logbooks

Provide metadata that allows others to understand your experiment.

Logbooks are an essential part of the scientific method. All scientists should keep a logbook. E-logbooks replace paper logbooks.

- E-logbook advantages
  - Shared editing online
  - Powerful search facilities
  - Access rules during embargo period
  - Allows others to understand what you did during the experiment
- E-logbook is metadata and will be part of the open data

Further reading: <https://guides.library.oregonstate.edu/research-data-services/data-management-lab-notebooks>



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# ESRF e-logbook example – ID21 / EV-280

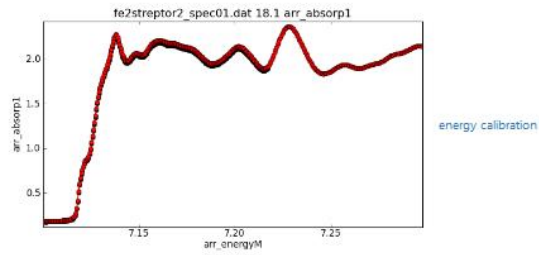
ID21 / EV-280 Beneficial symbiosis in tomato plants: its role on Fe translocation and speciation

Dataset List 90 Logbook Shipping

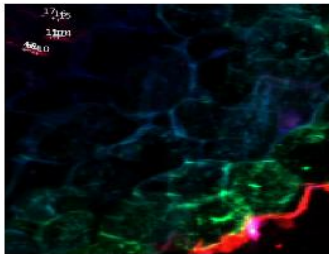
+ New Take a photo View PDF Help 0 new log(s) arrived. Everywhere Everywhere 72 found

November 5th 2018

10:18:40 OPTICS> zapenergy 7.1 7.3 400 0.1 1 2 0 2000 (zap: #2, spec: #19)



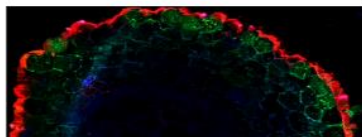
09:58:09 OPTICS> Fexanes\_ev280



Fe2 strepto r2 Main Root: XANES Points

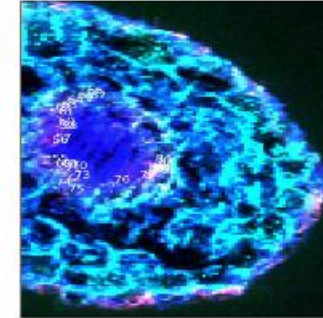


00:18:27 OPTICS> zapxiaimage samy 7.904 7.324 580 samz 25.476 26.025 549 100 0 (zap: #1, spec: #2)



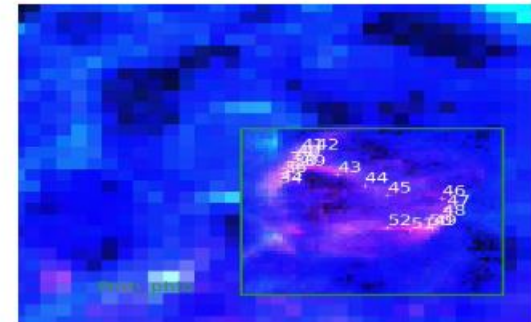
Fe [0.749]  $\mu\text{g/g}$   
Mn [0.121]  $\mu\text{g/g}$   
S [0.6692]  $\mu\text{g/g}$

23:50:29 OPTICS> Fexanes\_ev280



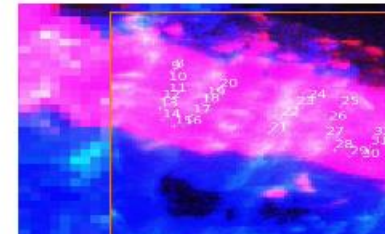
Fe3 prio r3 Sec Root: XANES Points

22:48:31 OPTICS> Fexanes\_ev280



Fe3 prio r3 Main Root prim phlo: XANES Points

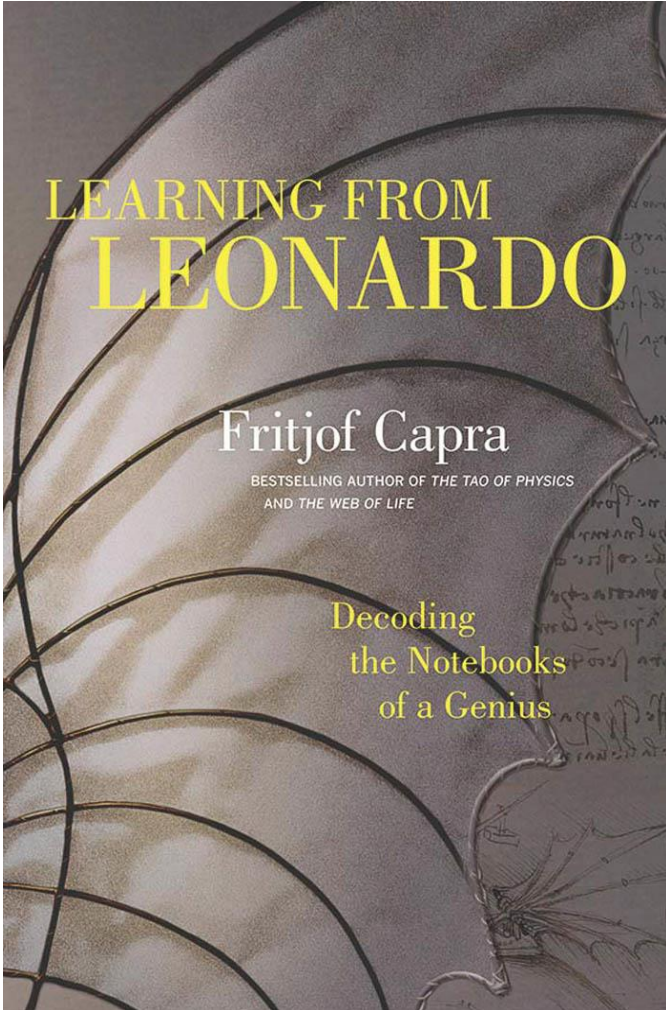
22:25:02 OPTICS> Fexanes\_ev280



ment No. 1



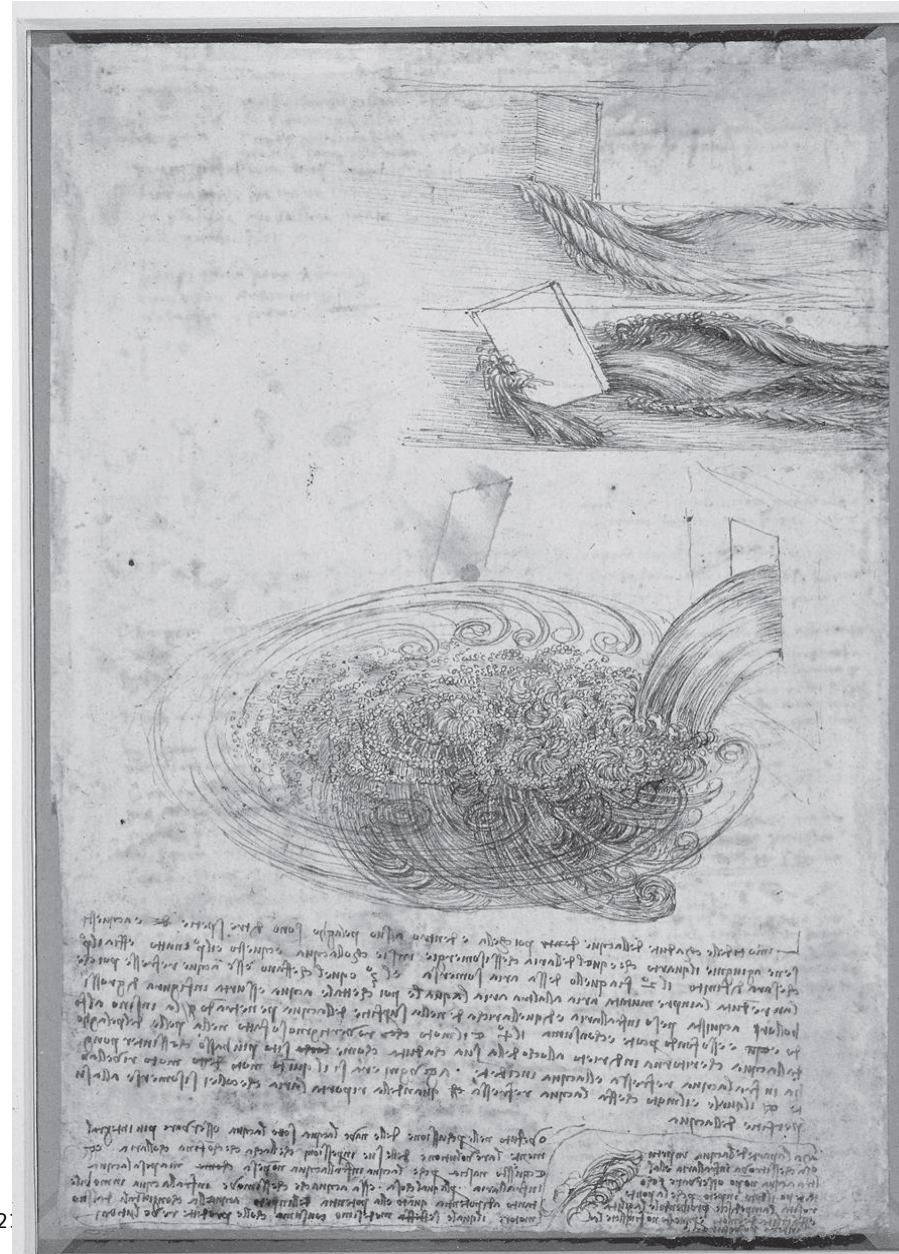
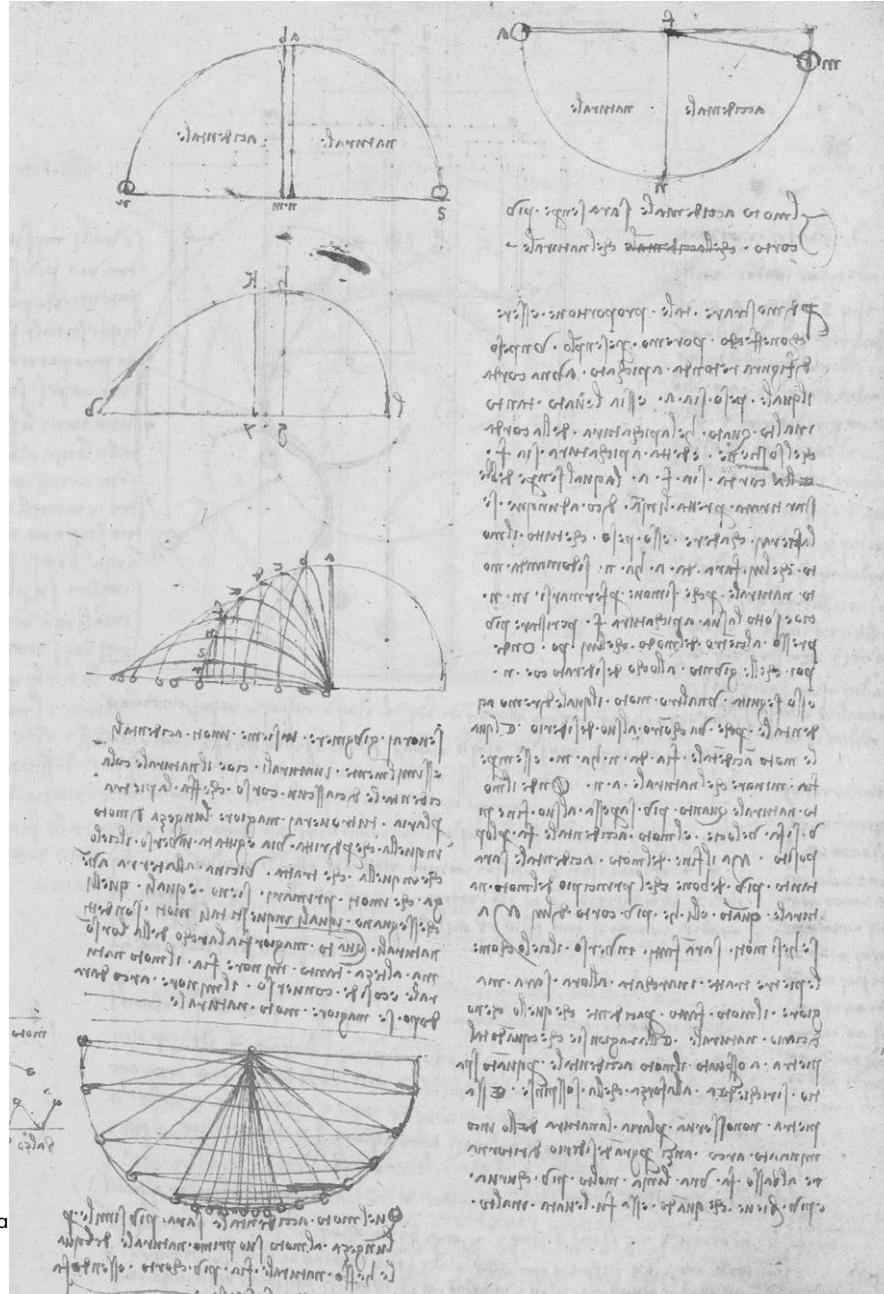
# Notebooks can inspire Logbooks e.g. Leonardo da vinci's notebooks



**notebooks can be very useful for posterity...**



This project has received funding from the European





# Open Source Software

Software is an essential part of a scientists toolset. Many scientists have learned to program so they can analyse their data. The resulting software is part of the outcomes of the research.

- Wherever possible use Open Source software
- When writing software :
  - Follow best practices for software
  - Publish it under an Open Source license
  - Store it in an open ([Git](#)) repository with version control
- Cite your software in your publications



GitHub.com



Gitlab.com



# E-Life author guide



<https://reviewer.elifesciences.org/author-guide/full>

- Source Code:
  - *Relevant software or source code should be deposited in an open software archive. Where appropriate, authors can upload source code files to the submission system (for example, MATLAB, R, Python, C, C++, Java). Any code provided should be properly documented, in line with these instructions (courtesy of PLOS). Please also refer to our Software sharing policy.*



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852





# Software tools

Many specific and generic tools exist. One common tool which is being adopted widely is JupyterLab and the Python language.

- Python has become the de facto programming language in science

- Jupyter notebooks enable reproducible publications

<https://jupyter.org>

- Binder service can preserve and run the software for an analysis - <https://mybinder.org/>

Jun 2021	Jun 2020	Change	Programming Language	Ratings	Change
1	1		 C	12.54%	-4.65%
2	3	▲	 Python	11.84%	+3.48%
3	2	▼	 Java	11.54%	-4.56%
4	4		 C++	7.36%	+1.41%
5	5		 C#	4.33%	-0.40%
6	6		 Visual Basic	4.01%	-0.68%
7	7		 JavaScript	2.33%	+0.06%



# Data Management Plans (DMP)

2. Go online for help in developing a data-management plan. A useful guide outlining UK funder expectations can be found at [go.nature.com/2tnohla](https://go.nature.com/2tnohla).

12. Revisit your plan frequently and update it if necessary.

- DMP document the data management steps in a more formal manner
- Funders are requiring DMPs to ensure RDM is planned
- Facilities will require DMPs more and more to be sure Users can deal with the research data
- DMPs are living documents which need to be updated throughout the project
- Examples of DMPs can be found on [DMPonline](#)



# Typical questions to be answered by the DMP

- What data will be created during research.
- Which policies might apply to the data, such as legal, institutional and funding requirements.
- Which data standards will be used, including metadata standards.
- How data will be documented.
- Ownership, copyright and intellectual property rights in data.
- Data security aspects.
- Data storage and backup measures and required equipment or infrastructure.
- Plans for sharing data, who will have access and whether there are any embargoes or restrictions.
- Data management roles and responsibilities.
- Costing or resources needed over and above usual research and dissemination activities to enable data sharing (certainly for the shorter term following the end of any funded research project).

“Managing and Sharing Research Data: A Guide to Good Practice” by Louise Corti et al

<https://study.sagepub.com/corti2e>



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Data repositories

6. Look for data repositories used by your research community or your host institution (see [www.re3data.org](http://www.re3data.org) for examples).

A data repository stores data for citing, accessing and archiving data over the long term. Repositories can be provided by facilities or community based. Choose the right repository with the service you expect

- Facilities offer repositories for raw and (sometimes) processed data e.g. <https://data.esrf.fr>
- Choose repository which is certified e.g. <http://go.nature.com/2eLHBFP> )
- Use an institute or community archive which is sustainable



# Data archiving

9. Make clear how and when your data can be shared with scientists outside your group.
  10. If your research involves sensitive data, explain any legal and ethical restrictions on data access and reuse.
  11. Assign responsibility for long-term data curation to a suitable office.
- Data need to be archived for long term future use
  - You don't know when and how your data could turn out to be useful
  - The meaning of long term depends on the data e.g. is 10 years enough?





# ESRF data portal - <https://data.esrf.fr>

← → ↻ data.esrf.fr/investigations?page=1

Data Portal My Data Open Data Closed Data Shipping ▾ My Beamlines ▾ Manager ▾

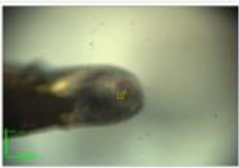
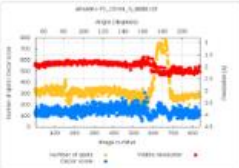
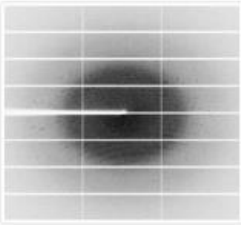
### My Data

HC-3800	ID01	10/09/2018	Strain imaging in suspended GeSn micro-Bridges for laser application using multi-angle Bragg projection Ptychography	0 0 Bytes	0	14/09/2021	DOI <a href="https://doi.org/10.1515/ESRF-ES-119464351">10.1515/ESRF-ES-119464351</a>
MI-1328	ID16A	08/05/2018	High resolution, high throughput pink beam far field Ptychography	209 9.1 MB	209	11/05/2021	DOI <a href="https://doi.org/10.1515/ESRF-ES-100129017">10.1515/ESRF-ES-100129017</a>
MA-3864	ID01	09/03/2018	Strain in operando AlGaIn/GaN High-Electron-Mobility Transistor	13 12.4 GB	140	13/03/2021	DOI <a href="https://doi.org/10.1515/ESRF-ES-91421585">10.1515/ESRF-ES-91421585</a>

19:29 Sep 26, 2018 AFAMIN-75\_15min AFAMIN-75\_15min\_5\_1874873 835 1 GB Download

Summary Crystallography Instrument Files (33) Metadata List

Name	AFAMIN-75_15min_5_1874873	Resolution	1.81887 Å
Start	7:29:00 PM	Wavelength	0.966 Å
Sample	AFAMIN-75_15min	Exposure Time	0.148 s
Images	835	Flux start	4.05e-11
Transmission	100 %	Flux end	4.07e-11
Prefix	AFAMIN-75_15min_5_XXXXX.cbf	X Beam	128.966 mm
		Y Beam	146.86 mm



[Download](#)

ICAT project collaboration <https://github.com/icatproject>

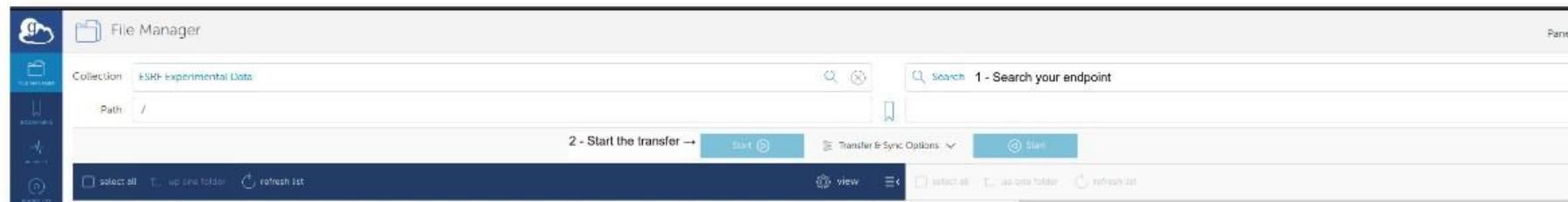
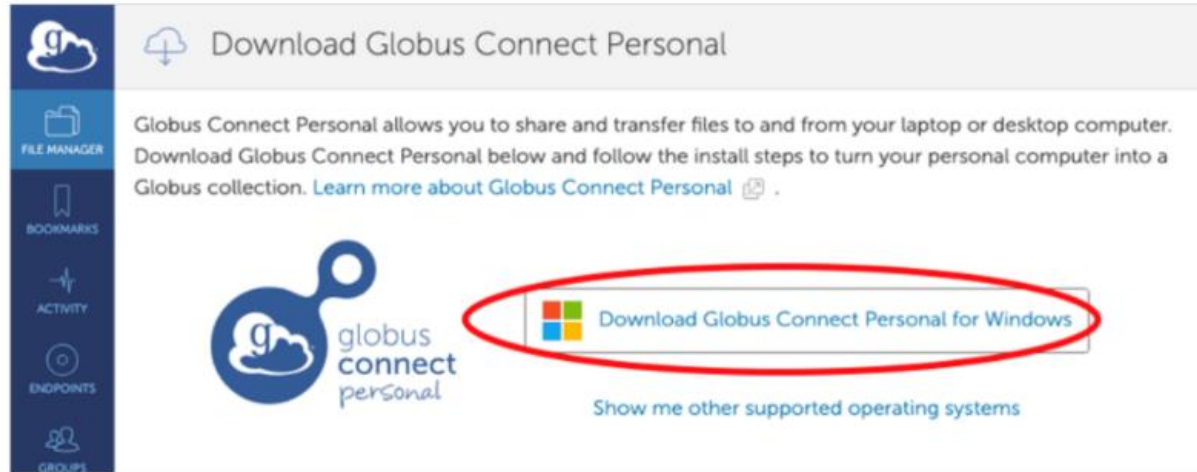


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Downloading large data: globus online

For users that want to download large volume of experimental data (**largest transfer so far 50TB**)



The service opened in fall 2021 for all users and all data

Data access is protected using Access Control Lists (ACLs) on the storage – users cannot see others data.



# Digital Object Identifier (DOI)



A DOI or Digital Object Identifier, is a string of numbers, letters and symbols used to permanently identify any object and link it to the web. DOIs were originally used for publications and are now used for many things including movies, samples, instruments and scientific DATA.

- A DOI is one implementation of a PID (Persistent Identifier)
- A web address (url) is not a PID because it is not guaranteed
- Make sure the data you want to cite has a DOI
- Cite the instrument, samples etc. you used



# Journal require datasets accessible

More and more journals require datasets used in the publication to be cited and accessible. For example eLife, Nature, Plos, Science, ...

- eLife – <https://reviewer.elifesciences.org/author-guide/full>



*All datasets used in a publication should be cited in the text and listed in the reference section and/or data availability statement. References for data sets and program code should include a persistent identifier, for example a Digital Object Identifier (DOI) or accession number.*

...

*Relevant software or source code should be deposited in an open software archive.*



# Example of article correctly citing data

nature neuroscience

Explore content ▾ Journal information ▾ Publish with us ▾ Subscribe

nature > nature neuroscience > technical reports > article

Technical Report | Published: 14 September 2020

## Dense neuronal reconstruction through X-ray holographic nano-tomography

Aaron T. Kuan, Jasper S. Phelps, Logan A. Thomas, Tri M. Nguyen, Julie Han, Chiao-Lin Chen, Anthony V Azevedo, John C. Tuthill, Jan Funke, Peter Cloetens, Alexandra Pacureanu ✉ & Wei-Chung Allen Lee ✉

*Nature Neuroscience* **23**, 1637–1643 (2020) | Cite this article

5492 Accesses | 8 Citations | 196 Altmetric | Metrics

<https://doi.org/10.1038/s41593-020-0704-9>

<https://data.esrf.fr/doi/10.15151/ESRF-DC-217728238>

DOI: [doi.esrf.fr/10.15151/ESRF-DC-217728238](https://doi.org/10.15151/ESRF-DC-217728238)



This project has received funding from the European Union's Horizon 2020 research and i

Open Data / 10.15151/ESRF-DC-217728238

Dataset List 4

Search

<input type="checkbox"/>	Date ↕	Sample ↕	Dataset ↕	Definition ↕	Files ↕	Size ↕	Download ↕	🔍
<input type="checkbox"/>	🕒 18:34 3 Jul 2020	Drosophila	drBrain		11	152.6 GB	<a href="#">Download</a>	🔍

Summary Files 11 Metadata List

Name **drBrain**

Definition

Start **6:34:54 PM**

Sample **Drosophila**

Description



[/data/id16a/inhouse2/staff/ap/dataNatNeuro2020/Drosophila/drBrain](#)

[Download](#)

<input type="checkbox"/>	🕒 18:35 3 Jul 2020	Drosophila	drLeg		11	133.5 GB	<a href="#">Download</a>	🔍
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Summary Files 11 Metadata List

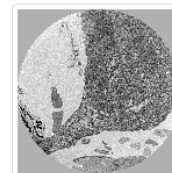
Name **drLeg**

Definition

Start **6:35:00 PM**

Sample **Drosophila**

Description



[/data/id16a/inhouse2/staff/ap/dataNatNeuro2020/Drosophila/drLeg](#)

[Download](#)



# Data storage

## 4. Decide what data and research materials require archiving and determine how much storage space you will need.

- Data volumes are constantly increasing (up to Petabytes)
- You could be faced with more data than you can store locally
- Very hard for individuals to maintain access to local storage for years
- **Research facilities provide services to keep raw data at the facility/cloud**
- Many free services exist now for scientific data e.g. Zenodo, Figshare, ...
- Commercial cloud offer practically unlimited resources at a cost
- Data stored on commercial cloud disappear when you stop paying



# File naming conventions

3. List the various types of data and research outputs that you expect to produce.

Adopt a directory and file naming convention which will allow you to know what the file contains.

- For example:

Proposal/Beamline/Sample\_name\_Scan\_type.ext

MA1234/ID56/Gold\_50\_nm\_ptycho\_scan.h5



# Own your identity in the digital world

In a digital world you need to control your identity and not give it away to the corporate world to exploit. It is highly recommended to create your own identity using ORCID – a free non-commercial service

- Benefits of an [ORCID](#) identity:
  - You will be distinguished from every other researcher, even researchers who share your same name,
  - Your research outputs and activities will be correctly attributed to you,
  - Your contributions and affiliations will be reliably and easily connected to you,
  - You will save time when filling out forms, (leaving more time for research!),
  - You will enjoy improved discoverability and recognition,
  - You will be able to connect your record to a growing number of institutions, funders, and publishers,
  - Your ORCID record is yours, for free, forever.



## Achieving 100% Open Identifiers:

1. All scientists encouraged to create an ORCID
2. Encourage the use of ORCID for users for publications



Dataset List 0 Logbook Shipping Proposal

### Suppression of charge-density wave order in 2H-TaSe2 by pressure

05/10/2022 08:00 - 08/10/2022 08:00 - on beamline: ID15B - release date: 08/10/2025

#### Abstract

This is new evidence that many materials feature superconducting phases when a CDW phase is suppressed by extrinsic parameters such as pressure or magnetic fields. In this work, we study the phase space of emergent superconductors in Ta-doped TMDCs. We propose to determine the CDW quantum critical point in 2H-TaSe2 under pressure. We will study the evolution of the soft phonon mode at the CDW transition in 2H-TaSe2 (unpublished) and determine if it has a CDW quantum critical point closely connected to the emergent superconducting phase. These transitions are mediated by the same mechanism, electron-phonon coupling of the phonon in its most crucial but still unexplored area.

Name: **Gaston Garbarino**

	ORCID
Investigator	<a href="https://orcid.org/id/00000000347809520">id/00000000347809520</a>
Participant, Scientist	<a href="https://orcid.org/id/00000000312931067">id/00000000312931067</a>
Participant, Scientist	<a href="https://orcid.org/id/00000000242561354">id/00000000242561354</a>

Yuliia TYMOSHENKO	Participant, Scientist	
Tom Laurin LACMANN	Participant, Scientist	<a href="https://orcid.org/id/0000000017795306X">id/0000000017795306X</a>
Amir-Abbas HAGHIGHIRAD	Participant, Scientist	<a href="https://orcid.org/id/00000000347234966">id/00000000347234966</a>



This project has received funding from the European Union's Horizon 2020



# Open Training – <https://pan-learning.eu>

<https://e-learning.pan-training.eu/moodle/course/view.php?id=11>

**PaNOSC summerschool FAIR session**

e-Learning | My courses | PaNOSC summerschool FAIR session

Turn editing on

### Making FAIR data a reality

**Making FAIR data a reality for the PaN community**

- Full FAIR compliance of PaN scientific data
- Support in shaping EOSC services for users needs
- Increase of RIs' impact by encouraging data reuse
- Innovative data services at RIs and as part of the EOSC
- Collaboration with EOSC projects to share outcomes
- Sharing of best practices for open data policies

? What are Science, Open Science, EOSC and PaNOSC

Please answer to the questions below to start the course.

Announcements

### Trust in Science

- Why trust
- Why trust science quiz

### What is Open Science

- Open Science definition
- Pillars of Open Science
- Process of Openness in Research
- Open Science Schools of Thought
- Open Science Resources

### What is EOSC

- The European Open Science Cloud
- EOSC Projects and Ecosystem

### What is PaNOSC + ExPaNDS

- PaNOSC + ExPaNDS projects

### Outcomes of PaNOSC + ExPaNDS

- PaNOSC + ExPaNDS FAIR Outcomes

### What is Scientific Data and Metadata

- Scientific Data and Metadata



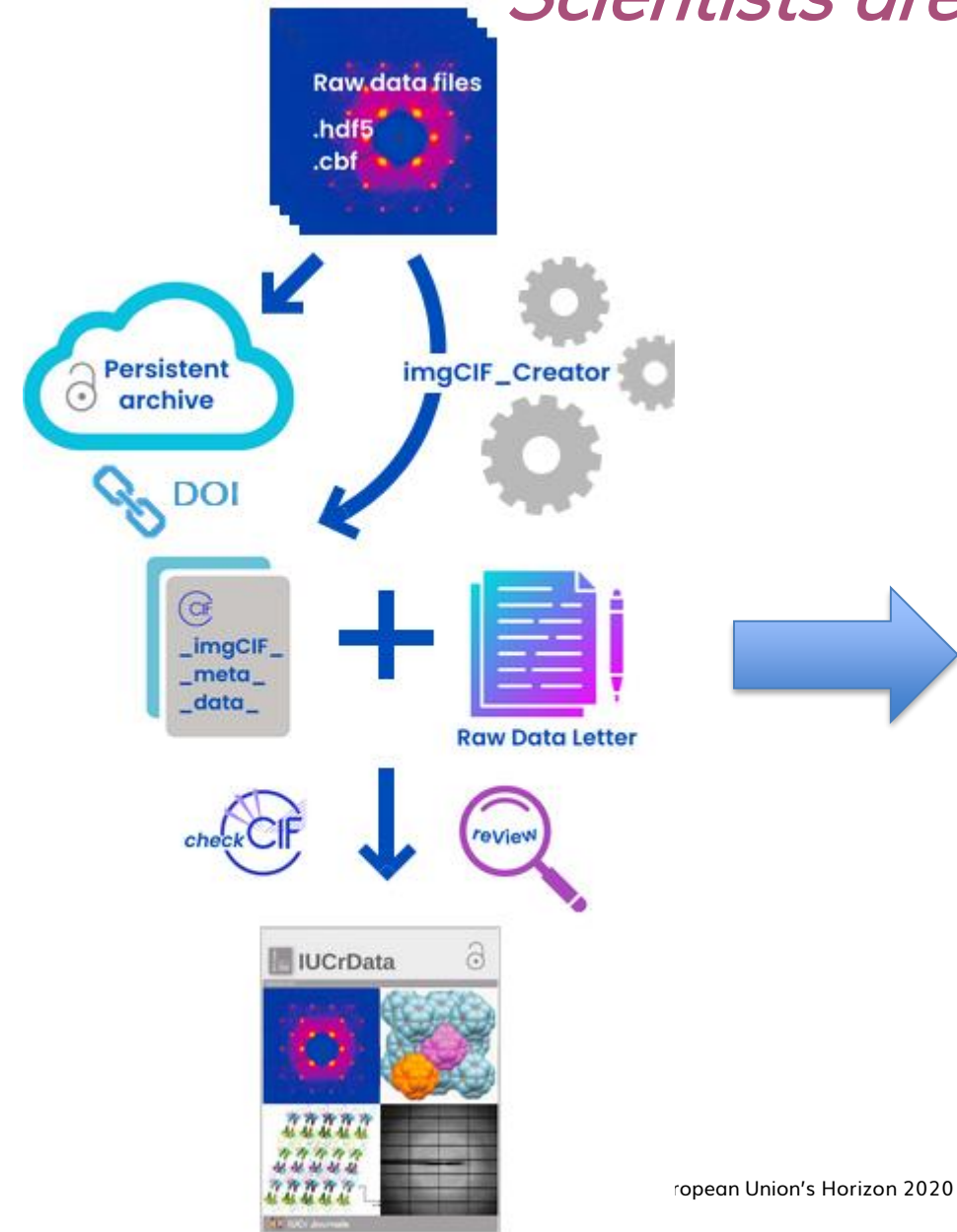
# What are the advantages of producing FAIR Data?

- Better data and metadata means better science
- Saves you time and improves your results
- Allows you to use standard data services
  - Remote data analysis
  - Data archiving
  - DOI
- Publications with open data are cited more often
- You get more credit for your work
- Science is more reproducible and replicable



# IUCr Journals have launched IUCrData's Raw Data Letters

## Scientists are encouraged to publish raw data



European Union's Horizon 2020 research

IUCrData  
ISSN 2414-3146

### Crystal structure of the second extracellular domain of human tetraspanin D9: twinning and diffuse scattering

Viviana Neviani, Martin Lutz, Wout Oosterheert, Piet Gros and Loes Kroon-Batenburg\*

Received 20 April 2021  
Accepted 1 May 2021

Keywords: twinning; diffuse scattering; tetraspanin CD9<sub>EC2</sub>

Department of Chemistry, Structural Biochemistry, Bijvoet Centre for Biomolecular Research, Faculty of Science, Utrecht University, Utrecht, The Netherlands. \*Correspondence e-mail: l.m.j.kroon-batenburg@uu.nl

Remarkable features are reported in the diffraction pattern produced by a crystal of tetraspanin CD9<sub>EC2</sub>, the structure of which was described previously [Oosterheert *et al.* (2020), *Life Sci. Alliance*, **3**, e202000883]. CD9<sub>EC2</sub> crystallized in space group *P1* and was twinned. Concurrent with the twinning, diffuse streaks were seen in the direction perpendicular to the twinning interface. Preliminary conclusions are made on packing disorder and potential implications for the observed molecular structure. It is envisaged that the raw diffraction images could be very useful for methods developers in trying to remove the diffuse scattering to extract accurate Bragg intensities or by using it to model the effect of packing disorder on the molecular structure.

Raw data	Structure

Raw diffraction data  
HDF5 data file, DOI: <https://doi.org/10.5281/zenodo.1234567>  
Metadata ImgCIF file, DOI: <https://doi.org/10.1107/S2414314622000384/me6134.cif>



# Estimated carbon footprint of experiment

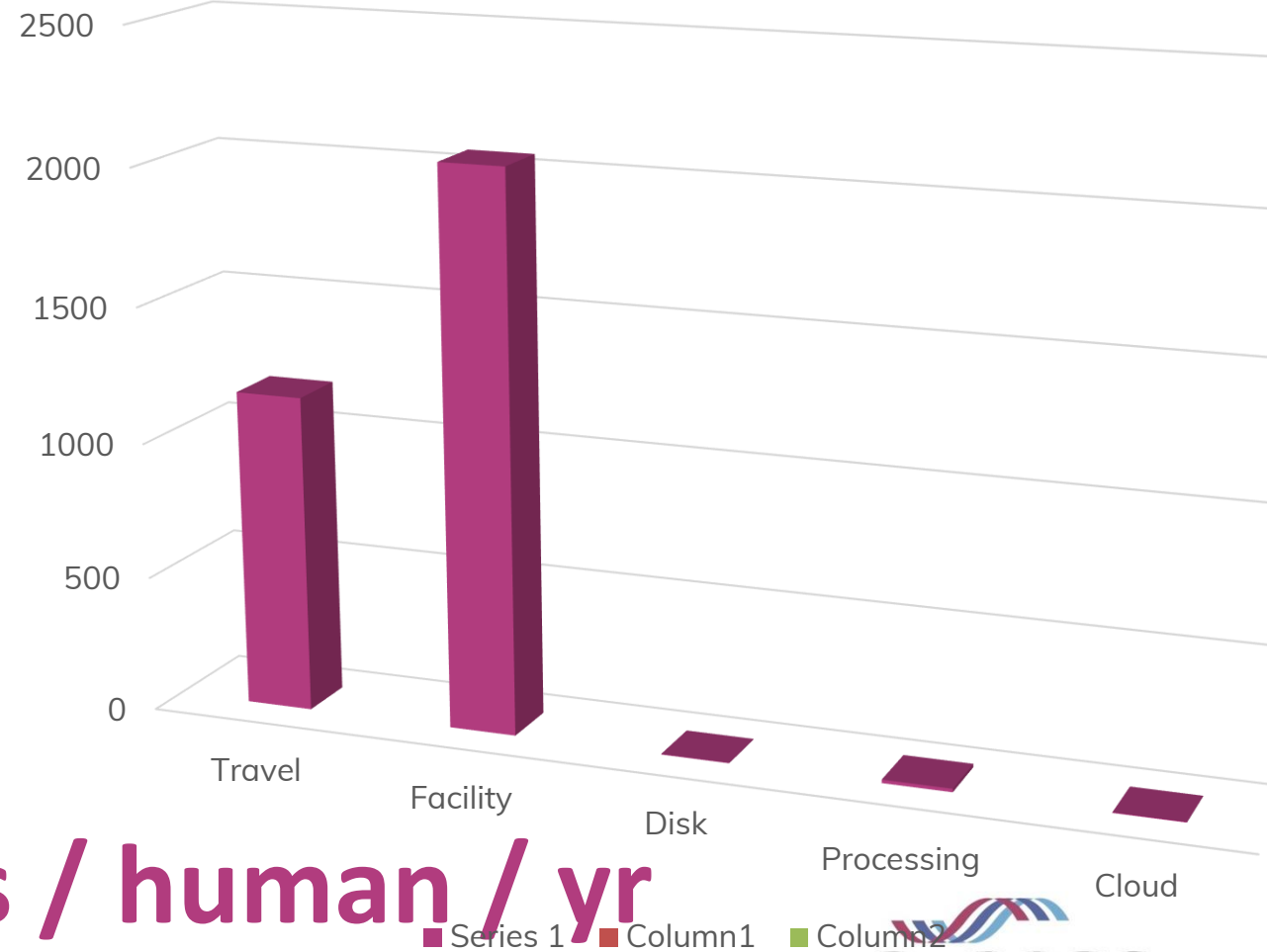
- User Travel = **1170 kg**
- Beamtime energy consumption = **2056 kg**
- Data stored on disk = **1.8 kg**
- Data processing on site = **12.6 kg**
- Cloud transfer = **2.3 kg**

CO<sub>2</sub>e per kWh in France = **75 g/kWh**

**TOTAL = 3.253 tons !**

**Sustainable Goal = 5 tons / human / yr**

Carbon footprint for 1 week experiment @ ESRF



# Carbon footprint of archiving data

- 200 GB Data archived on tape for 10 years (full tape library)  $\sim 13 \text{ g} * 10 \text{ yrs} = 130 \text{ grams}$

- ARCHIVING raw data for 10 years  
0.000004 % of CO<sub>2</sub>eq needed  
to acquire the raw data!



# Data availability – the wrong + right way



Data availability

Data available on reasonable request to the authors.



Open Research

## Data Availability Statement

The data that support the findings of this study are openly available in Zenodo at <https://doi.org/10.5281/zenodo.6993871> , reference number 6993871.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852





# Another reason for FAIR data is to distinguish from AI generated data

heart

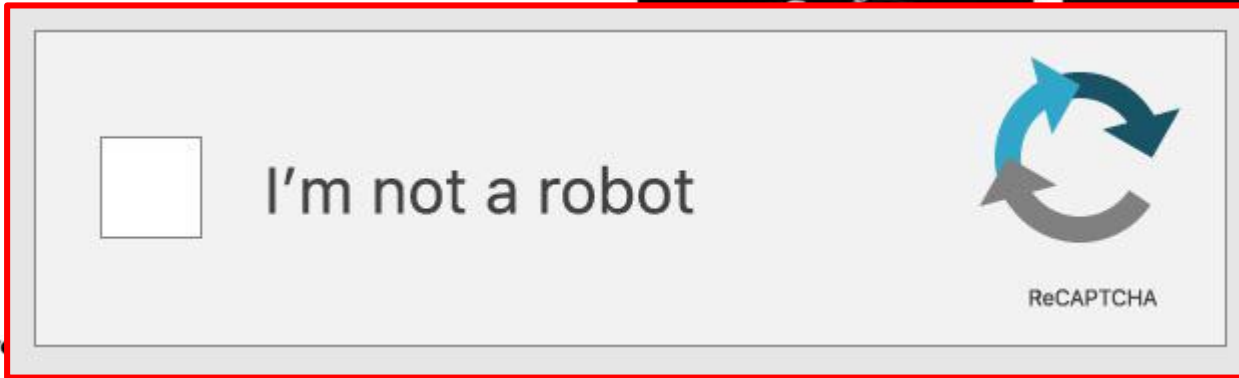
An MRI of the



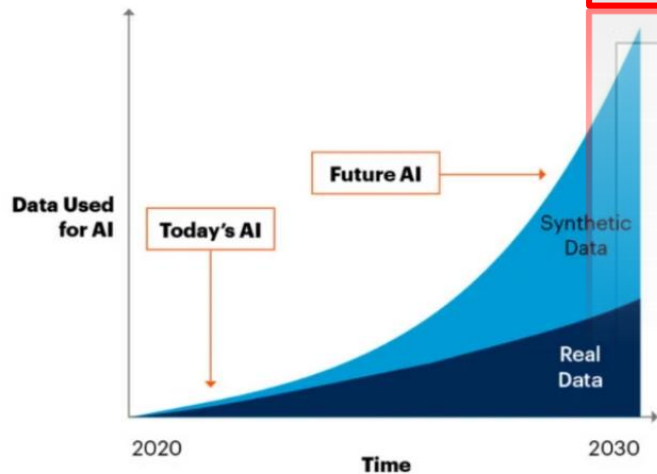
A CT of the



Ultrasound of the



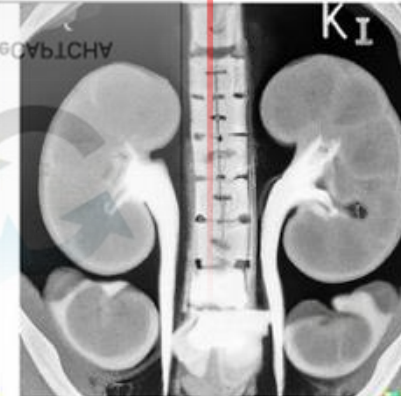
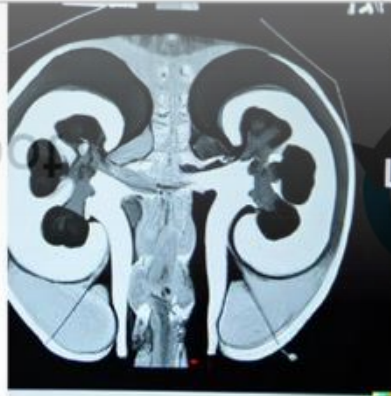
By 2030, Synthetic Data Will Completely Overwhelm Real Data



- Artificially Generated Data
- Generated From Simple Rules, Statistical Modelling, Simulation and Other Techniques

- Obtained From Direct Measurements
- Constrained by Cost, Logistics, Privacy Reasons

kidney



Examples of text-to-image-generated anatomical structures in CT, MRI, and ultrasound images created with DALL-E 2.

Image source: Adams et al., Journal of Medical Internet Research 2023 (CC BY 4.0)

# Conclusions #1

Adopting best practices for Open Science and FAIR Data has many benefits especially helping **MAKE BETTER + REPRODUCIBLE SCIENCE**

- Make sure you follow a checklist which covers the following topics:
  - Data Management Plan, Data Policy, Data Outputs, File types, File Formats, Software, Workflows, e-Logbooks, Data Storage, Data Archiving, Data DOI
  - Spend time with your data to make it FAIR by **adding rich metadata, your orcid, and then releasing it, publishing it, citing the data DOI !**
- Many **digital tools** exist for treating your data seriously + publishing them
- Learn about the data you will produce before going to the synchrotron




# Conclusions #2

1. Scientific results are much more than the publications
2. Data Availability - DO NOT use the phrase “data available on reasonable request” in publications
3. Instead make sure you cite the data DOIs !!!



# Acknowledgements

- [RDMKit](#) Elixir online guide 
- University of Saskatchewan
  - <https://library.usask.ca/studentlearning/workshops/grad-research.php#panel-section-3-ResearchDataManagementWhatYouNeedtoKnow>
- Nature magazine, Scientific Data
- PaNOSC, ExPaNDS are EOSC H2020 projects
- OSCARS, OSTRails are EOSC Horizon Europe projects
- Wikipedia, Internet, ChatGPT



# Tools to help you manage your research

A non-exhaustive list of tools to explore

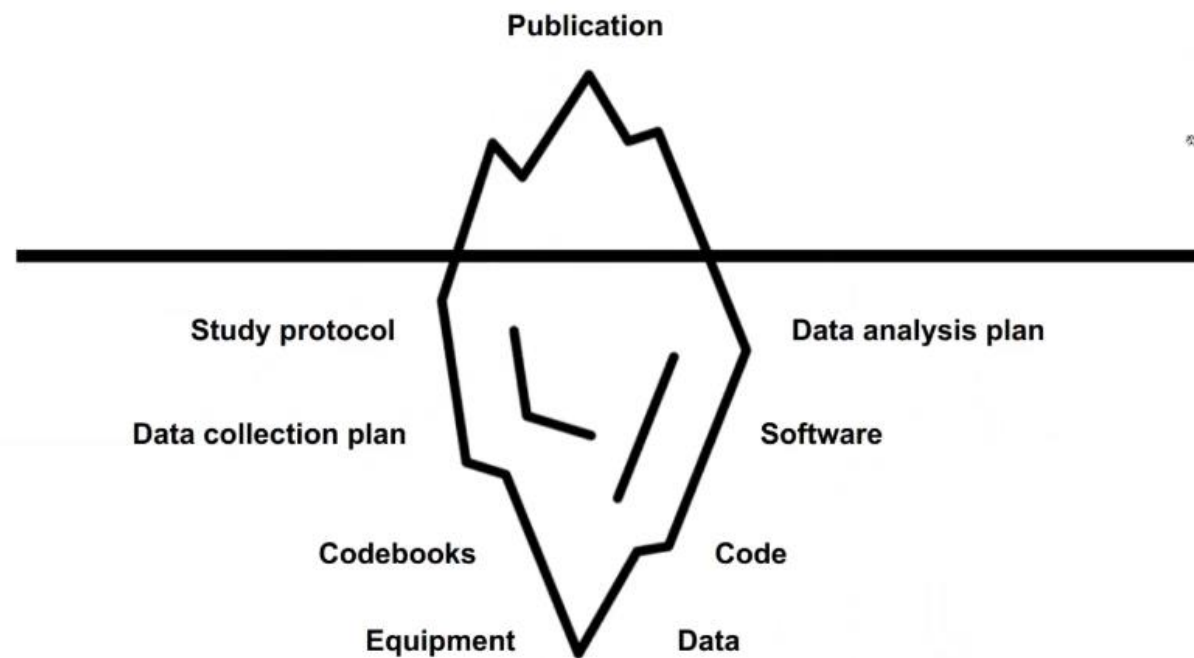
- Elixir training course on “FAIR, Open Data and Open Science”  
<https://oceantraining.eu/moodle/course/view.php?id=29>
- Open science framework – [osf.io](https://osf.io)
- [Protocols.io](https://protocols.io)
- [Fairsharing.org](https://fairsharing.org)
- [Jupyter.org](https://jupyter.org) notebooks





# Thank you

[andy.gotz@esrf.fr](mailto:andy.gotz@esrf.fr)



# Benefits of data sharing

## Benefits of Data Sharing for Different Players in the Research Environment

### Benefits for researchers:

- increases visibility of scholarly work;
- likely to increase citations rates, for example, open access journal articles are cited more;

*(Continued)*

*(Continued)*

- enables new collaborations;
- encourages scientific enquiry and debate;
- promotes innovation and potential new data uses;
- establishes links to next generation of researchers.

### Benefits for research funders:

- promotes primary and secondary use of data;
- makes optimal use of publicly funded research;
- avoids duplication of data collection;
- maximizes return on investment.

### Benefits for the scholarly community:

- maintains professional standards of open inquiry;
- maximizes transparency and accountability;
- promotes innovation through unanticipated and new uses of data;
- enables scrutiny of research findings;
- improves quality from verification, replication and trustworthiness;
- encourages the improvement and validation of research methods;
- provides resources for teaching and learning.

### Benefits for research participants:

- allows maximum use of contributed information;
- minimizes data collection on difficult-to-reach or over-researched populations;
- allows participants' experiences to be understood as widely as ethically possible.

### Benefits for the public:

- advances science to the benefit of society;
- adopts emerging norms such as open access publishing;
- to be, and appear to be, open and accountable;
- complies with openness laws and regulations.

“Managing and Sharing Research Data: A Guide to Good Practice” by Louise Corti et al

<https://study.sagepub.com/corti2e>



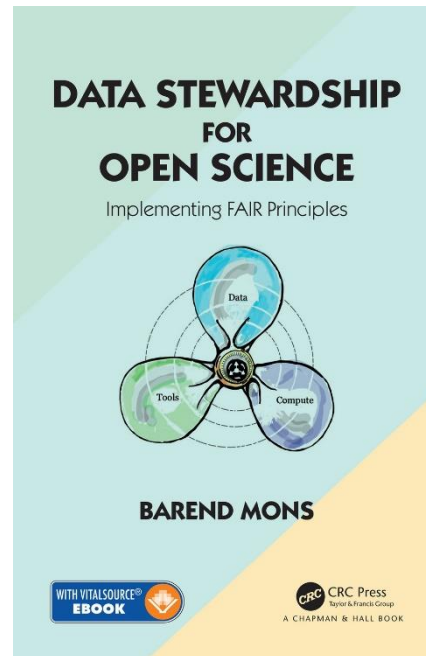
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# Learning more about FAIR RDM for data managers

- RDMKit - <https://rdmkit.elixir-europe.org/index.html>
  - Provides a rich set of resources for all aspects of RDM mainly for researchers working in the Life Sciences but also for other Sciences. Very comprehensive overview, pragmatic approach, up-to-date. An excellent place to start and/or find information.

- Recommended reading:



# OStails – an EOSC project to build Knowledge Graphs from Data Management Plans

## Project

### OStails

OStails aims to advance processes and instruments for Planning, Tracking, and Assessing scientific knowledge production beyond state-of-the-art, working with various national and thematic contexts, improving existing infrastructure, and connecting key components. For the Plan stage, OStails aims to increase the efficacy of Data Management Plans, turning them from static narrative to living, interconnected “machine actionable” resources, making them the instrument of choice for improving quality of RDM. For the Track stage, OStails is set to establish an open, interoperable and high-quality ecosystem of Scientific Knowledge Graphs, enriching them to become evidence of communities’ FAIR implementations.

The logo for OStails features a stylized 'O' composed of two overlapping semi-circles, one purple and one orange. To the right of this symbol, the word 'stails' is written in a lowercase, sans-serif font. The 's' is purple, and the remaining letters 't', 'r', 'a', 'i', 'l', 's' are black.

# Data management made simple

# Data management made simple

Keeping your research data freely available is crucial for open science – and your funding could depend on it.

[Quirin Schiermeier](#) in Nature (2018)

<https://doi.org/10.1038/d41586-018-03071-1>

1. Check the research-data requirements of your funding agency and field of research.
2. Go online for help in developing a data-management plan. A useful guide outlining UK funder expectations can be found at [go.nature.com/2tnohla](https://go.nature.com/2tnohla).
3. List the various types of data and research outputs that you expect to produce.
4. Decide what data and research materials require archiving and determine how much storage space you will need.
5. Define appropriate data file formats (see <https://fairsharing.org/> for formats).





# Data management made simple

[Quirin Schiermeier](#) in Nature (2018)

# Data management made simple

Keeping your research data freely available is crucial for open science – and your funding could depend on it.

<https://doi.org/10.1038/d41586-018-03071-1>

6. Look for data repositories used by your research community or your host institution (see [www.re3data.org](http://www.re3data.org) for examples).
7. Check what data format and structure the chosen archive might request.
8. Provide metadata that allows others to understand, cite and reuse your data files.
9. Make clear how and when your data can be shared with scientists outside your group.
10. If your research involves sensitive data, explain any legal and ethical restrictions on data access and reuse.
11. Assign responsibility for long-term data curation to a suitable office.
12. Revisit your plan frequently and update it if necessary.

