





Open Data and Open Science

Spotlight on Publishing and Open Science
15th November, 2021
by Andy Götz (ESRF)
PaNOSC coordinator



Outline of Talk

This talk will address the topic of Open Data for scientists doing research with an emphasis on data from life sciences @ ESRF

What you should learn from this talk:

What is the Global, European, Local view?
What are Open and FAIR Data?
What do you as scientists get?
What should you as scientists do?
What services are available?
What services are planned

My background in Open Data

- Software developer and manager @ ESRF since 30+ years
- Co-author of the ESRF data policy + leading the ESRF data policy implementation
- Coordinator of the <u>PaNOSC</u> project for making data from photon and neutron sources FAIR https://panosc.eu
- Member of the IUCr Committee on Data





from
deleting all
data
to
preserving
all raw
data
in
30 years



Definition of Open Data

Data that are freely available to all for re-analysis and re-use



Some questions raised by Open Data

How to access to Open Data?

How to attribute Open Data to give credit?

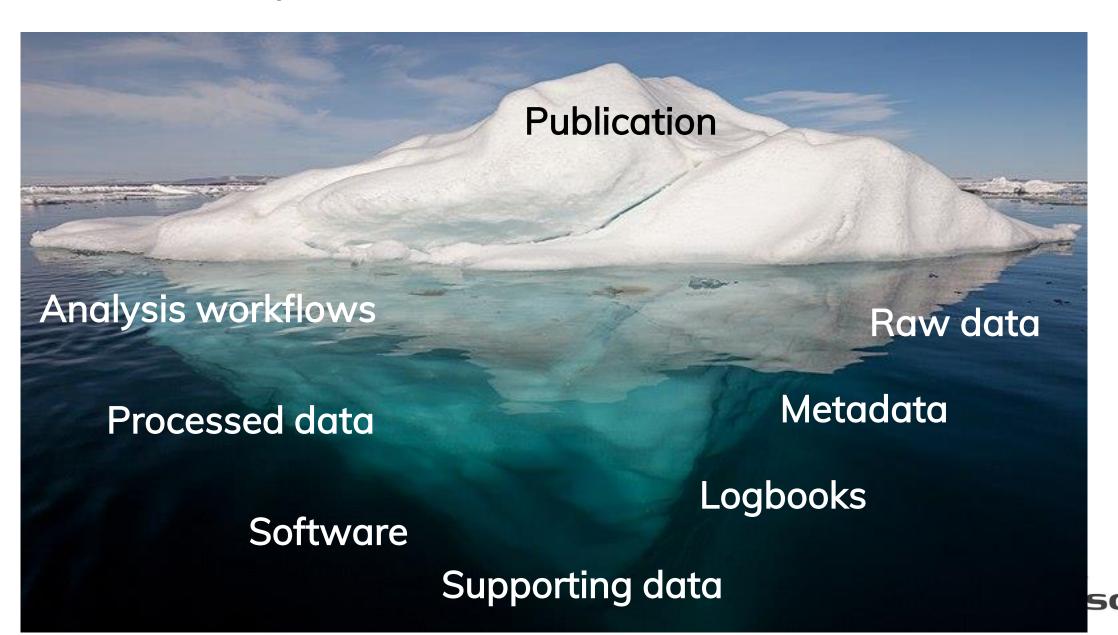
How to ensure Open Data are preserved?

How to ensure Open Data are useful?

Who owns Open Data?



Science produces much more than Publications



nttps://en.wikipedia.org/wiki/File:Iceberg_in_the_Arctic_

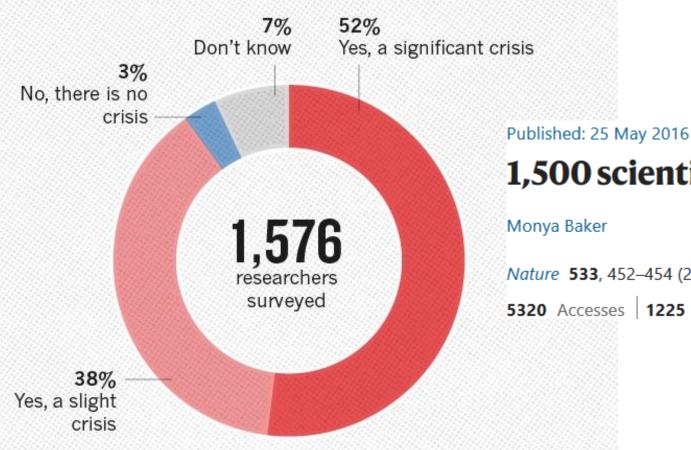
Why make data open?

- 1. Improve the reproducibility of scientific publications
- 2. Improve the quality of scientific data by curation
- 3. Save time for scientists by managing data
- 4. Managing data enable data services to be developed
- 5. Publicly funded research should be public
- 6. Allow data to be re-used by other scientists
- 7. Preserving data prevents data loss
- 8. Data can be used for developing new software
- 9. AI/ML algorithms can be trained on open data
- 10.Difficult to interpret data can get help from community



Open Data are a fundamental part of addressing the **Reproducibility Crisis**





1,500 scientists lift the lid on reproducibility

Nature **533**, 452–454 (2016) Cite this article

5320 Accesses | 1225 Citations | 3871 Altmetric | Metrics



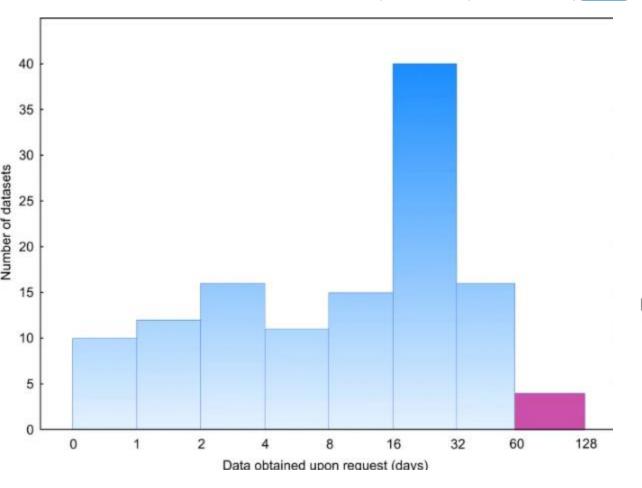


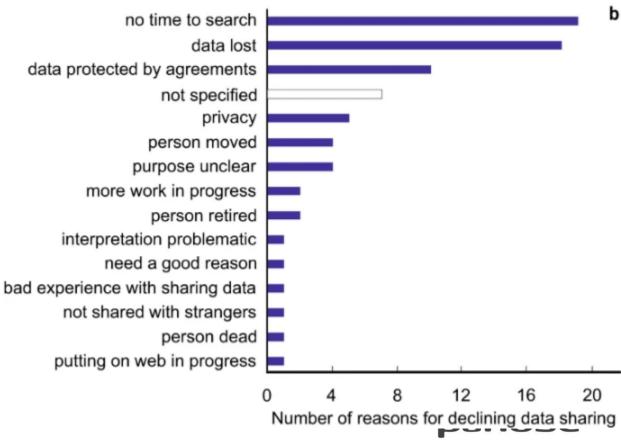
Data sharing practices and data availability upon request differ across scientific disciplines

<u>Leho Tedersoo</u> Margus Pedaste, Marju Raju, Anastasiya Astapova, Heli Lukner, Karin Kogermann & Tuul Sepp

Scientific Data 8, Article number: 192 (2021) Cite this article

6029 Accesses | 1 Citations | 237 Altmetric | Metrics





Recent study on Data availability in Science + Nature

... critical data are still unavailable for re-analysis or metaanalysis for more than half of the papers published in Nature and Science in the last decade.

While the majority of data are eventually available, it is alarming that less than a half of the data clearly stated to be available upon request could be effectively obtained

Our experience shows that receiving data typically required long email exchanges with the authors



FAIR guiding principles

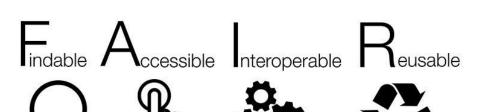
Open Access | Published: 15 March 2016

The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson, Michel Dumontier, [...] Barend Mons

Scientific Data 3, Article number: 160018 (2016) Cite this article

354k Accesses 2959 Citations 1910 Altmetric Metrics



What is FAIR DATA?



Data and supplementary materials have sufficiently rich metadata and a unique and persistent identifier.



Metadata and data are understandable to humans and machines. Data is deposited in a trusted repository. ACCESSIBLE



Metadata use a formal, accessible, shared, and broadly applicable language for knowledge representation.



Data and collections have a clear usage licenses and provide accurate information on provenance.





FAIR Principles

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

$m{T}$ indable

- 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

<u>Interoperable</u>

- 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
- 13: (Meta)data include qualified references to other (meta)data

$extcolor{R}$ eusable

- 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



https://www.rd-alliance.org/group/fair-data-maturity-model-wg/outcomes/fair-data-maturity-model-specification-and-guidelines-0

European Open Science Cloud – a cloud of FAIR data

- EC has spent 260 million euros on the EOSC so far
- The main aim of the EOSC is to make FAIR data a reality
- 4 of the 7 goals of the EOSC concern data
 - Opening up scientific data: The implementation of data management plans to make research data findable, accessible, interoperable and re-usable (FAIR principles).
 - Federation of existing scientific data infrastructures with new provisioning schemes, such as the cloud or specialised facilities, and the development of nodes to link existing national data centres, European e-infrastructures, external providers and research infrastructures.
 - Development of specifications for application interoperability (APIs), data
 portability and data sharing: To enable data to be shared across disciplines and
 infrastructures, more standardisation of meta-data and, perhaps, the actual
 data itself will be needed.
 - Creation of search tools: New software will be required to enable scientists to search, browse and access research data.





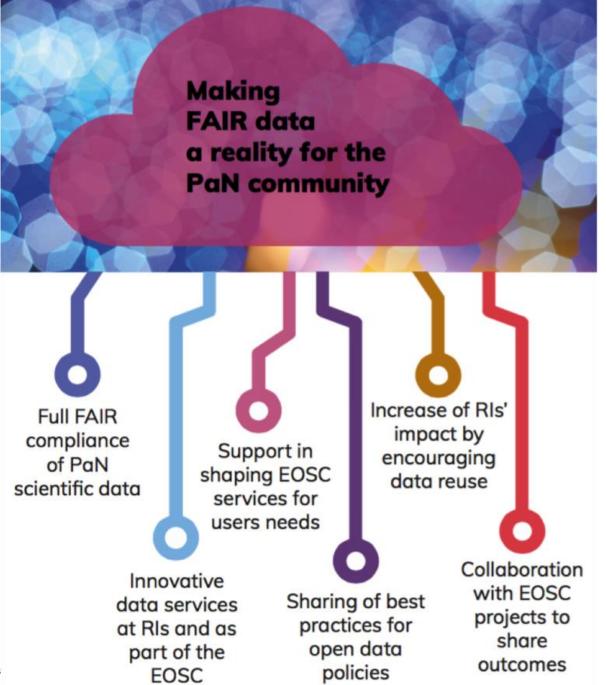
H2020 financed projects - PaNOSC and ExPaNDS

EU Call	HORIZON 2020 INFRA-EOSC-04	HORIZON 2020 INFRA-EOSC-5B
Description	Cluster of ESFRI PaN Sources	EOSC PaN Data Services
Partners	ESRF, ILL, ESS, EU-XFEL, CERIC-ERIC, ELI-DC, EGI	DESY, ALBA, DLS, ELETTRA, EGI, HZB, HZDDR, Max IV, PSI, Soleil, UKRI
Observers	GEANT EU-DAT National RI's	
Linked 3 rd Party	DESY STFC CESNET	
Start – End (Duration)	2018-12-01 - 2022-11-30 [4 Years]	2019-09-01 - 2023-02-28 [3 ½ Years]
Coordinators	A. Götz, G. Bodera	P. Fuhrmann, S. Servan
Budget	12 M Euros	6 M Euros
Home Page	https://panosc.eu	https://expands.eu
Twitter	@PaNOSC_eu #PaNOSC	@ExPaNDS_eu #ExPaNDS
GitHub	github.com/panosc-eu	github.com/expands-eu





PaNOSC objectives







FAIR == **AI**-ready

No-one really argues against the idea that data, as well as the accompanying workflows and services should be findable, accessible under well-defined conditions, interoperable without data munging, and thus optimally reusable.

Being FAIR is not a goal in itself; FAIR Data and Services are needed to enable data intensive research and innovation and (thus) have to be "AI-ready¹" (= future proof for machines to optimally assist us).

However, the fact that science and innovation becomes increasingly "machine-assisted" and hence the central role of machines, is still overlooked in some cases when people claim to implement FAIR.

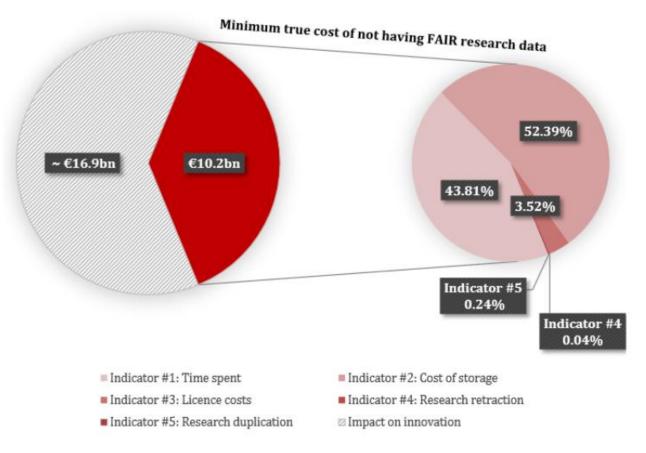
https://doi.org/10.1162/dint_e_00023 The FAIR Principles, B.Mons et al

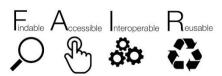




The cost of not having FAIR data = estimated €10.2bn / year

Likely cost of not having FAIR research data





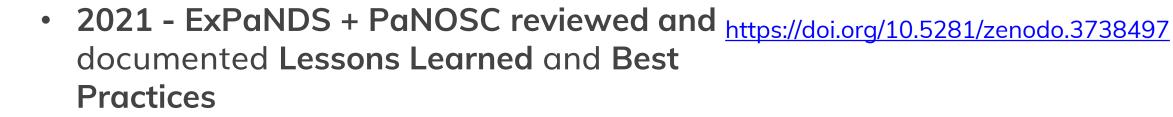
"Cost-benefit analysis for FAIR research data " (https://op.europa.eu/s/pevt)

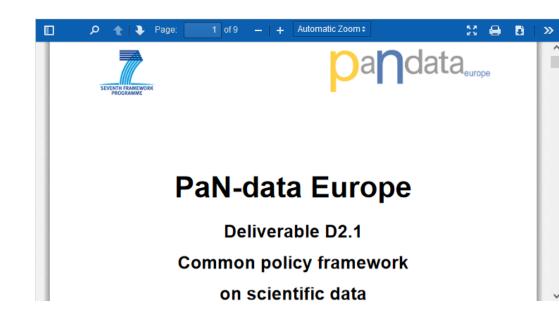




Photon and Neutron Sources – Open Data policies

- 2010 drafted the so-called PaNdata
 Data Policy Framework
- The framework was used for ALL PaN open data policies
- 2020 updated by PaNOSC





Implementing the data policies at PaNs remains challenging



EU Research facilities Data Policies

- ESA open data policy for most data (since 2010)
- ISIS open data policy (since 2010)
- ILL open data policy (since 2012)
- EMBL open access policy (since 2015)
- ESRF open data policy (since 2015)
- ESO open data policy (updated in 2016)
- EuXFEL open data policy (since 2017)
- CERN open data policy for LHC (since 2020)
- HZDR open data policy (since 2018)
- ELI-ERIC open data policy (December 2021)

•





ESRF Data Policy

https://www.esrf.fr/datapolicy



30 November 2015

The ESRF Data Policy

The ESRF aims to implement a Data Policy starting as soon as possible in 2016. The main elements of this policy comprise:

- Data ownership
- Data curation
- Data archiving
- Open access to data

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)





Main elements of ESRF Data Policy

- Data are under embargo for 3 years but can be released earlier by the experimental team
- All data have a DOI assigned automatically at the session level with appropriate high-level metadata from proposal
- Experimental team can register a DOI for a subset or superset of the data on provision of high-level metadata e.g. abstract
- PI can request an extension to the embargo period
- DOI must be cited when data are re-used
- Processed data can be uploaded to data portal
- Data can be downloaded from https://data.esrf.fr
- After embargo period and/or on creation of bespoke DOI Data are available under CC-BY-4.0 licence as Open Data









Findable Accessible Interoperable Re-usable (FAIR) diffraction data are coming to protein crystallography

John R. Helliwell, ** Wladek Minor, ** Manfred S. Weiss, ** Elspeth F. Garman, ** Randy J. Read, ** Janet Newman, ** Mark J. van Raaij, ** Janos Hajdu***, ** and Edward N. Baker** ** Baker** ** Baker** ** And Edward N. Ba

The structural biology community has always been at the forefront of sharing processed, *i.e.* analysed, results (the PDB was started in 1971)

- (i) Authors should provide a permanent and prominent link from their article to the raw data sets
- (ii) A registered Digital Object Identifier (doi) should be the persistent identifier of choice



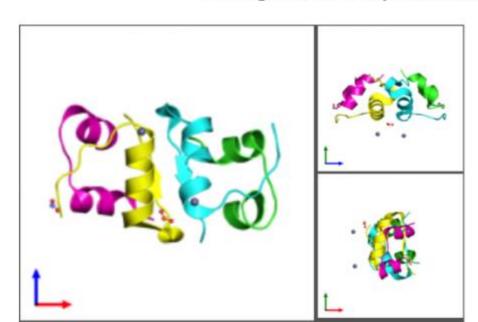
PaNOSC Use Cases - https://www.panosc.eu/all-use-cases/

Use Case 10 – Linking raw data to the Protein Data Bank in Europe (PDBe)

The OneDep deposition system enables depositors to provide the location of raw datasets as a 'digital object identifier' (doi), within their mmCIF file in the PDB archive and this DOI is now directly linked from an entry page at PDBe

PDB 6gv0 coloured by chain and viewed from the front

1145 PDB depositions from data taken at ESRF since 2020



Experimental raw data

Links to raw experimental data available for this entry are listed below

Raw experimental data related to PDB entry 6gv0:

Data DOI: 10.5281/zenodo.4456817

B

Dataset type: diffraction image data

Making data FAIR

- The ESRF Data Policy implementation implements
 - Findable by ensuring all data have a DOI
 - Accessible by making data open and downloadable

- Scientists help is needed to ensure
 - Interoperability by providing complete metadata
 - Reusability by providing complete e-logbooks, auxiliary information on the sample





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





Digital Object Identifiers (DOIs)

- All data must be referenced by a DOI
- First DOI minted on request of a scientist (Matt Bowler) was for ID30A1
- Create DOIs for data which you reference in publications
- Make your data count!



DOI > 10.15151/ESRF-DC-142893590

Data collection

Dataset Open access

Licence (for files)

Creative Commons Attribution 4.0

STRUCTURAL EVIDENCE FOR A ROLE OF THE MULTI-FUNCTIONAL HUMAN GLYCOPROTEIN AFAMIN IN

Andreas Naschberger; Bernhard Rupp.

Contributors

Matthew W. Bowler.

Afamin, a human plasma glycoprotein and putative transporter of hydrophobic molecules, has been shown to act as extracellular chaperone for poorly soluble, acylated Wnt proteins, forming a stable, soluble complex with functioning Wnt proteins. The 2.1-Å crystal structure of glycosylated human afamin reveals an almost exclusively hydrophobic binding cleft capable of harboring large hydrophobic moieties. Lipid analysis confirms the presence of lipids, and density in the primary binding pocket of afamin was modeled as palmitoleic acid, presenting the native O-acylation on serine 209 in human Wnt3a. The modeled complex between the experimental afamin structure and a Wnt3a homology model based on the XWnt8-Fz8-CRD fragment complex crystal structure is compelling, with favorable interactions comparable with the crystal structure complex. Afamin readily accommodates the conserved palmitoylated serine 209 of Wnt3a, providing a structural basis how afamin solubilizes hydrophobic and poorly soluble Wnt proteins

Proposals	Beamlines	Publication year 2018
OPID-1	ID30A1	1 20.0

Experimental report

The filename list is not available.

Experimental data

The data can be accessed by clicking on the link below

Access data

Below is the recommended format for citing this work in a research publication.

Naschberger A., Rupp B. (2018). Structural Evidence for a Role of the Multi-functional Human Glycoprotein Afamin in Wnt Transport. European Synchrotron Radiation Facility (ESRF).

https://doi.esrf.fr/10.15151/ESRF-DC-142893590

European Synchrotron Radiation Facility



Access to data is governed by the ESRF data policy.





Digital Object Identifiers (DOIs)

First DOI minted by a scientist (Matt Bowler) cited in the article ->



DOI > 10.15151/ESRF-DC-142893590

Data collection

Dataset Open access

DOI 10.15151/ESRF-DC-1428

Licence (for files)

Creative Commons Attribution 4.0

STRUCTURAL EVIDENCE FOR A ROLE OF THE MULTI-FUNCTIONAL HUMAN GLYCOPROTEIN AFAMIN IN WNT TRANSPORT

Andreas Naschberger; Bernhard Rupp.

Supporting information

3D view

PDB references: afamin, 6fak; complex with Gd-DO3A, 6rq7

Link https://doi.esrf.fr/10.15151/ESRF-DC-142893590

Raw diffraction images for the monoclinic (non-dehydrated) crystal form of afamin

Link https://doi.esrf.fr/10.15151/ESRF-DC-142915526

Raw diffraction images of the orthorhombic dehydrated crystal form of afamin

Link https://doi.esrf.fr/10.15151/ESRF-DC-186857652

Raw diffraction images for afamin with gadoteridol

Supplementary Movie S1. DOI: https://doi.org//10.1107/S2059798319013500/di5032sup1.wmv

Supplementary Movie S2. DOI: https://doi.org//10.1107/S2059798319013500/di5032sup2.mp4

Video



European Synchrotron Radiation Facility

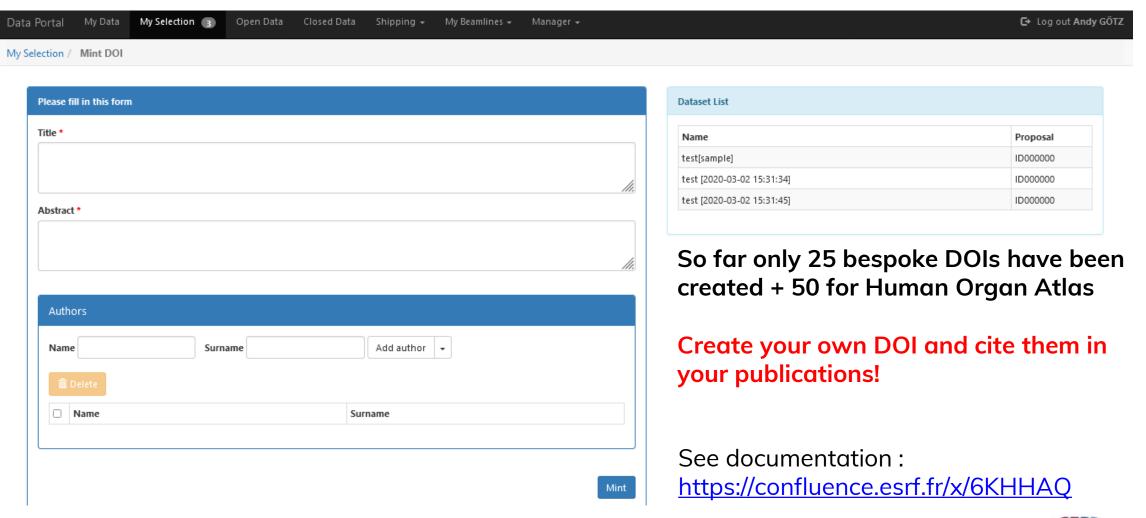


Access to data is governed by the ESRF data policy.





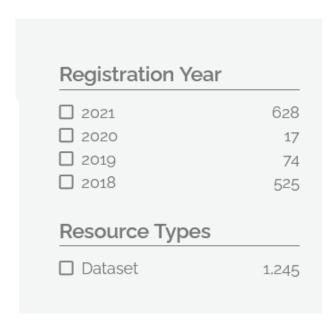
Creating your own DOIs on data.esrf.fr







Data DOIs minted et ESRF



 Total of 1245 DOIs created so far (1170 automatically)

 294 proposals are available as Open Data i.e. not under embargo





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 goal is to replace paper logbooks.

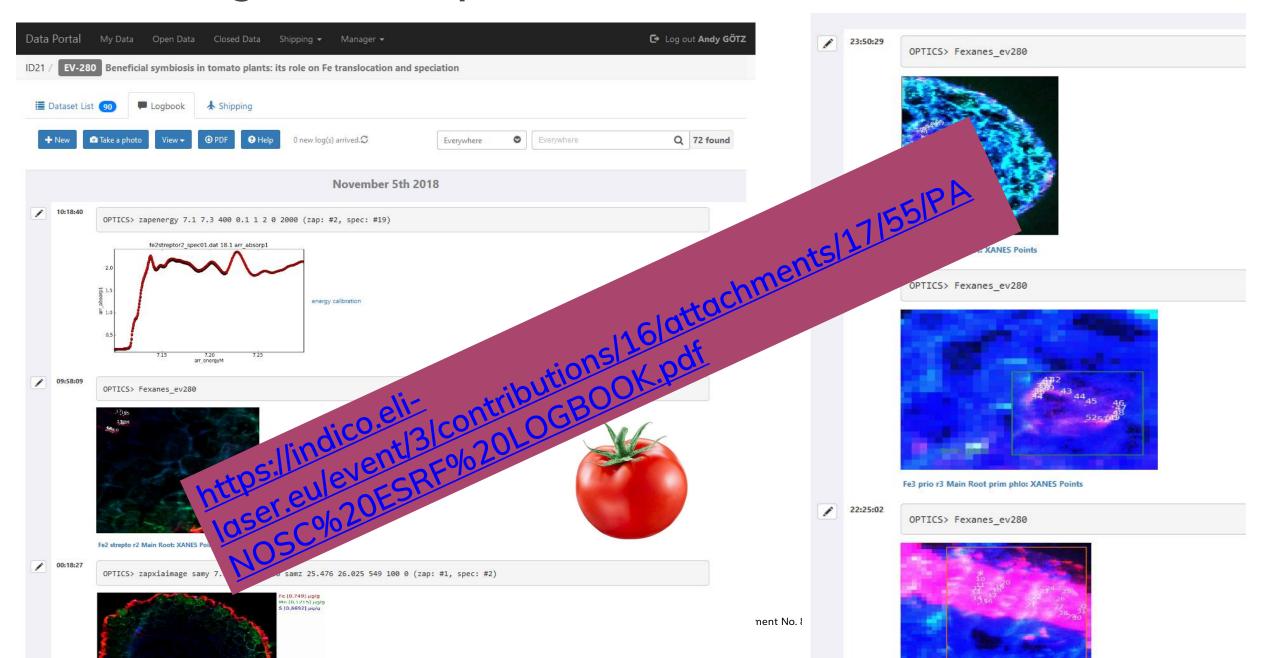
- E-logbook advantages
 - Shared editing online
 - Powerful search facilities
 - Access rules during embargo period
 - Allows others to understand what you did during the experiment
- E-logbook is metadata and will be part of the open data

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





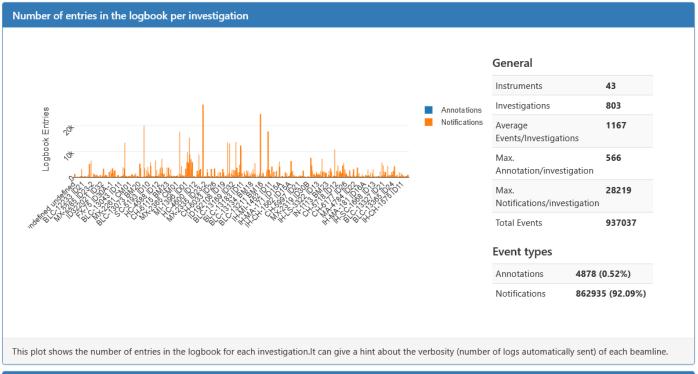
ESRF e-logbook example – ID21 / EV-280

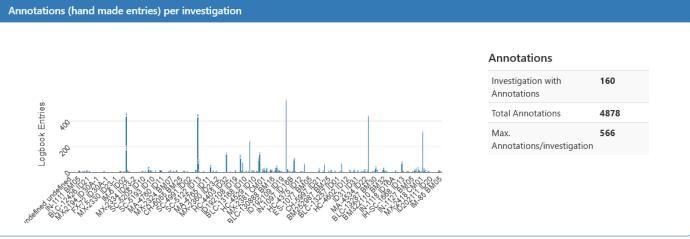


- E-Notebooks are still not used extensively
- SB sessions not making use of e-notebooks at all
- Ideas for future
 - Link e-notebooks to LIMS (ISPyB)
 - Train scientists

Logbook Usage for period 2021-08-01 and 2021-11-15

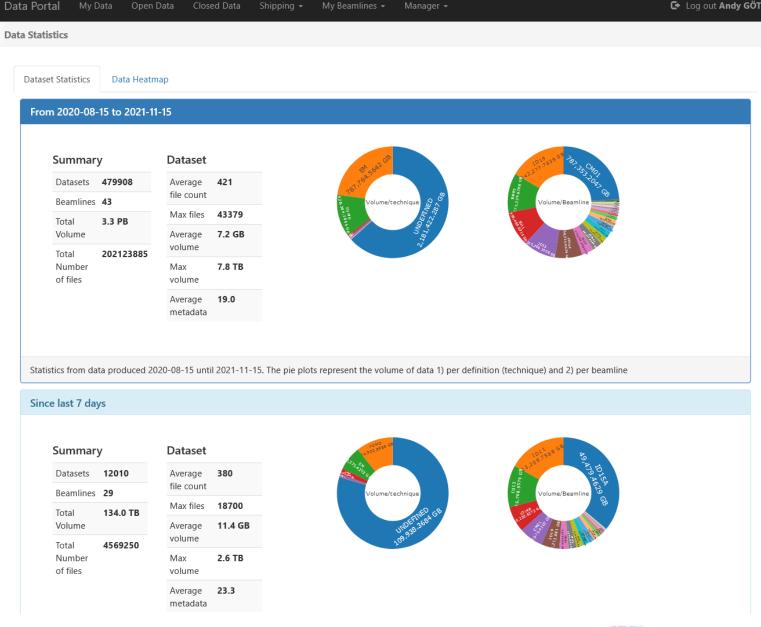
Change url parameters, startDate and endDate to change manually the range of dates. Example: /manager/starts/logbook?startDate=2020-08-01&endDate=2020-09-01







- Total of 3.3 PB
- CryoEM 22%
- Tomography 12%
- Other 63%
- Some beamlines are still missing

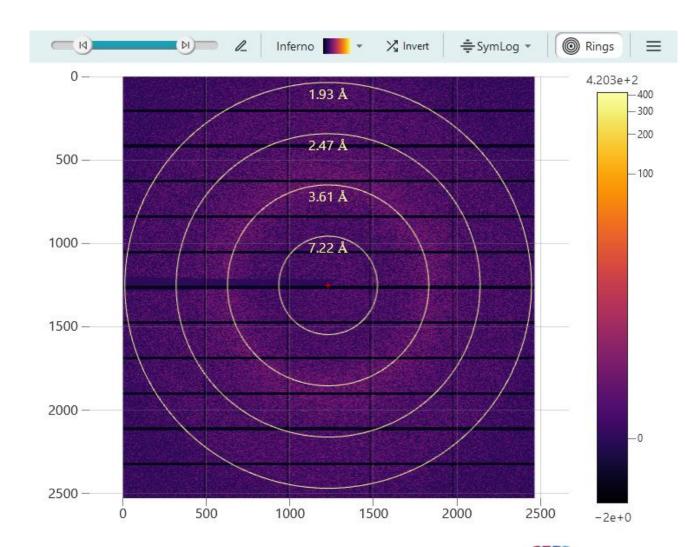






Data services planned for the future

- 1. Braggy diffraction image viewer on the web
- 2. Linking raw data to PDB
- 3. Remote analysis desktop (VISA)
- 4. Gold standard data format
- 5. Link e-logbook to LIMS
- 6. Analysis workflows
- 7. Improved metadata







Human Organ Atlas

- FAIR data i.e. can be re-used
- 50 Datasets already Open
- Opened immediately after processing (<18 months)

Goal is to create open data for an atlas of the entire human body at micron scale **Human Organ Atlas**

EXPLORE

SEARCH

HELP

https://human-organ-atlas.esrf.eu/

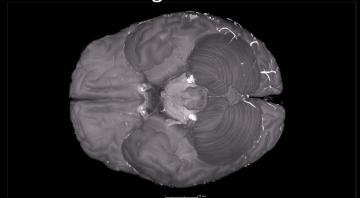
Welcome to the Human Organ Atlas

The Human Organ Atlas uses **Hierarchical Phase-Contrast Tomography** to span a previously poorly explored scale in our understanding of human anatomy, the micron to whole intact organ scale.

Histology using optical and electron microscopy images cells and other structures with sub-micron accuracy but only on small biopsies of tissue from an organ, while clinical CT and MRI scans can image whole organs, but with a resolution only down to just below a millimetre. <u>HiP-CT</u> bridges these scales in 3D, imaging intact organs with ca. 20 micron voxels, and locally down to microns.

We hope this open access Atlas, enabled by the ESRF-EBS, will act as a reference to provide new insights into our biological makeup in health and disease. To stay up to date, follow

HIP-CT ST



Funding

This project has been made possible by funding from:

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





Reference

Walsh, C.L., Tafforeau, P., Wagner, W.L. *et al.* Imaging intact human organs with local resolution of cellular structures using hierarchical phase-contrast tomography. *Nat Methods* (2021). https://doi.org/10.1038/s41592-021-01317-x

Collaborators

- <u>UCL</u>, 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
- Diamond Light Source, Harwell, UK: Andy Bodey, Robert C Atwood
- Imperial College London, UK: JL Robertus



Aknowledgements

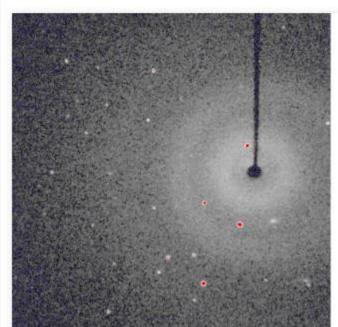
The development of this portal has been done as part of the <u>PaNOSC project</u>. PaNOSC has received funding from the European Union's <u>Horizon 2020</u> research and innovation programme under grant agreement No. 823852. The following people were involved in the development: Paul Tafforeau, Alejandro De Maria Antolinos, Axel Bocciarelli, Marjolaine Bodin and Andrew Götz from the ESRF, Jiří Majer from ELI, as well as the broader PaNOSC and ICAT communities.

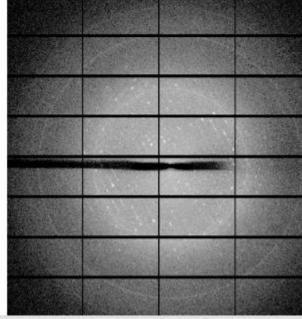


IUCrData to publish Raw Data Letters in 2022 – another motivation for Open Data with good metadata

IUCrData to publish Raw Data Letters

IUCrData is launching a new section for authors to describe their unprocessed or `raw' diffraction images. The new section will publish short descriptions of crystallographic raw data sets in the biological, chemical or materials science fields and provide a persistent link to the location of the raw data.





Read more



Received 20 April 2021 Accepted 1 May 2021

Keywords: twinning; diffuse scattering; tetraspanin CD9_{EC2}.

Raw data reference: the doi will appear here.
The raw data have been checked with checkCIF and an ImgCIF file of metadata is available from incredata increase.

PDB reference: tetraspanin CD9, 6rlr

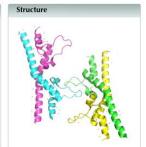
The extracellular domain of human tetraspanin CD9: twinning and diffuse scattering

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

Department of Chemistry, Structural Biochemistry, Bijvoet Centre for Biomolecular Research, Faculty of Science, Utrecht University, Utrecht, The Netherlands, "Correspondence e-mail: 1.m.i.ku natenburg@uu.nl

We describe remarkable features in the diffration pattern produced by a crystal of tetraspanin CD9_{EC2}-CD9_{EC2} crysts dized in pace group P1 and was twinned. Concurrent with the twinning, lifting dreaks were seen in the direction perpendicular to the twinning in a face. We make preliminary conclusions on packing disorder and polynoid indications for the observed molecular structure. We envis in that the lift diffraction images can be very useful for methods of velopers to symbol or remove the diffuse scattering to extract accurate Bragg into these by y using it to model the effect of packing disorder on the molecular structure.





raw data letters



What you need to do to CARE for your DATA – 10 rules

- Rule 1. Love Your Data, and Help Others Love It, Too
- Rule 2. Share Your Data Online, with a Permanent Identifier
- Rule 3. Conduct Science with a Particular Level of Reuse in Mind
- Rule 4. Publish Workflow as Context
- Rule 5. Link Your Data to Your Publications as Often as Possible
- Rule 6. Publish Your Code (Even the Small Bits)
- Rule 7. State How You Want to Get Credit
- Rule 8. Foster and Use Data Repositories
- Rule 9. Reward Colleagues Who Share Their Data Properly
- Rule 10. Be a Booster for Data Science







https://doi.org/10.1371/journal.pcbi.1003542

Ten Simple Rules for the Care and Feeding of Scientific Data

Alyssa Goodman¹, Alberto Pepe¹*, Alexander W. Blocker¹, Christine L. Borgman², Kyle Cranmer³, Merce Crosas¹, Rosanne Di Stefano¹, Yolanda Gil⁴, Paul Groth⁵, Margaret Hedstrom⁶, David W. Hogg³, Vinay Kashyap¹, Ashish Mahabal⁷, Aneta Siemiginowska¹, Aleksandra Slavkovic⁸

Conclusion

Adopting best practices for Open Data has many benefits but especially helping MAKE BETTER SCIENCE

- Some of the elements for generating Open Data:
 - Data Management Plan, Data Policy, Data Outputs, File types, File Formats, Software, Workflows, e-Logbooks, notebooks, Data Storage, Data Archiving, Data DOI
- Apply the FAIR principles ask yourself if you or someone else will be able to use or understand your data
- Make your Data count cite your data DOIs (raw and processed data)
- Open Data is not a goal on its own, reproducibility and data re-use are
- The Open Data movement has a lot to offer scientists and science

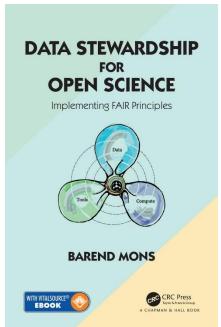




Learning more about Research Data Management

- 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.

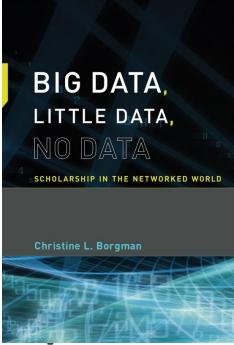










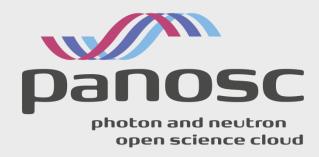




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- ICAT collaboration
- Wikipedia
- Internet









Thank you

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