

## The STORE database; towards FAIR

Paul Schofield, University of Cambridge







### **Open Science**

- Open publication access
- Open scholarly communication
- Open research data



### **Open Science**

"Open science is an approach based on open cooperative work and systematic sharing of knowledge and tools as early and widely as possible in the process"





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### EC Requirements

- Must manage the digital research data in line with the **FAIR principles** (Findable, Accessible, Interoperable, Reusable)
- Data Management Plan (DMP) is required by M6; updated midproject and at end of project
- **Deposit (meta)data as soon as possible** after production/generation or after processing and quality controls
- Deposit data in a trusted repository and make them open as soon as possible (deadlines set in DMP), following the "as open as possible, as closed as necessary" (open by default) principles
- Data closed if necessary, but metadata must be FAIR and unde r CCO (trusted repositories will automatically share metadata in CCO)
- Open licence, preferentially CC-BY or CC0 licence
- Detailed information about research outputs or tools/instruments needed to re-use or validate the data (e.g. data, software, algorithms, protocols, models, workflows, electronic notebooks)



Examples of metadata author(s) name, author(s) ORCID, DOI, licence, language, journal, title, etc.





### Why do we need to share data?

Evidence support for publications Reproducibility Accountability Data and resource reuse and reanalysis Resilience New discovery Prevention of duplication Supports RRRs Value for funding Coordination and integration of projects Training and education resources







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### FAIR sharing

Article Accesses

### Use of data at scale by humans and machines

Attention Score

CrossRef

SCIENTIFIC DA SPRINGER NATURE **OPEN** Comment: The FAIR Guiding SUBJECT CATEGORIES » Research data Principles for scientific data » Publication characteristics 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, Jaap Heinga, Peter A.C. 't Hoen, Rob Hooft, Tobias Kuhn, Ruben Kok, Joost Kok, Scott J. Lusher, Maryann E. Martone, Albert Mons, Abel L. Packer, Bengt Persson, Philippe Rocca-Serra, Marco Roos, Rene van Schaik, Susanna-Assunta Sansone, Erik Schultes, Thierry Sengstag, Ted Slater, George Strawn, Morris A. Swertz, Mark Thompson, Johan van der Lei, Erik van Mulligen, Jan Velterop, Andra Waagmeester, Peter Wittenburg, Katherine Wolstencroft, Jun Zhao, and Barend Mons SCIENTIFIC DATA | 3:160018 | DOI: 10.1038/sdata.2016.18 1958 Access & Citations 3993 451k 3173

Web of Science

Findable Accessible Interoperable Reusable Device Community defined terminologies Terms of access Community defined terminologies

# OPEN AND FAIR ARE NOT THE SAME THING

"Open" is about data rights and licensing. "FAIR" is about mechanics.

Anne Raugh

# FAIR IS PRIMARILY CONCERNED WITH PROGRAMMATIC PROCESSING

*FAIR* recognizes that data is diverse and scattered across cyberspace. Software processing levels the playing field.

Anne Raugh

The FAIR Principles at *go-fair.org* 



### FAIR is not a binary state

FAIRness is a spectrum. There are various ways to increase FAIRness and they can be applied incrementally.

#### BUT

- Use of generic data repositories is not very FAIR
- Lack of granularity in metadata
- Lack of metadata standards relevant to theme or community
- Non-grounded



The FAIR Principles at go-fair.org

#### **Open Science Projects**

Open Science Projects primary goals aim to increase collaborative scientific data sharing, analysis and more rapid scientific advancement.

#### GeneLab

GeneLab, an open science multi-omics repository, covering transcriptomics, metagenomics, epigenomics, proteomics, and metabolomics. Studies comprise of data from model organisms including microbes, plants, fruit flies, rodents and humans.



Learn more GeneLab

#### ALSDA

Ames Life Sciences Data Archive (ALSDA) collects, curates, and makes available space-relevant higher-order phenotypic datasets. Datasets that enable scientists to perform retrospective analysis across missions, experiments, life science disciplines, research subjects, and species.





NBISC

Learn more about BSP

**BSP** 

The NASA Space Biology Biospecimen

biospecimens to maximize the scientific

associated ground investigations and to

encourage and broaden participation from the scientific community in space biology-

return from biological spaceflight and

Sharing Program (BSP) collects

related research.

NASA Biological Institutional Scientific Collection (NBISC) is a biorepository of non-human samples collected from NASA-funded spaceflight investigations and correlative ground studies. The purpose of NBISC is to receive, store, document, preserve, and make the collection available to the scientific community.



Learn more about ALSDA

### GeneLab Data System



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**NASA** Institutional

Scientific Collection (ISC)

PI/Missions/

**Experiments** 



- 1. NASA GeneLab the first comprehensive space-related omics database (https://genelab.nasa.gov/)
- 2. Investigators can search, download, submit, privately share, and/or analyze omics data from spaceflight and corresponding ground-analog experiments.
- 3. GeneLab Data Systems users can explore GeneLab datasets in the Data Repository, submit omics data through the Submission Portal, analyze data using GeneLab Analysis Platform tools, and Visualize study results through Visualization Portal.
- 4. GeneLab also offers biospecimen processing services and NASA's Institutional Scientific Collection is a space-research biobank that offers potential investigators hundreds of biospecimens for further analysis.

# NASA Life Sciences Data Archive (LSDA)



and Situation Awareness

+ Program

15

The LSDA is a collection of NASA's life sciences research data and information, consisting of human, animal, microbe, and plant studies conducted from 1958 to present.

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Search/Filter

### Standardisation of metadata

### Ontologies

Comprised of standardised hierarchical concepts and relationships

Capture semantic data and metadata





radiobiology study type

Holistic approaches to governance study

### Radiation Biology Ontology (RBO)

data transformation

 Facilitates data retrieval and query expansion from NASA's GeneLab 'omics datab STORE



- Contains over 200 annotated classes instances specific to the study of rad biological systems, as well as import than 3500 additional classes from 13 Foundry ontologies
- Published through the OBO Foundry
- Available through NCBI Bioportal web site and application programming interface at https://bioportal.bioontology.org/ontologies/RBO

Whitney test followed by Benjamini-Hochberg correction for multiple comparisons. We used permutations of the phenotype vector that provid distribution to set rational thresholds that were calculated to be -10.6.5 for FPG and -10-5 for Background phenotypes and generally match in previously published GWAs using CC mice Pathway-phenotype associations were analyzed using Reactome database, which applies the followed by Benjamini-Hochberg adjustment for multiple comparisons.

Taxon

SAMPLES					N		
Source Name :	Sample Name :	col REF	Factor Value: : Ionizing Radiation	Factor Value: ÷ Particle Charge	Factor Value: i HZE	Parameter V ionizing radiation en	
C57BLF3	C57BLF3_P258_G4_C57	protocol	highly charged energetic nuclei	18	Ar-40 ion radiation	350 megaelectron nucleon	
C57BLM1	C57BLM1_P237_G3_C57	protocol	highly charged energetic nuclei	18	Atomic nuclei, each with 18 protons and 22 neutrons with kinetic energy imparted by natural or artificial means (such as by a particle accelerator)		
C57BLM2	C57BLM2_P237_H3_C57	protocol	highly charged energetic nuclei	18	Ar-40 ion radiation	350 megaelectron nucleon	
C57BLM3	C57BLM3_P237_E4_C57	protocol	highly charged energetic nuclei	18	Ar-40 ion radiation	350 megaelectron nucleon	
C57BLM1	C57BLM1_P258_G3_C57	protocol	highly charged energetic nuclei	18	Ar-40 ion radiation	350 megaelectron nucleon	
		protocol	highly charged energetic	18	Ar-40 ion radiation	350 megaelectro	

#### ionizing electromagnetic radiation

- gamma radiation
- Cesium-137 gamma radiation
- Cobalt-57 gamma radiation
- Cobalt-60 gamma radiation
- ultraviolet radiation
- x-ray radiation

ionizing radiation categorized by source

- nuclear reactor radiation
- particle accelerator radiation mixed radiation field

space radiation

ė.

- cosmic radiation
   galactic cosmic radiation
  - solar cosmic radiation

ionizing radiation energy low linear energy transfer radiation particle radiation

charged particle radiation delta ray

heavy ion radiation

- Ag-107 ion radiation
- Ar-40 ion radiation
- Au-197 ion radiation
- C-12 ion radiation
- Fe-56 ion radiation
- He-4 ion radiation
- Kr-84 ion radiation
- N-14 ion radiation
- Nb-93 ion radiation
- Ne-20 ion radiation
- Si-28 ion radiation
- Ta-181 ion radiation
- Ti-48 ion radiation
- Xe-129 ion radiation
- light ion radiation
- fast neutron

### How FAIR is STORE?

- Unique identifier  $\checkmark$
- Identifier persistence  $\checkmark$
- Resolvable identifier (identifiers.org)  $\checkmark$
- Structured metadata  $\checkmark$
- Grounded metadata (resolvable metadata IDs)  $\checkmark$
- Data identifier explicitly in metadata ٠
- Metadata identifier explicitly in metadata ٠
- Programmatic access  $\checkmark$
- Licenses  $\checkmark$

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### Work to be done

- Full implementation of the RBO ontology
- Implementation of the REST services
- Implementation of automated versioning
- Refinement of user interface
- Implement ISA-TAB to add licences, metadata and data IDs etc to data header.
- Investigate automatic extraction of candidate metadata classes from data record using NLP.



## Using open data to create new knowledge

Semantic data standards and metadata

- Discovering and integrating data between databases
- Federated queries and query expansion
- Semantic integration
- Ontologies permit the assertion of defined relationships between concepts

RBO cross references 13 OBO ontologies directly providing semantic linkage to most relevant databases

- Construction of Knowledge Graphs
- Graph embeddings for data representation
- Classification and similarity
- Inductive inference
- Learning over graph convolutional neural networks

Wilson et. Al. (2023) Machine intelligence for radiation science: International Journal of Radiation Biology, DOI: <u>10.1080/09553002.2023.2173823</u>



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