

## Overview of FAIR data publishing and RO-Crate



The University of Manchester

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Leyla Jael Castro, ZB MED Information Centre for Life Sciences Bioschemas

### Bioschemas: metadata for (life) sciences websites and data feeds

Community initiative built on top of schema.org

Aim

Improve data discoverability and interoperability in Life Sciences

Approach

Add Life Science types to schema.org Provide usage guidelines and examples Minimum, recommended, optional Link to domain ontologies Support software





### How does it work?

"@context": "https://schema.org", "http://purl.org/dc/terms/conformsTo": "https://bioschemas.org/profiles/Dataset/0.3-RELEASE-2019\_06\_14", "@type": "Dataset", "@id": "https://d-nb.info/gnd/121881389X", "identifier": "https://d-nb.info/gnd/121881389X", "name": "DaMaLOS 2020", "description": "First workshop on Research data\* management for linked open science - DaMaLO5 \* and other research objects", "keywords": "Research objects, Open Science, Data Management, Linked Data", "url": ["https://d-nb.info/gnd/121881389X", "https://repository.publisso.de/resource?query[0][term]=%22https://d-nb.info/gnd/121881389X%22"] "subjectOf": { "@type": "Event", "@id": "https://zbmed.github.io/damalos/docs/2020", "url": "https://zbmed.github.io/damalos/docs/2020", "location": { "@type": "VirtualLocation", "url": "https://zbmed.github.io/damalos/docs/2020" "name": "DaMaLOS 2020", "description": "First workshop on Research data\* management for linked open science - DaMaLOS \* and other research objects", "startDate": "2020-11-02". "endDate": "2020-11-02". "image": "https://zbmed.github.io/damalos/img/damalos.jpg", "eventAttendanceMode": "https://schema.org/OnlineEventAttendanceMode"

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linked open science - DaMaLOS \* and other research objects", "startDate": "2020-11-02", "endDate": "2020-11-02", "image" "https://zbmed.github.io/damalos/img/damalos.jpg", "eventAttendanceWode": "https://schems.org/OnlineEventAttendanceWode" ), "creator": (
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"https://repository.publisso.de/resource?query[0][tern]=K22https://d-nb.info/gnd/121881389XN22"], "subjectof": ["@type": "Event", "@id":

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Dataset/0.3-RELEASE-

d/121881389X", "name":

and other research objects",



DaMaLOS 2023 Call for papers

Important dates

Submission process

Workshop schedule

Program committee

Organizing committee

DaMaLOS 2020 proceedings

DaMaLOS 2021 proceedings

ESWC

JBMS

Contact

Camera-ready submission

### DaMaLOS 2020 - Workshop proceedings

DaMaLOS 2020 took place on the 2nd of November 2020 13:30 to 17:30 CET @ ISWC

Proceedings available at PUBLISSO Fachrepositorium DaMaLOS 2020 collection

- ODI:10.4126/FRL01-006423280 Editorial note
- Keynote by Prof. Dr. Carole Goble (The University of Manchester)
- Data management plans Chair Sören Auer (TIB)
  - ODI:10.4126/FRL01-006423282 ASIO: a Research Management System based on Semantic technologies, presented by Jose Emilio Labra Gayo
  - ODI: 10.4126/FRL01-006423283 Data Management Plans and Linked Open Data: exploiting machine actionable data management plans through Open Science Graphs, presented by Elli Papadopoulou
- DOI:10.4126/FRL01-006423289 Towards semantic representation of machine-actionable Data Management Plans, presented by João Cardoso
- ODI:10.4126/FRL01-006423291 Research Object Crates and Machine-actionable Data Management Plans, presented by Maroua Jaoua and Tomasz Miksa
- Data, Life Sciences and beyond Chair Dietrich Rebholz-Schuhmann (ZB MED)
  - OWDAT is ORKG? Invited talk, presented by Yaser Jaradeh (TIB)



knowledge acquisition for research data nted by Max Schröder Semantic Search on Scientific Repositories: by Thiago Gottardi

agement to Access Patient Data, presented by





### **FAIRness support in Bioschemas**







- F1, F3. Promote - use of unique identifiers
- F2. Provide rich metadata specifications
- F4. Promote use of registries

- A1. Use -HTTP(S)
- A2. Promote use of registries

- I1. Use JSON-LD
- I2. Use schema.org
- I3. Provide metadata specifications linking objects to each other



- R1. Provide metadata specifications (minimum, recommended, optional)
- R1.1. Promote use of licenses
- R1.2 Promote provenance and attribution
- R.1.3 Provide community standards

### **FAIRness limitations in Bioschemas**

- Focus on findability
- Focus on structured metadata via markup on webpages (but also options for data feeds/dumps)
- Lightweight rather than strong (e.g., ontology level) semantics
- Separation between metadata and data not always clear
- One profile per type (some use cases could need multiple profiles)
- Some tooling but (maybe) not enough

### **FAIRness evaluation and Bioschemas validation**

#### June 2023, new release v123

FAIR-Checker Improve the FAIRness of your web resources



#### Welcome

FAIR-Checker is a tool aimed at assessing FAIR principles and empowering data provider to enhance the quality of their digital resources.

Data providers and consumers can check how FAIR are web resources. Developers can explore and inspect metadata exposed in web resources.

### Check 🗹 🛛 Inspect 🔍

Step 1: fetch RDF metadata from the r	resource URL		
Examples: Dataset Dataverse Workflow Publication	on Datacite Dataset <u>Tool</u>		
% https://workflowhub.eu/workflows/18			Build Knowledge Gr
	Step 3: Metadata quality checks		
	Controlled vocabularies P Bioschemas		
	Bioschemas is a community effort aimed at reusing and extending resources, specifying minimal, recommended or optional informatic	Schema.org for better life science digital resource findability. Several profiles are defined for each kind of Life Science on. Are minimal information missing ? Should other information be provided for better findability ? Check BioSchemas	
	https://workflowhub.eu/workflows/18?version=1 has type **	Information (ComputerowWeak-	
	Required missing properties	Improvements	
	http://kitema.ren/witeit must be provided	https://science.org/consultentrol/	
	in the protocol	http://scheme.org/creativeWorkSatury should be provided	
		the line contraction and the second	

https://schema.org/lunding thoold be provided

### https://fair-checker.france-bioinformatique.fr/

**How are Bioschemas used?** Bioschemas define domain-specific **profiles** to add structured metadata to Life Science resources on the Web by using and expanding **schema.org:** *ChemicalSubstance, Gene, MolecularEntity, Protein, ProteinStructure, Sample, Taxon* 

**General-purpose profiles** are being lifted for use *beyond* life sciences (<u>https://schemas.science/</u>) including *Dataset, Course, ComputationalWorkflow, ComputationalTool, TrainingMaterial.* 

Bioschemas are **deployed** widely with >180 profile deployments overall

Bioschemas are developed and maintained by working groups in an active **community** (>150 members)

lame	Group	Use Cases	Cross Walk	Task & Issues	Exam
	Group	030 0303	CIUSS Mark	103K & 1350C5	LAUIN
hemicalSubstance /0.4-RELEASE) 7 April 2020	Chemicals		×.		:</td
ComputationalTool v1.0-RELEASE) 1 October 2021	Tools		×,		
omputationalWorkflow v1.0-RELEASE) 9 March 2021	Workflow		Ŕ		
iourse v1.0-RELEASE) 3 September 2022	Training		Ŕ		2</td
ourseInstance v1.0-RELEASE) 3 September 2022	Training		Ŕ		:</td
DataCatalog v0.3-RELEASE-2019_07_01) 1 July 2019	Data Repositories		Ŕ		:</td
Pataset v1.0-RELEASE) 2 July 2022	Datasets		×.		
ormalParameter v1.0-RELEASE) 9 March 2021	Workflow		×,		:</td
<mark>iene</mark> v1.0-RELEASE) 7 April 2021	Genes		¢,		:</td
<b>folecularEntity</b> /0.5-RELEASE) 7 April 2020	Chemicals		×,		
rotein /0.11-RELEASE) 7 April 2020	Proteins		×,		
ample /0.2-RELEASE-2018_11_10) 0 November 2018	Samples		¢,		
axon	Biodiversity		*		

https://bioschemas.org/profiles/

# Building FAIR data packages with RO-Crate



## Is it FAIR to use all these repositories?

## registry of Research Data Repositories

FAIRCOOKBOOK G GITHUB Search Wizard. F Findability A) Accessibility R Reusability Subjects Interoperability ransferring data with SFT Unique, persistent identifie Data licenses Gearch engine optimization Selecting terr Declaring data's permitted Content Types Creating a metadata profil LEARN MORE Archived data (504) LEARN MORE LEARN MORE FEADN MODE Audiovisual data (335) Assessments Maturity model Configuration data (45) Infrastructure Applied Examples 泪 -Databases (473) all Images (1090) LEARN MORE LEARN MOR LEARN MORE Networkbased data (111) Plain text (926)

https://faircookbook.elixir-europe.org/



Researchers are asked to make their research outputs FAIR – where to publish?

**Thousands** of public, institutional and domainspecific repositories

Help from guidance and **catalogues** (FAIRsharing, re3data, FAIR Cookbook)

..but how to gather and reference outputs across multiple repositories?

What about **contextual** information?

### https://www.re3data.org/

Scientific and statistical data formats (1429)

Raw data (979)

Source code (126)

other (769)

Software applications (368)

Structured graphics (792) Structured text (735)

Standard office documents (1262)

# Gathering diverse research outputs

Building a collection of compounded objects



## Aims of FAIR Research Objects

**Describe** and **package** data collections, datasets, software etc. with their **metadata** 

Platform-independent object exchange between repositories and services Support reproducibility and analysis: link data with codes and workflows Transfer of sensitive/large distributed datasets with persistent identifiers Aggregate citations and persistent identifiers Propagate provenance and existing metadata Publish and archive mixed objects and references Reuse existing standards, but hide their complexity



Findable Reusable Accessible Interoperable

IR



## **RO-Crate: Practical and general purpose**



Infrastructure independent – avoiding repository/service silos *Practical, lightweight, robust* 



Familiar, developer friendly, web native, machine- and humanreadable, search-engine accessible Adoptable Linked Data JSON and PIDs



Embrace diversity, legacy, unknowns, open-ended, multiinterpretation, self-describing, interlingua Adaptable Metadata Profiles



https://www.researchobject.org/ro-crate/

## **Realizing FAIR Digital Objects with RO-Crate**

id

id

type description datePublished

creator size

format

. . .

PTD

files

type

description

datePublished



https://www.researchobject.org/ro-crate/specification.html

https://doi.org/10.4225/59/5a4d9b76d79f4

https://data.research.uts.edu.au/examples/ro-crate/0.2/Victoria\_Arch\_pub/

### Dataset: Survey of Victoria Arch, Wombeyan Caves NSW Download this Dataset Download all the metadata for Survey of Victoria Arch, Wombeyan Caves NSW in JSON-LD format Check this crate ICheck this crate

@id	https://dx.doi.org/10.4225/59/5a4d9b76d79f4	
name	Survey of Victoria Arch, Wombeyan Caves NSW	
@type	Dataset	
description	This data is part of a project by Michael Lake and supported Caves by Robert Zlot in January 2014 using the Zebedee 3	by the Australian Speleological Federation. Data was acquired at Wombeyan D Mapping System developed by CSIRO.
datePublished	2017-10-01	
creator	<ul><li> Robert Zlot</li><li> Mike Lake</li><li> Lukas Kaul</li></ul>	
path	./	
contactPoint	Contact Mike Lake	https://www.npmjs.com/package/ro-crate-htr

## Guidance by examples



Search Research Object Crate (RO-Crate)

RO-Crate on

RO-Crate 1.1	RO-Crate Metadata Specification 1.1
Introduction	Permalink: https://w3id.org/ro/crate/1.1
Terminology	<ul> <li>Published: 2023-04-26</li> </ul>
RO-Crate Structure	Publisher: researchobject.org community
Metadata of the RO-Crate	Status: Recommendation
Root Data Entity	<ul> <li>JSON-LD context: https://w3id.org/ro/crate/1.1/context</li> </ul>
Data Entities	This version: https://w3id.org/ro/crate/1.1
Contextual Entities	Alternate formats: Web pages, single-page HTML, PDF, RO-Crate JSON-LD, RO-Crate HTML
Provenance of entities	<ul> <li>Previous version: https://w3id.org/ro/crate/1.0</li> </ul>
Workflows and scripts	<ul> <li>Cite as: https://doi.org/10.5281/zenodo.7867028 (this version) https://doi.org/10.5281 /zenodo.3406497 (any version)</li> </ul>
Appendix 🗸 🗸	<ul> <li>Editors: Peter Sefton, Eoghan Ó Carragáin, Stian Soiland-Reves</li> </ul>

https://www.researchobject.org/ro-crate/specification

RO-Crate is used by multiple international projects

Applied across research domains – from **life sciences** to **cultural heritage** 

## RO-Crate in practice

https://www.researchobject.org/ro-crate/in-use/



australian text analytics platform

Peter Sefton et al: <u>https://ptsefton.com/2022/11/25/Idaca-metadata-ecosystem-eresearch-</u>2022/index.html

# ROHub: Earth observation data

The EOSC project **RELIANCE** use RO-Crate to package data cubes of **earth observation data**, along with documentation, images and workflows

Connects to related **infrastructures** for interactive execution/analysis.

Metadata includes temporal coverage, spatial coverage and vertical coverage.

**ROHub** publishes the archived RO-Crates to general-purpose repositories (Zenodo, B2Share) for longevity and PIDs.

https://reliance.rohub.org/

https://www.researchobject.org/ro-crate/in-use/rohub.html

CAMS European air quality forecasts: REC		16.03.2023 (15:48)
My datacube project1		17.03.2023 (13:14)
https://reliance.adamplatform.eu/?dataset=69628:EU_CAMS_SURFACE_REC_Ce eature=61a8b7865e7d1c79f36e35da	6&f	17.03.2023 (14:39)
□ 😚 My DC product 3		17.03.2023 (14:41)
Screenshot 2023-03-27 at 14.46.39.png	136Kb	28.03.2023 (09:26)
Created: 16.03.2023 (15	5:48), last modifie	d: 16.03.2023 (15:48)
DATA CUBE COLLECTION       REMOTE         Image: Collection ID: EU_CAMS_SURFACE_REC_G         Identifiers:         Collection ID: EU_CAMS_SURFACE_REC_G         Description:         CAMS SURFACE RESIDENTIAL ELEMENARY CARBON	!o⊢	lub
SPATIAL COVERAGE	ige Helšink Stockholm Eesti	Санкт- Петербург

https://w3id.org/ro-id/6fa27870-c1a4-4386-8d51-855d5ac932e2

## Building an EOSC ecosystem of FAIR Workflows

 EOSC projects BY-COVID, EOSC-Life, EuroScienceGateway, BioDT exchange rich Workflow RO-Crates within an emerging EOSC ecosystem of workflow services

### Workflow Crates transfer

- identifiers, authors, license, workflow system
- executable workflows in their native format (e.g. Galaxy)
- interoperable CWL description of the workflow
- software citations (e.g. tools used)
- required data sources
- test suites
- workflow execution provenance



## Importance of profiles

*" Brian*: Look, you've got it all wrong! You don't need to follow me. You don't need to follow anybody! You've got to think for yourselves! You're all individuals!

Crowd: Yes! We're all individuals! Brian: You're all different! Crowd: Yes, we are all different! Man in crowd: I'm not...

Monty Python's Life of Brian (1979)

https://www.researchobject.org/ro-crate/profiles

Yes, we're all different!

## OPEN MEET. SHARE. INSPIRE. CARE. SCIENCE FESTIVAL

### #0SF2023DE

## Thank you!

Stian Soiland-Reyes The University of Manchester RO-Crate community co-chair ZB MED Information Centre for Life Sciences Bioschemas