How can data journals support data sharing and discovery?

Guy Jones, Chief Editor, Scientific Data

07 December 2023

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SCIENTIFIC DATA



What needs to change?

"The webinar series will focus on how data is enabling research – the current challenges and examples and how a better future can be created using chemistry data.

It will showcase current and planned initiatives to develop standards and tools, research infrastructures, and developing cultures to support Findable Accessible Interoperable Reusable (FAIR) chemistry data preparation, publication and reuse."

What can we use in the meantime?



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https://blogs.rsc.org/chemspider/2023/09/22/chemspider-webinars-helping-you-embrace-digital-chemistry-data-with-expert-insights https://digitalscience.figshare.com/articles/report/The State of Open Data 2023/24428194

Journal publishing

Modifying extant infrastructure to solve a new(ish) problem



Journal Data publishing

Modifying extant infrastructure to solve a new(ish) problem



Technical checks, peer review, typesetting, publication

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Start with a dataset

Deposited within a repository

The State of Open Data 2022		
Cite Download (6.51 MB) Share Embed + Collect		
DataCite Science, Digital; Goodey, Gregory; Hahnel, Mark; Zhou, Yuanchun; Jiang, Lulu; Chandra (2022). The State of Open Data 2022. Digital Science. Report. https://doi.org/10.6084/m Copy citation	amouliswaran, Ishwar; et al. 9.figshare.21276984.v5	TIPS Select your citation style and then place your mouse over the citation text to select it or use the Copy button.
https://doi.org/10.6084/m9.figshare.21276984.v5 Copy DOI		
Version 5 ✓ Report posted on 2022-10-18, 12:46 authored by Digital Science, Gregory Hahnel, Yuanchun Zhou, Lulu Jiang, Ishwar Chandramouliswaran, Amy Hafez, Taunton Gregurick, Samuel Simango, Juan Miguel Palma Peña, Holly Murray, Matt Cannon, Ret McKellar, Laura Day	Goodey, Mark USAGE Paine, Susan 30563 ecca Grant, Kate views	METRICS 12 6445 4 downloads citations 12
We're proud to release our seventh State of Open Data report.		0
$\mathbf{Published} \longrightarrow \mathbf{Search results} \longrightarrow$	SCIENTIF	
Query (keywords)	Data Desc	riptor
4		

Data citation

References

- 1. Lei, L. *et al*. A dynamic anomaly detection n 125575 (2023).
- Faustine, A., Pereira, L. & Klemenjak, C. A monitoring. *IEEE Trans. Smart Grid* 12, 398
- 3. Afzalan, M. & Jazizadeh, F. Residential loads
- segments. Appl. Energy 254, 113693 (2019).

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What else does a Data Descriptor do?

Practical details on provenance, contents, and trustworthyness



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Support FAIR via (data) publishing policy

Data deposition in repository

- Supports the use of persistent identifiers DOIs for datasets, registered with a suitable metadata registration agency (e.g. DataCite)
- Embargos during peer review, anonymous access for reviewers and no barriers to access upon publication (e.g. application processes, paywalls)
- "Download All" search, visualisation, dashboards, et all provide useful functionality and save time for certain tasks, but repositories should offer the full datasets

Clear, Open Licences

• CC0 and CC-BY, or their equivalents

Data citation

• Built on DOIs and metadata deposition with CrossRef and DataCite

Community data standards, useable formats, and share raw and processed data

Legal and ethical protection - personal data, third party data, sensitive human data



Subject breadth

Physical, biological, social, environmental, medical, computational science & engineering

Scienti

MIMIC-III, a freely accessible critical care database		
<u>Alistair E.W. Johnson, Tom J.</u>	Pollard ^[27] , Lu Shen, Li-wei H. Lehman, <u>Mengling Feng</u> , <u>Mohammad</u>	
<u>Ghassemi</u> , <u>Benjamin Moody</u>	Peter Szolovits, Leo Anthony Celi & Roger G. Mark	
<u>Scientific Data</u> 3 , Article nu	Database Credentialed Access	
MIMIC-III Clinical Database		
	Alistair Johnson 🚯 , Tom Pollard 🚯 , Roger Mark 🚯	
	Published: Sept. 4, 2016. Version: 1.4	

Quantum chemistry structures and properties of 134 kilo molecules

Raghunathan Ramakrishnan, Pavlo O. Dral, Matthias Rupp & O. Anatole von Lilienfeld 🏼



Surface energies of elemental crystals

Richard Tran, Zihan Xu, Balachandran Radhakrishnan, Donald Winston, Wenhao Sun, Kristin A. Persson & Shyue Ping Ong

Data from: Surface energies of elemental crystals

A database framework for rapid screening of structure-function relationships in PFAS chemistry

<u>An Su</u> & <u>Krishna Rajan</u> 🗹

Scientific Data 8, Article number: 14 (2021) Cite this article

A Database Framework for Rapid Screening of Structure-Function Relationships in PFAS Chemistry

Peer review

... In the absence of Results

Experimental Rigor and Technical Data Quality

Was the data produced in a rigorous and methodologically sound manner?

Please Select 🗸

Was the technical quality of the data supported convincingly with technical validation experiments and statistical analyses of data quality or error, as needed?

Please Select V

Are the depth, coverage, size, and/or completeness of these data sufficient for the types of applications or research questions outlined by the authors?

Please Select 🗸

Completeness of the Description

Are the methods and any data processing steps described in sufficient detail to allow others to reproduce these steps?

Please Select V

Did the authors provide all of the information needed for others to reuse this dataset, or integrate it with other data?

Please Select 🗸

Is this Data Descriptor, in combination with any repository metadata, consistent with relevant minimum information or reporting standards?

Please Select 🗸

Integrity of the Data Files and Repository Record

To the degree that you have viewed the actual data files, did they appear complete and do they match the descriptions in the Data Descriptor?

Please Select V

Have these data files been deposited in the most appropriate available data repository?

- Readers can download and use the data without bias
- It provides an alternative channel for research publication
- Counterbalances the extra steps
- Sound science publishing model we don't make editorial assessments on perceived impact

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Please Select 🗸

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2022 Journal Impact Factor: 9.8

Article processing charges : £1690.00/\$2190.00/€1890.00

