



Applying FAIR Principles to Articles and Preprints

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ACS: Championing Research and Data Integrity

High standards – deliver trust in science

- Rigorous peer review process is critical
- ✓ ACS editors are active researchers

Define and adhere to clear policies

- ✓ ACS Ethical Guidelines
- Committee on Publications Ethics (COPE)
- Each journal adopts relevant policies for own community

Dedicated resources to support ethics

✓ ACS staff, editors, and vendor support

Technology to support identification, evaluation, guidance

Exploring tools to assist with research integrity

ACS Publishing Integrity Office (PIO)

Advancing trusted science by ensuring research is reliable, reproducible, and ethical

Publication Ethics

- ✓ Pre- and post-publication scientific and ethical concerns
- ✓ ACS Ethical Guidelines
- ✓ Committee on Publication Ethics (COPE)
- ✓ Editor-in-Chief ethics training course
- ✓ Ombudsperson for unbiased evaluations of reported issues

Research Data Integrity

- ✓ ACS Research Data Policy
- ✓ Promoting FAIR data principals
- ✓ Sub-field standardization and guidelines
- ✓ Specific journal data checks
- ✓ Data and image integrity investigations





ACS Research Data Policy and Data Guidelines Pages

ACS Publications > ACS Publishing Center > ACS Research Data Policy

ACS Research Data Policy

The open exchange of information and ideas is critical to scientific progress and ACS' mission of improving people's lives through the transforming power of chemistry. ACS Publications' portfolio of journals offer the highest levels of rigor in the review and publication of scientific articles and research data. Transparency and the open availability of research data are essential to enhancing both scientific progress and the public trust of those research results.

ACS strongly endorses The FAIR Data Principles and believes that where ethically and legally feasible, all research data should be findable, accessible, interoperable, and reusable. ACS supports the Center for Open Science's Transparency and Openness Promotion (TOP) Guidelines, the Joint Declaration of Data Citation Principles, and the STM Brussels Declaration. ACS is a member of the Research Data Alliance. Through engagement with these community initiatives, we strive to promote best practices in research data availability and to bring those best practices to its community of researchers and journal authors to help improve the execution, communication, and reproducibility of science.

Open availability of research data offers the following benefits:

For authors of ACS journal articles

- Open availability of data makes the related research more trustworthy and enhances scientific reputation.
- · Research funders are increasingly recognizing data as a valuable research output.

ACS Publications > ACS Publishing Center > ACS Research Data Guidelines

ACS Research Data Guidelines

ACS Publications portfolio of journals offer the highest levels of rigor in the review and publication of scientific articles and research data. To assist authors to include data as a prioritized publication component, we have developed ACS Research Data Guidelines.

ACS Research Data Policy

Browse data guidelines for reporting

- Biological data
- · Simulations, Machine Learning, Computational Data
- · Organic chemistry data
- . Coming Soon Nanoscience / Materials science / Energy (in 2022)
- ➡ Simulations, Machine Learning, Computational Data
- 母 Organic chemistry data





Overview of ACS Research Data Levels

Research Data Policy Levels

All policy levels are subject to potential ethical and legal restrictions on the public release of data (see section below on Exceptions). Authors are advised to check the Author Guidelines for the journal to which they plan to submit for journal-specific data guidelines.

Level 1 Public data availability encouraged	The journal encourages all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are encouraged to provide a Data Availability Statement describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be cited appropriately.
Level 2 Public data availability encouraged; Data Availability	The journal encourages all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are required to provide a Data Availability

Level 2

Public data availability
encouraged; Data Availability
Statement required

The journal encourages all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are required to provide a Data Availability
Statement describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be cited appropriately.

Level 3 Public data availability required; Data Availability Statement required The journal requires, as a condition of publication, all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are required to provide a Data Availability Statement describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be cited appropriately.

Level 4 Public data availability required and data will be peerreviewed; Data Availability Statement required Availability Statement describing the public available data sets should be cited appropriately. The journal requires, as a condition of publication, all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. The data will undergo peer review along with the manuscript. Authors are required to provide a Data supporting the article's conclusions. Publicly available data sets should be cited appropriately.



Level 1: All ACS journals encourage data sharing

Level 2: Data Availability Statements at *Organic Letters* and *Journal of Organic Chemistry*

Level 3: Some journals require specific data types (i.e. CIF data) be shared publicly

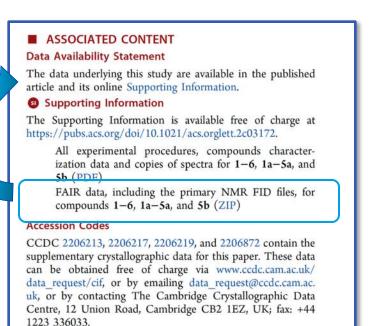




Data Availability Statement Pilot

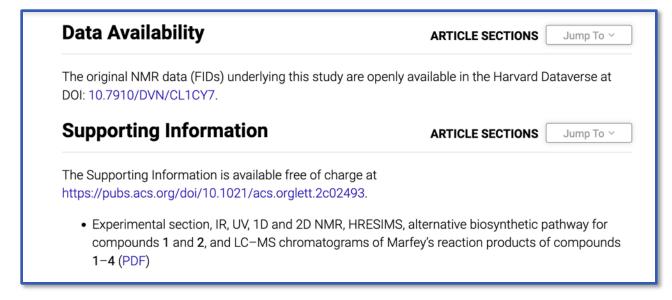


- Required for publication but not required at initial submission
- ✓ Meet Level 2 of the ACS Research Data Policy



Features of the PDF view:

- Consistent statement and placement
- CCDC Accession codes remain separate



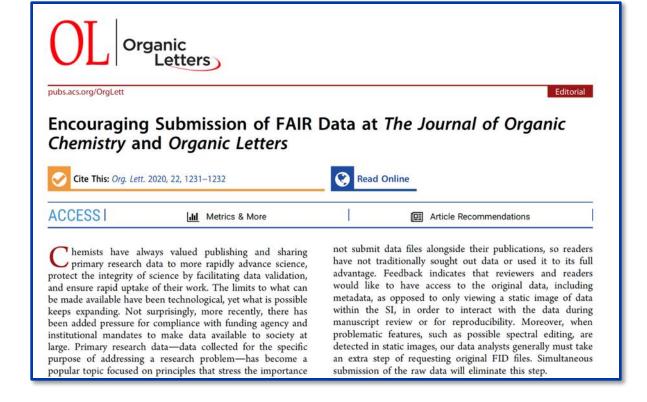
Features of the HTML view:

- New Header: Data Availability
- DAS is a 'Jump To' section Located above the SI Header
- Repository is hyperlinked

FAIR Data Pilot

Organic Letters and The Journal of Organic Chemistry







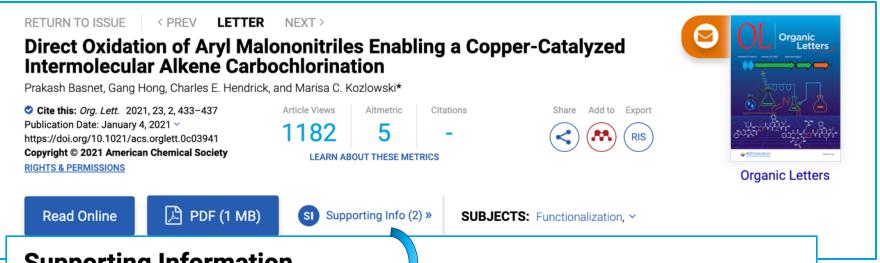
NMR packager connects raw data with meta data

ACS data packager was developed in-house

- X It was not user friendly:
 - too much time for authors
 - too many files

Example of an ACS Publication with FAIR Data





Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.orglett.0c03941.

- Experimental procedures and spectral data (PDF)
- FAIR data, including the primary NMR FID files, for compounds 3a-u, 4a-i, 6, 7, 9-13 (ZIP)

☐ Published in Article

ASSOCIATED CONTENT

Supporting Information

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ChemRxiv Overview



- ✓ ChemRxiv is a free submission, distribution, and archive service for unpublished preprints in chemistry and related areas.
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- √ 92 million+ views and downloads

Key Metrics						
35,113	66,062,045	26,045,799	11,276			
Live Content	Abstract Views	Content Downloads	Citations			

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Data on ChemRxiv



- ChemRxiv allows authors to upload any data files as supplementary materials or link to external resources.
- All content on ChemRxiv is free to post and read. Preprints are given DOIs and Creative Commons licenses, allowing reuse.
- ChemRxiv supports FAIR data principles, but there is currently no strict policy around inclusion or formatting of raw data.

	Supporting information	Integrative experimental details and characterization data.	Download (3 MB)
Supplementary weblinks	LINGO-1[1-20] 10 best models	Atom coordinates of 10 best models of LINGO-1[1-20] determined by NMR	Download (0.23 MB)
Supplementary weblinks	LINGO-1[1-20] 10 best models	Atom coordinates of 10 best models of LINGO-1[1-20] determined by NMR	

Title Description Actions

MDDG GitHub repository This is the repository for the code presented View ☑

in the preprint.





ACS Chemistry Databank (CDB)

Launched: January 2025

Purpose:

A home for chemistry data not suited for niche repositories

► Platform:

- Custom build on top of Dryad
- Free for authors
- Assigns a separate DOI for data

► Pilot Journal: *Organic Letters*

- Available only through the manuscript submission process for this journal
- Starting small to refine workflows
- Authors deposit data prior to manuscript submission
- Data sharing is optional, but a data availability statement is required
- Authors may choose any alternative repository or CDB





CDB Ensures FAIR Data

- README (Usage notes / documentation) enable others to use the data
 - Critical for Reusability and Interoperability: clear documentation helps others interpret and use the data correctly.
- Express preference for open-source file types for specific analytical methods
 - ► Enhances Interoperability and Accessibility: open formats reduce barriers to use and ensure compatibility across platforms.
- Data files can be opened with readily accessible software (no encryption or corruption)
 - ▶ Directly supports <u>Accessibility</u>: users can access and work with the data without proprietary or restrictive tools.
- The data contain no personally identifiable info or sensitive information
 - Ensures <u>Accessibility and Reusability</u>: data can be shared openly without legal or ethical constraints.





ACS Promoting Ethical Behavior and Data Integrity

Data Integrity:

- Expanded support for data cases (PIO)
- ✓ Launched the ACS Research Data Policy
- Data Availability Statement (DAS) required for a subset of journals
- ✓ Collaborative effort to support ChemRxiv
- ✓ Launched the Chemistry Data Bank

Publication Ethics:

- ✓ Expanded support for ethics cases (PIO)
- ✓ Published a policy page on use of Al
- Revised authorship change process to address paid authorship concerns
- ✓ New training course on publication ethics for Editor in Chiefs and Associate Editors





Questions

