

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)

[+ Biological data](#)

[+ Simulations, Machine Learning, Computational Data](#)

[+ 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 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 peer-reviewed; 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. The data will undergo peer review along with the manuscript. 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 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

■ ASSOCIATED CONTENT

Data Availability Statement

The data underlying this study are available in the published article and its online [Supporting Information](#).

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.orglett.2c03172>.

All experimental procedures, compounds characterization data and copies of spectra for **1–6**, **1a–5a**, and **5b** (PDF)

FAIR data, including the primary NMR FID files, for compounds **1–6**, **1a–5a**, and **5b** (ZIP)

Accession Codes

CCDC 2206213, 2206217, 2206219, and 2206872 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Data Availability

ARTICLE SECTIONS

Jump To ▾

The original NMR data (FIDs) underlying this study are openly available in the Harvard Dataverse at DOI: [10.7910/DVN/CL1CY7](https://doi.org/10.7910/DVN/CL1CY7).

Supporting Information

ARTICLE SECTIONS

Jump To ▾

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.orglett.2c02493>.

- Experimental section, IR, UV, 1D and 2D NMR, HRESIMS, alternative biosynthetic pathway for compounds **1** and **2**, and LC–MS chromatograms of Marfey's reaction products of compounds **1–4** (PDF)

Features of the HTML view:

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

Features of the PDF view:

- Consistent statement and placement
- CCDC Accession codes remain separate

FAIR Data Pilot

Organic Letters and The Journal of Organic Chemistry



A screenshot of the Organic Letters journal website. The header shows the 'OL' logo and 'Organic Letters' text. Below the header, the URL 'pubs.acs.org/OrgLett' is visible on the left and 'Editorial' on the right. The main title of the article is 'Encouraging Submission of FAIR Data at The Journal of Organic Chemistry and Organic Letters'. Below the title, there is a 'Cite This' button with a checkmark icon and a 'Read Online' button with a globe icon. The 'Cite This' button contains the text 'Org. Lett. 2020, 22, 1231–1232'. Below the buttons, there is a navigation bar with 'ACCESS |' on the left, 'Metrics & More' in the center, and 'Article Recommendations' on the right. The main text of the article is visible, starting with 'Chemists have always valued publishing and sharing primary research data to more rapidly advance science, protect the integrity of science by facilitating data validation, and ensure rapid uptake of their work. The limits to what can be made available have been technological, yet what is possible keeps expanding. Not surprisingly, more recently, there has been added pressure for compliance with funding agency and institutional mandates to make data available to society at large. Primary research data—data collected for the specific purpose of addressing a research problem—has become a popular topic focused on principles that stress the importance not submit data files alongside their publications, so readers have not traditionally sought out data or used it to its full advantage. Feedback indicates that reviewers and readers would like to have access to the original data, including metadata, as opposed to only viewing a static image of data within the SI, in order to interact with the data during manuscript review or for reproducibility. Moreover, when problematic features, such as possible spectral editing, are detected in static images, our data analysts generally must take an extra step of requesting original FID files. Simultaneous submission of the raw data will eliminate this step.'

A blue banner for the ACS Research Data Center. The text 'ACS RESEARCH DATA CENTER' is written in large, white, bold letters. Below this, a paragraph of text reads: 'ACS has developed a data packaging tool to assist you in zipping FID files, acquisition data, and processing parameters along with other appropriate FAIR metadata such as a SMILES or InChi for submission'. At the bottom of the banner, there is a yellow button with the text 'Submit your NMR Data' in black.

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

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Direct Oxidation of Aryl Malononitriles Enabling a Copper-Catalyzed Intermolecular Alkene Carbochlorination

Prakash Basnet, Gang Hong, Charles E. Hendrick, and Marisa C. Kozlowski*

Cite this: *Org. Lett.* 2021, 23, 2, 433–437
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<https://doi.org/10.1021/acs.orglett.0c03941>
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Organic Letters

Read Online  **PDF (1 MB)**  **Supporting Info (2) »** **SUBJECTS:** Functionalization, ▾

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

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](#))

ChemRxiv Overview

ChemRxiv[®]

- ✓ ChemRxiv is a free submission, distribution, and archive service for unpublished preprints in chemistry and related areas.
- ✓ **35,000+** preprints posted from authors in **100+** countries
- ✓ **92 million+** views and downloads

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

• *ChemRxiv is co-owned and managed by:*



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.

Supplementary weblinks

	Supporting information	Integrative experimental details and characterization data.	Download (3 MB)
	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)

Title

Description

Actions



MDDG GitHub repository

This is the repository for the code presented in the preprint.

[View](#) 

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 Accessibility: users can access and work with the data without proprietary or restrictive tools.
- **The data contain no personally identifiable info or sensitive information**
 - ▶ Ensures Accessibility and Reusability: 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 AI
- ✓ Revised authorship change process to address paid authorship concerns
- ✓ New training course on publication ethics for Editor in Chiefs and Associate Editors

Questions

