

# 論文とプレプリントへの FAIR原則の適用

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## ACS：研究とデータインテグリティを推進

### 高い基準 – 科学への信頼を確立する

- ✓ 厳格な査読プロセスが不可欠
- ✓ ACS編集者は現役の研究者

### 明確な方針を定め遵守する

- ✓ ACS倫理ガイドライン
- ✓ 出版倫理委員会（COPE）
- ✓ 各ジャーナルは自コミュニティに適合した方針を採用

### 倫理支援のための専用リソース

- ✓ ACSスタッフ、編集者、ベンダーによるサポート

### 特定・評価・指導を支援する技術

- ✓ リサーチインテグリティを支援するツールの模索

# ACS出版倫理室 (PIO/Publishing Integrity Office)

研究の信頼性、再現性、倫理性を確保することで、信頼できる科学を推進

## 出版倫理

- ✓ 出版前および出版後の科学的・倫理的懸念事項
- ✓ ACS倫理ガイドライン
- ✓ 出版倫理委員会 (COPE)
- ✓ 編集長向け倫理研修コース
- ✓ 報告された問題の公平な評価のためのオンブズパーソン

## 研究データインテグリティ

- ✓ ACS 研究データ方針
- ✓ FAIRデータ原則の推進
- ✓ サブ分野の標準化とガイドライン
- ✓ 特定ジャーナルのデータ検証
- ✓ データおよび画像のインテグリティ調査

# ACS研究データポリシーおよびデータガイドラインのページ

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](#)

# ACS研究データ レベルの概要

| <b>Research Data Policy Levels</b><br>All policy levels are subject to potential ethical and legal restrictions on the public release of data (see section below on <a href="#">Exceptions</a> ). Authors are advised to check the Author Guidelines for the journal to which they plan to submit for journal-specific data guidelines. |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Level 1</b><br>Public data availability encouraged                                                                                                                                                                                                                                                                                   | The journal <b>encourages</b> 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 <b>encouraged</b> to provide a <a href="#">Data Availability Statement</a> describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be <a href="#">cited appropriately</a> .                                                                                           |
| <b>Level 2</b><br>Public data availability encouraged; Data Availability Statement required                                                                                                                                                                                                                                             | The journal <b>encourages</b> 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 <b>required</b> to provide a <a href="#">Data Availability Statement</a> describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be <a href="#">cited appropriately</a> .                                                                                             |
| <b>Level 3</b><br>Public data availability required; Data Availability Statement required                                                                                                                                                                                                                                               | The journal <b>requires</b> , 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 <b>required</b> to provide a <a href="#">Data Availability Statement</a> describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be <a href="#">cited appropriately</a> .                                                              |
| <b>Level 4</b><br>Public data availability required and data will be peer-reviewed; Data Availability Statement required                                                                                                                                                                                                                | The journal <b>requires</b> , 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 <b>required</b> to provide a <a href="#">Data Availability Statement</a> describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be <a href="#">cited appropriately</a> . |



**レベル1:** すべてのACSジャーナルはデータ共有を推奨

**レベル2:** 『*Organic Letters*』および『*Journal of Organic Chemistry*』におけるData Availability Statement

**レベル3:** 一部のジャーナルでは特定のデータ形式(例: CIFデータ)の公開共有を要求

# Data Availability Statement パイロット版

- ✓ 出版には必須だが、初回提出時には必須ではない
- ✓ ACS研究データポリシーのレベル2を満たす

## ■ 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](http://www.ccdc.cam.ac.uk/data_request/cif), or by emailing [data\\_request@ccdc.cam.ac.uk](mailto: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)

## HTML表示の特徴:

- 新しいヘッダー: Data Availability
- DAS (Data Availability Statement) は「ジャンプ先」セクション - SIヘッダーの上に配置
- リポジトリはハイパーリンク化

## PDF表示の特徴:

- 一貫した記述と配置
- CCDCアクセスコードは分離されたまま

# FAIRデータパイロット

Organic LettersおよびThe Journal of Organic Chemistry





pubs.acs.org/OrgLett

Editorial

## Encouraging Submission of FAIR Data at *The Journal of Organic Chemistry* and *Organic Letters*

Cite This: *Org. Lett.* 2020, 22, 1231–1232

Read Online

ACCESS | Metrics & More | Article Recommendations

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.

## ACS RESEARCH DATA CENTER

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

Submit your NMR Data

NMRパッケージャーが生データとメタデータを連携

ACSデータパッケージングツールは自社開発

- ✕ ユーザーフレンドリーではなかった:
- 時間がかかりすぎる
  - ファイル数が多すぎる

# FAIRデータを含むACS出版物の例

RETURN TO ISSUE | < PREV LETTER NEXT >

## 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  
Publication Date: January 4, 2021  
<https://doi.org/10.1021/acs.orglett.0c03941>  
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Organic Letters

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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](#))

## 論文記事に掲載

### 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の概要

ChemRxiv<sup>®</sup>

- ✓ ChemRxivは、化学および関連分野における未発表のプレプリントを無料で投稿・配布・保存できるサービス
- ✓ 100ヶ国以上の著者から投稿された35,000件以上のプレプリント
- ✓ 9,200万回以上の閲覧・ダウンロード

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

• ChemRxiv は以下の組織が共同で所有・運営しています：



# ChemRxiv上のデータ



- ChemRxivでは、著者が補足資料として任意のデータファイルをアップロードしたり、外部リソースへのリンクを掲載したりできます。
- ChemRxiv上の全コンテンツは投稿・閲覧が無料です。**プレプリントにはDOIとクリエイティブ・コモンズ・ライセンスが付与され、再利用が可能です。
- ChemRxivはFAIRデータ原則をサポートしていますが、現時点では生データの包含やフォーマットに関する厳格なポリシーは存在しません。**

## Supplementary weblinks

|                                                                                   |                              |                                                                       |                                    |
|-----------------------------------------------------------------------------------|------------------------------|-----------------------------------------------------------------------|------------------------------------|
|  | Supporting information       | Integrative experimental details and characterization data.           | <a href="#">Download (3 MB)</a>    |
|  | LINGO-1[1-20] 10 best models | Atom coordinates of 10 best models of LINGO-1[1-20] determined by NMR | <a href="#">Download (0.23 MB)</a> |

Title

Description

Actions



MDDG GitHub repository

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

[View](#) 

# ACS Chemistry Databank (CDB)

▶ 開始時期 : 2025年1月

▶ 目的 :

- ▶ ニッチなりポジトリには適さない化学データの拠点

▶ プラットフォーム :

- ▶ Dryadを基盤とした独自構築
- ▶ 著者の費用負担なし
- ▶ データごとに個別のDOIを付与

▶ パイロットジャーナル: *Organic Letters*

- ▶ 本ジャーナルの原稿投稿プロセスを通じてのみ利用可能
- ▶ 小規模から開始しワークフローを洗練
- ▶ 著者は原稿提出前にデータを登録
- ▶ データ共有は任意ですが、Data Availability Statementは必須
- ▶ 著者は代替リポジトリまたはCDBを選択可能

# CDBは公正なデータ（FAIR）を確保します

- README（使用上の注意／ドキュメント）は他者がデータを利用できるようにする
  - ▶ 再利用性と相互運用性にとって重要：明確なドキュメントは他者がデータを正しく解釈・利用する助けとなります。
- 特定の分析手法にはオープンソースファイル形式を推奨
  - ▶ 相互運用性とアクセシビリティの向上：オープンフォーマットは利用障壁を低減し、プラットフォーム間の互換性を確保します。
- データファイルは容易に入手可能なソフトウェアで開くことができる（暗号化や破損なし）
  - ▶ アクセシビリティを直接支援：ユーザーは、専有ツールや制限のあるツールを使用せずにデータにアクセスし、作業できます。
- データには個人を特定できる情報や機密情報が含まれていない
  - ▶ アクセシビリティと再利用性を保証：法的・倫理的制約なくデータを自由に共有可能。

# ACS 倫理的行動とデータ完全性の促進

## データ完全性：

- ✓ データ関連事例への支援拡充（PIO）
- ✓ ACS研究データポリシーを開始
- ✓ 特定ジャーナル群におけるData Availability Statement（DAS）の義務化
- ✓ ChemRxiv支援のための共同取り組み
- ✓ Chemistry Data Bankの立ち上げ

## 出版倫理：

- ✓ 倫理事例への支援拡充（PIO）
- ✓ AI利用に関する方針ページを公開
- ✓ 有料執筆者問題への対応として著作者変更プロセスを改訂
- ✓ 編集長および副編集長向け出版倫理新研修コース

# Questions

