



Data Availability Statements in The Journal of Organic Chemistry, Organic Letters, and ACS Organic & Inorganic Au

Géraldine Masson

► To cite this version:

Géraldine Masson. Data Availability Statements in The Journal of Organic Chemistry, Organic Letters, and ACS Organic & Inorganic Au. ACS Organic & Inorganic Au, 2022, 2, pp.370 - 372. 10.1021/acsorginorgau.2c00049 . hal-03854728

HAL Id: hal-03854728

<https://hal.science/hal-03854728>

Submitted on 16 Nov 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Data Availability Statements in *The Journal of Organic Chemistry*, *Organic Letters*, and *ACS Organic & Inorganic Au*

Cite This: *ACS Org. Inorg. Au* 2022, 2, 370–372

Read Online

ACCESS |

Metrics & More

Article Recommendations

Data are increasingly being viewed as a valued research output, and making all data that go into reporting scientific results openly available increases trust in the research. Ultimately, when research data is findable, readable, and reusable, the impact of the research and associated publications receives a boost. In addition, data sharing and citation align with increasing funder mandates on reporting data. Here we address a new requirement for all articles containing primary research in *The Journal of Organic Chemistry*, *Organic Letters*, and *ACS Organic & Inorganic Au* to include a Data Availability Statement alerting readers on where and how to access all the related data.

Among the main disciplines of science, chemistry is a leader in the proportion of articles reporting original raw data, yet chemistry lags other disciplines in the proportion of articles that fully share original data.¹ ACS Publications has been developing a portfolio-wide data framework to address this shortcoming, which includes an [ACS Research Data Policy](#) and [standardized Data Guidelines](#) located in the [ACS Publishing Center](#). The main goal of the framework is to provide our authors with clear guidelines that help ensure results reported in our journals are verifiable, reproducible, and easily accessible to researchers. Building upon this framework, our next step forward in improving the quality and transparency of data is requiring authors to include a Data Availability Statement in their articles, pointing readers to where the original data may be found, either in the article or its Supporting Information file(s) or in publicly available repositories. We describe below a pilot project with the core ACS organic chemistry journals to implement and fine-tune Data Availability Statements before launching this initiative more broadly across the entire ACS family of journals.

■ ACS RESEARCH DATA POLICY

The first element in this data framework is our overarching [ACS Research Data Policy](#), in which ACS Publications lays out the principles that we as an organization value and provides the basis for subfield- or journal-specific policies. This policy applies to all ACS journals and was developed in partnership with ACS Editors and external experts. It provides recommendations for best-practice data citation, Data Availability Statements, and the use of appropriate data repositories.

Based on [Transparency and Openness Promotion \(TOP\) Guidelines](#), each ACS journal will occupy one of four policy levels ([Figure 1](#)). Each level features a set of best practices, giving each journal the flexibility to implement them as appropriate for the needs of its research community. All ACS

journals are currently at Level 1—that is, encouraging a Data Availability Statement and encouraging that data be made available.

■ SUBFIELD-SPECIFIC DATA GUIDELINES

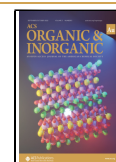
The second element of the data framework is a set of guidelines related to a specific subfield or data type. These guidelines provide specific instructions, explain what an author needs to do to make their data available, and how an author should report their data to comply with ACS standards. The goal of these subfield-specific guidelines is to have a single guideline for each type of data that is uniform across all journals publishing that data type. For example, an author publishing a manuscript that characterizes an organic compound with NMR data will be able to review one set of [organic data guidelines](#), which will explain which data should be made available, how to report the data, and how to make the data available.

These data standards intersect with the broader framework, because although the subfield-specific guidelines lay out best practices for a given data type across all ACS Publications journals, each journal will determine which policy level it will use. These guidelines also serve as a minimum requirement, and journals will be free to have additional requirements as needed for particular techniques used by different research communities.

■ DATA AVAILABILITY STATEMENT PILOT

Building off the ACS data framework, our next step forward in improving the quality and transparency of data is a pilot project undertaken by *The Journal of Organic Chemistry*, *Organic Letters*, and *ACS Organic & Inorganic Au* to require each peer-reviewed article to feature a [Data Availability Statement](#). Formally, this means these journals will be Level 2 in the [ACS Research Data Policy](#)—the journal encourages authors to publicly share all the data underlying the results reported in the article, preferably via archiving in an appropriate publicly available repository. This statement may refer to data that is new and original or may refer to third-party

Published: September 12, 2022



POLICY LEVEL	Level 1	Level 2	Level 3	Level 4
Encourages Data Sharing	X	X	X	X
Encourages Data Availability Statement	X	X	X	X
Requires Data Availability Statement		X	X	X
Requires Data Sharing			X	X
Requires Peer Review of Data				X

Figure 1. ACS Research Data Policy levels.

Sample Data Availability Statements	
Data Availability	Example Text
All underlying data available in the article itself and its supplementary materials	The data underlying this study are available in the published article and its online supplementary material.
Data openly available in a public repository	The data underlying this study are openly available in [Repository Name] at [Persistent Link to data in Repository, e.g., DOI, Accession Number].
Data used in the article available from a source in the public domain	The data underlying this study are openly available in [Repository Name] at [Persistent Link to data in Repository, e.g., DOI, Accession Number]. These data were derived from sources in the public domain [list sources, including URLs].
Data available upon request due to legal/ethical reasons	The data underlying this study are not publicly available due to [explanation of reasons for not sharing, e.g., patient privacy issues]. The data are available from the corresponding author upon reasonable request [list any registration or other requirements for access].
Data owned by a third party	The data underlying this study were provided by [Third Party] under license/by permission. Data are available from the corresponding author upon reasonable request with the permission of [Third Party].
No new data generated, or article describes entirely theoretical research	No new data were generated or analyzed in support of this study.
Author elects not to make data available*	The data underlying this study are not publicly available [include rationale preventing public release of data].
Sample Data Availability Statements marked with an asterisk () are not allowed in journals under Level 3 or Level 4 Research Data Policies.	

Figure 2. ACS sample Data Availability Statements.

data that was involved in the analysis of the work. Authors **must include** a Data Availability Statement, which can be selected from a prewritten set (Figure 2), describing the public availability of the data supporting the article's results and conclusions. These statements can be combined if multiple statements apply and customized as needed. Publicly available data sets should also be cited, and instructions on appropriate citation are provided.

The Data Availability Statement is a standalone piece of text presented in the Associated Content section at the end of a published article (Figure 3). Data Availability Statements should include confirmation that the data underlying the publication exists and specify where the data can be found, all

■ ASSOCIATED CONTENT

Data Availability Statement

The data underlying this study are openly available in [Repository Name] at [Persistent Link to data in Repository, e.g., DOI, Accession Number].

Supporting Information

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

Experimental procedures and characterization (PDF)

Figure 3. Sample Data Availability Statement.

persistent identifiers (Accession Numbers, DOIs, or URLs), and any relevant information on licensing restrictions. As a

Data Availability Statement	
A Data Availability Statement is required for publication. See the ACS Research Data Policy for additional information, sample statements, and appropriate repositories. When will you provide this statement?	
☐	Now - the statement is included in the manuscript
☐	Later - the statement will be provided during the revision process

Figure 4. New Custom Question in ACS Paragon Plus.

result, “data is available upon request” will no longer qualify as a Data Availability Statement. ACS also encourages the deposition of data in open repositories. Authors may refer to re3data.org and FAIRsharing.org for information on available repositories, their certification status, and services offered.

As part of the pilot, authors at participating journals will have a new custom question at submission asking when the Data Availability Statement will be provided (Figure 4). While it is preferable to have the Data Availability Statement in the manuscript at submission, the statement can be provided during the revision process. A Data Availability Statement is required for all peer-reviewed articles, and may be included but is not required for Addition/Correction, Editorial, Expression of Concern, or Retraction article types. The Data Availability Statement will be reviewed at first decision to make sure that available links work and the data is available as described in the statement; any missing sections will be noted in the decision letter for the author. Manuscripts will not be accepted without a Data Availability Statement.

These are the first steps that *The Journal of Organic Chemistry*, *Organic Letters*, *ACS Organic & Inorganic Au*, and ACS Publications more widely are taking to embrace the future of open science. The success of making data available rests with our authors to ensure the original data from FIDs to elemental analysis results are available in raw form in the article and Supporting Information or in freely available repositories, which then offers a greater opportunity for the impact of research to be recognized. ACS is committed to continuously developing our platform to make this as easy as possible for our authors. We hope you as an author, reviewer, and reader share our passion for this initiative and that this experiment in requiring Data Availability Statements will have a positive impact on transparency and openness in the field of chemistry.

Géraldine Masson, Deputy Editor orcid.org/0000-0003-2333-7047

Marisa C. Kozłowski, Editor-in-Chief orcid.org/0000-0002-4225-7125

Scott J. Miller, Editor-in-Chief orcid.org/0000-0001-7817-1318

AUTHOR INFORMATION

Complete contact information is available at:

<https://pubs.acs.org/10.1021/acsorginorgau.2c00049>

Notes

This Editorial is jointly published in *The Journal of Organic Chemistry*, *Organic Letters*, and *ACS Organic & Inorganic Au*.

REFERENCES

(1) Womack, R. P. Research Data in Core Journals in Biology, Chemistry, Mathematics, and Physics. *PLoS One* **2015**, *10* (12), No. e0143460, DOI: [10.1371/journal.pone.0143460](https://doi.org/10.1371/journal.pone.0143460).