

Review of Supporting Information at Organic Letters

In our continuing effort to ensure that we publish the very best, high quality research, Organic Letters began conducting a closer examination of the Supporting Information (SI) submitted with our Letters. We added a staff member fully devoted to this task in 2012 to focus on a more consistent and systematic SI review prior to publication. We would like to update you on some of the common problems we have encountered, describe our process, and provide some guidance for those preparing materials for submission to Organic Letters.

Since enhanced SI review began at Organic Letters, we have found that the submitted SI routinely contains numerous errors such as missing data, incorrect data, inconsistency between the manuscript and the SI, and occasionally, data manipulation. We now examine all manuscripts that are on track for acceptance to ensure they comply with Organic Letters standards and to address any concerns from a Reviewer or Editor. All data requirements must be addressed before a manuscript is accepted. Our goal is to present your work in the best possible light and to provide our readers with an accurate record of the research reported.

When examining the experimental procedure section, we often request additional information such as physical description, isolated amounts of final products, and purification details. Further, Organic Letters requires isolated yields for all new or improved reaction conditions—not a gas chromatographic or spectroscopically determined yield. This benefits our readers when they attempt to repeat the published reaction.

To that end, we review the spectra and work with authors to improve both the image quality and the required details. Specifically, we confirm that the spectra are displayed with the appropriate range, include peak integration, are properly labeled, are legible, and are the correct size. This analysis also safeguards against fraudulent and/or manipulated data. Occasionally, during SI review, we find spectra that appear to be edited. While this is not the primary focus of our SI review, it has come to our attention that it is happening in the community. Organic Letters is taking action not only to increase awareness of this issue but also to advise and assist authors to correct their data prior to publication [see Data Integrity Editorial]. Spectral editing is a serious violation of ACS Ethical Guidelines.

Pleasingly, we have integrated this analysis into our evaluation process over the past three years with little to no impact on the speed of manuscript review and publication. The feedback we have received from authors has been overwhelmingly positive, and authors are grateful to have their data reviewed and corrected prior to publication.

With the amount of data generated and the number of coauthors involved (often working collaboratively across multiple institutions and/or companies), it is understandable how errors may occur prior to submission. There are a few ways authors can avoid these issues and improve the data quality in their manuscripts. A thorough review of the final submitted manuscript and SI will improve the quality of the submission before peer review and decrease the revision time if accepted.

In addition, we encourage you to review the Organic Letters Guidelines for Authors during manuscript and SI preparation.

To assist authors further, we have prepared a checklist to assist in avoiding the most common issues found during SI review (see next page). This checklist is also provided as Supporting Information for your benefit. There is no need to include it with the submission documents. Rather, we encourage you to use it as a tool in reviewing the final manuscript and SI. Please share the checklist with coauthors, colleagues, postdoctoral fellows and students and ask them to review the SI prior to submission. This document will also be incorporated into the Organic Letters Guidelines for Authors in 2016.

While our approach to SI review continues to evolve, we have already seen significant improvements in submitted manuscripts and published Letters since Organic Letters began the enhanced review. As chemists, we understand the importance of high quality, reliable, and reproducible publications. With continuous development of our SI review process, we aim to assist authors when errors are found in the SI and to provide the best possible SI for Organic Letters readers.

Organic Letters is exactly where you want to be!

Angela M. Hunter, Data Analyst Amos B. Smith, III, Editor-in-Chief

ASSOCIATED CONTENT

Supporting Information

Supporting Information checklist. The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.orglett.5b01700.

AUTHOR INFORMATION

Notes

Views expressed in this editorial are those of the author and not necessarily the views of the ACS.

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2867

Organic Letters Editorial

ORGANIC LETTERS DATA PREPARATION CHECKLIST

<u>Ma</u>	nuscript/SI Consistency
Ш	Compounds are labeled consistently between the manuscript and SI:
	Compound numbers
	Experimental details and spectra in the SI are in the sequence that corresponds
	to the manuscript
	<u>General</u>
	Pages are numbered in all files for publication
	Manuscript title and authors names are listed on the first page of each SI file
	A table of contents is included
	Files are combined (do not submit a series of files containing individual images
_	or structures)
Ш	An Introductory Section is present and describes:
	☐ Standard techniques
	☐ Instruments (NMR, microwave reactors, etc.)
	☐ Suppliers for commercial compounds or citations to references for non-
	commercial known compounds
	☐ Hazardous reactions or toxic compounds
_	perimental Details
Ш	Synthetic procedures/data include:
	☐ Reactant quantities
	Detailed purification techniques
	Product quantities
	\square Isolated yields
	\square Physical state/description of the compounds (i.e., color, solid, etc.)

Organic Letters Editorial

☐ Data is reviewed for typos and omissions:
☐ Molecular formula
☐ HRMS data:
☐ HRMS actual values are within the ±10 ppm error limit
☐ HRMS molecular weight matches the structure shown
☐ Elemental Analysis:
\square Elemental analysis values are within the ±0.4% error limit
☐ Reported formula matches the structure shown
☐ Spectral data:
\square 1 H and 13 C atoms have been accounted for
Reported data corresponds to the spectra provided in the SI
<u>Spectra</u>
☐ Spectra are labeled with an image of the structure and a compound number
Spectra are legible and images are not faint or blurry
☐ Spectra are at least a half page in size
☐ NMR baseline is displayed with the minimum chemical shift range [and can be extended if needed]:
-1-9 ppm for ¹ H spectra
-10-190 ppm for ¹³ C spectra
Peaks in the ¹ H NMR are integrated
☐ Chemical shift values are included for all peaks in the ¹H NMR and ¹³C spectra
one made and mediate and parties of an experience of a second of the
Data Requirements - New Compounds
☐ ¹H and ¹³C spectra
☐ HRMS data or elemental analysis data
<u>Data Requirements – Known Compounds</u> (synthesized by a new/improved method)
A reference in the experimental details section
\square One or more of the following: 1 H, 13 C, elemental analysis, HPLC, GC