



Last updated: September 17, 2024 View the latest guidelines online

Manuscript Submission Requirements Checklist

Author Checklist. In lieu of a cover letter, we request that authors fill out the provided <u>Submission</u> <u>Cover Letter and Author Checklist</u>.

Note on all Submissions. An editorial was published on guidelines for publishing papers in <u>JCIM</u>: <u>J. Chem. Inf. Model. 2015, 55, 719</u>. Submissions should follow these guidelines.

Requirements for Data and Software Availability. An editorial was published on requirements for publishing papers beginning on January 1, 2021. Please refer to: <u>https://pubs.acs.org/doi/10.1021/acs.jcim.0c01389</u>.

Manuscripts must be submitted electronically via the secure Web site at <u>http://pubs.acs.org/page/4authors/submission/index.html</u>. Guidelines for this method are provided here. If substantially the same manuscript has been previously submitted to this Journal or to another ACS journal, the author should include copies of the reviews with the submission and explain any revisions in the cover letter. The Editor may accept the manuscript on the basis of those reviews and author remarks or may seek additional reviews.

For further inquiries contact the Editor-in-Chief, Prof. Kenneth M. Merz, Jr., Department of Chemistry, Michigan State University, 578 S. Shaw Lane, East Lansing, MI 48824-1322. Phone: 517-355-9715. Fax: 517-353-7248. E-mail: <u>merz-office@jcim.acs.org</u>.

Scope of the Journal

The *Journal of Chemical Information and Modeling (JCIM*) publishes papers reporting new methodologies in chemical informatics and molecular modeling and its applications with experimental validation. Specific topics include the representation and computer-based searching of chemical databases, molecular modeling, computer simulation using molecular dynamics and free energy methods, machine learning on chemical and biological data, combined quantum mechanical/molecular mechanical (QM/MM) multi-scale simulations, computer-aided molecular design of new materials, catalysts, or ligands, development of new computational methods or efficient algorithms for chemical software, and biopharmaceutical chemistry including analyses of biological activity and other issues related to drug discovery. JCIM will not consider straightforward applications of molecular docking methods to a single target system without adequate experimental validation.

Chemists, computer scientists, and information specialists look to *JCIM* for insightful research studies, programming innovations, reviews, perspectives, and viewpoints to keep current with advances in this integral, multidisciplinary field.

As a member of this community – author, reader, or reviewer -- you'll stay abreast of advances and applications in molecular modeling, developments in multi-scale modeling, use of mathematical theory and computer science techniques in chemical problems, substructure search systems, pattern recognition, and clustering, analysis of chemical and physical data, database search systems, graphics, and natural language interfaces, bibliometric and citation analysis, and synthesis design, and reaction databases.

Manuscript Types

Viewpoints. General commentaries on current issues in the computational chemistry field, or scholarly comment on papers appearing in the Journal. Viewpoints must contain a Table of Contents graphic and an abstract, which should be a 2-5 sentence executive summary. Suggested limits for Viewpoints are 2000 words and no more than 2 figures, with no restriction on the number of references. Viewpoints will be rigorously editorially reviewed by at least two *JCIM* editors for content and the importance of the topic. Following the editorial review procedure, select articles will be sent out for peer review for final assessment according to Editors discretion.

Comments on articles must raise scientific or technical questions about an article; correspondence that is mainly opinion will not be accepted. Correspondence should be submitted within six months of the date of publication of the original article. The author(s) of the original article will be allowed to respond. Contributions may be edited for length and clarity.

Articles. Full-length research manuscripts, consistent with the objectives of *JCIM*, are the principal focus of the Journal. Authors must follow the instructions for preparation and submission given below.

Perspectives. Perspectives are interpretive accounts on subjects of current interest to the JCIM community. This series is intended to be a forum for experts to present their perspectives on emerging or active areas of research. Manuscripts must be ~10,000 words. There is no limit to the number of references. You may approximate the length of figures, schemes, and tables by counting single-column images as 300 words and double-column as 600 words (this count assumes that they will occupy ¼ and ½ page, respectively, at final production size). If a table was created using the Tables function in Word it will be included in the word count; subtract the word count for the table, and estimate the space as you would for a scheme or figure. The use of graphics to illustrate key concepts (3–5 display items) is strongly encouraged. A submission should include ~8–10 keywords extracted from the text as well as a graphical Table of Contents entry consisting of a colorful figure that represents the topic of the paper.

• *Perspectives: Best Practices Series.* This special series aim to capture and articulate best practices in different areas of cheminformatics and computational chemistry, e.g., molecular simulations, docking, or implementation of sophisticated algorithms for solving practical problems around chemical design/bioactivity prediction. Authors should follow the same instructions as given below for preparation and submission of Reviews. Authors are encouraged to send a pre-submission inquiry for approval prior to submitting a *Perspectives: Best Practice* to the journal. The pre-submission inquiry should contain a brief summary of the proposed topic. For pre-submission inquiries, please email the journal at <u>eic@jcim.acs.org</u>.

Reviews. Reviews are topical, brief, and of general interest to the *JCIM* community. These papers critically evaluate existing work and make the material more easily comprehendible to those not expert in the subject matter. Manuscripts must be ~10,000 words (excluding the References and all graphics). There is no limit to the number of references, but please ensure citations are appropriate. You may approximate the length of figures, schemes, and tables by counting single-column images as 300 words and double-column as 600 words (this count assumes that they will occupy ¼ and ½ page, respectively, at final production size). If a table was created using the Tables function in Word it will be included in the word count; subtract the word count for the table, and estimate the space as you would for a scheme or figure. The use of graphics to illustrate key concepts (3–5 display items) is strongly encouraged. A submission should include ~8–10 keywords extracted from the text as well as a graphical Table of Contents entry consisting of a colorful figure that represents the topic of the paper. Authors are encouraged to send a pre-

submission inquiry to the editorial team for approval prior to submitting a review to the journal. The pre-submission inquiry should contain a brief summary of the proposed review and its significance to the field. For pre-submission inquiries, please email the journal at <u>eic@jcim.acs.org</u>.

Letters. Letters are intended for rapid publication of preliminary reports on important findings of novel and timely significance. The major concepts of the paper should not have been published previously. Manuscripts are limited to four journal pages (approximately 3500 words, including the text, references, author names, and all graphics). You may approximate the length of figures, schemes, and tables by counting single-column images as 300 words and double-column as 600 words (this count assumes that they will occupy ¼ and ½ page, respectively, at final production size). If a table was created using the Tables function in Word it will be included in the word count; subtract the word count for the table, and estimate the space as you would for a scheme or figure. The abstract is limited to 75 words and should briefly state the purpose of the research, principal results, and major conclusions. Supporting Information can be provided detailing procedures or providing supplementary data.

Application Notes. Application notes are informative peer-reviewed reports on novel software packages, databases, and web servers. Submissions should be no longer than 5000 words and contain at least one figure. This word count includes the abstract, text, and graphics only. References do not count towards the word limit. You may approximate the length of figures, schemes, and tables by counting single-column images as 300 words and double-column as 600 words (this count assumes that they will occupy 1/4 and 1/2 page, respectively, at final production size). If a table was created using the Tables function in Word, it will be included in the word count; subtract the word count for the table, and estimate the space as you would for a scheme or figure. Authors will be expected to abide by this rule and to submit a statement from the corresponding author indicating the word count of the article and how it was obtained. Articles with word counts over 5000 words will be returned to the authors for editing before going through the review process. The name of the application being described should be clearly stated in the manuscript title. The scientific, technical, or other usability advancements of the software should be clearly described. As far as possible, the software packages and web servers should be operating system agnostic (Windows, Linux, and OSX). All submitted manuscripts will be reviewed by an editor prior to being sent out for peer-review. The software should be generally available for evaluation or purchase at the time of publication for academic and commercial use. The software must be made available for testing by reviewers to address specific data or claims in the manuscript, upon request by reviewers, while preserving reviewer anonymity. Articles viewed to be unsuitable for the journal or inconsistent with the above guidelines will be returned after editorial review.

Additions and Corrections. Additions and Corrections may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the ACS Paragon Plus environment by the corresponding author for publication in the "Addition/Correction" section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction or provide evidence that such approval has been solicited. The Addition and Correction should include the original article title and author list, citation including DOI, and details of the correction. For proper formatting, see examples in a current issue of the Journal.

Retractions. Articles may be retracted for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon

may be retracted in order to correct the scientific record. Retractions may be requested by the article author(s) or by the Journal Editor(s) but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of Retraction will be published containing information about the original article title, author list, and the reason for the Retraction. Retracted articles will be accompanied by the related Retraction notice and will be marked as "Retracted". The originally published article will remain on the web except in extraordinary circumstances (e.g., where deemed legally necessary or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information, see http://publicationethics.org/.

Expressions of Concern. The American Chemical Society (ACS) follows guidance from the Committee on Publication Ethics (COPE) when considering expressions of concern; for more information see: <u>http://publicationethics.org/</u>. In accordance with COPE guidelines, expressions of concern may be issued if:

- there is inconclusive evidence of research or publication misconduct by the authors;
- there is evidence that the findings are unreliable but the authors' institution will not investigate the case;
- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
- an investigation is underway but a judgment will not be available for a considerable time.

Expressions of concern are published at the discretion of the Editor-in-Chief. Upon completion of any related investigation, and when a final determination is made about the outcome of the article, the expression of concern may be replaced with a retraction notice or correction.

ACS Researcher Resources

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit <u>ACS</u> <u>Researcher Resources</u> for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- <u>Mastering the Art of Scientific Publication</u>, which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on <u>how to prepare and submit a manuscript</u> to ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, including details on selecting the applicable <u>Journal Publishing Agreement</u>.
- <u>Sharing your research</u> with the public through the ACS Publications open access program.
- <u>ACS Reviewer Lab</u>, a free online course covering best practices for peer review and related ethical considerations.
- <u>ACS Author Lab</u>, a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- <u>ACS Inclusivity Style Guide</u>, a guide that helps researchers communicate in ways that recognize and respect diversity in all its forms.

Manuscript Preparation

Submit with Fast Format

All ACS journals and partner journals have simplified their formatting requirements in favor of a streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers <u>here</u>.

Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- When required by a journal's structure or length limitations, manuscript templates should be used.
- References can be provided in any style, but they must be complete, including titles. For information about the required components of different reference types, please refer to the <u>ACS Style Quick Guide</u>.
- Supporting Information must be submitted as a separate file(s).

Document Templates and Format

The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates <u>here</u>.

General information on the preparation of manuscripts may also be found in the <u>ACS Guide to</u> <u>Scholarly Communication</u>.

Acceptable Software, File Designations, and TeX/LaTeX

See the list of <u>Acceptable Software</u> and appropriate <u>File Designations</u> to be sure your file types are compatible with ACS Paragon Plus. Information for manuscripts generated from <u>TeX/LaTeX</u> is also available.

Cover Letter

A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

For *JCIM*, we request that authors fill out the provided RTF <u>Submission Cover Letter and Author</u> <u>Checklist</u> and submit as their cover letter.

Manuscript Text Components

Title. The title of the paper should be brief—preferably 12 words or fewer. Readers rarely read and absorb longer titles, so it should be concise. An abstract of 3–4 sentences is required, and as with the title, it should be concise, touching on just the major points about which the author wants to alert the reader.

Note on all Submissions. An <u>editorial</u> was published on guidelines for publishing papers in *JCIM*: *J. Chem. Inf. Model.* 2015, *55*, 719. Submissions should follow these guidelines.

Supporting Information

This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of <u>Acceptable Software by File</u> <u>Designation</u> and confirm that your Supporting Information is <u>viewable</u>.

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief, nonsentence description of the actual contents of each file, including the file type extension, is required. This description should be labeled Supporting Information and should appear before the Acknowledgement and Reference sections. Examples of sufficient and insufficient descriptions are as follows:

Examples of sufficient descriptions: "Supporting Information: ¹H NMR spectra for all compounds (PDF)" or "Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)".

Examples of insufficient descriptions: "Supporting Information: Figures S1-S3" or "Additional figures as mentioned in the text".

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

Research Data Policy

All ACS journals strongly encourage authors to make the research data underlying their articles publicly available at the time of publication.

Research data is defined as materials and information used in the experiments that enable the validation of the conclusions drawn in the article, including primary data produced by the authors for the study being reported, secondary data reused or analyzed by the authors for the study, and any other materials necessary to reproduce or replicate the results.

The <u>ACS Research Data Policy</u> provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

<u>ACS Math Style Sheet</u>. Authors including math, display or in-text, in their manuscripts are encouraged to consult the <u>ACS Guidelines for Presenting Mathematical Information</u>. This style sheet provides brief discussion of formatting related to the presentation of mathematical formulas, complete with examples of ACS style and layout. This document was developed to help authors anticipate how mathematical expressions will be formatted in the published version of the paper.

Compound Characterization. If the submission contains reports of new experimental data, the same <u>guidelines</u> as required by the *Journal of Medicinal Chemistry* must be followed. Supporting evidence must be provided for identification of the chemical structure and purity of any compound that is reported to be active in an assay. This normally requires inclusion of NMR spectra, molecular weight verification by high-resolution mass spectrometry, and HPLC data verifying purity at the 95% or greater level.

QSAR/QSPR Submissions. An editorial was published on guidelines for QSAR/QSPR papers: J.

Chem. Inf. Model. 2006, 46, 937. Submissions in this area need to follow the guidelines.

Language and Editing Services

A well-written paper helps share your results most clearly. ACS Publications' <u>English Editing</u> <u>Service</u> is designed to help scientists communicate their research effectively. Our subject-matter expert editors will edit your manuscript for grammar, spelling, and other language errors so your ideas are presented at their best.

Preparing Graphics

The quality of illustrations in ACS journals and partner journals depends on the quality of the original files provided by the authors. Figures are not modified or enhanced by journal production staff. All graphics must be prepared and submitted in digital format.

Graphics should be inserted into the main body whenever possible. Please see Appendix 2 for additional information.

Any graphic (figure chart, scheme, or equation) that has appeared in an earlier publication should include a <u>credit line</u> citing the original source. Authors are responsible for <u>obtaining written</u> <u>permission</u> to re-use this material.

Figure and Illustration Services

The impact of your research is not limited to what you can express with words. Tables and figures such as graphs, photographs, illustrations, diagrams, and other visuals can play a significant role in effectively communicating your findings. Our <u>Artwork Editing</u> and <u>Graphical Abstract</u> services generate publication-ready figures and Table of Contents (TOC) graphics that conform to your chosen journal's specifications. For figures, this includes changes to file type, resolution, color space, font, scale, line weights, and layout (to improve readability and professional appearance). For TOC graphics, our illustrators can work with a rough sketch or concept or help extract the key findings of your manuscript directly for use as a visual summary of your paper.

Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through <u>ACS Paragon Plus</u>, which requires an ACS ID to log in. Registering for an ACS ID is fast, free, and does not require an ACS membership. Please refer to Appendix 1 for additional information on preparing your submission

Prior Publication Policy

The *Journal of Chemical Information and Modeling* authors are allowed to deposit an initial draft of their manuscript in a preprint service such as arXiv, bioRxiv, or <u>ChemRxiv</u>. Please note any use of a preprint server in the cover letter, and as appropriate, state how the manuscript has been adjusted/updated between deposition and submission. All other prior/redundant publication is forbidden. Upon publication in the Journal of Chemical Information and Modeling, authors are advised to add a link from the preprint to the published paper via the Digital Object Identifier (DOI). For further details, contact the <u>Editorial Office</u>.

Editorial Policies

To help *JCIM* authors prepare high-quality manuscripts, we propose the extended guidelines listed in Table 1 of our published 2015 <u>Editorial</u>, reproduced here.

More Likely To Succeed in Review:

- Modeling study leading to a design that enables new and successful experiments (e.g., new potent compounds) irrespective of the modeling technique.
- Models (with clearly outlined availability, e.g., implemented as a web service) of important new endpoints and demonstrably better models (e.g., larger and/or much higher quality) than any other existing models. Models for a known endpoint but a new biological target (e.g., human vs rodent data) confirmatory vs primary assay that leads to clearly outlined design strategies.
- Provocative papers criticizing/rejecting existing paradigms; should be very well grounded and preferably must provide the reader some idea(s) how to solve the problem. Methodological papers summarizing best practices.
- New approaches for modeling, clustering, similarity estimation, etc. Must be benchmarked against multiple different tasks and consistently show superiority. These approaches could be developed and tested using simulated data sets but applied to several real tasks, and actual compounds should be designed using them.
- Manuscripts describing databases/data sets; should contain some unique features—the biggest existing data set, user-friendly database, etc.
- Perspectives on "hot" or important topics.
- New nontrivial analyses/concepts of all related fields including med chem, drug design, tox, etc., approached from the molecular modeling point of view.
- Papers describing innovative application of existing cheminformatics techniques to new types of substances (nanomaterials, materials, mixtures, polymers, macromolecules, texts) that lead to new testable hypotheses.

Less Likely To Succeed in Review:

- Routine modeling studies or modeling of thoroughly explored biological endpoints (LogP or well-studied inhibitor classes such as ACE inhibitors).
- Models for a known endpoint, or an old data set, that do not show any advantage over existing models or models that are not OECD-compliant viz (1) a defined endpoint, (2) an unambiguous algorithm, (3) a defined domain of applicability,(4) appropriate measures of goodness-of-fit, robustness, and predictivity, or (5) a mechanistic interpretation, if possible.
- Any paper without a section on data curation.
- Any paper containing proprietary data without making an explicit argument why the data should be protected and yet why in the absence of the data the manuscript is still valuable.
- New approaches for modeling, clustering, similarity estimation, etc. without benchmarking, or if benchmarked, showed results similar to existing methods.
- Papers with innovative applications but not demonstrating predictive or instructional value (e.g., application of chemical graph-based descriptors to proteins without a clear indication of their value to structural biology).

Providing Potential Reviewer Names

Please suggest 5 reviewers. Authors are encouraged to avoid suggesting reviewers from the authors' institutions. Do not suggest reviewers who may have a <u>real or perceived conflict of</u>

interest. Whenever possible, suggest academic email addresses rather than personal email addresses.

Manuscript Transfer

If your submission is declined for publication by this journal, the editors might deem your work to be better suited for another ACS Publications journal or partner journal and suggest that the authors consider transferring the submission. <u>Manuscript Transfer</u> simplifies and shortens the process of submitting to another ACS journal or partner journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied by ACS Paragon Plus to the new draft submission. Authors are free to accept or decline the transfer offer.

Note that each journal is editorially independent. Transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor of the next journal.

PRODUCTION AND PUBLICATION

Proofs via ACS Direct Correct

Correction of the galley proofs is the responsibility of the Corresponding Author. The Corresponding Author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via <u>ACS Direct Correct</u>. Extensive or important changes on page proofs, including changes to the title or list of authors, are subject to review by the editor.

It is the responsibility of the Corresponding Author to ensure that all authors listed on the manuscript agree with the changes made on the proofs. Galley proofs should be returned within 48 hours in order to ensure timely publication of the manuscript.

Publication Date and Patent Dates

Accepted manuscripts will be published on the ACS Publications Web site as soon as page proofs are corrected and all author concerns are resolved. The first date on which the document is published on the Web is considered the publication date.

Publication of manuscripts on the Web may occur weeks in advance of the cover date of the issue of publication. Authors should take this into account when planning their patent and intellectual property activities related to a document and should ensure that all patent information is available at the time of first publication, whether ASAP or issue publication.

All articles published ahead of print receive a unique Digital Object Identifier (DOI) number, which is used to cite the manuscript before and after the paper appears in an issue. Additionally, any supplemental information submitted along with the manuscript will automatically be assigned a DOI and hosted on Figshare to promote open data discoverability and use of your research outputs.

ASAP Publication

Manuscripts will be published on the "ASAP Articles" page on the web as soon as page proofs are corrected and all author concerns are resolved. ASAP publication usually occurs within a few working days of receipt of page proof corrections, which can be several weeks in advance of the cover date of the issue.

Post-Publication Policies

The American Chemical Society follows guidance from the <u>Committee on Publication Ethics</u> (COPE) when considering any ethical concerns regarding a published article, Retractions, and Expressions of Concern.

Additions and Corrections

Additions and Corrections may be requested by the author(s) or initiated by the Editor to address important issues or correct errors and omissions of consequence that arise after publication of an article. All Additions and Corrections are subject to approval by the Editor, and should bring new and directly relevant information and corrections that fix scientific facts. Minor corrections and additions will not be published. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work.

Additions and Corrections must be submitted as new manuscripts via ACS Paragon Plus by the Corresponding Author for publication in the "Addition/Correction" section of the Journal. The corresponding author should obtain approval from all coauthors prior to submitting or provide evidence that such approval has been solicited. The manuscript should include the original article title and author list, citation including DOI, and details of the correction.

Retractions

Articles may be retracted for scientific or ethical reasons and may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. When an article is retracted, a notice of Retraction will be published containing information about the reason for the Retraction. The originally published article will remain online except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks).

Expressions of Concern

Expressions of Concern may be issued at the discretion of the Editor if:

- there is inconclusive evidence of research or publication misconduct by the authors;
- there is evidence that the findings are unreliable but the authors' institution will not investigate the case;
- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
- an investigation is underway but a judgment will not be available for a considerable time.

Upon completion of any related investigation, and when a final determination is made about the outcome of the article, the Expression of Concern may be replaced with a Retraction notice or

Correction.

Sharing Your Published Article

At ACS Publications, we know it is important for you to be able to share your peer reviewed, published work with colleagues in the global community of scientists. As sharing on sites known as scholarly collaboration networks (SCNs) is becoming increasingly prevalent in today's scholarly research ecosystem, we would like to remind you of the many ways in which you, a valued ACS author, can <u>share your published work</u>.

Publishing open access makes it easy to share your work with friends, colleagues, and family members. In addition, ACS Publications makes it easy to share your newly published research with ACS Articles on Request (see below). Don't forget to promote your research and related data on social media, at conferences, and through scholarly communication networks. Increase the impact of your research using the following resources: <u>Altmetrics</u>, <u>Figshare</u>, <u>ACS Certified Deposit</u>

E-Prints

When your article is published in an ACS journal or partner journal, corresponding authors are provided with a link that offers up to 50 free digital prints of the final published work. This link is valid for the first 12 months following online publication, and can be shared via email or an author's website. After one year, the access restrictions to your article will be lifted, and you can share the <u>Articles on Request</u> URL on social media and other channels. To access all your Articles on Request links, log in to your ACS Researcher Resources account and visit the "My Published Manuscripts" page.

Reprints

Article, journal, and commercial reprints are available to order.

Appendix 1: PREPARING FOR SUBMISSION

We've developed ACS' publishing and editorial policies in consultation with the research communities that we serve, including authors and librarians. Browse our policies below to learn more.

Ethical Guidelines

ACS editors have provided <u>Ethical Guidelines</u> for persons engaged in the publication of chemical research—specifically, for editors, authors, and reviewers. Each journal also has a specific <u>policy</u> <u>on prior publication</u>.

OFAC Compliance

As a U.S.-based non-profit organization, the American Chemical Society (ACS) is required to comply with U.S. sanctions laws and regulations administered by the <u>U.S. Treasury Department's</u> <u>Office of Foreign Assets Control</u> (OFAC). While these laws and regulations permit U.S.-based publishers like ACS to engage in publishing-related activities with authors located in sanctioned regions in many cases, ACS may be prohibited under U.S. law from engaging in publishing-related

activities in some cases, including, but not limited to, instances where an author or the institution with which an author is affiliated is located in a particular sanctioned region or has been designated by OFAC as a <u>Specially Designated National</u> (SDN) pursuant to certain U.S. sanctions programs. ACS reserves the right to refrain from engaging in any publishing-related activities that ACS determines in its sole discretion may be in violation of U.S. law.

Safety Considerations

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the <u>Safety Statement</u> <u>Style Sheet</u> and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* is freely available here.

Conflict of Interest Disclosure

A statement describing any financial conflicts of interest or lack thereof is published in each ACS journal and partner journal article.

During the submission process, the Corresponding Author must provide a statement on behalf of all authors of the manuscript, describing all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest. If the manuscript is accepted, the statement will be published in the final article.

If the manuscript is accepted and no conflict of interest has been declared, the following statement will be published in the final article: "The authors declare no competing financial interest."

Plagiarism

In publishing only original research, ACS is committed to deterring plagiarism, including selfplagiarism. ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process.

Further information about plagiarism can be found in Part B of the <u>Ethical Guidelines to Publication</u> <u>of Chemical Research</u>. See also the <u>press release</u> regarding ACS' participation in the CrossCheck initiative.

Authorship, Author List, and Coauthor Notification

Authors are required to obtain the consent of all their coauthors prior to submitting a manuscript. The submitting author accepts the responsibility of notifying all coauthors that the manuscript is being submitted.

During manuscript submission, the submitting author must provide contact information (full name, email address, institutional affiliation, and mailing address) for all of the coauthors. Because all of the author names are automatically imported into the electronic <u>Journal Publishing Agreement</u>, the names must be entered into ACS Paragon Plus. (Note that coauthors are not required to register

in ACS Paragon Plus.) Author affiliation should reflect where the work was completed, even if the author has since left that institution. Authors may include a note with a current address if their institution has changed since the work was completed.

To expedite the processing of your manuscript, please format your author and affiliation information according the guidelines in this link: https://pubsapp.acs.org/paragonplus/submission/author-address-information.pdf.

Criteria for authorship can be found in Part B of the <u>Ethical Guidelines to Publication of Chemical</u> <u>Research</u>. Artificial intelligence (AI) tools do not qualify for authorship. The use of AI tools for text or image generation should be disclosed in the manuscript within the Acknowledgment section with a description of when and how the tools were used. For more substantial use cases or descriptions of AI tool use, authors should provide full details within the Methods or other appropriate section of the manuscript.

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Appendix 2: Preparing Graphics

Resolution

Digital graphics pasted into manuscripts should have the following minimum resolutions:

- Black and white line art, 1200 dpi
- Grayscale art, 600 dpi
- Color art, 300 dpi

Size

Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (allow 12 pts. For each line of caption text). Lettering should be no smaller than 4.5 points in the final published format. The text should be legible when the graphic is viewed full-size. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

Color

Color may be used to enhance the clarity of complex structures, figures, spectra, and schemes, etc., and color reproduction of graphics is provided at no additional cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

Consult the Guidelines for Table of Contents/Abstract Graphics for specifications.

Our team of subject-matter experts and graphical designers can also help generate a compelling TOC graphic to convey your key findings. Learn more about our <u>Graphical Abstract service</u>.

Figures

A caption giving the figure number and a brief description must be included below each figure. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

Charts

Charts (groups of structures that do not show reactions) may have a brief caption describing their contents.

Tables

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter-relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

Schemes

Each scheme (sequences of reactions) may have a brief caption describing its contents.

Chemical Structures

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

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