

## Manuscript Submission Requirements Checklist

- **Submit with Fast Format:** ACS journals have simplified formatting requirements with a streamlined and standardized review-ready format for an *initial* manuscript submission. Include article titles in references.
- **Scope:** *JACS Au* publishes manuscripts reporting significant discoveries in all fields of chemistry.
- **Cover Letter:** must include a paragraph explaining why your manuscript is appropriate for *JACS Au*, clearly indicating what key advance(s) are described in the work relative to the state-of-the-art, and a statement confirming the manuscript has not been previously published by any of the authors and/or is not under consideration for publication in another journal at the time of submission.
- **Suggested Reviewers:** Submit names and email addresses of at least six scientists from at least three different countries who could evaluate the work. These suggested reviewers must not be former mentors or mentees nor collaborators or co-authors from the past five years.
- **Disclosure of previous submissions:** If the manuscript was previously rejected by *JACS Au*, provide the manuscript number and a detailed response to each reviewer's comments. If the manuscript was previously declined by any other journal, even without external peer review, this must be disclosed; however, providing the journal name and additional information is optional.
- **Disclosure of prior publication & JACS Au preprint policy:** Submitted work must not be published elsewhere or concurrently submitted to another journal. Posting submitted manuscripts on a pre-print server is permitted in accordance with *JACS Au* policy and must be disclosed upon submission to the journal.
- **Author list with affiliations:** List of authors, order of authors, author affiliations, and manuscript title must be the same on all pieces of the submission and match the electronic entry at submission.
- **Manuscript Type:** Article, Letter, Perspective, Correspondence/Rebuttal, or Addition and Correction
- **Title and Abstract:** Be clear and concise, reflect the emphasis and content of the manuscript. Titles and abstracts of manuscripts may not contain the words "New", "Novel", or "First"; "Superb", "Excellent", "Exceptional", "Outstanding" or other similar descriptive words discouraged unless rigorously supported by a thorough comparison with the state-of-the-art in the manuscript. Acronyms and abbreviations are not permitted in manuscript titles, unless they are broadly familiar to readers in all disciplines of chemistry.
- **Graphics (Figures/Tables/Schemes):** Text should be clear and legible, ideally with Arial or Helvetica fonts, with fonts no smaller than 8 pt. Chemical structures should be presented in ACS format. Authors should use drawing packages with journal-based templates, if possible. These contain the appropriate bond widths, bond lengths, fonts, and other settings recommended by *JACS Au*. Figures must be mentioned in the text in consecutive order and number with Arabic numerals. Avoid inset figures.
- **References:** Include article titles in references.
- **Safety:** Authors must emphasize any unexpected, new, and/or significant hazards associated with the work.
- **Table of Contents graphic:**
  - required, dimensions of 3.25 inches by 1.75 inches (approx. 8.25 cm by 4.45 cm)
- **Cover Art (optional):** Authors may submit images to be considered for the cover (TIF, JPG, PNG or EPS files with a resolution of at least 300 dpi for pixel-based images). The image size is 8.19 inches (20.8 cm) wide × 10 inches (25.4 cm) high at 300 ppi.
- **Supporting Information (if any):** must be included at the time of electronic submission. Include the heading "Supporting Information" followed by the manuscript title, author list, and affiliations. Tables, Schemes, and Figures should be written as Table S1, Figure S1, Scheme S1, etc. All pages of the PDF Supporting Information should be numbered consecutively. Copies of all related works that are "in press", "accepted", or "submitted" for publication or in the late stages of preparation

must be uploaded as Supporting Information for Review Only at the time of submission.

References that are only available online should be cited by the Digital Object Identifier (DOI).

- **Administrative considerations:** All manuscripts must not be under consideration or published elsewhere; manuscripts will be screened with plagiarism software; information on whether the manuscript has been previously considered elsewhere must be provided; do not forget to list funding sources and utilize ORCID.

Correspondence should be addressed to the Editor-in-Chief at [eic@jacsau.acs.org](mailto:eic@jacsau.acs.org).

## Scope of the Journal

[\*JACS Au\*](#) is a monthly open access multi-disciplinary journal devoted to the publication of manuscripts reporting significant research discoveries in all fields of chemistry. The journal considers submissions in traditional core fields such as analytical, physical, inorganic, and organic chemistry, as well as areas such as biological, medicinal, environmental, catalytic, computational, and theoretical chemistry; materials and nanoscience; chemical engineering, chemical education, and other multidisciplinary research as it applies to chemistry. Articles, Letters, and Perspectives are published. More information can be found [here](#).

## Manuscript Types

**Articles** should report a significant advance in a subfield of chemistry, being characterized by the editor and referees as an advance representing the top 10% of articles published annually in that field. Articles must be of high scientific quality, originality, significance, and conceptual novelty. Articles that mainly expand findings that were previously published as Letters in *JACS Au* or elsewhere and that only incorporate experimental data, without greatly expanded scope and without providing new insights or conceptual breakthroughs, will be declined or recommended for Manuscript Transfer to specialized journals. Similarly, articles that are mainly routine extensions of previously published related work will be declined or recommended for Manuscript Transfer to specialized journals.

Use of the template for Articles is strongly encouraged but is not required. If an author chooses not to use a template to prepare an Article, only Times and Symbol fonts and 1.5 or double line spacing should be used. Other fonts may cause problems when the PDF files used for review are created. Also, if the template is not used, the document mode or its equivalent in the word-processing program should be used; i.e., files should not be saved in "Text Only" (ASCII) mode. If a non-Western version of word-processing software is used to prepare the manuscript, the file should be saved in rich-text format (RTF).

Articles should cover their subjects with thoroughness, clarity, and completeness but should be as concise as possible. Abstracts to Articles are typically limited to 300 words and should summarize the significant results and conclusions.

**Letters** are short publications that report results whose immediate availability to the science and engineering community is deemed important. A Letter must convey the scientific findings concisely in a brief abstract, main text, and graphical elements as determined by word count not exceeding 2,200 words, including titles/footnotes/captions of approximately five graphics (typically 2 inches long in a single column). References are not included in word count to allow article titles to be included at submission. To calculate word count within the word processing application, select all text from abstract through end of main text (excluding title, authors, affiliations, and content after main text) and view the

word processor's word count data. Letters exceeding the word count limit must be shortened before acceptance. Note: *JACS Au* encourages submission of Letters ranging from approximately 1,200-2,200 words (equivalent to 2-4 formatted journal pages), with more concise submissions appropriate for the most urgent new findings of exceptional significance.

All graphics and tables must be placed near the point of first mention in the text of the manuscript (not grouped at the end of the document) and must be sized according to current guidance. Long notes are not permitted in the References section; information not directly germane to the Letter can be included as Supporting Information. Letters can be complete publications, but follow-up publication may be justified when the research is continued and a more complete account of the work is deemed necessary, especially for the most urgent concise Letters noted above. Special efforts will be made to expedite the reviewing and the publication of Letters. The time for proofreading the galley proofs is relatively short. For this reason, authors of Letters should ensure that manuscripts are in final, error-free form when submitted. A [template for Letters](#) is available.

**Perspectives** are personal reviews of a field or area by one or a small team of authors, and they are focused rather than comprehensive. Perspective authors are asked to assess the current status of the field with an emphasis toward identifying key advances being made or those advances that are needed, and with an eye to the future. The *JACS Au* Perspective should touch base with the current literature, including key contributors and references, but will primarily serve to inspire and help direct future research efforts. Authors may be invited by the Editor to submit Perspectives. Authors interested in submitting a Perspective are strongly encouraged to contact the Editor prior to manuscript preparation and submission, to seek conditional approval of the proposed topic. One-page proposals should be sent to the Editorial office ([eic@jacsau.acs.org](mailto:eic@jacsau.acs.org)), for consideration. Perspectives may not exceed 10,000 words in abstract, main text, and graphical elements.

**Correspondence/Rebuttal.** Correspondence is a technical contribution providing, with supporting material, a respectful but alternative point of view to a publication that has appeared in *JACS Au*. The author of the original publication may be invited to write a Rebuttal. The Correspondence and Rebuttal will appear in the same issue of the journal, when possible.

**Methods/Protocols** are manuscripts that provide a platform for researchers to report innovative experimental and computational methods and best laboratory practices relevant to their disciplines that would be of interest to the broader scientific community. The goal of this manuscript type is to encourage and promote reproducibility and facile duplication of research by those skilled in the art, and to promote high scientific standards in the reporting of scientific methods. We consider both invited and unsolicited Methods/Protocols submissions describing either experimental or computational protocols from all areas of chemistry and allied fields. These Methods/Protocols manuscripts should begin with a brief review of the area, followed by detailed descriptions of procedures and/or in-depth information about computational methods. They may include helpful insights, "insider" advice, and warnings about potential pitfalls and safety concerns. There is no set length, and authors are asked to include videos and photographs of experiments and apparatuses in the Supplementary Information, as well as additional details to ensure reproducibility. The manuscript and any supplementary materials will undergo the usual rigorous peer review process of the journal.

Please feel free to contact the Editorial Office at [eic@jacsau.acs.org](mailto:eic@jacsau.acs.org) for more details regarding the format and preparation of a Methods/Protocols manuscript.

# 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 [ACS Researcher Resources](#) for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- [Mastering the Art of Scientific Publication](#), which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on [how to prepare and submit a manuscript](#) to the ACS Publications manuscript submission and peer review system, including details on selecting the applicable [Journal Publishing Agreement](#).
- [Sharing your research](#) with the public through the ACS Publications open access program.
- [ACS Reviewer Lab](#), a free online course covering best practices for peer review and related ethical considerations.
- [ACS Author Lab](#), a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- [ACS Inclusivity Style Guide](#), 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 [here](#).

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 [ACS Style Quick Guide](#).
- 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 [here](#).

General information on the preparation of manuscripts may also be found in the [ACS Guide to Scholarly Communication](#).

### Acceptable Software, File Designations, and TeX/LaTeX

See the list of [Acceptable Software](#) and appropriate [File Designations](#) to be sure your file types are compatible with the submission system. Information for manuscripts generated from [TeX/LaTeX](#) 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.

The letter must provide the corresponding author's name, title, affiliation, and e-mail address. All Editorial correspondence concerning receipt, status, review, revision, and publication of a manuscript will be sent only to one person who has been designated as the corresponding author during the evaluation period. The corresponding author is responsible for communicating the manuscript status to all co-authors of the manuscript and for obtaining the co-authors' assent to any substantial changes of content or interpretation made during revision. While a cover letter with designate a single corresponding author who serves as the primary contact during the submission and review process, additional corresponding authors may be designated with asterisks in collaborative manuscripts, with the number of corresponding authors not to exceed three.

The cover letter must include a paragraph explaining why your manuscript is appropriate for *JACS Au*. This paragraph should clearly indicate what key advance(s) is/are described in the work. The letter may suggest the name of an appropriate *JACS Au* Associate Editor. However, manuscript assignment to an Associate Editor is ultimately at the discretion of the Editor-in-Chief. Non-preferred Associate Editors and reviewers may be denoted in the cover letter, along with a reason for their designation.

The cover letter should provide explicit assurance that the manuscript is not under consideration for publication and has not been published elsewhere. Please note any submission to a preprint server such as ChemRxiv, bioRxiv, or arXiv in the cover letter and include a link to the preprint, and as appropriate, state how the manuscript has been adjusted/updated between deposition and submission.

## Manuscript Text Components

**Title.** Titles should clearly and concisely reflect the emphasis and content of the manuscript. Titles are of great importance for current awareness and information retrieval and should be carefully constructed for these purposes. Titles of manuscripts may not contain the words "New" or "Novel" nor any part number or series number without permission from the Editor. Claims of precedence should not be made in a title, so use of "First" in titles for this purpose is prohibited. Additionally, "Superb", "Excellent", "Exceptional", "Outstanding" or other similar descriptive words, are strongly discouraged. Acronyms and abbreviations are not permitted in manuscript titles, unless they are broadly familiar to readers in all disciplines of chemistry. Titles should not be phrased as a question.

**Author List.** Bylines should include all those who have made substantial contributions to the work. To facilitate indexing and retrieval and for unique identification of an author, use first names, initials, and surnames or first initials (e.g., Jody R. Smith), second names, and last names (e.g., J. Riley Smith). Do not use only initials with surnames (e.g., J. R. Smith). Deceased persons who meet the criteria for inclusion as coauthors should be included, with an Author Information note indicating the date of death. Do not include professional or official titles or academic degrees. At least one, or optionally more than

one but fewer than four authors must be designated with an asterisk as the author(s) to whom reader correspondence regarding the published manuscript may be addressed.

The full names and e-mail addresses of all co-authors must be provided on the Authors & Institutes page upon submission of the manuscript via the ACS Publishing Center. Use of ORCID identifiers is encouraged.

Addition or deletion of an author or authors after submission of the manuscript requires justification from the corresponding author and is subject to approval by the Editor.

**Institution Address.** The author affiliation(s) listed should be the institution(s) where the work was conducted. If the present address of an author differs from that at which the work was done, that address should be given in an Author Information note.

Many Funders and Institutions require that institutional affiliations are identified for all authors listed in the work being submitted. ACS facilitates this requirement by collecting institution information during manuscript submission under Step 2: Authors and Affiliations in the ACS Publishing Center.

**Abstract.** All Articles, Letters, and Perspectives) must be accompanied by an abstract, including an Abstract (TOC) graphic, which should state briefly the purpose of the research, the principal results, and major conclusions. Abstracts of manuscripts may not contain the words “superb”, “excellent”, “exceptional”, “outstanding”, or other similar descriptive words unless rigorously supported by a thorough comparison with the state-of-the-art in the manuscript. Like manuscript titles, the words “New”, “First”, or “Novel” are also generally disallowed in the abstract. The abstract should not generally exceed 200/300 (Letter/Article) words. Pasting the abstract in the text box on the Web submission page does not replace the need for including an abstract in the manuscript document.

**Keywords.** All Articles, Letters, and Perspectives must be accompanied by 5–8 keywords. These keywords will appear in the PDF version of the article and will also be used as a search term in the HTML version of the article.

**Text (Articles).** The first paragraphs of an Article should explain the motivation for and import of the work, where it fits in the development of the field and of chemistry, and perhaps why it should be of interest to chemists in other areas. It should be possible to do this without excessively increasing the length of the Article. Extensive reviews of the literature cannot be accepted. Thoughtful use of schemes and figures (with well-composed captions) is recommended, so that even casual browsers can discern the nature of the work. Well-known procedures should be designated by name, or literature references to them should be given. Experimental results are of lasting value and should be clearly and logically presented in a separate section. Standard Article format must be used for preparing a manuscript for submission as an Article, including section headings and a proper Introduction, a complete Experimental Section (unless placed in the Supporting Information), Results, and Discussion. The addition of a

Conclusion section at the end of the manuscript, which briefly summarizes the principal conclusions of the work, is recommended. If desired for clarification, section headings may be given Arabic numbers and subsections numbered in decimals (e.g., subsection 2.1 and subsection 2.2).

**Text (Letters).** Section headings (Introduction, Experimental Section, Conclusion, etc.) should not be used in a Letter.

**Safety.** Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. For each manuscript that reports experimental procedures, authors must include an affirmative statement about safety in the Experimental Section of the full article or the main text of a Letter. Further information may be included or re-introduced in the Supporting Information.

**Appendices.** Appendix sections must be placed in the Supporting Information.

**Dedications.** All dedications must appear in the Acknowledgment section and are subject to approval by the Editor.

**Abbreviations.** Acronyms and abbreviations that are not broadly familiar to readers in all disciplines of chemistry should be introduced in parentheses following the full term on its first appearance in the text. Do not include a separate Abbreviations list.

**Acknowledgment.** Dedications and notes acknowledging financial or professional assistance to the conduct of research or indicating presentation at a meeting should be brief and placed in the Acknowledgment section.

**Author Information Notes.** The e-mail address(es) of the corresponding author or authors must be provided as a Corresponding Author note. Present addresses for individual authors that differ from the address(es) at which the work was done should be given in a Present Address(es) note.

Statements about author contributions to the work or equal contributions of work should be included as a separate statement.

**References and Footnotes.** *All the references and footnotes must be placed together in a list at the end of the manuscript text.* In the Web edition, many of them will have links to other Web resources, such as the corresponding abstracts in *Chemical Abstracts* and the full text from other American Chemical Society journals. Because of this electronic linking, and to aid scientific research, *it is crucial that authors verify the accuracy of all references.*

Unnecessarily long lists of references should be avoided, and excessive self-citation is not permitted. However, authors must reference all previous publications in which portions of the present work have appeared. Each literature reference should be assigned one number and placed in the text as a superscript Arabic numeral. Footnotes to the text should be combined with references and numbered in ordinal sequence. Long footnotes should be avoided in Articles and are not permitted in Communications; additional data and peripheral discussion should be placed in the Supporting Information rather than in footnotes.

Bibliographic references to classified documents and reports or references to unpublished materials that are not generally available to the scientific public should not be used. Authors must obtain written permission from any person whose work is cited as a personal communication, unpublished work, or work in press. Copies of letters of permission and documentation should be appended to the cover letter file. If the manuscript is accepted but the necessary permissions have not been received, the Editor will ask the author to remove the reference(s) and dependent text.

List submitted articles as “in press” only if they have been formally accepted for publication. Otherwise, use “unpublished work” with the name of the place where the work was done and the date. For work published online (ASAP, in press), the DOI should be furnished in addition to the author name(s), article title, journal name, and year. DOI is an accepted form of citation before and after the article appears in an issue.

Example of a journal reference:

Yue, Q.; Liu, W.; Zhu, X. n-Type Molecular Photovoltaic Materials: Design Strategies and Device Applications. *J. Am. Chem. Soc.* **2020**, *142*, 11613–11628.

Example of an in-press journal reference:

Ham, J. S.; Park, B.; Son, M.; Roque, J. B.; Jurczyk, J.; Yeung, C. S.; Baik, M.-H. ; Sarpong, R. C–H/C–C Functionalization Approach to N-Fused Heterocycles from Saturated Azacycles. *J. Am. Chem. Soc.* **2020**, DOI: 10.1021/jacs.0c04278.

Example of a reference to a book with no editors:

Desiraju, G. R.; Vittal, J. J.; Ramanan, A. *Crystal Engineering: A Textbook*. World Scientific Publishing Co Pte Ltd: Singapore, 2011.

Example of a reference to a book with editors:

Byrn, S. R.; Stowell, J. G. Impurities in Drug Substances and Drug Products. In *Validation of Active Pharmaceutical Ingredients*; Berry, I.R., Harpaz, D., Eds.; CRC Press: Boca Raton, 2001; pp 271–292.



Authors should consult the [ACS Guide to Scholarly Communication](#) for the appropriate style to use in citations of journal articles, books, and other publications. In literature references, article titles must be included and journal abbreviations should be those used in the [Chemical Abstracts Service Source Index \(CASSI\)](#).

## 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 [Acceptable Software by File Designation](#) and confirm that your Supporting Information is [viewable](#).

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:  $^1\text{H}$  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 [ACS Research Data Policy](#) provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

## Data Requirements

### Compound Characterization, Experimental, and Computational Data

Authors are required to provide sufficient information (as described in more detail below) to establish the identity of a new compound, its purity, and its yield. Sufficient experimental details must also be included to allow another researcher to reproduce the synthesis. Safety: Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the full article or communication. Characterization data and experimental details must be included in either the manuscript or the Supporting Information. [Guidelines for reporting NMR data](#) are available online. Note that, when possible, unambiguous peak assignments should be given for all NMR spectra.

**Characterization of New Substances.** Adequate evidence to firmly establish both identity and purity should be provided. Recommended criteria vary according to substance categories. A summary of the detailed criteria may be found below.

### ***Guidelines for Characterization of Organometallic and Inorganic Compounds***

Authors are required to provide sufficient information (as described in more detail below) to establish the identity of a new compound, its purity, and its yield. Sufficient experimental details must also be included to allow another researcher to reproduce the synthesis. Characterization data and experimental details must be included in either the manuscript or the Supporting Information. It must be emphasized that the following is only a general guideline and authors are encouraged to present as much data as possible to support their structure assignments. In some cases, a reviewer or Editor may require authors to submit additional data to satisfy themselves of the validity of a proposed formulation.

#### *Characterization Data*

##### **(a) Routine Compounds**

Compounds in this category are those that have either literature precedents or are obtained by a logical synthesis in close to quantitative yield. Because of potential misidentification of atoms, an X-ray diffraction structure alone will not typically be considered to provide sufficient characterization for these molecules. Diamagnetic compounds must also be characterized by NMR spectroscopy, preferably for at least two different nuclei. In addition, at least one other characterization technique must be used to support the proposed formulation. Preferably, this would be a technique that provides definitive identification of a key functional group or chromophore. For example, IR spectroscopy may be used to support the presence of carbonyl, acyl, dinitrogen, carbonyl, and hydride moieties.

Paramagnetic compounds of this category present a further complication if NMR spectroscopy does not furnish clear evidence for the proposed formulation (note that NMR spectroscopy of paramagnetic complexes can be useful if sufficiently large sweep widths are used). In many cases, X-ray diffraction may provide the most unambiguous characterization of such complexes, but this will not suffice as the only means of characterization. In the absence of an X-ray structure determination, evidence for elemental constitution must be provided by elemental analysis (e.g., combustion analysis, microprobe analysis), or mass spectrometry. Magnetic moment and/or ESR spectroscopic data should also be given for paramagnetic compounds if it is considered that the spin state of the molecule is of special interest.

##### **(b) Novel or Unexpected Compounds**

Compounds in this category are those that either (i) exhibit an unprecedented type of structure, or (ii) are obtained by unexpected reaction. Such compounds require more detailed characterization to ensure their validity. In select instances, a variety of definitive spectroscopic techniques may provide sufficient characterization (for example, if many of the nuclei are NMR active), but in the majority of cases evidence for elemental constitution must be provided by either elemental analysis (e.g., combustion analysis, microprobe analysis), or mass spectrometry. While an X-ray diffraction structure is not considered definitive proof of elemental composition, it is acceptable evidence for composition providing that the results of other physical methods concerning the characterization are conclusive.

### **(c) Solid State Materials**

Compounds in this category are those that have no existence in solution. These materials must be characterized in such a way as to sufficiently describe their structure and composition. Atomic ratios and elemental compositions must be provided for solid state materials. X-ray diffraction data should be provided for crystalline materials.

### **(d) Compounds That Have Not Been Isolated**

Compounds that have not been isolated in pure form (e.g., reaction intermediates or intractable mixtures, or unstable species) may be published. However, in these circumstances, an explicit statement must be given indicating that the compounds have not been isolated. Only in exceptional circumstances will an article be published in which none of the new compounds reported has been isolated and fully characterized.

#### *Purity and Yield*

The yield and purity of all compounds must be reported, including the methods used to determine them. The yield of a compound obtained in an NMR tube reaction should be determined using an internal standard.

### ***Guidelines for Characterization of Organic Compounds***

#### *Sample Quality*

For new substances, evidence of the homogeneity the purified sample should be included. Elemental analysis is sufficient. If no analysis was performed, then other evidence ( $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, HPLC, gel electrophoresis, etc.) should be included as figures in the Supporting Information.

#### *Molecular Weight*

Evidence of molecular weight should be provided, especially if elemental analysis was not performed. Low resolution MS data under conditions that minimize fragmentation are acceptable. If there is a specific need to distinguish alternative formulas with the same molecular mass (within one amu), then HRMS data are necessary.

## *Miscellaneous*

Numerical listings of characteristic spectroscopic data should be included to support assigned structures, changes in functionality, unusual chromophores, properties, etc. Methods of purification used to prepare samples for characterization should be described. For crystalline samples, information about the method of crystallization should be included (solvents; mp; etc.). For non-racemic, chiral substances, data to allow correlation of absolute configuration should be given, preferably including  $[\alpha]_D$  values. If correlation data are provided based on HPLC or related methods, then retention times for both enantiomers must be provided, together with solvent and flow rate information, and identification of the chiral support.

## *Intermediates on Solid Phase; Combinatorial Chemistry*

Validation of methods and characterization of new substances in a statistically significant sampling should be provided. Resin-bound intermediates need not be characterized if acceptable end product quality (as defined in three section above) is demonstrated.

## ***Guidelines for Reporting Biological Data***

These guidelines are intended to facilitate the manuscript preparation process for prospective authors and to improve the transparency and reproducibility of published results in ACS journals. Please note that there are requirements specific to different journals and the purpose of this document is to provide guidance on important topics relevant to biological chemistry research. For more detailed information on each topic, please consult the provided links and references.

## *Data Presentation*

Data should be presented in a way that makes interpretation clear to the reader. Authors should use the appropriate data presentation method based on the characteristics of the data. Where possible, authors should plot all individual data points in addition to error bars and other statistical information. As an example, rather than showing a [bar graph](#), a [box-and-whisker](#) plot is more appropriate for large sample sizes ( $n > 100$ ). However, bar graphs where all individual data points are displayed are acceptable for small samples. Univariate scatterplots, boxplots, and histograms are best for continuous data. Figure captions should provide all statistical information, including the method used, error calculation, and exact P values. All data must be included in the reporting unless significance testing shows that a given data point can be reliably excluded.

For more information on data presentation, see:

1. [Quantifying the Interactions between Biomolecules: Guidelines for Assay Design and Data Analysis](#)
2. [Beyond Bar and Line Graphs: Time for a New Data Presentation Paradigm](#)
3. [Reporting standards and availability of data, materials, code and protocols.](#)

## *Statistics*

Appropriate statistical assessment is important for both experimental and computational studies. The following points should be considered:

- a. Statistical analyses must adhere to acceptable statistical and scientific standards
- b. Use of the term “significant” should be reserved for describing a relationship evaluated by appropriate statistical analysis. Please consider these resources:
  - [Moving to a World Beyond “ \$p < 0.05\$ ”](#)
  - [It’s time to talk about ditching statistical significance](#)
- c. A clear and comprehensive description of experimental data or computed data underlying the analysis is required.
- d. Appropriate statistical tests must be used for given data sets and attention should be given to data that are not normally distributed. In these cases, the appropriate non-parametric test should be used. Please see this resource for further information on this topic:
  - [Parametric and Nonparametric: Demystifying the Terms](#)
- e. Statistical methods used must be clearly identified, including whether they were one- or two-tailed. Non-standard statistical methods should be described in detail or precisely referenced.
- f. Underlying assumptions of statistical methods should be specified. For example, many statistical tests assume the presence of normal data distributions, which is often an approximation.
- g. Depending on the type of data, either confidence limits (CL), standard deviations (SD), or standard errors of the mean (SEM) must accompany a mean value provided in either graphical or tabular form. The experimental section for each assay performed should indicate the number of replicates and independent experiments as well as the statistical method used for data analysis. For example, assay curves must contain error bars derived from multiple measurements.
- h. For regression curves, uncertainty must be assessed by plotting original data along the curve or by establishing experimental or calculation confidence limits.
- i. If average values are reported from computational analysis, their variance must be documented. This can be accomplished by providing the number of times calculations have been repeated, mean values, and standard deviations (or standard errors). Alternatively, median values and percentile ranges can be provided. Data might also be summarized in scatter plots or box plots.
- j. Reporting averages of data assigned to pre-defined value ranges and ‘averages of average values’ must be avoided.
- k. For data that are not normally distributed, or for small sample sizes, appropriate statistical tests should be used.
- l. Standard measures (mean, median) and error bars must be stated for each dataset. If a sample size is small and/or not normally distributed, then mean or standard deviation calculations are not appropriate. In data tables, errors associated with the means presented need to be provided.
- m. Provide exact  $p$  values regardless of overall significance.

a. **Antibodies:** Authors are required to report the name of the antibody, the host species in which the antibody was produced and whether it is monoclonal or polyclonal. For commercial antibodies, report the company and catalog or code number and the antibody identifier obtained from [The Antibody Registry](#). For academic antibodies, report the source laboratory and relevant reference. Clearly state the application for each antibody used in the manuscript. Include batch numbers for experiments in which variability is found among different antibody batches. Clearly state the final antibody concentration or dilution. Whenever possible, report the antigen or antigen location.

b. **Cell Lines and Microorganisms:** To avoid inadvertent use of cross-contaminated or misidentified cell lines/microorganisms, authors are urged to validate each cell line/microorganism used. Authors must report the source of all cell lines/microorganisms in their manuscript, the date of authentication (must be within a year of manuscript submission date) and a description of the authentication method. Authors should be able to provide the authentication test results upon request. If no testing was done, provide the date when cells/microorganisms were purchased from authenticated source. For mammalian cell lines, authors must state whether the cell line has recently been tested for mycoplasma contamination. Resources for using cell lines as biological models:

- [Cell and Microbial Authentication](#)
- [Cell Lines as Biological Models: Practical Steps for More Reliable Research](#)
- [A resource for cell line authentication, annotation and quality control](#)

c. **Human subjects:** A statement confirming that the research has been approved by relevant ethical committees and performed under The Code of Ethics of the World Medical Association (Declaration of Helsinki) must be provided. Details listed in the latest version of the STROBE ([Strengthening the Reporting of Observational Studies in Epidemiology](#)) guidelines and description of informed consent protocols must also be provided. Authors reporting clinical trials should follow the [CONSORT Statement](#) for recommendations regarding the reporting of clinical trial results.

d. **Animal subjects:** Research involving animals must be performed in accordance with institutional guidelines as defined by the [Institutional Animal Care and Use Committee](#) for U.S. institutions or an equivalent regulatory committee in other countries. A statement confirming that all animal experiments performed for the manuscript were conducted in compliance with these guidelines is required. In the experimental section, the source, age, sex, species, and strain of animals should be included. For each treatment group, the number of animals used and sex should be clearly stated. Appropriate statistical methods should be used to test the significance of differences in results, and claims thereof. It is encouraged that all figure and table captions include the number of animals and sex for each treatment group, the method of statistical analysis as well as the corresponding p-values where significant differences are found.

- Further information on research involving animal and human subjects can be found in the following resources:
  - [Ethics and biosecurity](#)
  - [ACS Ethical Guidelines](#)
- For key reagents and tools, we recommend the use of Research Resource Identifiers:
  - <https://www.force11.org/group/resource-identification-initiative>
  - <https://scicrunch.org/resources>

e. **Biological Assays:** Assay interference can cause misleading results. Thus, appropriate controls experiments should be performed to exclude common artefacts caused by reactive molecules (covalent and redox activity), colloidal aggregation, decomposition, and interference with the spectroscopic

method. Authors should consult the recent ACS [Editorial](#) on assay interference compounds. The routes of administration of test compounds and vehicles should also be indicated. Benchmarks should be included in the form of appropriate positive or negative control substances or reference materials. Especially for studies on nanomaterials, additional steps and controls are needed such as sterilization procedures, checking assays for optical or chemical interferences, reporting different measuring units related to dose (e.g., surface area, mass, particle number per surface area, volume, cell number), and others as described in:

1. [Minimum information reporting in bio-nano experimental literature](#)
2. [ARRIVE \(Animal Research: Reporting of In Vivo Experiments\) guidelines](#)

f. **Kinetic and Equilibrium Data.** For publication in *JACS Au*, steady-state, pre-steady-state, or approach-to-equilibrium kinetic data and equilibrium binding data for proteins, nucleic acids, and other species must include a description of the identity of the catalyst or binding molecule, its origin, purity of composition, and any modifications such as mutations, post-translational modifications, or other modifications made to facilitate expression and purification. The assay method and the exact experimental assay conditions should be provided as a reference to previous work, with or without modifications, or fully described if a new assay. Regardless of whether previously reported, the temperature, pH, and pressure (if other than atmospheric) must be included. Terms such as “not detectable” (ND) should be avoided. Instead, an estimate of the limit of detection based on the sensitivity and error analysis of the assay should be provided. First-order and second-order rate constants (including steady-state values of  $k_{\text{cat}}$  and  $k_{\text{cat}}/K_{\text{M}}$  for enzymes and nucleic acids) should be reported in units of  $\text{s}^{-1}$  and  $\text{M}^{-1}\text{s}^{-1}$ , respectively. Equilibrium constants describing a binding interaction should be reported as equilibrium dissociation constants with units of concentration (e.g., M, mM, #M, etc.). Steady-state enzyme activity (specific activity) should be optimally reported as  $k_{\text{cat}}$  or, if there is uncertainty in the molar concentration of the catalyst, as a  $V_{\text{max}}$  (e.g., nmol, #mol) of product formed per amount of protein per unit time. All reported parameters should be given with a calculated estimate of error and a description of the software used in the data analysis. Authors are referred to the STRENDA (Standards for Reporting Enzymology Data) Commission of the Beilstein Institut (<http://www.beilstein-institut.de/en/projects/strenda/guidelines>) for an example of detailed guidelines.

### *Sequence Data*

Authors should submit sequence data to a public repository prior to submission and include accession numbers in their manuscript where appropriate.

1. High-throughput sequencing data: [GEO](#)
2. DNA and RNA sequences: [GenBank](#) or [Protein DataBank](#)
3. Nucleic acid sequencing data: [NCBI Trace Archive](#) or [NCBI Sequence Read Archive \(SRA\)](#)

### *Reporting and Stewardship of NMR Data*

The [NMR Guidelines](#) recommend a standard baseline for the submission of NMR data to ACS journals. They are intended to promote accuracy and consistency. The guidelines are divided into three sections: NMR text, which outlines the preferred format for NMR data included in the Experimental Section; NMR spectra, which outlines the preferred format for inclusion of hard copies of spectra in the Supporting Information; and primary NMR data files, which outlines the procedure for submitting FID files, acquisition data, and processing parameters to include in the Supporting Information. Authors are strongly encouraged to provide all three sets of data for all new and/or key compounds described in a manuscript submission.

In the Experimental Section, the compound must be clearly identified, for example in a header at the beginning of the synthetic procedure or the summary of spectroscopic data. List the nucleus being measured, any nucleus being broad-band decoupled, the solvent used (formula preferred, e.g., C<sub>6</sub>D<sub>6</sub> over benzene-*d*<sub>6</sub>), the standard used, and the field strength. Field strength should be noted for each spectrum, not as a comment in the general Experimental Section. The standard(s) may be specified in the general Experimental Section; as an example, <sup>1</sup>H NMR data recorded in C<sub>6</sub>D<sub>6</sub> listed as “residual internal C<sub>6</sub>D<sub>5</sub>H (# 7.15)”. Indicate solvent or peak suppression protocols used in collecting data. List the probe temperature when it is accurately known; ambient probe temperature is otherwise understood. Give <sup>1</sup>H NMR chemical shifts to two digits after the decimal point. Include the number of protons represented by the signal, peak multiplicity, and coupling constants as needed (*J* italicized, reported with up to one digit after the decimal). The number of bonds through which the coupling is operative, <sup>x</sup>*J*, may be specified by the author if known with a high degree of certainty. Accepted abbreviations for multiplicities and descriptors are s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet (denotes complex pattern), dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, and br = broad signal.

Chemical shifts should be listed consistently in a single article, starting either from downfield to upfield or vice-versa. Assign peak identities under the following circumstances: non-decoupled or equivalent spectra have been collected (<sup>13</sup>C, <sup>31</sup>P, etc.); 2-D experiments have been performed; or unambiguous assignment is possible without additional experiments, such as in the case of an organometallic metal-hydride <sup>1</sup>H signal, PF<sub>6</sub> vs MPPh<sub>3</sub> <sup>31</sup>P signal, etc. Give <sup>13</sup>C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks. Include peak multiplicities for <sup>1</sup>H-coupled <sup>13</sup>C NMR spectra or for signals in <sup>1</sup>H-decoupled spectra that are coupled to other magnetically active nuclei. A <sup>13</sup>C NMR signal will be considered a singlet if the multiplicity is not assigned. Only rarely is a true multiplet observed in a <sup>13</sup>C{<sup>1</sup>H} NMR spectrum. However, a certain region may contain a group of unresolved peaks or signals. Mention of unobserved resonances is encouraged.

Submission of spectra (.doc, .docx, .txt, .pdf, .tif) is strongly recommended for all new and/or key compounds, following these guidelines:

- A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g. C<sub>6</sub>D<sub>6</sub> over benzene-*d*<sub>6</sub>) and the field strength.
- A representation of the compound should be included on the spectrum—please use ChemDraw or a related program. The compound identifier used in the manuscript should be included.
- The largest peak in the <sup>1</sup>H NMR spectrum should normally arise from the compound, not the solvent.
- All peaks in the <sup>1</sup>H NMR spectrum should be integrated. Chemical shift values should be included.
- The solvent peak should be clearly labeled on the spectrum.
- All peaks should be visible on the spectrum. Insets are encouraged to show expanded regions. At minimum, the spectral window should be #1 ppm to 9 ppm for <sup>1</sup>H NMR and #10 ppm to 180 ppm for <sup>13</sup>C NMR.
- Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is encouraged for all new and/or key compounds. When submitting these files, please consider the following guidelines:



- One folder should be created for each compound. The folder should be named clearly, using the compound name (if available) and compound identifier, as referenced in the Experimental Section or Supporting Information. Include the FID files, acquisition data, and processing parameters for each experiment.
- Name each spectrum according to the type of nucleus measured.  $^1\text{H}$ ,  $^{13}\text{C}$ , DEPT, COSY, etc. NMR files should be compressed into zip files—please use multiple zip files if necessary. Files must be submitted in their native format. In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e., 300 MHz  $^1\text{H}$  or 50 MHz  $^{13}\text{C}$ ). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

### *Nuclear Magnetic Resonance Pulse Sequences*

For manuscripts that present new NMR pulse sequences, authors are requested to supply as “Supporting Information for Publication” a file that includes the original working pulse sequence information required to record data. This will typically include the pulse sequence code, parameter set, and other associated files, such as tables of gradient or pulse shapes.

### *Structural and Chemical Shift Data for Proteins and Nucleic Acids*

Any set of atomic coordinates referred to in the manuscript, including atomic coordinates and structure factors for proteins determined by X-ray crystallography and coordinates determined by NMR, should be deposited with the Protein Data Bank, Research Collaboratory for Structural Bioinformatics at Rutgers University whenever appropriate. (Theoretical model depositions are no longer accepted for inclusion in the PDB archive.) If the coordinate files are not deposited in the PDB, or if the PDB files are on hold until publication, then the coordinate files must be included in the Supporting Information submitted concurrently with the manuscript. Requirements are similar for structures of nucleic acids, which should be deposited with the Nucleic Acid Database. A manuscript that does not provide coordinates at the time of submission will not be sent out for review. It is the responsibility of the author to obtain a file name (PDB ID or NDB ID) for the molecule; the file name must appear in the published manuscript. If a file name has not yet been obtained upon acceptance of a manuscript, it must be added in proof. Atomic coordinates and structure factors for all structures mentioned must be available immediately upon publication of the article, either directly in the Supporting Information or as a data bank deposition. Similar requirements also apply to any chemical shifts referred to in the manuscript, whether they are only for assignment of resonances or used for any form of structure calculation. Those chemical shifts must be available to the reviewer at time of submission, either as an available entry in the Biological Magnetic Resonance Data Bank or included directly as Supporting Information.

### **Biomolecule Structures:**

1. Protein Structures: The atomic coordinates and related experimental data associated with a structure reported in ACS journals must be deposited at a member site of the [Worldwide Protein Data Bank](#): [RCSB PDB](#), [PDBe](#), [PDBj](#), or [BMRB](#). The PDB ID should be included in the manuscript. Authors must upload map density files, PDB files and PDB validation reports as Supporting Information for Review only. Authors must agree to release the atomic coordinates and experimental data when the associated article is published. A manuscript will be accepted only after receipt from the submitting author of a written statement that the coordinates have been deposited. Coordinates must be released immediately upon publication.

2. **X-Ray Crystallographic Structures of Small Molecules:** Crystallographic data on nucleosides, nucleotides, and other small molecules should be submitted upon publication to the [Cambridge Structural Database](#). Crystal structures of nucleic acids should be deposited with the Nucleic Acid Database (NDB) at [Nucleic Acid Database \(NDB\)](#) or with the RCSB PDB at [RCSB Protein Data Bank - RCSB PDB](#).
3. **NMR Studies of Biopolymers:** Deposition of relevant NMR assignments and related experimental data at the [BioMagResBank](#) is required. The author is responsible for obtaining a BMRB entry accession number, which should appear in a data deposition paragraph. The data must be released upon publication.
  - **Biological Macromolecules from Electron Microscopy Experiments:** Density maps should be deposited at either the [Protein Data Bank in Europe](#) (UK) or RCSB (USA) [EMDB deposition site](#). Once the map has been deposited, any fitted atomic coordinates should be deposited with the Protein Data Bank (PDB) by following the link provided from the EMDB deposition session. The EMDB and PDB IDs should be included in the manuscript. Both the map and the coordinate data will be made public when the associated article is published.
  - **Structures from Sequence Homology:** Manuscripts dealing with the development of structures from sequence homology are generally not considered unless significant experimental tests of the model also are presented.

### *Single Crystal Diffraction Data*

Manuscripts reporting the determination of one or more structures by X-ray diffraction must adhere to the following requirements:

*Abstract.* The abstract may summarize geometric features of unusual interest but should not contain unit cell parameters.

*Main Body of Manuscript.* Tables of essential interatomic distances and angles are *not required* but may be submitted (metric information for standard structural components should not be included).

For structures with anisotropically refined atoms, a figure displaying the thermal ellipsoids should ordinarily be presented; a spherical-atom representation may be substituted if necessary for clarity. If a spherical atom view is chosen for the manuscript, a thermal ellipsoid figure should be included in the Supporting Information. In cases where intermolecular interactions are relevant to the discussion, a view of the unit cell may be included.

An article should list for each structure the formula, formula weight, crystal system, space group, color of crystal, unit cell parameters, temperature of data collection, and values of  $Z$ ,  $R$ , and GOF; a brief description of data collection and solution and refinement of the structure should be placed in the Experimental Section. Tables of atom coordinates and thermal parameters will not be printed.

*Supporting Information.* Complete detailed data for each structure must be submitted in the electronic Crystallographic Information File (CIF) format. Deposition of CIF files in the Cambridge Crystallographic Data Centre (CCDC) does not eliminate the *JACS Au* requirement to submit the CIF file (s) as Supporting Information.

Authors are requested to combine multiple CIFs for a given manuscript into a single file. The individual structures in the combined file are to be separated from each other by the sequence #===END at the beginning of a new line. *JACS Au* requires authors to run the CheckCIF program for each crystallographic structure and to correct any syntax errors in the CIF file prior to submission. Authors should consult the CIF Submission Instructions listed below during manuscript preparation.

Structure factors (except for proteins and nucleic acids) should not be submitted as Supporting Information. However, one printed table of structure factors should be retained in case it is requested by the Editor for review purposes only.

## CIF Submission Instructions

Authors are encouraged to submit X-ray crystallographic data to be published as Supporting Information. The information required for each structure should be submitted in the electronic CIF format. Such files should be submitted electronically as described below.

CIFs must be uploaded at the same time the manuscript is submitted via the Web, with the file designation Supporting Information for Publication. The CIF for each structure should be uploaded as a separate Supporting Information file. CIFs should be saved in the text-only (plain ASCII) format, with a .cif extension before being submitted. No information other than the CIF itself should be included inside the file. CIFs may NOT be furnished as Microsoft Word, Corel WordPerfect, or PDF files.

Before submission, CIFs must be checked using the CheckCIF utility on the Web at <http://checkcif.iucr.org/>. A copy of the output should be retained in case it is requested by an Editor. Authors with appropriate software may alternatively use IUCRVAL or the CHECK validation tool in PLATON.

If CIFs are not available, the required data should be furnished in neatly formatted tables with informative titles that identify the name or the structure number of the compound.

**Powder Diffraction Data.** The presentation of X-ray powder diffraction data for new materials or for materials previously uncharacterized by this technique is encouraged. Data from X-ray powder measurements should be accompanied by details of the experimental technique: source of X-rays, the radiation, its wavelength, filters or monochromators, camera diameter, the type of X-ray recording, and the technique for measuring intensities. In cases of unindexed listing of the data, the  $d$  spacings of all observed lines should be listed in sequence, together with their relative intensities. In cases where filtered radiation is used, every effort should be made to identify residual  $\#$  lines. Where resolution into  $\#_1$ - $\#_2$  doublets occurs, the identification of the  $d$  spacing for each line as  $d\#_1$ ,  $d\#_2$  gives a measure of the quality of the diffraction pattern. When an indexing of the data is offered, the observed and calculated  $1/d^2$  values should be listed along with the observed relative intensities (it is superfluous to give  $d$  spacings in this instance). All calculated  $1/d^2$  values should be listed (exclusive of systematic absences), to the limit of the data quoted. If possible, the crystal system should be specified. Possible space groups may also be listed if the data warrant it. Relevant information about the specimen used should be included.

## *Magnetic Measurements*

Fits of magnetic data [ $\chi(T)$ ,  $\chi^{-1}(T)$ ,  $\chi T(T)$ ,  $\chi(T)$ ,  $M(H)$ , etc.] to an analytical expression must include both the Hamiltonian from which the analytical expression is derived and the final analytical expression and fitting parameters. When the value of an exchange coupling constant,  $J$ , is given in the abstract, the form of the Hamiltonian must also be included. The expressions may be included in the manuscript or, if long and complex, as Supporting Information; if the latter method is used, it should be noted in the Supporting Information paragraph at the end of the manuscript. In addition, how the sample was measured (in a gelatin capsule, Teflon capsule, etc.) and the diamagnetic correction for the sample holder, as well as the diamagnetic correction for the material, must be provided and the manner in which it was calculated (Pascal's constants) or measured must be stated.

## *Computations*

When computational results are part of a manuscript, sufficient detail must be given, either within the manuscript or in the Supporting Information, to enable readers to reproduce the calculations. This includes data such as force field parameters and equations defining the model (or references to where such material is available in the open literature). If the software used for calculations is generally available, it must be properly cited in the References and Footnotes. References to the methods upon which the software is based must also be provided. Results obtained from methods or parameters that are not adequately described in the manuscript or in the literature are not acceptable for publication. Authors who report the results of electronic structure calculations are requested to provide as Supporting Information the geometries (either as Cartesian coordinates or  $Z$  matrices) of all the stationary points whose relative energies are given in the manuscript. The absolute energies in hartrees that are computed at these geometries should not be given in the manuscript but should be included in the Supporting Information. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states.

# Contributor Roles Taxonomy (CRediT)

[CRediT](#) is a high-level taxonomy used to identify and acknowledge the roles played by contributors to scientific scholarly output. During original submission and/or revision, there are 14 standard roles from which the submitting author can select to describe the specific contributions of each author. At this time, CRediT is optional for authors. Please note that author CRediT information will not transfer if the manuscript is transferred to a non-pilot journal. [Click here to learn more about the ACS CRediT pilot.](#)

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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 [credit line](#) citing the original source. Authors are responsible for [obtaining written permission](#) to re-use this material.

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## Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through [ACS Publishing Center](#), 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

Submission of a manuscript to *JACS Au* is contingent upon the agreement by all the authors that the reported work has not received prior publication and that no portion of this or any other closely related work is under consideration for publication.

*JACS Au* authors may deposit an initial draft of their manuscript in a preprint service such as [ChemRxiv](#), [bioRxiv](#), [arXiv](#), or the applicable repository for their discipline before the manuscript is accepted for publication in *JACS Au*. Authors may revise the preprint version of their manuscript up until a final acceptance decision has been issued. Please note any use of a preprint server in the cover letter and include a link to the preprint, 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 *JACS Au*, authors should add a link from the preprint to the published article via the Digital Object Identifier (DOI). Some preprint servers, including ChemRxiv and bioRxiv, add this link for authors automatically after publication. For further details, contact the Editorial Office. For the ACS Publications policy on theses and dissertations, click [here](#).

## Editorial Policies

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Pricing details [can be found here](#). For assistance with open access, please contact [support@services.acs.org](mailto:support@services.acs.org).

**Audience.** Manuscripts submitted to *JACS Au* should be written in a style that addresses a wider audience than for manuscripts prepared for more specialized journals. Authors should present their materials with the utmost conciseness and clarity. Articles that exceed the norm of ~10 journal pages, and Letters that exceed 2,200 words, often contain a level of detail that is not appropriate for a broad audience.

**Initial Editorial Review.** *JACS Au* is devoted to the publication of original, fundamental research of unusual urgency and significance in all fields of chemistry, such that the Editor(s) and referees assess the work to represent an advance commensurate with top 10% of articles published in chemistry annually. When a manuscript is submitted to *JACS Au*, Editors must make an initial editorial judgment regarding its suitability for the journal's multidisciplinary readership. Editorial triage is a necessary step in our review process to expedite the peer review of those manuscripts that most clearly communicate significant innovations in chemistry and allied fields. Our current process entails an initial scrutiny by at least two *JACS Au* Editors before a manuscript is declined or recommended for Manuscript Transfer.

**Presubmission Inquiries.** If an author is unsure of the fit of their manuscript in *JACS Au*, the editorial board is willing to examine manuscripts prior to formal submission via inquiry to the editorial office via email ([eic@jacsau.acs.org](mailto:eic@jacsau.acs.org)).

**Back-to-Back Publication.** Manuscripts intended for back-to-back publication will be considered. These manuscripts will be judged independently on their individual merit to ensure that they meet the qualifications outlined herein and that back-to-back presentation actually enhances the pedagogy and impact of the work. As such, manuscript submitted for back-to-back publication undergo a higher degree of scrutiny than conventional submissions.

**Incomplete Manuscripts.** Manuscripts that are incomplete at the time of submission must be revised to include the missing items or corrected files before peer review. The official date of receipt of the manuscript will be recorded as the date that the revised manuscript is received in the Editor's office in the complete and proper format.

**Related Work by Authors.** All related work under consideration for publication in any medium must be cited in the manuscript, and the Editor must be informed at the time of submission. When related work by any of the authors is not available to the editors or referees because it is in press (accepted), submitted, or in preparation for submission to *JACS Au* or another journal, a copy of each related article should be uploaded as “Supporting Information for Review Only” at the time of submission. If a cited reference has already appeared on the Web, indicate that it is published electronically (“ASAP” for ACS journals) and give the DOI number for convenient access. The full journal citation should be completed during manuscript revision or page proof correction, if possible.

**Peer Review.** Submitted manuscripts should not be published or under consideration elsewhere and may be examined using software to detect duplication of previously published material. Reviewers will evaluate the manuscript on the basis of originality, technical quality, clarity of presentation, and importance to the field. Reviewer identities are confidential, and the names of reviewers will not be revealed to an author.

Reviewers may be asked to review subsequent versions of the manuscript, especially if new data have been added to the paper, to evaluate whether the authors have addressed the scientific concerns appropriately. In such cases, anonymized copies of all reviewers’ comments are normally sent to the reviewers. The Editors will expedite any additional rounds of review to ensure timely publication.

The Editors strongly disapprove of any attempts by authors to determine the identity of reviewers or to confront potential reviewers. The editorial policy of this journal is neither to confirm nor to deny any speculation about the identities of our reviewers. Authors whose manuscripts are published in *JACS Au* are expected to review manuscripts submitted by other researchers from time to time. More information about peer review at ACS Publications can be found here: ([https://researcher-resources.acs.org/publish/peer\\_reviews](https://researcher-resources.acs.org/publish/peer_reviews)).

**Reject after Editorial Review.** The Editors may identify submissions that in their expert opinions would not fare well during the review process; these manuscripts may be rejected without additional external review. Multiple editors will typically be consulted during this initial screening. This process shortens the time to decision and ensures a manageable workload and prevents overburdening our reviewers. Examples of situations where manuscripts may not be externally peer reviewed include but are not limited to the following: the paper is a routine extension or minor technical improvement of research already published; the science lies outside the scope of *JACS Au*; the science does not meet *JACS Au*’s standards; insufficient data are provided to properly substantiate the claims and conclusions made; closely related work has already been published and few, if any, new insights are provided; the work is not of general appeal to the readership of *JACS Au*; the manuscript is a resubmission of a paper that has been previously declined without the addition of adequate new science and/or without notification in the cover letter of previous submission.

**Editorial Decision.** The Editors will evaluate the reviewers’ comments in the context of the scope and aims of the journal and make the final decision on each manuscript. The possible decisions include: accept; revise to address the concerns of the reviewers before the editors make a final decision; decline but consider a resubmission if significant additional work is completed; or decline on the grounds of major technical or interpretational flaws, insufficient advance, or lack of novelty and broad interest.

In cases when reviewers make different or conflicting recommendations, the Editors may request additional information from the reviewers, consult other experts, and/or ask the authors to clarify the sections in question. Some manuscripts that are declined may be considered upon resubmission if significant additional work is completed, but authors are required to let the Editor know that the work is being resubmitted for reconsideration.

**Revised Manuscripts.** When a revision is requested after peer review, the authors must return the revised manuscript promptly. Requests for extensions should be sent to the Assigned Editor for consideration. After the allotted time, a revised manuscript will be handled as a new submission and will be given a new receipt date.

**Resubmission to *JACS Au*.** The resubmission of manuscripts previously considered and declined for publication in *JACS Au* is strongly discouraged and will only be considered under extraordinary circumstances unless revision and resubmission is explicitly invited in the decision letter.

Well-reasoned appeals of decisions may be considered, but must first be directed to the Associate Editor who handled the original submission and not to the Editor-in-Chief. Such appeals should cc the Editorial office ([eic@jacsau.acs.org](mailto:eic@jacsau.acs.org)).

If a manuscript has been declined by *JACS Au* and the author wishes to submit a revised version, the author is required to first gain consent from the Associate Editor who handled the initial submission. If the Associate Editor's consent to resubmit is received (which does not guarantee ultimate acceptance), the cover letter must explicitly state that permission was obtained from the Associate Editor and must describe the changes that have been made in the manuscript and include justification for reconsideration. The manuscript will be assigned to the same Associate Editor who handled the initial submission.

**Self-Citations.** The use of excessive self-citations, as assessed by the referees and editor(s), is not permitted.

**Nomenclature.** Registered trademark names should be capitalized whenever used. Trade and trivial names should not be capitalized. It is not necessary to use the trademark, registered trademark, or service mark symbol to ensure legal protection for the trademark.

## **Providing Potential Reviewer Names**

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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.

Avoid relying on color alone to represent information. Use indicators such as symbols, text labels, or patterns to ensure the data is accessible to those with color vision deficiency or other visual conditions. If color is necessary to understand data, such as in heat maps or fluorescence images, choose accurate and

accessible color combinations. For additional guidance and suggested color schemes, see [How to Make Scientific Figures Accessible to Readers with Color-Blindness](#) and [Coloring Chemistry—How Mindful Color Choices Improve Chemical Communication](#).

Ensure the content within graphics has sufficient contrast against adjacent colors, including the background. Contrast ratios measure the difference in brightness between two adjacent colors, helping make text and images readable. The Web Content Accessibility Guidelines (WCAG) define [minimum contrast requirements](#) of 4.5:1 for text and 3:1 for nontext elements, with [some exceptions](#) for elements like large text.

Two tools to measure contrast are TPGi's [Colour Contrast Analyzer](#) and Web Accessibility in Mind's [Contrast Checker](#). To improve low contrast, increase the saturation of one of the colors, or use borders or other visual separators between adjacent colors. For additional information and examples, see [Color to convey meaning](#) and [Choosing color in data visualizations](#) in the ACS Inclusivity Style Guide.

## **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 [Graphical Abstract service](#).

### **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, so avoid merging or splitting cells.

### **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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