ACS Publications
Most Trusted. Most Cited. Most Read.

ACS BIO & MED CHEM Au
AN OPEN ACCESS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Last updated: March 26, 2024 View the latest guidelines online

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.
- **Cover Letter**: must include a paragraph explaining why your manuscript is appropriate for *ACS Bio & Med Chem 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 *ACS Bio & Med Chem 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- **Disclosure of prior publication & *ACS Bio & Med Chem Au* preprint policy**: Submitted work must not be published elsewhere or concurrently submitted to another journal.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 *ACS Bio & Med Chem 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, Review, 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 *ACS Bio & Med Chem 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.

Scope of the Journal

ACS Bio & Med Chem Au is a broad scope, open access journal, which publishes short letters, comprehensive articles, reviews, and perspectives in all aspects of biological and medicinal chemistry. Studies providing fundamental insights or describing novel syntheses, as well as clinical or other applications-based work, are welcomed.

This broad scope includes experimental and theoretical studies on the chemical, physical, mechanistic, and/or structural basis of biological or cell function in all domains of life. It encompasses the fields of chemical biology, synthetic biology, disease biology, cell biology, agriculture and food, natural products research, nucleic acid biology, neuroscience, structural biology, and biophysics.

The journal publishes studies that pertain to a broad range of medicinal chemistry, including compound design and optimization, biological evaluation, molecular mechanistic understanding of drug delivery and drug delivery systems, imaging agents, and pharmacology and translational science of both small and large bioactive molecules. Novel computational, cheminformatics, and structural studies for the identification (or structure-activity relationship analysis) of bioactive molecules, ligands, and their targets, are also welcome. The journal will consider computational studies applying established computational methods, but only in combination with novel and original experimental data (e.g., in cases where new compounds have been designed and tested).

Also included in the scope of the journal are articles relating to infectious diseases research on pathogens, host-pathogen interactions, therapeutics, diagnostics, vaccines, drug-delivery systems, and other biomedical technology development pertaining to infectious diseases. 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 *ACS Bio & Med Chem 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: *ACS Bio & Med Chem 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.

Reviews are topical, forward looking, and of general interest to the readership. Length is flexible (6–20 or more pages). A good review critically evaluates existing work of multiple groups in a field or across disciplines, provides a logical organization, and makes the material more easily available to those not expert in the area through clear text and figures. Reviews should lay out the challenges and opportunities that lie ahead. Reviews should contain an abstract and appropriate references. The use of graphics to illustrate key concepts is strongly encouraged. Reviews include a graphical Table of Contents entry. Reviews also include ~8–10 keywords and a vocabulary section in which 5–7 terms extracted from the text are defined in one or two sentences.

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. An *ACS Bio & Med Chem 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. Perspectives may not exceed 10,000 words in abstract, main text, and graphical elements.

Authors interested in submitting a Review or Perspective are strongly encouraged to contact the Editor prior to manuscript preparation and submission, to seek conditional approval of the proposed topic. Authors interested in contributing a Review or Perspective should email the Editor, Squire Booker (booker-office@biomedchemau.acs.org), providing a single document that includes the following information for consideration:

1. Proposed Review or Perspective title
2. Corresponding author names, affiliations, and websites
3. A short (~400 word) description of the focused topic
4. A list of 5-10 lead references that will form the foundation of the manuscript
5. A list of recent review articles published on this topic, written by the submitting authors or others, and an explanation of how the proposed review will differ in focus and advance the literature on the subject.

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 *ACS Bio & Med Chem 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.

ACS Publishing Center

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 the ACS Publishing Center 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 ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, 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

ACS Bio & Med Chem Au does not require the use of any document templates. General information on the preparation of manuscripts may 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 ACS Paragon Plus. 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 *ACS Bio & Med Chem 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 *ACS Bio & Med Chem 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 in ACS Paragon Plus. 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 ACS Paragon Plus.

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}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.

ACS Bio & Med Chem Au applies ACS Research Data Policy **Level 1**, meaning the journal encourages all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are also encouraged to provide a Data Availability Statement describing the public availability of the data supporting the article’s conclusions. Publicly available data sets should be cited appropriately.

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

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.

Data Requirements

1. Accession Codes.

ACS Bio & Med Chem Au is committed to improving the functional annotation of protein databases

to improve their value to the biological chemistry community. To achieve this goal, we ask that **all proteins** referred to in a manuscript published in *ACS Bio & Med Chem Au* be linked to an accession ID from a public domain database (UniProt or NCBI) to facilitate the transfer of functional information reported in the manuscript to the database. Accession IDs may be listed as a separate section at the end of the manuscript; e.g.,

- SPBP: Q9UGU0
- TOPBP1: Q92547
- ETS1: P27577

Alternatively, the accession ID may also be indicated in parenthesis after the protein name when it is first mentioned in the manuscript, e.g., “Stromelysin-1 PDGF responsive element binding protein (SPBP, UniProtKB Q9UGU0)…”

Accession IDs should be as accurate as possible, e.g., an isoform identifier can be used if the full sequence of the molecule is known or can unambiguously be inferred, e.g., UniProtKB Q9UGU0-2. However, for example, if the protein is identified by a peptide which may be present in more than one isoform, only the entry-level, canonical identifier should be given (UniProtKB Q9UGU0).

Sequence-level features such as domains, variants or site-directed mutations should be mapped to the version of the sequence in the database.

2. Biological Data.

Quantitative biological data are required for all tested compounds. Biological test methods must be referenced or described in sufficient detail to permit the experiments to be repeated by others. Detailed descriptions of biological methods should be placed in the experimental section. Required information includes the source (if purchased or lab from which originally obtained, if applicable), description of cell line used (e.g., HEK293, COS-1, COS-7), etc., and experimental conditions necessary for those trained in the art to reproduce the experiments as detailed in the manuscript and under identical conditions. Standard compounds or established drugs should be tested in the same system for comparison. Data may be presented as numerical expressions or in graphical form; biological data for extensive series of compounds should be presented in tabular form. Significant figures should be appropriate for the data presented. Tables consisting primarily of negative data will not usually be accepted; however, for purposes of documentation they may be submitted as Supporting Information for Publication. Clearly state in the experimental section how many replicates and independent experiments were performed for the tested compounds to generate the biological data presented.

Active tested compounds obtained from combinatorial syntheses should be resynthesized, analytically characterized, and percent purity determined (with values provided) and retested in the biological assay to verify that the biology conforms to the initial observation. To increase the scientific rigor of the finding and the manuscript's contribution to the field, conformation in an orthogonal assay of the lead molecule(s) biological activity are highly encouraged. Judgment regarding if an orthogonal experiment is critical to the significance of the research presented are at the discretion of the Editors.

Statistical limits (statistical significance) for the biological data are usually required. If statistical limits cannot be provided, the number of determinations and some indication of the variability and reliability of the results should be given. References to statistical methods of calculation should be included. Concentrations should be expressed as molar quantities (e.g., mM, nM) and doses in

animals should be expressed in weight/weight or molar quantities (e.g., mg/kg, mmol/kg). The routes of administration of test compounds and vehicles used should be indicated, and any salt forms used (hydrochlorides, sulfates, etc.) should be noted. The physical state of the compound dosed (crystalline, amorphous; solution, suspension) and the formulation for dosing (micronized, jet-milled, nanoparticles) should be indicated. For those compounds found to be inactive, the highest concentration (in vitro) or dose level (in vivo) tested should be indicated. See section 8 below on *Statistical Criteria* for more detailed requirements.

Cytotoxicity mean graphs from the National Cancer Institute (NCI) should appear in Supporting Information for Publication and not in the main body of the manuscript. Numerical data derived from a limited number of cell lines may be tabulated in the text of the manuscript.

If human cell lines are used, authors are strongly encouraged to include the following information in their manuscript in accordance with NIH guidelines:

- the cell line source, including when and from where it was obtained;
- whether the cell line has recently been authenticated and by what method;
- whether the cell line has recently been tested for mycoplasma contamination.

3. Use of Human or Animal Subjects.

Manuscripts must comply with the ACS Ethical Guidelines to Publication of Chemical Research. Sufficient information must be provided so that results can be reproduced and tested by other laboratories. For research involving animals or humans, Editors reserve the right to request additional information from authors.

Animals: Research involving animals must be performed in accordance with institutional guidelines as defined by 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 in 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. The term "significant" should not be used unless the appropriate statistical analysis was performed and the probability value (p-value) used to identify significance (generally $p<0.05$) is consistent with the scientific rigor of the field. Authors are encouraged to include in all figure and table captions 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.

Humans: Research studies involving humans must have institutional review board approval. Authors are requested to identify the institutional or licensing committee that has approved the experiments.

4. Purity of Tested Compounds.

Methods: All scientifically established methods (e.g., HPLC, combustion analysis, absolute quantitative ^{1}H NMR [qHNMR; see Purity by Absolute qNMR instructions] following the established Journal protocol or equivalent qHNMR methods) of establishing purity are acceptable. Documentation is required for qHNMR. If the target compounds are solvated, the quantity of

solvent should be included in the compound formulas. When HPLC is the method for determination of compound purity, HPLC traces are required only for key target compounds. Documentation is required to be uploaded as Supporting Information for Publication.

Purity Percentage: All tested compounds, whether synthesized or purchased, should possess a purity of at least 95%. Tested compounds must have a purity of at least 95%. In exceptional cases, authors can request a waiver when compounds are less than 95% pure. For solids, the melting point or melting point range should be reported as an indicator of purity.

Elemental analysis: Found values for carbon, hydrogen, and nitrogen (if present) should be within 0.4% of the calculated values for the proposed formula.

Statements/Documentation: Include the specific analytical method used to determine purity in the general part of the experimental section together with a statement confirming 95% purity. If the purity of a particular compound is less than 95%, specify the percentage of purity at the end of the description of its synthesis in the experimental section. For qHNMR experiments, additional documentation is required. For purchased compounds, provide proof of purchase as Supporting Information for Publication.

Author Submission Checklist: Specify the method employed for establishing purity and percentage of purity in the checklist. Waivers for compounds of less than 95% purity should be requested on the checklist.

5. Confirmation of Structure.

Adequate evidence to establish structural identity must accompany all new compounds that appear in the experimental section of *Articles* and *Drug Annotations*. Sufficient spectral data should be presented in the experimental section to allow for the identification of the same compound by comparison. Generally, a listing of ^{1}H or ^{13}C NMR peaks is sufficient. However, when the NMR data are used as a basis of structural identification, the peaks must be assigned. Proton NMR shifts, reported to 0.01 ppm precision, should be accompanied by an abbreviation for any multiplet structure, the number of atoms represented by the peak or multiplet, and coupling constraints where applicable. *J* values are in hertz (Hz) and have one decimal place. Give 13C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks. See NMR Guidelines for ACS Journals.

List only infrared absorptions that are diagnostic for key functional groups. If a series contains very closely related compounds, it may be appropriate merely to list the spectral data for a single representative member when they share a common major structural component that has identical or very similar spectral features. HRMS data may be supplied as an additional criterion of compound identity. For the first member of a new class of oligomers containing up to 10 residues, ^{1}H NMR (300-500 MHz) and HRMS are a requirement.

Specific optical rotations should be reported for isolated natural products, enantiopure compounds, and enantioenriched isomer mixtures when sufficient sample is available. Specific rotations based on the equation [] = (100)/(*lc*) should be reported as unitless numbers as in the following example: $[]^{20}_{D}$ 25 (*c* 1.9, $CHCl_3$), where the concentration *c* is in g/l00 mL and the path length *l* is in decimeters. The units of the specific rotation, (deg*mL)/(g*dm), are implicit and are not included with the reported value.

6. Combinatorial Chemistry.

When combinatorial chemistry has been employed to generate molecules, which become prototypes for a subsequent focused SAR investigation, the lead compounds and any other compounds that are key to the analysis and interpretation of the SAR of the focused series must conform to the appropriate criteria for purity and structural identity required by this Journal. However, the combinatorial chemistry methodology, screening data, and *preliminary* SAR which led to the generation of the lead molecule(s) may be reported as Supporting Information for Publication without confirmation of structure or demonstration of purity. These data may be briefly summarized in the main manuscript when they clarify the SAR discussion of the focused series.

7. Computational Chemistry.

7.1 Manuscript Categories. When computational chemistry is a major component of a study, manuscripts must fall into one or more of the following categories:

(A) Practical applications of existing computational methods combined with original experimental data. Manuscripts that report prospective computational design, synthesis, and experimental evaluation of new chemical entities are highly encouraged.

Applications of existing computational methods are not considered without original experimental data that assess the computational predictions. QSAR modeling is acceptable only if a significant number of new compounds is predicted, prepared, and tested. Avoid overinterpretation of computational predictions and conclusions drawn from molecular models as if they represent experimental data.

(B) Substantially novel methods along with evidence for utility in medicinal chemistry with significant potential for advancing the field.

Clearly describe computational methods to be accessible to a general medicinal chemistry audience and clarify the relevance of the new method to medicinal chemistry. Present sufficient information to allow the method to be reproduced and tested in other laboratories.

(C) Statistical analysis or mining of publicly available databases or data sets that provide unprecedented insights into the advancement of medicinal chemistry problems.

Such investigations must be based upon large data sets. Small series of compounds whose properties are reinvestigated using computational methods do not qualify for this category.

7.2 Proprietary Data. Normally, the use of proprietary data for computational modeling or analysis is not acceptable because it is inconsistent with the ACS Ethical Guidelines. All experimental data and molecular structures used to generate and/or validate computational models must be reported in the paper, reported as supporting information, or readily available without infringements or restrictions. The Editors may choose to waive the data deposition requirement for proprietary data in rare cases where studies based on large corporate data sets provide compelling insight unobtainable otherwise.

7.3 Virtual Screening Studies. Prospective virtual screen studies must meet the following acceptance criteria.

1. In order to validate virtual screening hits obtained from any source, provide proof of dose-response behavior, confirmation of IC_{50} or K_i values, and controls for nonspecific or artificial inhibition (i.e., proof of reversibility, detergent controls). Submit structure confirmation (^1H NMR and MS; see section 4) for active compounds.
2. For target-directed virtual screens, evidence for direct binding/inhibition must be provided; the exclusive use of cell-based/functional/reporter gene assays is insufficient.
3. Include explicit support for the significance of experimental findings. Identifying weakly potent compounds for a given target is not considered a significant advance if many potent compounds acting by the same or a similar mechanism are already available.
4. Virtual screening hits must be filtered for Pan Assay Interference Compounds (PAINS; Baell and Holloway, *J. Med. Chem.* 2010, *53,* 2719-2740) and the results must be reported in the manuscript (exemplary online filter: http://zinc15.docking.org/patterns/home/).
5. For virtual screens that produce compound rankings, provide as Supporting Information for Publication the total number of compounds that were screened and the ranks of identified hits before application of any further manual or other subjective selection steps.
6. Complex virtual screening protocols are not validated by identifying a few active compounds. Evidence must be provided that much simpler approaches would not have yielded comparable results (e.g., 2D similarity or substructure searching).
7. Reported calculations must be limited to those that were essential for the identification of novel active compounds. In virtual screening studies, retrospective computational studies such as benchmarking or similar *in silico* validation attempts should not be reported. All computational studies that do not directly contribute to the identification of novel active compounds must be omitted.
8. For virtual screening studies, computational models of targets (e.g. homology models) and ligand/target complexes such as docked/modeled complexes of active compounds must be made freely available as PDB coordinate files as Supporting Information for Publication (see also 6.7).

7.4 Retrospective Use of Computational Methods. Manuscripts that contain experimental studies with a retrospective computational component will be considered only under the following conditions:

1. Computational work must lead to a clearly stated message, either an improved understanding of the experimental work or a well-defined experimentally testable hypothesis.
2. Clearly distinguish models and hypothetical statements from experimental observations both in the text and in figure captions.
3. Describe computational methods in sufficient detail for the reader to reproduce the results.
4. Draw conclusions from modeling with an appropriate amount of caution in light of assumptions made and within the accuracy limitations of the applied computational methods. The overall amount of space (text and figures) devoted to retrospective computational work must be proportionate to its significance.

7.5 Predicted Compound Binding Modes. The prediction of compound binding modes by docking is a frequent computational application submitted to the Journal in combination with experimental data. Provide PBD IDs of crystal structures used as starting points for molecular modeling in the legends of figures depicting the resulting molecular models. In the absence of supporting structural information demonstrate that putative binding modes are consistent with structure-activity relationships for a series of analogues.

QSAR, pseudo-receptor, or machine learning models that are occasionally applied retrospectively to analyze biological activities observed in the context of experimental SAR studies are acceptable only when used to illustrate a point of central relevance for a manuscript.

7.6 Benchmark Calculations. Benchmark investigations, such as comparisons of virtual screening algorithms, are considered only if they provide particularly clear and generally relevant conclusions that set new standards in the field. General relevance and new standards must be clearly stated.

7.7 PDB Coordinates for Computational Models. If three-dimensional computational models of targets, binding sites, or target-ligand complexes are reported, PDB coordinates of hydrogen-suppressed atomic models must be included as Supporting Information for Publication at submission to ensure reproducibility of calculations and reported findings.

8. QSAR/QSPR and Proprietary Data.

The following are general requirements for manuscripts reporting work done in this area:

1. Authors should explicitly state in the abstract, introduction, and/or results sections of the paper what is novel about the quantitative structure–activity relationships/quantitative structure–property relationships (QSAR/QSPR) study being reported.
2. If a new method/theory is reported, it should be compared to and “validated” against at least one other common method that is widely used in the field.
3. All data and molecular structures used to carry out a QSAR/QSPR study are to be reported in the paper and/or as Supporting Information for Publication. The use of proprietary data is generally not acceptable.
4. Standard QSAR/QSPR studies are considered only if the predictions are experimentally tested and if the experimental data are novel and significant. Only QSAR/QSPR analyses that provide new insights into the activity are considered.

Specifically discouraged are (i) QSAR and QSPR modeling for data sets that have already been extensively modeled, (ii) model development featuring high ratios of descriptors to data points, and (iii) reports of new descriptors without clear evidence for their superiority in QSAR/QSPR modeling to existing, commonly used alternatives.

9. Statistical Criteria.

Appropriate statistical assessment is equally important for experimental and computational studies in medicinal chemistry. Reported results generally require statistical validation such as the use of the probability value (p-value) used to identify significance (generally $p < 0.05$). Statistical analyses of compound data are also frequently presented, which must adhere to acceptable statistical and scientific standards. Specifically:

1. A clear and comprehensive description of experimental data or computed data underlying the analysis is required.
2. Statistical methods used must be clearly identified. Non-standard statistical methods should be described in sufficient detail or precisely referenced.
3. 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 in practice.
4. Depending on the type of experiments reported, 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 in vitro and in vivo assay performed should indicate the number of independent experiments as well as the statistical method used for data analysis. For example, assay curves must contain errors bars derived from multiple measurements.

5. For regression curves, their uncertainty must be assessed by plotting the original data along the curve or by establishing experimental or calculation confidence limits.
6. 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.
7. Reporting averages of data assigned to pre-defined value ranges and 'averages of average values' must be avoided.

10. Software.

Software used as a part of computer-aided drug design should be readily available from reliable sources, and the authors should specify where the software can be obtained.

11. Structural Data.

For papers describing structures of biological macromolecules, the atomic coordinates and the related experimental data (structure factor amplitudes/intensities and/or NMR restraints) must be deposited at a member site of the Worldwide Protein Data Bank (www.wwpdb.org): RCSB PDB (www.pdb.org), Protein Databank in Europe (PDBe) (http://www.ebi.ac.uk/pdbe/docs/References.html), PDBj (www.pdbj.org), or BMRB (www.bmrb.wisc.edu). The PDB ID must appear before the references (under Manuscript Text Components see section B.7) and in the figure legend. Authors must release the atomic coordinates and experimental data when the associated article is published. Questions related to deposits should be sent to info@wwpdb.org. Papers that utilize coordinates of molecules already in the database should specify the PDB ID as a reference.

For X-ray diffraction of structures of small molecules 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. Articles should list for each structure the formula, formula weight, crystal system, space group, unit cell parameters, temperature of data collection, and values of Z, R, and GOF in the experimental section. Tables of atom coordinates and thermal parameters will not be printed. CIF files must be deposited with Cambridge Crystallographic Data Centre (CCDC).

12. Compound Characterization Checklist.

When manuscripts report the synthesis of compounds, submission of a completed Compound Characterization Checklist (CCC) is recommended *but not required*. The CCC form can be completed on-screen and saved for uploading with the submission of the manuscript as Supporting Information for Review Only. The CCC will be provided to reviewers to help them assess the overall thoroughness of the characterization of synthesized compounds.

13. Electron Microscopy Data.

No formal requirement exists for deposition of molecular envelope reconstruction from electron microscopy data, but the journal encourages authors to deposit relevant information in appropriate databases. Approved databases for deposition of electron microscopy data are the Worldwide Protein Data Bank (www.wwpdb.org), the Protein Data Bank Japan (www.pdbj.org), or the Protein Databank in Europe (PDBe, www.ebi.ac.uk/pdbe).

14. Microarray Data.

Data must be submitted to the GEO (www.ncbi.nlm.nih.gov/geo) or ArrayExpress (www.ebi.ac.uk/arrayexpress) databases and the inclusion of relevant accession numbers in the published manuscript. Please reference the Microarray Gene Expression Data (MGED) open letter specifying microarray standards at www.mged.org/Workgroups/MIAME/miame_checklist.html.

15. Genetically Modified Organisms and Mutants.

Use established repositories such as the Jackson Laboratory, the Mutant Mouse Regional Resource Center, the American Type Culture Collection, the UK Stem Cell Bank, or another public storage area whenever possible. Large datasets for which an approved database has not yet been established must be housed as online Supporting Material at *ACS Bio & Med Chem Au*.

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.

Language and Editing Services

A well-written paper helps share your results most clearly. ACS Publications' English Editing Service 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 credit line citing the original source. Authors are responsible for obtaining written permission 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 Artwork Editing and Graphical Abstract 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 ACS Paragon Plus, 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 *ACS Bio & Med Chem 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.

ACS Bio & Med Chem 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 *ACS Bio & Med Chem 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 *ACS Bio & Med Chem 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

Open Access and Article Publishing Charges at *ACS Bio & Med Chem Au*:

ACS Bio & Med Chem Au is a fully open access journal, with all content published under an open access license. There is therefore no subscription charges and no charge to access, read, and download articles published in the journal. Authors of accepted manuscripts will need to pay an Article Publishing Charge (APC) to publish their research in *ACS Bio & Med Chem Au*. The default

license for authors will be CC BY-NC-ND, with the option to upgrade to CC BY. Discounts are available for ACS Members and further country discounts apply for authors based in countries with lower-income economies, detailed here. Authors from institutions with ACS Read + Publish Agreements are eligible to have their APC covered through these agreements. Information can be found here.

Pricing details can be found here. For assistance with open access, please contact support@services.acs.org.

Anonymity of Peer Review

All manuscripts are subject to critical, single-anonymized peer review. It is to be understood that the final decision relating to a manuscript's suitability rests solely with the Editor. The journal disapproves of attempts by authors to determine the identity of reviewers. This journal's policy is to neither confirm nor deny speculation about the identities of reviewers.

Providing Potential Reviewer Names

Authors are required to provide the names of at least four reviewers, working in at least three different countries, competent to referee their manuscripts. They may also suggest in their cover letter that certain individuals not be used as referees along with justification for the request. Such requests will generally be honored by the Editors, unless it is believed that the specific individual's opinion is vital in the consideration of the manuscript. Authors are encouraged to avoid suggesting reviewers from the authors' institutions. Do not suggest reviewers who may have a real or perceived conflict of 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. Manuscript Transfer 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 ACS Direct Correct. 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, all author concerns are resolved, and payment has been received. ASAP publication typically occurs within 1-2 working days of receipt of page proof corrections (provided payment has been resolved), which can be a few weeks in advance of the cover date of the issue.

Post-Publication Policies

The American Chemical Society follows guidance from the Committee on Publication Ethics (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.

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

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.S. Treasury Department's Office of Foreign Assets Control (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 Specially Designated National (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 Safety Statement Style Sheet 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 self-plagiarism. 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 Ethical Guidelines to Publication of Chemical Research. See also the press release 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 Journal Publishing Agreement, 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 Ethical Guidelines to Publication of Chemical Research. 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.

If any change in authorship is necessary after a manuscript has been submitted, confirmation is required that all of the authors (including those being added or removed) have been notified and have agreed to the change. To provide this confirmation, authors are asked to complete and sign an authorship change form and provide the completed form to the appropriate editorial office.

Authors with a single name: If you, or any of your coauthors, have only one name, please follow these steps for proper submission to ACS Paragon Plus:

1. First (Given) Name Field: Enter an asterisk (*) into the "First (Given) Name" field.
2. Last (Family) Name Field: Enter your single name into the "Last (Family) Name" field.

If your paper is accepted, the asterisk (*) will be removed from the published version of the paper.

Patent Activities and Intellectual Property

Authors are responsible for ensuring that all patent activities and intellectual property issues are satisfactorily resolved prior to first publication (ASAP or in issue). Acceptance and publication will not be delayed for pending or unresolved issues of this nature.

Open Researcher and Contributor ID (ORCID)

Authors submitting manuscript revisions are required to provide their own personal, validated ORCID iD before completing the submission, if an ORCID iD is not already associated with their ACS Paragon Plus user profiles. This ID may be provided during original manuscript submission or when submitting the manuscript revision. All authors are strongly encouraged to register for an ORCID iD, a unique researcher identifier. The ORCID iD will be displayed in the published article for any author on a manuscript who has a validated ORCID iD associated with ACS when the manuscript is accepted.

ORCID iDs should not be typed into the manuscript. ACS publishes only those ORCID iDs that have been properly verified and linked **before the manuscript is accepted**. After your ORCID iD is linked, it will be displayed automatically in all subsequently accepted manuscripts for any/all ACS journals. We do not publish ORCID iDs provided during proof review or via other communications after a manuscript is accepted for publication.

With an ORCID iD, you can create a profile of your research activities to distinguish yourself from other researchers with similar names, and make it easier for your colleagues to find your publications. If you do not yet have an ORCID iD, or you wish to associate your existing ORCID iD with your ACS Paragon Plus account, you may do so by clicking on “Edit Your Profile” from your

ACS Paragon Plus account homepage and following the ORCID-related links. Learn more at www.orcid.org.

Copyright and Permissions

To obtain forms and guidelines for completing the Journal Publishing Agreement or obtaining permissions from copyright owners, and to explore a Copyright Learning Module for chemists, click here.

Funder Reporting Requirement

Authors are required to report funding sources and grant/award numbers. Enter **ALL** sources of funding for **ALL** authors in **BOTH** the Funder Registry Tool in ACS Paragon Plus and in your manuscript to meet this requirement.

Open Access Compliance

Authors publishing in *ACS Bio & Med Chem Au* retain copyright of their published research and may publish via a choice of CC BY-NC-ND or CC BY license. ACS offers options by which authors can fulfill the requirements for open access and deposition into repositories for funded research. Visit our Open Science site to see how to fulfill requirements for specific funders and to find out if you are eligible to publish under a read and publish agreement between ACS and your institution. You can also find out more about Open Access Compliance and ACS Open Science initiatives.

Diversity and Inclusion Statement

During manuscript submission, ACS journal authors have the option to submit a statement sharing information related to diversity and inclusion that is relevant for their paper. If supplying a diversity and inclusion statement, the corresponding author must provide this on behalf of all authors of the manuscript during the submission process. These statements include but are not limited to analysis of citation diversity and acknowledgment of indigenous land on which research was conducted. Statements expressing political beliefs are not permitted and may be removed by the journal office. All statements are subject to final review by the Editor.

- **Citation Diversity Statement:**The citation diversity statement should appear in the Acknowledgements section of the manuscript. ACS recommends including the following: (1) the importance of citation diversity, (2) the proportion of citations by gender and race/ethnicity for the first and last authors, (3) the method used to determine those proportions and its limitations, and (4) steps taken to by the authors to improve citation diversity in the article. We recognize that one limitation of the current methods is that it cannot account for intersex, non-binary, and transgender people, or Indigenous and mixed-race authors. (Adapted from BMES/Springer Guidelines)
- **Land acknowledgment:**The land acknowledgment statement should appear in the Acknowledgements section of the manuscript. The statement should link to the institutions' formal land acknowledgments on which the research took place, if possible. Further guidance for creating these statements can be found here: https://nativegov.org/news/a-guide-to-indigenous-land-acknowledgment/.

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 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.

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.

Cover Art

ACS Bio & Med Chem Au authors are encouraged to submit images to be considered for use on the journal's front cover or Supplementary Covers at the time of the submission of their revised manuscript. If your article is accepted for publication, your suggestion may also be selected for use on one of the journal's covers. If your art is selected for front cover, ACS will send you information about how to request one complimentary 18" by 24" printed poster featuring your work. Images chosen for the front cover will be published at no cost to the author.

Cover image submissions should be colorful and visually engaging, with minimal text. The cover image should not resemble a graphical abstract or data figure, but rather should be an artistic and scientifically accurate representation of the manuscript.

Image files should be submitted as TIF, JPG, PNG or EPS files (not PDF or PPT) with a resolution of at least 300 dpi for pixel-based images. Cover art should be 8.19 inches (20.80 cm) wide × 10 inches (25.4 cm) high at 300 ppi, and submission of "layered" artwork is encouraged. The journal's logo will obscure the top 3 inches (7.62 cm) of the image. Authors should submit the cover image, along with a short (< 50-word), clear legend explaining the image, as supplementary files to ACS Paragon Plus with their revised manuscript.

If you wish to be considered only for the front cover, and not a paid supplementary cover, please respond NO accordingly to the Supplementary Cover Art question in ACS Paragon Plus. For more information on the Supplementary Covers program, please see this webpage. All art submitted for consideration for a supplementary cover will also be considered for a front cover.

Web Enhanced Objects (WEO)

The Web editions of ACS journals allow readers to view multimedia attachments such as animations and movies that complement understanding of the research being reported.

WEOs should be uploaded in ACS Paragon Plus with 'Web Enhanced Object' selected as the file designation. Consult the list of compatible WEO formats.