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ACS Medicinal Chemistry Letters

Last updated: May 05, 2022 View the latest guidelines online

Scope of the Journal

Major Change: The *Letters to the Editor* manuscript type has been discontinued.

ACS Medicinal Chemistry Letters is interested in receiving manuscripts that discuss various aspects of medicinal chemistry. The journal will publish studies that pertain to a broad range of subject matter, including compound design and optimization, biological evaluation, drug delivery, imaging agents, and pharmacology of both small and large bioactive molecules. Specific areas include but are not limited to:

- Identification, synthesis, and optimization of lead biologically active molecules and drugs (small molecules and biologics)
- Biological characterization of new molecular entities in the context of drug discovery
- Computational, cheminformatics, and structural studies for the identification or SAR analysis of bioactive molecules, ligands and their targets, etc.
- Novel and improved methodologies with broad application to medicinal chemistry
- Discovery technologies for biologically active molecules from both synthetic and natural (plant and other) sources
- Pharmacokinetic/pharmacodynamic studies that address mechanisms underlying drug disposition and response
- Pharmacogenetic and pharmacogenomic studies used to enhance drug design and the translation of medicinal chemistry into the clinic
- Mechanistic drug metabolism and regulation of metabolic enzyme gene expression
- Chemistry patents relevant to the medicinal chemistry field

For more information, please see the journal website.

Manuscript Types

ACS Medicinal Chemistry Letters is an online publication that publishes original research in the form of Letters, Notes, and Technology Notes. The journal also invites publications that highlight recent and/or highly innovative developments in medicinal chemistry in the form of Viewpoints and Innovations. The Editors strongly encourage dialogue within the medicinal chemistry community this form of communication can be made in the form of Letters to the Editor. Descriptions of the aforementioned submission types are as follows:

Letters. Peer-reviewed reports of original research focused on an individual finding significant to a broad medicinal chemistry field.

Notes. Brief peer-reviewed reports of original research intended for the rapid dissemination of highly notable findings where existing limitations may preclude further development at the time of publication.

Technology Notes. Peer-reviewed descriptive manuscripts outlining new or improved "toolbox" innovations encompassing a myriad of technologies (high-throughput/high-content screening, robotics, structure-based drug design, fragment-based drug design, combinatorial

chemistry/parallel synthesis, etc.), which simultaneously facilitate and partially define modern medicinal chemistry.

Innovations. May include articles intended to tell the backstory of drug discovery campaigns relating to the development of new therapeutic agents or articles covering the discovery and development of new technologies that enable the identification of new therapeutic targets or advancement and acceleration of drug discovery programs. See the first published Innovations article as an example.

Topical Innovations are short, timely reviews of a topic of high interest to the medicinal chemistry community. Emphasis should be on a focused topic that is instructive, rather than comprehensive, so that a medicinal chemistry audience may understand the importance of the topic and next steps that will move the field forward. Topical Innovations should include a critical evaluation of the work they review. Topics can include inter alia specific sub-disciplines of medicinal chemistry, including development of new technologies that enable identification of new therapeutic targets or advancement and acceleration of drug discovery programs. Topical Innovations should include a single unnumbered high-resolution image without caption that is 7 in. wide x 9 in. high (vertical), 7 in. high x 9 in. wide (horizontal) or 504 pt x 648 pt. This or another graphic will serve as the TOC graphic.

Viewpoints. Invited general commentaries on current issues in the medicinal chemistry field, including views on new chemical patents and relevant patent laws and tutorials of immediate interest to the broad readership.

Patent Highlights. A journal section dealing with recently issued medicinal chemistry patents. The coverage will feature patents and published patent applications in high-interest areas with brief commentaries on their potential impact. The Patent Highlights are written by members of the Patent Panel appointed by the Editors and are not open to submission by other authors.

The following list summarizes the publication and formatting requirements for *ACS Medicinal Chemistry Letters* manuscript types.

- ***Letters***: 4500 words, 150 word abstract, 6-10 figures/tables, ~40 references, peer reviewed
- ***Notes***: 2500 words, 150 word abstract, 2-4 figures/tables, ~30 references, peer reviewed
- ***Technology Notes***: 4500 words, 150 word abstract, 6-10 figures/tables, ~40 references, peer reviewed
- ***Innovations***: 7000 words, 250 word abstract, <6 figures/tables, ~50 references, peer reviewed, **by invitation only**
- ***Topical Innovations***: 7000 words, ~250 word abstract, one graphic (see details above) ~50 references, peer-reviewed
- ***Viewpoints***: 2000 words, ~50 word abstract, 0-2 figures/tables, 5-12 references, editorial review, **by invitation only**

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.

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 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 cover letter should contain clear and precise information about the submission, highlighting the significance of the work and must contain the following elements:

- Manuscript title
- Name of the corresponding author, with contact information
- Paragraph explaining why the manuscript is appropriate for *ACS Medicinal Chemistry Letters*
- Short lay summary (1 paragraph) describing the significance of the study and its interest for a broad audience
- Suggestions for a minimum of five possible reviewers, as well as sufficient justification for excluding potential reviewers that might have a conflict of interest

If your manuscript is accepted for publication, *ACS Medicinal Chemistry Letters* may choose to modify, edit, and publish your lay summary in the ***In This Issue*** feature of the journal. The journal may also promote your research article through press communications.

Manuscript Text Components

Title. Titles are *limited to 120 characters, including spaces*, and should clearly and concisely reflect the emphasis and content of the manuscript and be accessible to a broad audience. Titles are of great importance for current awareness and information retrieval and should be carefully constructed for these purposes. One option that authors may wish to consider is to present a significant outcome in the title. Titles should not contain specialized abbreviations or jargon. Editors may request author revision of a title at any time prior to publication.

Author List. All those who have made substantial contributions to the work should be included. To facilitate indexing and retrieval and for unique identification of an author, first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and surnames (e.g., J. Robert Smith) should be used. At least one author must be designated with an asterisk as the person to whom correspondence should be addressed. 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 Letters, Notes, Technology Notes, Innovations and Viewpoints must contain an abstract, which should provide a succinct, informative summation of the most important results and conclusions. Abbreviations should be used sparingly and spelled out when first used. The abstract should be written in complete sentences without the use of subheadings or specialized jargon. It should be accessible to a graduate student in the field so as to be palatable to a broad audience.

Keywords. Authors should provide a list of four to six keywords to be displayed below the abstract of their publication.

Introduction. In this unheaded section, the purpose and significance of the research should be clearly stated and placed in the context of earlier work in the area. Historical summaries are seldom warranted. Attempts at a complete survey of the literature should not be made. If a recent article has summarized work on the subject, that article should be cited without repeating its individual citations. In general, the introductory section should be approximately 750 words for a Letter.

Results and Discussion. This section should be continuous with the Introduction and does not receive a heading. The first paragraphs should explain the motivation for the work and how it combines the chemistry and biology disciplines. Tables and figures should be used only if they contribute significantly to the comprehension of the data. The same data should not be presented in more than one figure or in both a figure and a table. The purpose of the discussion is to interpret the results and to relate them to existing knowledge in the field. Manuscripts reporting new 3D structures of small molecules from crystallographic analysis should include a structural figure with probability ellipsoids and a CIF file. Those reporting NMR or X-ray crystal structures of macromolecules must include a table with relevant data collection and refinement statistics. For manuscripts reporting structures derived from electron microscopy experiments, authors must provide one image showing the distribution of particles being analyzed, the percentage of the particles being used in the reconstruction, and a correlation coefficient plot (or equivalent data) to indicate the resolution of the presented structure. Upon request from the Editor, the authors must provide sequence, structure data (including coordinate files and structure), and/or microarray data in a MIAME-compliant format to the Editors and reviewers for the purpose of evaluating the manuscript.

Experimental Procedures. A clear, unambiguous description of materials, methods, and equipment should be provided in a format that permits repetition of the work elsewhere. Novel experimental procedures and characterization data for key compounds should be described in sufficient detail, but where pertinent, synthetic and bioassay protocols should refer to published procedures by literature citation of the original method and any later modifications used. The Experimental Procedures section can also contain subsections (with subheadings), but it is recommended that most procedural details be placed in Supporting Information. Manuscripts reporting data from experiments on live animals must include a statement identifying the approving committee and certifying that such experiments were performed in accordance with all national or local guidelines and regulations. Results from experiments involving humans or tissue samples must additionally include a statement that informed consent was obtained from the subject or from the next of kin. Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. Authors are encouraged to review the following publication for detailed standards on chemical laboratory safety practice: National Research Council. 2011. Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards, Updated Version. Washington, DC: The National Academies Press. https://doi.org/10.17226/12654

Author Information. The following information should be provided in these specific subheadings:

- **Author Addresses:** current address for each author if different from the location(s) where the research was conducted.
- **Author Contributions:** *ACS Medicinal Chemistry Letters* recommends that individual contributions of authors be listed.
- **Funding Sources**

Acknowledgments. Financial support, technical assistance, advice from colleagues, gifts, etc. should be included.

Funding Sources. Authors are required to report ALL funding sources and grant/award numbers relevant to this manuscript. Enter all sources of funding for ALL authors relevant to this manuscript in BOTH the Open Funder Registry tool in ACS Paragon Plus and in the manuscript to meet this requirement. See http://pubs.acs.org/page/4authors/funder_options.html for complete instructions.

Abbreviations. If nonstandard abbreviations (see *The ACS Style Guide*) are used within the manuscript, then a section should be added to identify the abbreviations. Such abbreviations

should also be defined on first appearance in the manuscript text.

References. All references should be compiled together in a list at the end of the manuscript text. During the publication process, many of them will have links added to other Web resources, such as the corresponding abstracts in *Chemical Abstracts* and the full text on publisher Web sites. Because of this electronic linking and because the references are not checked in detail by Editors or reviewers, it is crucial that authors verify their accuracy. Unnecessarily long lists of references should be avoided. However, authors must reference all previous publications in which portions of the present work have appeared, **including published patent applications and issued patents**. Long references with multiple citations within one reference number should be avoided. Each reference should be listed as a separate citation, and each should be assigned a unique reference number. Additional data and peripheral discussion should be placed in the Supporting Information rather than in the references. Supplementary references may be placed in the Supporting Information. Literature references must be numbered with Arabic numerals in the order of their first citation in the text, and the corresponding numbers must be inserted at the appropriate locations in the text. The following reference styles should be used.

For journals:

- Rich, D. H.; Green, J.; Toth, M. V.; Marshall, G. R.; Kent, S. B. H. Hydroxyethylamine Analogues of the p17/ p24 Substrate Cleavage Site Are Tight-Binding Inhibitors of HIV Protease. *ACS Med. Chem. Lett*. **2010**, *1*, 1285–1288.

For journal articles published online ahead of issue or online only:

- Liu, C.; Yang, S. Synthesis of Angstrom-Scale Anatase Titania Atomic Wires. *ACS Nano*, published online March 23, 2009; DOI: 10.1021/nn900157r.

For monographs:

- Casy, A. F.; Parfitt, R. T. *Opioid Analgesics*; Plenum Press: New York, 1986; pp 333–384.

For edited books:

- Rall, T. W.; Schleifer, L. S. Drugs Effective in the Therapy of the Epilepsies. In *The Pharmacological Basis of Therapeutics*, 7th ed.; Gilman, A. G., Goodman, L. S., Rall, T. W., Murad, F., Eds.; Macmillan Publishing Co.: New York, 1985; pp 446–472.

Titles of journals should be abbreviated according to *Chemical Abstracts Service Source Index* (CASSI, www.cas.org/products/print/cassipr/index.html). Letters accepted for publication should be cited as “in press”; the DOI should be given if the Letter is published online. Manuscripts that are in preparation or have been submitted, but have not yet been accepted, should be cited as unpublished results or personal communications.

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.

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

Nomenclature. Nonstandard abbreviations (see *The ACS Style Guide*) and acronyms should be used sparingly, and all usage should be defined at the first occurrence in the text. Whenever possible, systematic nomenclature as recommended by IUPAC and IUBMB for chemical compounds and biomolecules should be used. Names of organisms should comply with genetic conventions, with genus and species names written in italics and spelled out in full on first appearance. Gene symbols should conform to approved nomenclature and should be italicized, whereas corresponding protein products should start with a capital letter and should not be italicized. The available nomenclature databases (e.g., LocusLink) should be consulted for correct names and symbols. Enzyme names should be accompanied by their Enzyme Commission (EC) numbers (e.g., see http://www.expasy.org).

Chemical Compound Characterization. The knowledge of the purity of compounds employed in biological studies, whether they are synthesized, purchased, or received as gifts, is a crucial factor for obtaining reliable and reproducible results. For studies reported in *ACS Medicinal Chemistry Letters*, it is preferred that assayed compounds be at least 90% pure as judged by either HPLC, LC-MS, or NMR. The analytical methods used for compound characterization and purity assessment should be mentioned in the Experimental Procedures section. For novel compounds, it is important to obtain such data to confirm their structure and purity. Manuscripts for *ACS Medicinal Chemistry Letters* should *at least* provide exemplary characterization data for new compounds, including LC-MS, and ^{1}H NMR and full characterization, including ^{13}C NMR (peak lists), HPLC, and HRMS (see below for more details) for final products that are undergoing screening. For compounds prepared in a library format, a general experimental procedure should be provided, including full experimental details, with yields, for a representative selection of library

members. The synthesis protocols and selected characterized compounds must reflect the reliability and scope of the reaction sequence. The purity of all reported library compounds should be explicitly stated. The submission of manuscripts solely based on mixture synthesis and/or mixture analysis is strongly discouraged. Authors must be specific about the reagents used to obtain the final product so that the work can be reproduced by another laboratory.

***Key Compounds*.** Frequently, articles will present a series of compounds with analogous structures. In such a case, complete characterization data need not be reported for all compounds. However, complete data should be provided for key compounds, which are those compounds in a manuscript that receive extra attention beyond the primary or general screening of the entire set used for structure- activity analysis. Key compounds include those that are subject to: (a) additional or follow-up studies for bioactivity in functional cellular assays, isolated tissues, or in vivo systems; (b) advanced adsorption, distribution, metabolism, excretion, and toxicology (ADMET) studies; (c) in vivo pharmacokinetics/pharmacodynamics studies; or (d) studies identifying off-target effects. The relevant characterization data for **key compounds** are as follows:

HRMS and Elemental Analysis. For novel key compounds (excluding biomacromolecules and other polymers), HRMS data should be reported to support the molecular formula assignment. Elemental analysis data, which are optional, can serve as an alternative. The reported HRMS data should include the molecular formulas on which the theoretical (calcd) values are based. HRMS molecular formulas and calcd values should include any added atoms (usually H or Na). Found values should be close enough to the calcd values, and have sufficiently small estimated uncertainties, to exclude alternative plausible formulas. The ionization method and the mass detector type should be reported. Elemental analysis values found for carbon, hydrogen, and nitrogen (if present) should be within 0.4% of the calcd values for the proposed formula. Complexed solvents, including water, should be confirmed by an additional analytical method, such as NMR analysis for organic solvents and Karl Fischer titration for water.

***NMR Spectral Data*.** ^{1}H NMR and ^{13}C NMR resonances should be listed for each key compound, and the solvent and instrument frequency should be identified. ^{13}C NMR peak shifts should be rounded off to the nearest 0.1 ppm, except when greater precision is needed to distinguish between closely spaced peaks. If detailed peak assignments are made, the type of 2D NMR methods used to establish atom connectivities and spatial relationships should be identified in an Experimental Procedures paragraph in the Supporting Information. Authors are encouraged to place in the Supporting Information copies of well-resolved ^{1}H NMR and proton-decoupled ^{13}C NMR spectra for every new key compound. In cases where structure assignments of complex molecules depend heavily on NMR data interpretation, including isolated and synthesized natural products, copies of suitable 2D spectra should also be placed in the Supporting Information. For complete details and best practices on reporting NMR, please see http://pubs.acs.org/page/4authors/submission/index.html.

Melting Points. It is suggested that a melting point *range* be reported for crystalline solid products.

Isomers and Isomeric Mixtures. The composition of isomeric mixtures (regioisomers, diastereomers, and enantiomers) must be reported. Enantiomeric ratio (er) or diastereomeric ratio (dr) values are preferred over enantiomeric excess (ee) or diastereomeric excess (de) values. Specific optical rotations should be reported for enantiopure compounds, enantioenriched isomer mixtures, and isolated natural products, when a sufficient sample is available. Specific rotations based on the equation [] = (100)/(*lc*) should be reported as unitless numbers as in the following

example: $[]_D^{20}$ (*c* 1.9, MeOH), where the concentration *c* is in g/l00 mL and the path length *l* is in decimeters. The units of the specific rotation, (degmL)/(gdm), are implicit and are not included with the reported value.

Peptides and Biomacromolecules. For peptide materials, it is necessary to provide an amino acid composition analysis. For biomacromolecules, structures may be established by providing evidence about sequence and mass. Sequences may be inferred from the experimental order of amino acid, saccharide, or nucleotide coupling; from known sequences of templates in enzyme-mediated syntheses; or through standard sequencing techniques. Typically, a sequence will be accompanied by MS data that establish the molecular weight. Additional characterization and physical property data should be placed in the Supporting Information unless they are important to the main discussion.

Biological Results. Biological test methods must be referenced or described in sufficient detail (in the main text or preferably in the Supporting Information) to permit the experiments to be repeated by others. The methods used should be relevant to the purpose of the study. Authors should be cognizant of significant figures for their measurements when reporting biological data. A statement regarding inherent error, such as standard deviation, standard error of the mean (SEM), or the like, should be provided. The error limits themselves need not be presented in the main text but can appear in the Supporting Information. The number of experiments for a given data point (e.g., $N = 3$) should be indicated in some manner. In vivo biological data should be accompanied by statistical limits (statistical significance). Doses and concentrations should be expressed as molar quantities (e.g., mol/kg, nM) whenever possible. Exceptions include antibiotic concetrations for which µg/mL has been traditionally been used.

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

- Practical applications of computational methods including experimental data, in particular, experimental validation of computational predictions
- Substantially novel methods along with evidence for utility in medicinal chemistry and drug design and significant potential for advancing the field, with methods that must be described clearly and comprehensibly
- Computational, statistical, or other theoretical analyses of currently available data that provide unexpected or provocative insights into topical problems and advance medicinal chemistry knowledge

When manuscripts combine computational and experimental studies, both components must be significant. For example, computational analyses are not automatically validated by the addition of a minor experimental component. For manuscripts reporting virtual screening results, purity data should conform to journal purity requirements for all experimentally tested active compounds, and convincing experimental data should be provided that demonstrate true biological activity of identified hits. For manuscripts describing new methods, the scope of the method must be validated convincingly.

Sufficient information should be presented to allow the method to be reproduced and tested in other laboratories. All experimental data and molecular structures used to generate and/or validate computational models must be reported in the manuscript or Supporting Information or be readily available without infringements or restrictions.

QSAR/QSPR and Proprietary Data

***General Requirements*.** (1) Authors should explicitly state in the manuscript the novel features of the quantitative structure–activity relationships/quantitative structure–property relationships (QSAR/QSPR) study being reported. (2) If a new method/theory is being reported in the manuscript, it should be compared and "validated" against at least one other common data set for which a published study exists by using at least one other method/approach and preferably a method/approach that has been widely used in the field. The data set should not be small. (3) All data and molecular structures used to carry out a QSAR/QSPR study should be reported in the manuscript or Supporting Information or must be readily available without infringements or restrictions. The use of proprietary data is generally not acceptable. (4) Standard QSAR/QSPR studies will only be considered 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 mechanism of activity are encouraged.

***Guidelines for Prospective Authors*.** (1) 3D QSAR studies that overlap with and enhance structure-based design methods are encouraged. QSAR models that lead to subsequently validated experimental findings are encouraged. (2) Manuscripts reporting new and novel QSAR/QSPR methods and approaches for facilitating a mechanistic understanding of ADMET properties, and/or for reliable ADMET screening, are welcomed. (3) New QSAR/QSPR methods that interface with cheminformatics and bioinformatics methods and/or with data-mining techniques are encouraged. (4) QSAR/QSPR approaches for virtual screening must demonstrate distinct advantages or advances over current virtual screening schemes. (5) Specific studies that are *discouraged* include the following: QSAR and QSPR modeling for data sets that have already been extensively modeled, model development featuring high ratios of descriptors to data points, and reports of new descriptors without clear evidence for their superiority in QSAR/QSPR modeling to existing, commonly used alternatives.

Database Deposition

Sequence Data. Manuscripts reporting protein or nucleic acid sequences will not be published without an accession number to GenBank/EMBL/DDBJ, SWISS-PROT, or another appropriate database in the field that provides free access to the data for all scientists from the date of publication.

Crystal and NMR Structures. Small molecular crystallographic data should be submitted upon publication to the Cambridge Structural Database (www.ccdc.cam.ac.uk). Manuscripts reporting macromolecular NMR or crystal structures must specifically state that the atomic coordinates have been deposited in the Protein Data Bank (PDB) (www.rcsb.org/pdb/home/home.do) or the Nucleic Acid Database (http://ndbserver.rutgers.edu) and must list the accession code(s). These coordinates must be designated "for immediate release upon publication". Authors of manuscripts reporting X-ray crystal structures are encouraged to deposit the structure factor files in the PDB. No formal requirement exists for deposition of NMR assignments and constraints (see Biological Magnetic Resonance Data Bank at www.bmrb.wisc.edu).

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).

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 relevant accession numbers must

be included 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.

Genetically Modified Organisms and Mutants. 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 should be used whenever possible. Large data sets for which an approved database has not yet been established must be housed as online Supporting Information at *ACS Medicinal Chemistry Letters*.

Material and Data Availability

ACS Medicinal Chemistry Letters understands that communication and collaboration between scientists are significantly enhanced when materials and data can be exchanged. Therefore, authors are strongly encouraged to make experimental data and protocols available to readers through deposition in a publicly used database. The hosting of such information on an author's Web site is not an acceptable substitute. Authors should endeavor to make research materials reported in their manuscript that are not otherwise reasonably obtainable available to interested academic researchers. Any restrictions as to the availability of materials or information should be stated at the time of submission.

Policy Summary on Patent Citation. *ACS Medicinal Chemistry Letters* authors should cite issued patents or published patent applications when the material in the manuscript overlaps with or is significantly related to that in the patent literature. Due to the significant differences in the review of patents vs journal articles, however, we cannot accept a reference to the patent literature in lieu of experimental protocols (chemical and biological) and characterization data for novel and key compounds. For the same reasons, we cannot publish articles whose primary purpose is to dispute patent literature and which do not provide additional assay and/ or compound information that extends significantly beyond the patent scope of work. Authors who wish to raise concerns regarding data or statements reported in patents are advised to open a dialogue with the community by submitting Letters to Editors.

Web Enhanced Objects, Such as Movies. The use of multimedia attachments such as animations and movies is encouraged. These objects should complement a reader's understanding of the research being reported. Authors should submit Web-enhanced objects via the Paragon Plus Web site as part of their submissions and clearly indicate to the Editor that the material is Web-enhanced object content.

Descriptions of Web Enhanced Objects should be noted in the appropriate places within the graphic caption or text of the manuscript, noting the type of file and format. Example: "A 3D rotatable image in *xyz* format is available." For acceptable file formats and specifications, please refer to this webpage on Submission & Authoring in ACS Paragon Plus.

Frequent Reasons for Revisions

The following constitute examples of frequent reasons for revisions and should ideally be addressed before manuscript submission:

1. Standard deviations/SEM missing
2. Data reported not consistent with standard deviation/standard error of measurement
3. References in incorrect format

4. Purity assessment not included
5. Uncommon abbreviations section missing or incomplete
6. No section headings
7. Optical characterization missing

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 Figures service generates publication-ready figures that conform to your chosen journal's specifications. This includes changes to file type, resolution, color space, font, scale, line weights, and layout (to improve readability and professional appearance).

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

ACS Medicinal Chemistry Letters authors are allowed to deposit an initial draft of their manuscript in a preprint service such as ChemRxiv, arXiv or bioRxiv. A patent or a published patent application is not considered to be a prior "publication". Please note any use of a preprint server, patents, and dissertations in the cover letter, and as appropriate, state how the manuscript has been adjusted/updated between deposition and submission. All other prior/redundant publications are forbidden. Upon publication in *ACS Medicinal Chemistry Letters*, authors are advised to add a

link from the preprint to the published paper via the Digital Object Identifier (DOI).

Editorial Policies

Costs. *ACS Medicinal Chemistry Letters* does not impose submission or publication fees.

Presubmission Inquiries. Presubmission inquiries can be made to the Editor-in-Chief by e-mail at: eic@medchemlett.acs.org.

Review Process. The Editors evaluate submitted manuscripts, and only those judged to fall within the scope of the journal and to be of potential interest to our readers are sent to two or more reviewers for evaluation. Reviewers can suggest that a manuscript be published, revised, or rejected. Reviewers will evaluate the originality, technical quality (including appropriateness of compound characterization and quality of experimental data), clarity of presentation, and significance to the field. The Editors evaluate the reviewers' arguments in the context of the scope of the journal and make the final decision on each manuscript.

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Appendix 2: Preparing Graphics

Resolution

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

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

Size

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

Color

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

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

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

Figures

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

Charts

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

Tables

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

Schemes

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

Chemical Structures

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

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