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Journal of
Medicinal Chemistry

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Manuscript Submission Requirements Checklist

Please review the Editorial "Simplifying Submission Requirements for the *Journal of Medicinal Chemistry*" for an overview of recent changes.

MAJOR CHANGE:

The journal no longer requires the Author Submission Checklist for Articles and Drug Annotations. Submissions should be accompanied by a standard cover letter that should include the title of the manuscript, a short description of the research, and why it is appropriate for *JMC*. The letter should also contain the Journal purity statement (which should also be stated in the general experimental section of the manuscript) that "All compounds are >95% pure by HPLC analysis." HPLC traces should be included for all compounds that have in vivo data described in the manuscript or, if no in vivo data, a representative number of HPLC traces of compounds described with in vitro data in the SAR tables (HPLC traces should be in the Supporting Information, SI). Alternatively, other methods of purity determination (e.g. elemental analysis) that were used need to be indicated. Authors may suggest Associate Editor(s) to handle your manuscript, however, due to manuscript workload, the desired Editor may not be assigned.

Scope of the Journal

The *Journal of Medicinal Chemistry* (Journal) invites original research contributions dealing with chemical-biological relationships. The primary objective of the Journal is to publish studies that contribute to an understanding of the relationship between molecular structure and biological activity or mode of action.

Some specific areas that are appropriate include the following.

- Design, synthesis, and biological evaluation of novel biologically active compounds, diagnostic agents, or labeled ligands employed as pharmacological tools.
- Molecular modifications of reported series that lead to a significantly improved understanding of their structure-activity relationships (SAR). Routine extensions of existing series that do not utilize novel chemical or biological approaches or do not add significantly to a basic understanding of the SAR of the series will normally not be considered for publication.
- Structural biological studies (X-ray, NMR, etc.) of relevant ligands and targets with the aim of investigating molecular recognition processes in the action of biologically active compounds.
- Molecular biological studies (e.g., site-directed mutagenesis) of macromolecular targets that lead to an improved understanding of molecular recognition.
- Computational studies that analyze the SAR of compound series of general interest and lead to experimental studies or analysis of other available chemical and/or biological data that substantially advance medicinal chemistry knowledge.
- Substantially novel computational chemistry methods with demonstrated utility for the identification, optimization, or target interaction analysis of bioactive molecules.
- Effect of molecular structure on the distribution, pharmacokinetics, and metabolic transformation of biologically active compounds. This may include design, synthesis, and

evaluation of novel types of prodrugs.
- Novel methodology with *broad* application to medicinal chemistry, but only if the methods have been tested on relevant molecules.
- The Journal does not publish papers based on studies with crude extracts.

The Journal publishes 24 issues per year on the second and fourth Thursdays of each month.

Manuscript Types

Manuscripts can be submitted as *Articles*, *Perspectives*, or *Drug Annotations*.

- *Articles* are definitive, full accounts of significant studies.
- *Perspectives* are interpretive accounts on subjects of current interest to medicinal chemists. Perspectives differ from reviews, as they feature multiple “teaching moments” to inform and educate the community while providing an overview of an area or topic. This series is intended to be a forum for experts to present their perspectives on emerging or active areas of research that affect the practice of medicinal chemistry. Manuscripts are usually submitted at the invitation of the Perspectives Editor. However, experts are welcome to contact the Perspective Editor to ensure that a topic is suitable. Approval is recommended prior to submission. Additional information can be found here.
- *Drug Annotations* are reports of development candidates in phase I, II, and III clinical trials, as well as new approved drugs. These manuscripts should provide a description of the selected development candidate (including structure), target(s), mechanism of action, associated SARs, pre-clinical pharmacological properties and rationale for bringing the drug to clinical trial (for example, first-in-class or improvements over previous lead compounds). Reports on original research are also acceptable. Clinical data are highly desirable but not required. Authors are welcome to contact the *Drug Annotations* Editor to ensure that a topic is suitable. Approval is recommended prior to submission but is not required.
- *Letters to the Editor* are commentaries on previously published work from the journal, as well as on general issues that directly or indirectly impact medicinal chemistry research. Commentaries on previously published work should be submitted within 18 months of the ASAP publication date of the original material. The purpose of this manuscript type is to start a dialog between authors and should not be used to supplement prior publications with new data. The author(s) of the original material will be given an opportunity to reply. *Letters to the Editor* are typically not peer-reviewed, however, in cases where new data are presented, manuscripts may be sent out for peer review at the Editor’s discretion. Reviewing previously published examples of *Letter to the Editors* is strongly recommended.
- *Viewpoint* manuscripts are invited by the Editors. *Viewpoint* manuscripts are typically accompanied commentaries to *Featured Article*s.
- *Featured Articles* are selected by the Editors from accepted *Articles.*

Please note that *Journal of Medicinal Chemistry* no longer publishes *Brief Articles*.

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

Templates for the *Journal of Medicinal Chemistry* are available below for *Articles*. The template facilitates the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text.

A Sample Manuscript is available for reference on proper styling and construction of your manuscript.

Articles:

- Microsoft Word 2011 Template for Macintosh
- Microsoft Word 2010 Template for Windows | README file [PDF]

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

The journal no longer requires the Author Submission Checklist for Articles and Drug Annotations. Submissions should be accompanied by a standard cover letter that should include the title of the manuscript, a short description of the research, and why it is appropriate for *JMC*. The letter should also contain the Journal purity statement (which should also be stated in the general experimental section of the manuscript) that "All compounds are >95% pure by HPLC analysis." HPLC traces should be included for all compounds that have in vivo data described in the manuscript or, if no in vivo data, a representative number of HPLC traces of compounds described with in vitro data in the SAR tables (HPLC traces should be in the Supporting Information, SI). Alternatively, other methods of purity determination (e.g. elemental analysis) that were used need to be indicated. Authors may suggest Associate Editor(s) to handle your manuscript, however, due to manuscript workload, the desired Editor may not be assigned.

Manuscript Text Components

A. General Considerations

Manuscripts should be kept to a minimum length. Authors should write in clear, concise English, employing an editing service if necessary. The responsibility for all aspects of manuscript preparation rests with the authors. Extensive changes or rewriting of the manuscript will not be undertaken by the Editors. Please see the *ACS Guide to Scholarly Communication*, which provides helpful information for communicating research.

All text (including the title page, abstract, all sections of the body of the paper, figure captions, scheme or chart titles, and footnotes and references) and tables should be in *one* file.

Manuscripts that do not adhere to the guidelines may be returned to authors for correction.

1. *Articles*. *Article* format can be single column, double-spaced or double column, single spaced including text, references, tables, and legends. This applies to figures, schemes, and tables as well as text. Manuscripts do not have page limitations but should be kept to a minimum length. A template is not required. The experimental procedures for all of the steps in the synthesis of all tested compounds must be included in the experimental section of the manuscript.

2. *Perspectives.* *Perspectives* can be single column, double-spaced or double column, single spaced including text, references, tables, and legends. This applies to figures, schemes, and tables as well as text. A template is not required. Manuscripts do not have the same headings as other manuscript types. Author(s) biographies of less than 125 words each should be placed immediately before the references.

- *Perspectives* are no more than 25 journal pages (100 double-spaced manuscript pages) and should not contain more than 180 references.
- *Miniperspectives* are no more than 8 journal pages (32 double-spaced manuscript pages) and should not contain more than 70 references.
- *Award Perspectives* page limits are flexible, but they should conform to other requirements stated for *Perspectives* or *Miniperspectives*.

3. *Drug Annotations.* *Drug Annotations* can be single column, double-spaced or double column, single spaced including text, references, tables and legends. This applies to figures, schemes, and tables as well as text. In general, manuscripts should include design and chemistry, known biological targets, in vitro and in vivo biological activity, pharmacological properties, and available toxicity information. Clinical data are highly desirable but not required.

4. *Viewpoint.* Manuscripts are limited to 2000 words, including title page, abstract (~50 words), references, tables, and illustrations.

5. Nomenclature. It is the responsibility of the authors to provide correct nomenclature. Nomenclature should conform to current American usage. It is acceptable to use semisynthetic or generic names for certain specialized classes of compounds, such as steroids, peptides, carbohydrates, etc. In such a case, the name should conform to the generally accepted nomenclature conventions for the compound class. Chemical names for drugs are preferred. If these are not practical, generic names, or names approved by the U.S. Adopted Names Council or by the World Health Organization, may be used. Authors may find the following sources useful for recommended nomenclature:

- The *ACS Guide to Scholarly Communication*, which provides helpful information for communicating research.
- *Enzyme Nomenclature*; Webb, E. C., Ed.; Academic Press: Orlando, 1992.
- IUPHAR database of receptors and ion channels (http://www.guidetopharmacology.org/).

6. Compound Code Numbers. Code numbers (including peptides) assigned to a compound may be used as follows:

- Use is permitted but excessive use is discouraged. Authors are encouraged to assign bold Arabic numbers to compounds. If code number usage is cumbersome or detracts from the readability of the manuscript, editors may require the authors to limit usage by assigning bold Arabic numbers.
- Once in the manuscript title.
- Code numbers in the text must correspond to structures or, if used only once, the chemical name must be provided with the code number. Code numbers in the text referring to a previously published compound must have a citation to a publication or a patent on first appearance.

Compounds *widely* employed as research tools and recognized primarily by code numbers may be designated in the manuscript by code numbers without the above restrictions. Their chemical name or structure should be provided as above. Editors have the discretion of determining which code numbers are considered widely employed.

7. Trademark Names. Trademark names for reagents or drugs must be used only in the experimental section. *Perspectives* may use trademark names once in the manuscript. Do not use

trademark or service mark symbols.

8. Interference Compounds. Active compounds from any source must be examined for known classes of assay interference compounds and this analysis must be provided in the General Experimental section. Compounds shown to display misleading assay readouts by a variety of mechanisms include, but are not limited to, aggregation, redox activity, fluorescence, protein reactivity, singlet-oxygen quenching, the presence of impurities, membrane disruption, and their decomposition in assay buffer to form reactive compounds. Many of these compounds have been classified as Pan Assay Interference Compounds (PAINS; see Aldrich et al. *J. Med. Chem.* **2017,** *60*, 2165-2168 and webinar at bit.ly/jmcPAINS). Provide firm experimental evidence in at least two different assays that reported compounds with potential PAINS liability are specifically active and their apparent activity is not an artifact.

B. Manuscript Organization

Manuscripts can be submitted in a general double-column ACS template or as a general Word document, single-spaced. **Please insert figures/tables/schemes, etc. in the text where they should be located based on text references** and *not at the end of the Word document*. For chemical structures, ChemDraw with the ACS preferences selected is preferred; however, authors who do not have access to ChemDraw may use whichever available drawing program.

1. Title Page. *Title*: The title of the manuscript is of great importance and should be constructed with care for readability and should reflect the purposes and findings of the work in order to provide maximum information in a computerized title search. Minimal use of nonfunctional words is encouraged. Only commonly employed abbreviations (e.g., DNA, RNA, ATP) are acceptable. Code numbers for compounds may be used in a manuscript title. Avoid complex compound names as much as possible in the title by using generic names or code numbers, and spell out elements rather than using symbols unless part of a compound name. Neither the title nor any other text should indicate that the paper is part of a numbered series on a broader research topic, or a numbered contribution from a particular institution or research group. IUPAC names are not required in the title and actually not preferred.

Code numbers for compounds may be used in a manuscript title when placed in parentheses AFTER the chemical or descriptive name.

Authors' Names and Affiliations: The authors' full first and last names and affiliations with addresses (including postal codes) at time of work completion should be listed below the title. The name of the corresponding author should be marked with an asterisk (*).

2. Abstract. *Articles*, *Drug Annotations, Perspectives*, and *Viewpoints* must have an abstract following the title page. For *Articles, Drug Annotations,* and *Perspectives,* 150 words are usually adequate; for *Viewpoints*, 50 words are adequate. Abstracts should be presented in a findings-oriented format in which the most important results and conclusions are summarized. Descriptive names or code names may be used in the abstract.

3. Introduction. The rationale and objectives of the research should be discussed in this section. The background material should be brief and relevant to the research described.

4. Results. This section could include synthetic schemes and tables of biological data. The discussion of the chemistry and biology should be descriptive. Note that results and discussion

may be combined with a separate conclusions section.

5. Discussion and Conclusions. Authors should discuss the analysis of the data together with the significance of results and conclusions, if a separate conclusions section is not employed.

6. Experimental Section. Authors should be as concise as possible in experimental descriptions. General reaction conditions should be given only once. The title of an experiment should be followed by the parenthesized code number or bold Arabic identifier number.

The Experimental section must include the purity statement “All compounds are >95% pure by HPLC.” HPLC traces should be included for representative compounds that have in vitro data and for all compounds with in vivo data described in the manuscript. Reasons for any exceptions/exclusions should be explained.

The experimental procedures for all of the steps in the synthesis of target compounds must be included in the experimental section of the manuscript and not in the SI.

Molar equivalents of all reactants and percentage yields of products should be included.

A general introductory section should include general procedures, standard techniques, and instruments employed (e.g., determination of purity, chromatography, NMR spectra, mass spectra, names of equipment) in the synthesis and characterization of compounds described subsequently in this section. Provide analysis for known classes of assay interference compounds.

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the manuscript.

Abbreviations. Standard abbreviations should be used throughout the experimental section (see Standard Abbreviations and Acronyms). Please note that these are used in ACS Journals without periods. The preferred forms for some of the more commonly used abbrevations are mp, bp, ºC, K, min, h, mL, L, g, mg, g, cm, mm, nm, mol, mmol, mol, ppm, TLC, GC, NMR, UV, and IR. Units are abbreviated in table column heads and when used with numbers, not otherwise. For further information, refer to *The ACS Style Guide.*

7. Ancillary Information. Include pertinent information in the order listed immediately before the references.

Supporting Information: Provide brief descriptions in non-sentence format listing the contents of the files supplied as Supporting Information.

PDB ID Codes: Include the PDB ID codes with assigned compound Arabic number. Include the statement “Authors will release the atomic coordinates and experimental data upon article publication.”

Homology Models: Coordinates of homology models in PDB format should be submitted as Supporting Information for Publication.

Corresponding Author Information: Provide email addresses for each of the designated corresponding authors.

Present/Current Author Addresses: Provide information for authors whose affiliations or addresses have changed.

Author Contributions: Include a statement such as "These authors contributed equally."

Acknowledgment: Authors may acknowledge people, organizations, and financial supporters in this section.

Abbreviations Used: Provide a list of nonstandard abbreviations and acronyms used in the paper, e.g., "YFP, yellow fluorescent protein." Separate by semicolons. Do not include compound code numbers in this list. It is not necessary to include abbreviations and acronyms from the Standard Abbreviations and Acronyms list.

8. References and Notes. Number literature references and notes in one *consecutive* series by order of mention in the text. Footnotes are not used. Numbers in the text are non-parenthesized superscripts. The accuracy of the references is the responsibility of the corresponding author(s). Following are reference examples.

- 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. *J. Med. Chem.* **1990**, *33*, 1285-1288.
- Online early access: Rubner, G.; Bensdorf, K.; Wellner, A.; Kircher, B.; Bergemann, S.; Ott, I.; Gust, R. Synthesis and Biological Activities of Transition Metal Complexes Based on Acetylsalicylic Acid as Neo-Anticancer Agents. *J. Med. Chem.* [Online early access]. DOI: 10.1021/jm101019j. Published Online: September 21, 2010. *Note: If a citation is given, it should be provided in lieu of the DOI number.*
- Periodicals published in electronic format only: Zloh, M.; Esposito, D.; Gibbons, W. A. Helical Net Plots and Lipid Favourable Surface Mapping of Transmembrane Helices of Integral Membrane Proteins: Aids to Structure Determination of Integral Member Proteins. *Internet J. Chem.* [Online] **2003,** *6,* Article 2. http://www.ijc.com/articles/2003v6/2/2/ (accessed Oct 13, 2004).
- Web Sites: U. S. Environmental Protection Agency. http://www.epa.gov (accessed Nov 7, 2018).
- 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: New York, 1985; pp 446-472.
- Patents: Sheem, S. K. Low-Cost Fiber Optic Pressure Senor. U.S. Patent 6,738,537, May 18, 2004 *OR*2004. *(Date format needs to be consistent.)*

Excessive self-citations are discouraged.

List submitted manuscripts as “in press” only if formally accepted for publication. Manuscripts available on the Web with a DOI number are considered published. For manuscripts not accepted, use “unpublished results” after the names of authors.

Additional reference examples may be found on the Journal website.

Prior to acceptance of a manuscript, journal citations must include:

- All authors; do not use 'et al.'
- Titles with capitalization of first word only (excluding, for example, acronyms and trade names) OR capitalization of first letter of all main words. The chosen style should be used consistently throughout the references. *Note: This only pertains to Journals. All other publications should have initial capitalization of all main words.*
- Inclusive complete starting and ending page numbers (e.g., 711-731 NOT 711-31).

9. Tables. Tabulation of experimental results is encouraged when this leads to more effective presentation or to more economical use of space. Tables should be numbered consecutively in order of citation in the text with Arabic numerals. Footnotes in tables should be given italic lowercase letter designations and cited in the tables as superscripts. The sequence of letters should proceed by row rather than by column. If a reference is cited in both table and text, insert a lettered footnote in the table to refer to the numbered reference in the text. Each table must be provided with a descriptive title that, together with column headings, should make the table self-explanatory.

Titles and footnotes should be on the same page as the table. Tables may be created using a word program text mode or table format feature. The table format feature is preferred. Ensure each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a return at the end of each row. Tables should be inserted in the text where first mentioned.

10. Image Manipulation. According to ACS Ethical Guidelines, images should be free from misleading manipulation. Images included in an account of research performed or in the data collection as part of the research require an accurate description of how the images were generated and produced. Apply digital processing uniformly to images, with both samples and controls. Cropping must be reported in the figure legend. For gels and blots, use of positive and negative controls is highly recommended. Avoid high contrast settings to avoid overexposure of gels and blots. For microscopy, apply color adjustment to entire image and note in the legend. When necessary, authors should include a section on equipment and settings in supporting information to describe all image acquisition tools, techniques and settings, and software used. All final images must have resolutions of 300 dpi or higher. Authors should retain unprocessed data in the event that the Editors request them. Unprocessed data can also be part of the supporting information.

11. Table of Contents Graphic. A graphic entry for the table of contents (TOC) must be supplied as the last page of the manuscript and labeled “Table of Contents graphic.” This *small* graphic should capture the reader's attention and, in conjunction with the manuscript title, should give the reader an idea of the key target compounds or series discussed in the paper. The TOC graphic will also appear in the abstract of the published PDF file. Do not provide a separate abstract graphic.

- A chemical structure should be clearly depicted.
- The TOC graphic should be entirely original work created by one of the coauthors and should not be a duplicate of a graphic appearing elsewhere in the manuscript.
- The TOC graphic should be no wider than 3.25 inches by 1.75 inches (approximately 8.25 cm by 4.45 cm).

For additional information see the ACS Publications Guidelines for Table of Contents/Abstract

Graphics.

12. Molecular Formula Strings. Authors are required to submit SMILES string computer-readable identifiers of molecules discussed in the manuscript along with the associated biochemical and biological data, if applicable as Supporting Information for Publication. It is recognized that some molecules, including antibodies, peptides greater than six amino acids, proteins, etc., do not contribute to the spirit of molecular formula strings and are exempt from this requirement. Judgment regarding exemption of ligands are at the discretion of the Editors. Submission of molecular formula strings and associated data enables enhanced quality control at review and can increase an article's discoverability and citability.

Getting started:

- Creating a Molecular Formula Strings Spreadsheet
- Molecular Formula Strings Template
- Example SMILES Document
- Announcing the use of SMILES in *J Med Chem*

Learn more about SMILES from Dr. Michael Gilson in Digital Chemistry in the *Journal of Medicinal Chemistry* or watch the video.

Instructions for Authors:

1. Use your existing chemical drawing programs (e.g., ChemDraw, ACD ChemSketch, Marvin Sketch) to generate a computer-readable SMILES formula for each compound presented in your article.
2. Paste these formulas into the spreadsheet template, along with basic information about each compound. This spreadsheet will provide a machine-readable version of the key data presented in the article's tables.
3. Upload the final CSV document in ACS Paragon Plus at the time of manuscript submission as Supporting Information for Publication.

13. Supporting Information. Authors are encouraged to make use of this resource when manuscripts contain extensive tabulations of data that are of interest only to those readers who may need more complete data.

The first page of the supporting information file should contain the title of the manuscript, the names of all authors, and a table of contents including page numbers; label this page “Supporting Information”. The pages must be consecutively numbered S1 (the title page), S2, etc. Figure captions, titles to tables, and other identifying captions should appear on the same page as the figures or tables. Supporting information may be single-spaced. Generally, if one has difficulty reading the material as submitted, it is unacceptable.

All supporting information files of the same type should be prepared as a single file (rather than submitting a series of files containing individual images or structures with the exception of PDB files for computational models). For example, all supporting information available as PDF files should be contained in one PDF file. Author-created file names will be automatically replaced with standardized file names generated at the time of publication.

DO NOT UPLOAD FIGURES AND TABLES THAT ARE TO BE PUBLISHED IN THE MANUSCRIPT AS SUPPORTING INFORMATION FILES.

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

1. 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.

2. 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.

3. 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.

Cover Letter: The letter should contain the Journal purity statement (which should also be stated in the general experimental section of the manuscript) that “All compounds are >95% pure by HPLC analysis.” HPLC traces should be included for all compounds that have in vivo data described in the manuscript or, if no in vivo data, a representative number of HPLC traces of compounds described with in vitro data in the SAR tables (HPLC traces should be in the Supporting Information, SI). Alternatively, other methods of purity determination (e.g. elemental analysis) that were used need to be indicated.

4. 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.

5. 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.

6. Computational Chemistry.

6.1 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.

6.2 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.

6.3 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).

6.4 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.

6.5 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.

6.6 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.

6.7 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.

7. 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.

8. 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.

9. 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.

10. 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).

11. 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.

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.

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

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

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

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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

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Authors should submit only original work that has not been previously published and is not under consideration for publication elsewhere. Authors must note any use of a preprint server, patents, and dissertations in the cover letter. The following does not constitute prior publication:

- Academic theses, including those on the Web or at a college Web site.
- Patents
- Preprint servers. Upon publication in the Journal, authors are advised to add a link in the

preprint to the published paper via the Digital Object Identified (DOI).

Editorial Policies

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

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- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
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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.

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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."

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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.

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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.

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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.

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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

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