Scope of the Journal

*ACS Infectious Diseases* invites original articles that highlight the role of chemistry in the multidisciplinary and collaborative field of infectious disease research. The scope of the journal encompasses all aspects of chemistry relating to infectious diseases research including research on pathogens, host-pathogen interactions, therapeutics, diagnostics, vaccines, drug-delivery systems, and other biomedical technology development pertaining to infectious diseases. Authors are encouraged to read a recent Editorial on our scope [here](#).

Some specific areas that are appropriate include the following.

- **Pathogens and Host-Pathogen Interactions.** Use of structural biology, chemical biology, glycobiology, physical chemistry, nucleic acid chemistry, and biochemistry to elucidate molecular mechanisms of pathogenesis. Development of tools to dissect mechanisms of pathogenesis.

- **Therapeutics.** Use of target- and phenotypic-based approaches for discovery and development of new agents to treat infectious diseases, with an emphasis on establishing mechanism of action, understanding binding mode and inhibitory mechanism, and/or discussing pathogen-specific challenges to drug development. Development of new technologies to facilitate characterization, validation, and prioritization of potential drug targets or to assess the physicochemical bases for cellular penetration of anti-infectives.

- **Drug Resistance.** Mechanistic investigations of antimicrobial resistance.

- **Vaccines.** Discovery and development of synthetic vaccines and small molecule vaccine adjuvants. Structural and physical investigations of epitope binding.

- **Diagnostics.** Development of novel and improved diagnostics using physical, surface, analytical, and nano chemistry techniques. Use of structural biology, molecular biology, and chemical biology to investigate diagnostics targets.

- **Drug Delivery Systems.** Use of novel materials and technologies, such as nanotechnologies, for delivery of antimicrobial agents.

Manuscript Types

*ACS Infectious Diseases* publishes original Articles, Featured Articles, Letters, Reviews, Perspectives, and Viewpoints that highlight recent developments and further the understanding of infectious diseases. The Editors welcome the submission of manuscripts in the following categories:

- **Articles.** Concise, yet comprehensive, original research presenting an advance of immediate, broad, and lasting impact. Articles are not intended to be follow-up manuscripts, unless they contain new and extensive information that will advance the understanding of the system or biological process. Articles are peer-reviewed and contain an unreferenced abstract of 250 words or less. Abstracts should not contain abbreviations or acronyms unless essential. A referenced introduction should expand on the background of the work. Articles include the following headed sections (presented in this order): Results and Discussion (can be combined), and Methods. In general, Articles should be less than 6500 words in length and include 7–10 display items.
Featured Articles. The Editors may choose to give “Featured Article” status to any Article at the time of acceptance.

Letters. Short reports of original research focused on an individual significant finding. Letters are peer reviewed and begin with an unreferenced abstract of less than 150 words. Abstracts should not contain abbreviations or acronyms unless essential. Letters include unheaded sections for the Introduction and combined Results and Discussion and a headed section for Methods that can also contain subsections. Letters should contain 4–6 display items (figures/tables/schemes) and ~30 references. Letters should include sufficient experimental detail to allow others to reproduce the findings presented. Supporting Information is encouraged. Letters should be less than 4500 words in length, including the abstract, body text, methods, references, and figure/scheme legends. Letters include a graphical Table of Contents entry and a list of up to six keywords.

Reviews. Topical and of general interest to the readership. Reviews are peer-reviewed and contain an unreferenced abstract of 250 words or less that summarizes the main points. A good Review critically evaluates existing work, provides a logical organization, and makes the material more easily available to those not expert in the area through clear text and figures. The manuscript should contain the following components; a brief introduction of the field such that the general reader can understand (and/or appreciate) the questions that have been the focus of the field in the past 1-3 years, the progress that has been made addressing these questions in recent publications, and a summary putting the recent progress into context for the field. The scope of a Review should be broad enough that it is not dominated by the work of a single laboratory, and particularly not by the authors' own work. It should appeal to the wide readership of ACS Infectious Diseases (chemists, biochemists, molecular biologists, structural biologists & microbiologists). Reviews should be greater than 5000 words in length, include 4–8 display items (figures/tables/schemes), and contain ~100 references. Include a graphical Table of Contents entry consisting of a colorful figure that represents the topic of the Review. Authors may choose to divide the Review into sections preceded by headings. Finally, the journal recommends that authors define key words used in the Review and key concepts in a separate paragraph.

Perspectives. Submitted by invitation only. Perspectives are designed to provide an enlightened appraisal of a field of research in which experts review the “state of the art” for a given topic similar to Reviews. Unlike Reviews, however, authors have editorial freedom to express their views on the strategic directions of the field of research. Perspectives should include a brief introduction of the field such that the general reader can understand (and/or appreciate) the questions that have been the focus of the field in the past 1-3 years, the progress that has been made addressing these questions in recent publications, and a summary putting the recent progress into context of the field and highlighting new questions that may arise or are now within reach in the next 1-3 years. It is best if the authors briefly put the field in perspective and discuss which questions can now be answered by the data in recent publications. The authors should provide a brief statement at the end of the Perspective about where the new data take us and what we should expect in the coming years in this area of research. The scope of a Perspective should be 3000–6000 words in length, include 3–6 display items (figures/tables/scheme), and contain up to 100 references. Authors may choose to divide the Perspective into sections preceded by headings. Finally, the journal recommends that authors
define key words used in the Perspective and key concepts in a separate paragraph. We accept shorter forms of this manuscript type (“Miniperspective”) as long as they discuss emerging topics. Perspectives are submitted via a special link created in the author dashboard.

**Viewpoints. Submitted by invitation only.** Viewpoints are brief non-peer reviewed commentaries on current issues in the infectious diseases field, meant to call attention to a specific topic and encourage dialogue within the community. Responses to Viewpoints or other content will be considered. Viewpoint articles should be approximately 1500 words in length and contain a short abstract (100 words) to highlight the main point. Viewpoints can accommodate up to 2 smaller figures and/or tables. We strongly encourage the use of at least 1 figure. Please limit references to 8-12.

**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

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.

A letter must contain the following elements:
• Manuscript title
• Name of the corresponding author
• Name(s) of any other author(s)
• A paragraph explaining why the paper is appropriate for ACS Infectious Diseases, and
• Note whether the manuscript was discussed with an ACS Infectious Diseases Editor before submission
• A short (~150 word) lay summary (at the level of an undergraduate in chemistry or biochemistry) describing the significance of the study for a broad audience

Manuscript Text Components

Title Page. Titles 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. Include all those who have made substantial contributions to the work. To facilitate indexing and retrieval and for unique identification of an author, use first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and surnames (e.g., J. Robert Smith). 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.

During manuscript submission, the submitting author must provide contact information (full name, e-mail address, institutional affiliation, and mailing address) for each of the co-authors. Because all of the author names are automatically imported into the electronic Journal Publishing Agreement, all author names must be entered into ACS Paragon Plus. (Note that co-authors are not required to register in ACS Paragon Plus.) The author who submits the manuscript for publication accepts the responsibility of notifying all co-authors that the manuscript is being submitted. Deletion of an author after the manuscript has been submitted requires a confirming letter to the Editor-in-Chief from the author whose name is being deleted. For more information on ethical responsibilities of authors, see the Ethical Guidelines to Publication of Chemical Research.

Abstract. All Articles, Letters, Reviews, Perspectives, and Viewpoints must contain an abstract, which should provide a succinct, informative summation of the most important results and conclusions. Ideally, an abstract should be less than 150 words. References cannot be cited in the abstract. Abbreviations should be used sparingly and spelled out when first used. Abstracts display the same graphic provided for the TOC.

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

Introduction. 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. Do not attempt a complete survey of the literature. If a recent article has summarized work on the subject, cite that article without repeating its individual citations. In general, the introductory section should be ~750 words for a letter and ~1000 words for an article. This section does not have a heading.

Results and Discussion. Results should be presented concisely. Tables and figures should be referred to directly, and data should be presented in only one figure or table. In the interest of economy of space, Supporting Information (also subject to review) should be submitted as a separate file. The discussion should interpret the results, relate them to existing knowledge in the field, and clearly state their significance. To conserve space, please submit supplemental information as a single PDF as Supporting Information for Review. The Results and Discussion sections in Research Articles may be combined into a single section or described separately (preferred). Please use section headings.

Conclusion. Authors should write a brief conclusion that succinctly highlights the key findings of the paper and their significance.

Experimental Section. Provide a clear, unambiguous description of materials, methods, and equipment in sufficient detail to permit repetition of the work elsewhere. Describe novel experimental procedures in detail, but refer to published procedures by literature citation of both the original and any published modifications. Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the full article or communication. Experimental 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.

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 material 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.”
- **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 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., "Mtbb, Mycobacterium tuberculosis". 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 in The ACS Style Guide (http://pubs.acs.org/series/styleguide) or those accepted by the Journal of Medicinal Chemistry (http://pubs.acs.org/paragonplus/submission/jmcmar/jmcmar_abbreviations.pdf).

References and Notes. Number literature references and notes in one consecutive series by order of mention in the text. Numbers in the text are non-parenthesized superscripts. The accuracy of the references is the responsibility of the author. List all authors; do not use et al. Provide inclusive page numbers. Titles may have capitalization of first word only (excluding, for example, acronyms and trade names) or standard capitalization as shown below. The chosen style should be used consistently throughout the references. Double-space the references using the format shown below.

Compile all references together in a list at the end of the manuscript text. Many of them will have links to other web resources, such as the corresponding abstracts in Chemical Abstracts and the full text on publisher websites. 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. Avoid unnecessarily long lists of references. However, authors must reference all previous publications in which portions of the present work have appeared. Avoid long references; place additional data and peripheral discussion in the Supporting Information rather than in references. Supplementary references may be placed in Supporting Information. Literature references must be numbered with Arabic numerals in the order of their first citation in the text and the corresponding numbers inserted at the appropriate locations in the text.

Titles of journals are abbreviated according to Chemical Abstracts Service Source Index (CASSI, http://cassi.cas.org/search.jsp). Manuscripts accepted for publication are cited as “in press”; the DOI should be given if the paper is published online. Cite manuscripts that are in preparation or have been submitted but not yet accepted as unpublished experiments or personal communications.

- **Journals:** Gehrke, S. S., Kumar, G., Yokubynas, N. A., Côté, J. P., Wang, W., French, S.,

- Serial publications like Methods in Enzymology should be listed in the same form as journals.
- Journal articles published online ahead of print or online only, the DOI should be used:

**Tables.** Tabulation of experimental results is encouraged when this leads to more effective presentation or to more economical use of space. Titles and footnotes should be on the same page as the table. Tables may be created using a word processor’s 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. Submit within the body of the manuscript text file.

- Number consecutively using Arabic numbers.
- Include a descriptive heading that, together with the individual column headings, makes the table self-explanatory.
- Give footnotes letter designations and cite them in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column.
- When a reference is cited, insert a lettered footnote in the table and put the reference number in a footnote.
- When columns are used, arrange data efficiently to save space.
- Place crystallographic and NMR data tables last in a series of tables in a manuscript, because they are generally placed in the Methods section.

Include list of sections/components specific to Journal with any descriptions (if needed). Title, Author List, Abstract, Keywords, Main Text (Introduction, Experimental, Results, Discussion/Conclusion), Acknowledgement, References (NOTE: references upon submission must follow Review-Ready Submission requirements, graphics included in separate section).

**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**

**Web Enhanced Objects Such as Movies.** ACS Infectious Diseases encourages the use of multimedia attachments such as animations and movies. These objects should complement a reader’s understanding of the research being reported. For acceptable file formats and specifications please refer to the web page on Specifications for Web Enhanced Objects.

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

**Data Presentation**

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

For more information on data presentation, see:

a. Quantifying the Interactions between Biomolecules: Guidelines for Assay Design and Data Analysis
Purity of Tested Compounds. 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 Infectious Diseases*, it is required that assayed compounds be at least 95% pure. The analytical methods used for compound characterization and purity assessment should be described in the Methods section.

- **Methods**: All scientifically established methods to evaluate purity (e.g., HPLC, combustion analysis, absolute quantitative $^1$H NMR, qHNMR) are acceptable. If the target compounds are solvated, the quantity of solvent should be included in the compound formulas. No documentation is required with the exception of qHNMR (see Purity by Absolute qNMR instructions).

- **Purity Percentage**: All tested compounds, whether synthesized or purchased, should possess a purity of at least 95%. Compound purities less than 95% may be accepted on a case-by-case basis at the editor's discretion, if appropriate documentation is provided on the present impurities and/or the compound is inactive.

- **Elemental analysis**: Found values for carbon, hydrogen, and nitrogen (if present) should be within 0.5% 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 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.

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 (see this Editorial in *ACS Infectious Diseases* on the Ecstasy and Agony of Assay Interference Compounds). 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. Provide firm experimental evidence in at least two different assays that reported compounds with potential liability are specifically active and their apparent activity is not an artifact. The most common artifact in assays is due to colloidal aggregation, which can be evaluated by a number of methods as described in the above cited Editorial.

Compound Characterization. Manuscripts for *ACS Infectious Diseases* should provide characterization data for all compounds, including $^1$H NMR, $^{13}$C NMR (peak lists), and HRMS and preferably full characterization of all compounds described. Infrared absorbances (IR), specific optical rotation, and melting points may be included, but are not required. 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 purely based on mixture synthesis and/or mixture analysis is discouraged. Peptides should be characterized by HRMS and HPLC. Macromolecules and polymers should be characterized using established methods in their respective field. For nanomaterials, the stability and reactivity of the nanomaterials as well as influence of external parameters like the composition of cell culture media, buffers, etc., on nanomaterial properties should be addressed, for example by measuring dissolution, formation of reactive oxygen species...
or agglomeration under experimental conditions, and physical characterization techniques for nanomaterials should be sufficient, including description of algorithms and methods used to analyze the data. Please review the following resource:

- Minimum information reporting in bio-nano experimental literature

**Computational Chemistry.** Practical applications of existing computational methods combined with original experimental data will be considered for publication. Manuscripts that report prospective computational design, synthesis, and experimental evaluation of new chemical entities are highly encouraged. Applications of computational methods are not considered without original experimental data that assess the validity of computational predictions. QSAR modeling is acceptable only if a significant number of new compounds are predicted, prepared, and tested. 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, software, software parameters, and molecular structures used to generate and/or validate computational models must be described in the paper or reported in the Supporting Information. The use of proprietary algorithms and datasets (including force field parameters, descriptors, formulae, equations and constants) is not acceptable (if it limits the ability of the community to reproduce the results). Commercial software and datasets employed must be adequately described and cited to ensure reliable reproduction of results.

All three-dimensional models described in the manuscript must be included in the Supporting Information or adequately cited to ensure reproducibility of the calculations, models, and reported findings. This requirement includes models described in figures or tables (such as protein-ligand binding modes). In this case, the complete structure should be reported in the Supporting Information. Hydrogen-suppressed atomic models must be provided in standard PDB-formatted coordinate files. Models derived from known X-ray structures must provide the IDs of crystal structures used as starting templates applied in model building or docking studies.

Pure computational studies, algorithm comparisons, virtual screens, and statistical analyses of datasets will not be considered for publication.

**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 or strain used 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. Clearly state in the experimental section how many replicates and independent experiments were performed for the key target compounds to generate the biological data presented.

Active key target compounds obtained from high-throughput screening, combinatorial syntheses, etc… 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, confirmation in an orthogonal assay of the lead molecule(s) biological activity is 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., µM, nM) and doses in animals should be expressed in weight/weight or molar quantities (e.g., mg/kg, µmol/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 on Statistical Criteria for more detailed requirements.

Biological Specimens

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

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

1. A resource for cell line authentication, annotation and quality control
2. Cell Lines as Biological Models: Practical Steps for More Reliable Research
3. Cell and Microbial Authentication

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

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

i. Further information on research involving animal and human subjects can be found in the following resources:
   - ACS Ethical Guidelines
   - Ethics and biosecurity

ii. For key reagents and tools, we recommend the use of Research Resource Identifiers:
   - https://scicrunch.org/resources

e. Biological Assays: Assay interference can cause misleading results. Thus, appropriate controls experiments should be performed to exclude common artefacts caused by reactive molecules (covalent and redox activity), colloidal aggregation, decomposition, and interference with the spectroscopic method. Authors should consult the recent ACS Editorial on assay interference compounds. The routes of administration of test compounds and vehicles should also be indicated. Benchmarks should be included in the form of appropriate positive or negative control substances or reference materials. Especially for studies on nanomaterials, additional steps and controls are needed such as sterilization procedures, checking assays for optical or chemical interferences, reporting different measuring units related to dose (e.g. surface area, mass, particle number per surface area, volume, cell number), and others as described in:
   - ARRIVE (Animal Research: Reporting of In Vivo Experiments) guidelines
   - Minimum information reporting in bio-nano experimental literature

Statistical Criteria. Appropriate statistical assessment is equally important for experimental and computational studies in medicinal chemistry. Reported results generally require statistical validation. 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. Statistical analyses of compound data are also frequently presented, which must adhere to acceptable statistical and scientific standards. The following points should be considered:

a. Statistical analyses must adhere to acceptable statistical and scientific standards.

b. Use of the term “significant” should be reserved for describing a relationship evaluated by appropriate statistical analysis. Please consider these resources:
   - Moving to a World Beyond “p < 0.05
   - It’s time to talk about ditching statistical significance

c. A clear and comprehensive description of experimental data or computed data underlying the analysis is required.

d. Appropriate statistical tests must be used for given data sets and attention should be given to data that are not normally distributed. In these cases, the appropriate non-parametric test should be used. Please see this resource for further information on this topic:
   - Parametric and Nonparametric: Demystifying the Terms

e. Statistical methods used must be clearly identified, including whether they were one- or two-tailed. Non-standard statistical methods should be described in detail or precisely referenced.

f. Underlying assumptions of statistical methods should be specified. For example, many statistical tests assume the presence of normal data distributions, which is often an approximation.

g. Depending on the type of data, either confidence limits (CL), standard deviations (SD), or standard errors of the mean (SEM) must accompany a mean value provided in either graphical or tabular form. The experimental section for each assay performed should indicate the number of replicates and independent experiments as well as the statistical method used for data analysis. For example, assay curves must contain errors bars derived from multiple measurements.
h. For regression curves, uncertainty must be assessed by plotting original data along the curve or by establishing experimental or calculation confidence limits.

i. If average values are reported from computational analysis, their variance must be documented. This can be accomplished by providing the number of times calculations have been repeated, mean values, and standard deviations (or standard errors). Alternatively, median values and percentile ranges can be provided. Data might also be summarized in scatter plots or box plots.

j. Reporting averages of data assigned to pre-defined value ranges and ‘averages of average values’ must be avoided.

k. For data that are not normally distributed, or for small sample sizes, appropriate statistical tests should be used.

l. Standard measures (mean, median) and error bars must be stated for each dataset. If a sample size is small and/or not normally distributed, then mean or standard deviation calculations are not appropriate. In data tables, errors associated with the means presented needs to be provided.

m. Provide exact p values regardless of overall significance.

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

Sequence Data. We ask that all authors submit sequence data to a public repository prior to submission and include accession numbers in their paper where appropriate. Examples of suitable public repositories for DNA and RNA sequences include GenBank or Protein DataBank; nucleic acid sequencing data can be deposited in NCBI Trace Archive or NCBI Sequence Read Archive (SRA). High-throughput sequencing data can be submitted to GEO. Protein sequences can be submitted to Uniprot.

Structural Data. The atomic coordinates and related experimental data (structure factor amplitudes/intensities and/or NMR restraints) associated with a structure reported in ACS Infectious Diseases must be deposited at a member site of the Worldwide Protein Data Bank (www.wwpdb.org): RCSB PDB (www.pdb.org), PDBe (www.ebi.ac.uk/pdbe), PDBj (www.pdbj.org), or BMRB (www.bmrdb.wisc.edu). The PDB ID should be included in the manuscript. Authors must agree to release the atomic coordinates and experimental data when the associated article is.
Manuscripts that report X-ray crystallographic structures should include a table of data statistics that contains the number of reflections, data cutoff (e.g., $F > 0$), $R_{work}/R_{free}$, $I/\sigma(I)$, percent completeness, redundancy, $R_{merge}$, number of atoms per asymmetric unit, and $B$-factors for protein, waters, and ligands/ions. For papers that involve NMR studies in which complete or nearly complete resonance assignments of biopolymers have been carried out, authors are required to deposit relevant NMR assignments and related experimental data at the BioMagResBank (BMRB; Biological Magnetic Resonance Bank). These data may include assigned chemical shifts, coupling constants, relaxation parameters ($T_1$, $T_2$, and NOE values), dipolar couplings, or other data accepted by BMRB. The author is responsible for obtaining a BMRB entry accession number (e.g., 4248), which should appear in a data deposition paragraph. The data must be released upon publication.

Crystallographic data on nucleosides, nucleotides, and other small molecules should be submitted upon publication to the Cambridge Structural Database. Crystal structures of nucleic acids should be deposited with the Nucleic Acid Database (NDB) at Nucleic Acid Database (NDB) or with the RCSB PDB at RCSB Protein Data Bank - RCSB PDB.

For papers describing structures of biological macromolecules from electron microscopy experiments, the 3D map should be deposited at either the Protein Data Bank in Europe (UK) or RCSB (USA) EMDB deposition site. Once the map has been deposited, any fitted atomic coordinates should be deposited with the Protein Data Bank (PDB) by following the link provided from the EMDB deposition session. The EMDB and PDB IDs should be included in the manuscript. Both the map and the coordinate data will be made public when the associated article is published. Methods for Motion Correction and CTF estimation during image analysis and details of the process used for initial model generation should be provided. Authors should also provide the commands used to generate Masks for postprocessing of refined maps. Both the non-post-processed final maps and the corresponding sharpened maps should be submitted to the appropriate database.

Manuscripts dealing with the development of structures from sequence homology are generally not considered unless significant experimental tests of the model also are presented.

Animal Data. 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. It is encouraged that all figure and table captions include the number of animals and sex for each treatment group, the method of statistical analysis as well as the corresponding p-values where significant differences are found.

**Database Deposition**

**Sequence Data.** Papers 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. Authors should submit sequence data to a public repository prior to submission and include accession numbers in their paper where appropriate.

a. High-throughput sequencing data: GEO
b. DNA and RNA sequences: GenBank or Protein DataBank
c. Nucleic acid sequencing data: NCBI Trace Archive or NCBI Sequence Read Archive (SRA)
d. Protein sequences: Uniprot

Crystal and NMR Structures Structural Data. Small molecular crystallographic data should be submitted upon publication to the publication to the Cambridge Structural Database Cambridge Structural Database (www.ccdc.cam.ac.uk). Crystal structures of nucleic acids should be deposited with the Nucleic Acid Database (ND) at Nucleic Acid Database (ND) or with the RCSB PDB at RCSB Protein Data Bank - RCSB PDB. Papers reporting macromolecular NMR or crystal structures must specifically state that the atomic coordinates have been deposited at a member site of the Worldwide Protein Data Bank; RCSB PDB, PDBe, PDBj, or BMRB. The PDB ID should be included in the manuscript. Authors must upload map density files, PDB files and PDB validation reports as Supporting Information for Review only. Authors must agree to release the atomic coordinates and experimental data when the associated article is published. A manuscript will be accepted only after receipt from the submitting author of a written statement that the coordinates have been deposited. Coordinates must be released immediately upon publication 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 papers 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.bmrbrisc.edu).

a. Biomolecule Structures:
  i. NMR Studies of Biopolymers: Deposition of relevant NMR assignments and related experimental data at the BioMagResBank is required. The author is responsible for obtaining a BMRB entry accession number, which should appear in a data deposition paragraph. The data must be released upon publication.

b. Biological Macromolecules from Electron Microscopy Experiments: Density maps should be deposited at either the Protein Data Bank in Europe (UK) or RCSB (USA) EMDB deposition site. Once the map has been deposited, any fitted atomic coordinates should be deposited with the Protein Data Bank (PDB) by following the link provided from the EMDB deposition session. The EMDB and PDB IDs should be included in the manuscript. Both the map and the coordinate data will be made public when the associated article is published.

c. Structures from Sequence Homology: Manuscripts dealing with the development of structures from sequence homology are generally not considered unless significant experimental tests of the model also are presented.

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 (pdbj.org), or the Protein Data Bank 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 included in the published manuscript. Please reference the Microarray Gene Expression Data (MGED) open letter specifying microarray standards here.

**Genetically Modified Organisms and Mutants.** Use established repositories such as the Jackson Laboratory, the Mutant Mouse Regional Resource Center, the American Type Culture Collection, the UK Stem Cell Bank, or another public storage area whenever possible. Large datasets for which an approved database has not yet been established must be housed as online Supporting Information on the journal’s website.

**Material and Data Availability.** *ACS Infectious Diseases* understands that communication and collaboration between chemists and biologists are significantly enhanced when materials and data can be exchanged among scientists. Therefore, a condition of publication is that authors are required to make materials, data, and protocols available to readers through deposition in a publicly used database. Hosting on an author’s website is not an acceptable substitute. Authors also agree to make available to interested academic researchers for their own use any materials reported in their manuscript that are not otherwise obtainable. Any restrictions to the availability of materials or information must be stated at the time of submission.

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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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- Once in the abstract.
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- Will provide assurance that animals used in the study were cared for in accordance with institutional guidelines;
- Will verify that, in human studies, consent was obtained after the consequences of the studies had been explained to the experimental subjects (all research on humans must have IRB approval);
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Appendix 1: PREPARING FOR SUBMISSION

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

Ethical Guidelines

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

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As a U.S.-based non-profit organization, the American Chemical Society (ACS) is required to comply with U.S. sanctions laws and regulations administered by the U.S. Treasury Department’s Office of Foreign Assets Control (OFAC). While these laws and regulations permit U.S.-based publishers like ACS to engage in publishing-related activities with authors located in sanctioned regions in many cases, ACS may be prohibited under U.S. law from engaging in publishing-related activities in some cases, including, but not limited to, instances where an author or the institution with which an author is affiliated is located in a particular sanctioned region or has been designated by OFAC as a Specially Designated National (SDN) pursuant to certain U.S. sanctions programs. ACS reserves the right to refrain from engaging in any publishing-related activities that ACS determines in its sole discretion may be in violation of U.S. law.

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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.

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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.

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