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## Scope of the Journal

[ACS Infectious Diseases](#) is the first journal to highlight chemistry and its role 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. We encourage submissions covering all pathogens, including bacteria, viruses, parasites and fungi. We also encourage submissions related to microbial toxins and prions.

With editors well-versed in both chemistry and the biology of infectious diseases, the journal aims to bridge the gap between these two disciplines. *ACS Infectious Diseases* welcomes submission of articles reporting investigations into chemistry and biology of infectious diseases, and encourages discussions centered on specific pathogen- and disease-related issues. Manuscripts dealing with epidemiological studies, or clinical case reports are outside the scope of *ACS Infectious Diseases*.

Topics covered by the journal include but are not limited to the following:

- **Therapeutics.** Use of target-, phenotypic-, or computational-based approaches for discovery and development of new agents to treat infectious diseases or to regulate the host-pathogen interaction, 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. Chemistry-driven immunomodulatory therapeutics for mitigating infection associated inflammation. Host-directed antimicrobial therapeutics
- **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.
- **Anti-infective Biomaterials and Drug Delivery Systems.** Novel biomaterials to mitigate infections. Use of novel materials and technologies, such as nanotechnologies, for delivery of antimicrobial agents.
- **Drug Resistance.** Mechanistic investigations of antimicrobial resistance.
- **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. Mechanistic understanding of inflammation and infection interplay. Host-microbiome and pathogen interactions in context of infection, immunity, and inflammation.
- **Vaccines.** Discovery and development of synthetic vaccines and small molecule vaccine adjuvants. Structural, physical, or computational investigations of epitope binding.

## 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. An introduction should expand on the background of the work and should not have a header. Articles include the following headed sections (presented in this order): Results and Discussion (can be combined), and Methods (after the conclusion or at the end of the manuscript if there is no conclusion). In general, Articles should be less than 6500 words in length and include 7–10 display items (figures/tables/schemes) and ~50 references. Supporting Information may be included. Articles include a graphical Table of Contents entry and a list of up to six keywords.

## **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. Author should be a recognized expert in the field. 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 review should provide critical analysis of the topic, and insights about the challenges and future direction of 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. Potential authors are encouraged to write to the editor with a proposal/plan for the review.

## 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 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). Perspectives are peer-reviewed, contain an unreferenced abstract of 250 words or less, and include a graphical Table of Contents. Perspectives 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 Researcher Resources

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit [ACS Researcher Resources](#) for additional information on everything that is needed to prepare (and

review) manuscripts for ACS journals and partner journals, such as

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

## Manuscript Preparation

### Submit with Fast Format

All ACS journals and partner journals have simplified their formatting requirements in favor of a streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers [here](#).

Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- When required by a journal's structure or length limitations, manuscript templates should be used.
- References can be provided in any style, but they must be complete, including titles. For information about the required components of different reference types, please refer to the [ACS Style Quick Guide](#).
- Supporting Information must be submitted as a separate file(s).

### Document Templates and Format

The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates [here](#).

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

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

See the list of [Acceptable Software](#) and appropriate [File Designations](#) to be sure your file types

are compatible with the submission system. Information for manuscripts generated from [TeX/LaTeX](#) is also available.

## Cover Letter

A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

A cover letter must contain the following elements:

- Manuscript title
- Name of the corresponding author, with contact information
- Name(s) of all other author(s)
- Highlight of the manuscript, and its novelty and relevance in the field
- A paragraph explaining why the manuscript is appropriate for *ACS Infectious Diseases*
- Note whether the manuscript was discussed with an *ACS Infectious Diseases* Editor before submission
- Note any use of a preprint server, and as appropriate, state how the manuscript has been adjusted/updated between deposition and 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. Refer to the [Authorship, Author List, and Coauthor Notification](#) section in the Appendix of these Guidelines for complete information.

### 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. Figure captions (or table titles) must always accompany the respective 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. Please use section headings.

## **Conclusion**

Authors should write a brief conclusion that succinctly highlights the key findings of the manuscript 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. The section should be headed as “Materials and Methods” or “Methods”. 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.

## **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 manuscript, e.g., "*Mtb*, *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 Guide to Scholarly Communication](#) or those accepted by the *Journal of Medicinal Chemistry* ([http://pubs.acs.org/paragonplus/submission/jmcmr/jmcmr\\_abbreviations.pdf](http://pubs.acs.org/paragonplus/submission/jmcmr/jmcmr_abbreviations.pdf)).

## References and Notes

Number literature references and notes in one consecutive series by order of mention in the text. The accuracy of the references is the responsibility of the author. Compile all references together in a list at the end of the manuscript text. Authors must also cite any previously published work wherein portions of the submitted work have been disclosed. 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). Manuscripts accepted for publication are cited as "in press"; the DOI should be given if the article is published online. Cite manuscripts that are in preparation or have been submitted but not yet accepted as unpublished experiments or personal communications. Authors should consult [The ACS Guide to Scholarly Communication](#) for the appropriate style to use in citations of journal articles, books, and other publications.

## Supporting Information

This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of [Acceptable Software by File Designation](#) and confirm that your Supporting Information is [viewable](#).

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief, nonsentence description of the actual contents of each file, including the file type extension, is required. This description should be labeled Supporting Information and should appear before the Acknowledgement and Reference sections. Examples of sufficient and insufficient descriptions are as follows:

Examples of sufficient descriptions: "Supporting Information:  $^1\text{H}$  NMR spectra for all compounds (PDF)" or "Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)".

Examples of insufficient descriptions: "Supporting Information: Figures S1-S3" or "Additional figures as mentioned in the text".

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

## Research Data Policy

All ACS journals strongly encourage authors to make the research data underlying their articles publicly available at the time of publication.

*Research data* is defined as materials and information used in the experiments that enable the validation of the conclusions drawn in the article, including primary data produced by the authors for the study being reported, secondary data reused or analyzed by the authors for the study, and any other materials necessary to reproduce or replicate the results.

The [ACS Research Data Policy](#) provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

## Data Requirements

### 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 article.

## Data Presentation

Data should be presented in a way that makes interpretation clear to the reader.

For more information on data presentation, see:

- [Quantifying the Interactions between Biomolecules: Guidelines for Assay Design and Data Analysis](#)
- [Beyond Bar and Line Graphs: Time for a New Data Presentation Paradigm](#)

## Purity of Tested Compounds

Disclosure of structure and/or composition, with adequate characterization is essential for manuscripts which report antimicrobial activity. 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  $^1\text{H}$  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.



- *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 several methods as described in the above cited Editorial.

## Compound Characterization

The knowledge of the structure and 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 recommended to refer to the Compound Characterization requirements in the [Organic Chemistry ACS Research Data Guidelines](#) for comprehensive instructions. Reviewers will assess the overall thoroughness of the characterization of synthesized compounds using these guidelines.

## Computational Chemistry

When computational chemistry is a major component of a study, manuscripts must fall into one or more of the following categories. It is encouraged to include experimental validation of theoretical aspects.

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

When manuscripts combine computational and experimental studies, both components must be significant. For example, computational analyses are not automatically validated by the addition of a minor experimental component. For manuscripts reporting virtual screening results, purity data

should conform to journal purity requirements for all experimentally tested active compounds, and convincing experimental data should be provided that demonstrate true biological activity of identified hits. For manuscripts describing new methods, the scope of the method must be validated convincingly.

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

## Biological Data

Biological test methods must be referenced or described in sufficient detail (in the main text or preferably in the Supporting Information) to permit the experiments to be repeated by others. The methods used should be relevant to the purpose of the study. Authors should be cognizant of significant figures for their measurements when reporting biological data. A statement regarding inherent error, such as standard deviation, standard error of the mean (SEM), or the like, should be provided. The error limits themselves need not be presented in the main text but can appear in the Supporting Information. The number of experiments for a given data point (e.g.,  $N = 3$ ) should be indicated in some manner. *In vivo* biological data should be accompanied by statistical limits (statistical significance). Doses and concentrations should be expressed as molar quantities (e.g., mol/kg, nM) whenever possible. Exceptions include antibiotic concentrations for which  $\mu\text{g/mL}$  has traditionally been used. For further information regarding the use of biological specimens including antibodies, cell lines and microorganisms, human subjects, animal subjects, and biological assays, refer [here](#).

## 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 clear and comprehensive description of experimental data or computed data underlying the analysis is required.
- 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.
- 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.
- 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.
- Depending on the type of data, either confidence limits (CL), standard deviations (SD), or

standard errors of the mean (SEM) must accompany a mean value provided in either graphical or tabular form. The experimental section for each assay performed should indicate the number of replicates and independent experiments as well as the statistical method used for data analysis. For example, assay curves must contain error bars derived from multiple measurements.

- For regression curves, uncertainty must be assessed by plotting original data along the curve or by establishing experimental or calculation confidence limits.
- 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.
- Reporting averages of data assigned to pre-defined value ranges and 'averages of average values' must be avoided.
- 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/](http://www.beilstein-strenda-db.org/strenda/)) for detailed guidelines on how this data should be organized and formatted. For publication in *ACS Infectious Diseases*, reporting of 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. Conditions essential to reproduce the results such as the temperature, pH, and pressure (if other than atmospheric) of the assay should 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.

## 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](http://www.wwpdb.org)): RCSB PDB ([www.pdb.org](http://www.pdb.org)), PDBe ([www.ebi.ac.uk/pdbe](http://www.ebi.ac.uk/pdbe)), PDBj ([www.pdbj.org](http://www.pdbj.org)), or BMRB ([www.bmrwisc.edu](http://www.bmrwisc.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 published. Questions relating to depositions should be sent to [deposit@wwpdb.org](mailto:deposit@wwpdb.org). 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. Refer to the [NMR Guidelines for ACS Journals](#) for more information.

Manuscripts that report X-ray crystallographic structures should include a table of data statistics that contains the number of reflections, data cutoff (e.g.,  $F > 0$ ),  $R_{work}/R_{free}$ ,  $I(\sigma)$ , percent completeness, redundancy,  $R_{merge}$ , number of atoms per asymmetric unit, and  $B$ -factors for protein, waters, and ligands/ions. For manuscripts 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 manuscripts 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.

## Database Deposition

### Sequence Data

Authors should refer to the [Biological Data Guidelines](#) for information on submitting sequence data to the appropriate public repository.

### Crystal and NMR Structures Structural Data

Small molecular crystallographic data should be submitted upon publication to the [Cambridge Structural Database](#). Manuscripts reporting macromolecular NMR or crystal structures must specifically state that the atomic coordinates have been deposited in the [Protein Data Bank \(PDB\)](#) or the [Nucleic Acid Knowledgebase](#) and must list the accession code(s). These coordinates must be designated “for immediate release upon publication”. Authors of manuscripts reporting X-ray crystal structures are encouraged to deposit the structure factor files in the PDB. No formal requirement exists for deposition of NMR assignments and constraints (see the [Biological Magnetic Resonance Data Bank](#)).

- **Biomolecule Structures:** NMR Studies of Biopolymers: Deposition of relevant NMR assignments and related experimental data at the [BioMagResBank](#) is required. The author is responsible for obtaining a BMRB entry accession number, which should appear in a data deposition paragraph. The data must be released upon publication.
- **Biological Macromolecules from Electron Microscopy Experiments:** Density maps should be deposited at either the [Protein Data Bank in Europe](#) or RCSB [EMDB deposition site](#). Once

the map has been deposited, any fitted atomic coordinates should be deposited with the Protein Data Bank (PDB) by following the link provided from the EMDB deposition session. The EMDB and PDB IDs should be included in the manuscript. Both the map and the coordinate data will be made public when the associated article is published.

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

### **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](#), the [Protein Data Bank Japan](#), or the [Protein Databank in Europe \(PDBe\)](#).

### **Microarray Data**

Data must be submitted to the [Genome Expression Omnibus \(GEO\)](#) or [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.

### **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.

## **Language and Editing Services**

A well-written paper helps share your results most clearly. ACS Publications' [English Editing Service](#) is designed to help scientists communicate their research effectively. Our subject-matter expert editors will edit your manuscript for grammar, spelling, and other language errors so your ideas are presented at their best.

## **Preparing Graphics**

The quality of illustrations in ACS journals and partner journals depends on the quality of the original files provided by the authors. Figures are not modified or enhanced by journal production

staff. All graphics must be prepared and submitted in digital format.

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

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

## Figure and Illustration Services

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## Appendix 2: Preparing Graphics

### Resolution

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

- Color art, 300 dpi

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## 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.

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