

## Scope of the Journal

*Chemical Research in Toxicology* publishes Articles, Communications, Reviews, Perspectives, Letters to the Editor, and ToxWatch on a wide range of topics in Toxicology that inform a chemical and molecular understanding and capacity to predict biological outcomes on the basis of structures and processes. The overarching goal of activities reported in the Journal are to provide knowledge and innovative approaches needed to promote intelligent solutions for human safety and ecosystem preservation. The journal emphasizes insight concerning mechanisms of toxicity over phenomenological observations. It upholds rigorous chemical, physical and mathematical standards for characterization and application of modern techniques. Representative research includes:

1. Studies concerning the molecular mechanisms by which physical, chemical, or biological agents or materials, interact with and perturb the normal function and/or structure of biological systems, including living organisms, cells, or biomolecules.
2. Studies that address hypotheses concerning mechanisms of adverse or therapeutic responses, or contribute to the development of models of toxic/biological function on the basis of quantifying chemical, molecular and cellular responses to physical, chemical, or biological agents or materials.
3. Studies involving data resulting from high content characterization of molecular responses to agents from the use of bioanalytical approaches such as proteomics, metabolomics, lipidomics, genomics, high content imaging, multi-omics, etc. to characterize targeted patterns or global cellular responses, as well as studies that use novel or existing data to create new models for quantifying exposures or building predictive models of biological pathways or networks.
4. The identification and characterization of potentially hazardous agents such as environmental contaminants, industrial chemicals, drugs and drug-like molecules, natural products, biological toxins and engineered nanomaterials, and the development and application of novel methodologies for their detection and/or characterizations of their interactions with biological systems or biomolecules.
5. Studies concerning pathological biochemistry and molecular mechanisms of disease etiology involving exogenous as well as endogenous agents and/or molecular pathways or networks.

In the case of uncertainty regarding the suitability of a manuscript, authors may send a pre-submission inquiry to the Editor that includes an abstract and cover letter indicating the intended manuscript format by e-mail ([eic@crt.acs.org](mailto:eic@crt.acs.org)).

## Manuscript Types

Reviews, Perspectives, Letters to the Editor, and ToxWatch. See the Manuscript Organization section for details concerning the technical organization for each manuscript type.

- **Articles:** <300 word abstract; no limit on length, figures/tables, or references
- **Communications:** 3000 word limit; <100 word abstract; ~5 or fewer figures/tables; ~30 references

- **Reviews:** <300 word abstract; no limit on length, figures/tables, or references
- **Perspectives:** 3000-6000 words; <300 word abstract; no limits on figures/tables or references
- **ToxWatch:** 1000 words; 250-character abstract; maximum 5 references 1 figure: 7 in width x 9 in. height (or 504 pt x 648 pt)
- **Letters to the Editor:** 2000 words; no abstract; 0-1 figures/tables; maximum 5 references

## Articles

Comprehensive accounts of significant original research should be submitted as Articles.

## Communications

Timely topics that are important and of urgent interest should be submitted as Communications. We aim for a decision within three weeks of receipt. Only minor revisions, completed within ten days, are possible. Any manuscript deemed publishable but requiring a major revision may be further considered as an article. Authors should review the Journal's Preparation of Manuscripts (below) prior to submission of a manuscript. Communications are strictly limited to 3,000 words.

## Reviews

Comprehensive reviews of topics within the scope of the journal and supported by significant literature should be submitted as reviews. Short reviews of recent literature that update a topic are also considered. The information in Reviews should be presented objectively, not limited to the contributions of the authors, and written with the intent of familiarizing the general reader with the broad current state of knowledge of a topic of active interest. The length of reviews should be commensurate with the information available; there are no formal limitations on length.

## Perspectives

Manuscripts that discuss particular issues about which the author has expertise, for example introducing new concepts, proposing original models, offering the author's interpretation of statistical trends, or weighing in on a controversy, should be submitted as perspectives. Perspectives contain approximately 3,000-6,000 words and have no limitations on figures, tables or references.

## Letters to the Editor

Communication with the readership of the journal, for example, highlighting important concerns or differences of interpretation of scientific or policy matters relevant to all areas of Toxicology should be submitted as Letters to the Editor. In topics of controversy, contributions from investigators with differing viewpoints may be invited by the Editors. Letters to the Editor should be limited to 2,000 words and are subject to editorial, but not peer review.

## ToxWatch

Forum in which interesting perspectives and opinions on current issues in Toxicology including aspects of policy, risk assessment practices, and in explaining how particular research findings in toxicology are anticipated to impact society. These pieces are written in a way that they are accessible by a wide audience, clearly explaining key background information. These articles

should also provide a critical evaluation of policies, practices, or scientific work they are addressing. ToxWatch contain approximately 1000 words, a single unnumbered high resolution image without caption that is 7 in. width x 9 in. height (vertical), 7 in. height x 9 in. width (horizontal) or 504 pt x 648 pt graphic, and a maximum of 5 references. This graphic should be used as TOC graphic. ToxWatch is subject to editorial, but not peer review.

## 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.
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- [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](#).

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## 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.

We encourage you to view [Publishing Your Research 101- Episode 2 on Writing Your Cover Letter](#).

## Manuscript Text Components

**Title Page.** A brief and informative title (preferably fewer than 12 words) will aid in the classification and indexing of the paper. Do not use trade names of drugs, jargon, or abbreviations. Include keywords. List full names and institutional affiliations of all authors, and if differentiation is necessary, indicate the affiliations of each author by the superscript symbols <sup>†</sup>, <sup>‡</sup>, <sup>§</sup>, , , etc. These symbols should also be used to indicate author affiliations different from those stated on the title page and present address information. The author to whom correspondence should be addressed is indicated by an asterisk. It is implicit in listing a person as an author that this individual has agreed to appear as an author of the manuscript.

**Table of Contents Graphic.** A Table of Contents (TOC) graphic is published with each manuscript. It is submitted for use in the table of contents and is also used for multiple purposes, including the document abstract and other situations where a representative graphic is required. Create an image that represents the work while adhering to size constraints. Keeping in mind that various devices may be involved, some of the best images are simple, relatively free of text and technical characters, and make use of color for visual impact. It is best to avoid complex structure schemes and small-sized details. The author must submit a graphic in the actual size to be used for the TOC that will fit in an area 8.47 cm by 4.76 cm (3.33 in. by 1.88 in.). Larger images will be reduced to fit within those dimensions. Type size of labels, formulas, or numbers within the graphic must be legible at the specified size. Tables or spectra are not acceptable. Place the TOC graphic after the title page and before the abstract page of the manuscript. **All elements of the TOC graphic must be (1) entirely original and (2) created by one or more of the authors.** Lastly, this graphic should have no legend.

**Abstract.** An abstract should be included with all Articles, Communications, Reviews, and Perspectives. For Articles and Communications, the abstract should briefly (300 word maximum) present, in one paragraph, the problem and experimental approach and state the findings and conclusions. For Reviews and Perspectives, the abstract should introduce the topic, summarize key points, and state the major conclusions. In all cases, the abstract should be self-explanatory

and suitable for reproduction without rewriting. Footnotes or undefined abbreviations may not be used. Avoid the use of jargon, but include keywords relevant to the field to improve indexing and discoverability to potential readers. If a reference must be cited, complete publication data must be given.

Introduction. The introduction should state the purpose of the investigation and its relation to other work in the field. Background material should be brief and relevant to the research described. Detailed or lengthy reviews of the literature should be avoided.

Experimental Procedures. Procedures for experimental methods should be described in sufficient detail to enable other investigators to repeat the experiments. Names of product manufacturers (with city, state address, catalog number) should be included if alternate sources are deemed unsatisfactory or if the product is of limited availability. Novel experimental procedures should be described in detail, but previously published procedures should be referred to by literature citation of the original detailed explanation, and should include description of any modifications.

Results. The results should be presented concisely. Tables and figures should be designed to maximize the presentation and comprehension of the experimental data. The same data should not be presented in more than one figure or in both a figure and a table. Detailed interpretation of results should be reserved for the discussion section of an Article.

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Abbreviations. Abbreviations are used in ACS Journals without periods. Standard abbreviations should be used throughout the manuscript. All nonstandard abbreviations should be kept to a minimum and must be defined in the text following their first use.

Footnotes. When footnotes are necessary to express some relevant thoughts, these should be included as a parenthetical statement, placed next to the related text to ensure visibility. Footnotes should not be included in the reference list.

Tables. Tabulation of experimental results is encouraged when this leads to more effective presentation or to more economical use of space. 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 cell; no listing of data by using bullets or numbering. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row. Tables should be numbered consecutively with Arabic numerals. Provide a brief title with each

table and a brief heading for each column. Clearly indicate the units of measure (preferably SI). Data should be rounded to the nearest significant figure. Explanatory material referring to the whole table is to be included as a footnote to the title (a). Footnotes in tables should be given lower case letter designations and cited in the tables as italicized superscripts. All tables should be cited in the text in consecutive order.

Previously published tables that are being borrowed or adapted from another source require permission from the copyright holder. Once permission is obtained, the permission letter should be uploaded to the submission under the tag "Other Files for Editors Only." Also, the copyright holder's preferred credit line should be included in the table's legend.

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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: <sup>1</sup>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.

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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

*Chemical Identity and Purity.* The identity and purity of key compounds, including those used for toxicological testing, and description(s) of the method(s) used to determine purity, which should generally include HPLC and NMR, should be included in the experimental procedures section. Characterization data for key compounds should include HPLC,  $^1\text{H}$  NMR/ $^{13}\text{C}$  NMR (peak lists), and HRMS. For instructions on submitting NMR data, refer to ACS guidelines: [https://publish.acs.org/publish/manu\\_prep\\_sub](https://publish.acs.org/publish/manu_prep_sub). HRMS data should be reported to support the molecular formula assignment and should include the molecular formulas on which the theoretical (calcd) values are based. HRMS molecular formulas and calcd values should include any added atoms (usually H or Na). Found values should be close enough to the calcd values, and have sufficiently small estimated uncertainties, to exclude alternative plausible formulas. The ionization method and the mass detector type should be reported.

*Nanomaterials.* The physico-chemical properties of nanomaterials used for toxicological studies should be characterized appropriately in order to support the conclusions of the study. This applies to commercially available materials as well as to designed materials. Where applicable, the information included should comprise primary size and shape, aspect ratio, size distribution, agglomeration or aggregation state, rigidity, elemental composition, surface modification, zeta potential, redox potential, surface reactivity, and/or crystalline phase. A description or reference to the synthetic procedure used to prepare the materials should be included. Furthermore, the stability and reactivity of the nanomaterials as well as influence of external parameters like the composition of cell culture media, buffers etc. on the nanomaterials properties should be addressed, for example by measurements of dissolution or dissolution rate, formation of reactive oxygen species or agglomeration under experimental conditions. Finally, the techniques used to characterize the materials should be described sufficiently or referenced, including the description of algorithms and methods used to analyze the data.

*Hazardous Materials.* 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. All hazardous chemicals should be clearly identified as such. Precautions for handling dangerous materials or for performing hazardous procedures should be explicitly stated and referenced. Identification of and precautions for handling hazardous chemicals and dangerous procedures should be placed at the beginning of this section. An example would be: “**Caution:** *The following chemicals are hazardous and should be handled*

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**Biological models:** The identity and source of the biological model used (i.e. organism, cells) should be specified (collection and collection number) and referenced (primary description). Where appropriate, information on the state of cell lines (e.g. passage number, doubling number) and information regarding how they were authenticated to ensure identity and validity for use, should be given. A rationale for selecting the specific model relevant to the aims of the study should be given.

**Biological Assays.** Exposure protocols and methods must be referenced or described in sufficient detail to permit the experiments to be repeated by other investigators. This includes for example information on the preparation of the test materials, medium components, and duration of exposure. In addition, the applied dose or dose range should be given in a meaningful unit and the relevance of the applied dose should be substantiated. Doses and concentrations should be expressed as molar quantities (e.g., mol/kg, mM, etc.), particularly when comparisons of potencies are made on compounds having large differences in molecular weights. The routes of administration of test compounds and vehicles should be indicated. Benchmarks should be included in form of appropriate positive or negative control substances or reference materials. Especially for studies on nanomaterials, assays should be checked for interference induced by nanomaterials, e.g. optical or chemical interference, masking of the analyte or other interference mechanisms by inclusion of appropriate controls. Also for studies on nanomaterials, sterilization procedures and specification of dilution steps as well as the order of addition should be provided, and as far as possible, various measuring units related to dose (e.g. surface area, mass, particle number per surface area, volume, cell number) should be given to increase comparability with other studies. Data may be presented as numerical expressions or in graphical form. 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.

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Justifications for the doses used in the research should be included, and where appropriate, the relationship between these doses and relevant environmental or human exposure or intake levels is encouraged to be provided.

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**Data Deposition.** Large data sets, such as those from structure determination, omics or



sequencing data must be submitted to discipline-appropriate repositories recognized by the corresponding scientific community, and made publically available by the time of publication. A statement must appear in the submitted manuscript confirming submission of the data and indicating the data bank and any pertinent accession codes/ID.

Any set of atomic coordinates for structural data referred to in the manuscript, including atomic coordinates and structure factors for proteins determined by X-ray crystallography and coordinates determined by NMR, should be deposited with the Protein Data Bank, Research Collaboratory for Structural Bioinformatics at Rutgers University whenever appropriate. (Theoretical model depositions are no longer accepted for inclusion in the PDB archive.) If the coordinate files are not deposited in the PDB, or if the PDB files are on hold until publication, then the coordinate files must be included in the Supporting Information submitted concurrently with the manuscript. Requirements are similar for structures of nucleic acids, which should be deposited with the Nucleic Acid Database. A manuscript that does not provide coordinates at the time of submission will not be sent out for review. It is the responsibility of the author to obtain a file name (PDB ID or NDB ID) for the molecule; the file name must appear in the published manuscript. If a file name has not yet been obtained upon acceptance of a paper, it must be added in proof. Atomic coordinates and structure factors for all structures mentioned must be available immediately upon publication of the paper, either directly in the Supporting Information or as a data bank deposition. Similar requirements also apply to any chemical shifts referred to in the paper, whether they are only for assignment of resonances or used for any form of structure calculation. Those chemical shifts must be available to the reviewer at time of submission, either as an available entry in the Biological Magnetic Resonance Data Bank or included directly as Supplementary Information.

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## Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through [ACS Paragon Plus](#), which requires an ACS ID to log in. Registering for an ACS ID is fast, free, and does not require an ACS membership. Please refer to Appendix 1 for additional information on preparing your submission

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# Appendix 1: PREPARING FOR SUBMISSION

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## Appendix 2: Preparing Graphics

### Resolution

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

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

## Size

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

## Color

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

## Type of Graphics

### Table of Contents (TOC)/Abstract Graphic

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## 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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