Last updated: June 25, 2024 View the latest guidelines online

Scope of the Journal

Organic Letters invites original reports of fundamental research in all branches of the theory and practice of organic, physical organic, organometallic, medicinal, and bioorganic chemistry. *Organic Letters* provides rapid disclosure of the key elements of significant studies that are of interest to a large portion of the organic community. In selecting manuscripts for publication, the Editors place emphasis on the originality, quality and wide interest of the work. Authors should provide enough background information to place the new disclosure in context and to justify the rapid publication format. Back-to-back Letters will be considered. Full details should be reserved for an Article, which should appear in due course.

Scope Details

- *Organic Letters* is a communications journal focusing on rapid but brief reports of cutting-edge results, hence to keep article length within our four-page maximum the number of compounds required does not need to be exhaustive. While the number of compounds reported is not limited, for methods discoveries we generally recommend 10–20 diverse substrates including some that are unreactive or give low yields as sufficient, provided they are diverse and represent the true scope of each reported reaction.
- One-step organic transformations must be highly innovative and include one detailed complete method at the 1 mmol scale; exceptions may be discussed with the editor for certain materials chemistry and electrochemistry work.
- Designed structures: if the design, synthesis and spectral data of a new compound are not exceptionally novel, then data such as biological, binding, or materials properties must be included.
- Novel organic electronic materials need to illustrate either a novel synthetic method or interesting device properties.
- Supramolecular assemblies: a novel method should be demonstrated and/or the materials should have either interesting properties or a significant application.
- Analytical detection of a selected species (we are highly selective in this category): Letters must contain a novel synthetic protocol and/or demonstrate notable improvement on the limits of detection of the species.The synthesis of a novel compound or a significantly improved route to a known compound will only be considered if appropriate improved device or use data is provided.The synthesis of a known compound via known methods together with new sensing data will not be considered, unless the new binding or sensing data provides a significant advance on previously reported selectivity and/or sensitivity for a target species and/or a novel mode of binding for a particular species under consideration.Manuscripts focusing on mechanistic studies (experimental or theoretical) should show methodological advances or provide novel insight into the course of chemical reactions, rather than only confirming previously established mechanisms.

If you are a new *Organic Letters* author, or if you have not submitted a manuscript during the past year, please read and familiarize yourself with these complete Author Guidelines to ensure you are up to date with all of the journal's manuscript preparation and submission requirements.

Editors, Authors, and Reviewers should read the ACS Ethical Guidelines.

Emphasis on Chemical Safety

In 2021, in support of ACS's core value of "Professionalism, Safety, and Ethics," ACS Publications added a Safety Considerations requirement to the Author Guidelines of every ACS journal (Appendix 1):

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the Safety Statement Style Sheet and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* is freely available here.

Organic Letters is participating in a pilot program to further encourage use of Safety Statements in manuscripts, including details on how to mitigate hazards and risks. Reviewers and Editors will be more carefully checking manuscripts to determine whether an existing Safety Statement is accurate and complete, and if there is no Safety Statement in a manuscript whether there are any hazards or risks that require a Safety Statement be added. If a Safety Statement is needed, authors will be asked to include one in their manuscript at revision and before acceptance.

Manuscript Types

Organic Letters publishes only communications-length manuscripts. Authors are required to use the document template to help facilitate placement of figures and to determine whether your submission meets the journal's length requirements.

A manuscript may not exceed 2,200 words at submission. This word count includes the title, abstract, main text, and titles/footnotes of typically five graphics (one of which is the TOC graphic). Tables and graphics count toward the word-count limit at the rate of 20 words per vertical centimeter for one-column items and 50 words per vertical centimeter for wider items up to two columns. Large graphics or additional graphics will require a reduced amount of text. Authors are reminded that any graphics that are reduced in size to help adhere to the length limits need to be fully legible when the page is printed at 100% scale.

The goal for these length requirements is for manuscripts to fit within four pages, end matter (Supporting Information, Author Information, Notes, Acknowledgments) and references excluded — end matter and references are not included in the word count, and are the only part of the manuscript that will be allowed to extend beyond the end of the fourth page. Authors of submitted manuscripts that exceed the length requirements will be asked to adjust their manuscript by removing material, which can be placed in the Supporting Information. Note that authors should take care to not allow the length of their manuscript to exceed these requirements when making revisions.

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 the 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 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.

The cover letter should address the criteria of significance and the need for rapid disclosure and, if the author wishes, list the name of a suggested Associate Editor for consideration. Information regarding previous submission to *Organic Letters* or to any other ACS journal should be included. If back-to-back publication with another paper is desired, this should be stated, along with the desired order of publication in the cover letters of both manuscripts.

Manuscript Text Components

Letters contain a Title, Abstract, main text without section headings, a Data Availability Statement, and references/end matter.

The title should be descriptive of the topic of the article and as short as possible (not exceeding 20 words), using easily searchable keywords and avoiding/minimizing hyphenation. To that end, avoid using abbreviations and acronyms unless they are more commonly used than spelled out words. Also avoid complex compound names as much as possible in the title by using generic names, and spell out elements rather than using symbols unless part of a compound formula. Neither the title nor any other text should indicate that the article is part of a numbered series on a broader research topic, or a numbered contribution from a particular institution or research group.

The Abstract of 75 words or less of text should briefly state the purpose of the research, the principal results, and the major conclusions. A well-written Abstract along with its graphic figure can attract the attention of potential readers and increase the likelihood that the published article will be read and cited by other researchers. Summaries of numerical results should be quantitative, for example, “in yields of 65 to 90%” rather than “in good to excellent yields”).

A graphic must be included with each manuscript for display in Abstract and in the Table of Contents (TOC). The graphic should capture the reader’s attention and, in conjunction with the Title and Abstract text, should give the reader a quick impression of the essence of the article. In preparing the graphic, creativity is welcome, but avoid images of people living or from the past and avoid caricatures or parodies that could be socially/culturally insensitive or considered racist or discriminatory, especially when taken out of context. Ensure that cartoon depictions of machinery, nature, and processes do not indicate actions or settings that are improbable. The graphic must fit in an area no larger than 8.25 cm by 4.45 cm (3.25 inches by 1.75 inches); the Abstract and graphic together should not exceed the space required for 200 words. See Appendix 2 for full details on graphics requirements.

The introduction of the main text should include sufficient background information to provide appropriate context as to the novelty and importance of the new work and clearly state the purpose and objectives of the research. An extensive review of prior work is not appropriate, and documentation of the relevant background literature should be selective rather than exhaustive, particularly if reviews can be cited.

A Data Availability Statement is required for all peer-reviewed articles and is not required for the following non-peer-reviewed articles: Addition/Correction, Editorial, Expression of Concern, or Retraction. The ACS Research Data Policy provides additional information on Data Availability

Statements, Data Citation, and Data Repositories.

Claims of priority, originality, convenience, effectiveness, or value should be avoided or used with great restraint in the title and throughout the main text. For example, the words “concise,” “convenient,” “efficient,” “elegant,” “expedient,” “facile,” “first,” “new,” “novel,” “practical,” “simple,” “unique,” “unprecedented,” and “versatile” should not be used. The use of “free” should also be avoided, that is “metal-free,” “catalyst-free,” “light-free,” and so on, as these terms can be misleading. In addition, editors may ask authors to moderate or remove what they judge to be excessive use of subjective evaluative language elsewhere in the manuscript.

Abbreviations, Symbols, Units, Compound Names. Authors should use abbreviations and acronyms in the text to conserve space. A list of standard abbreviations is provided in the ACS Guide to Scholarly Publishing. Nonstandard abbreviations and acronyms must be defined the first time they are used in the abstract, text, and supporting information. The use of abbreviations should be consistent throughout the manuscript text and graphics. For example, either CH_3 or Me may be used for “methyl,” but not both. Full systematic names of compounds (see Part 4 and Part 5 of the ACS Guide to Scholarly Communication for guidance) should be included in the Experimental Section on first mention and for brevity assigned a molecule number for reference throughout the article. In other sections of the manuscript, authors should use their judgement on common usage of compound names or use a generic name or molecule numbers in lieu of full systematic names. As a courtesy to the research community, a list of abbreviations used in your manuscript if extensive can be included under Associated Content at the end of the manuscript and at the end of the Supporting Information before the References section.

References

Authors should be judicious in citing the literature; unnecessarily long lists of references should be avoided. If a number of publications are relevant to a statement in the text, not more than two or three of the most seminal or recent should be cited; if appropriate, the author may add “and references cited therein” following a reference. Authors must also cite any previously published work wherein portions of the submitted work have been disclosed. It is seldom necessary or appropriate for an author to cite more than 5 of their own publications. No reference should repeat a reference that appears elsewhere in the manuscript’s list of references. Authors are encouraged to include additional references cited in Supporting Information files in the main article reference list. Long endnotes should be avoided; peripheral discussion should be placed in the supporting information. Endnotes should not contain graphics, experimental procedures, or compound characterization data.

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

Supporting Information

Supporting Information (SI) is required and is reviewed for completeness and accuracy by a Data Analyst. Submissions without adequate SI will be inactivated and the authors will be asked to provide the requested information.

Introductory Section

An introductory section should include general procedures, standard techniques, and instruments employed in the synthesis and characterization of the compounds described in this section.

- General reaction conditions
- Instruments used (NMR, microwave reactors, etc.)
- Suppliers for commercial compounds
- Citations to references for noncommercial known compounds

Experimental Details Section

- New procedures should be fully described in detail to ensure reproducibility.
- When a new or improved synthetic method is described, at least one detailed complete method must be provided at the 1 mmol scale.
- The yields reported in key experimental examples, and yields used for comparison with existing methods, should represent amounts of isolated and purified products.
- Chromatographically or spectroscopically determined yields are not acceptable
- Reactant quantities and product yields should be reported in weight and molar units; percentage yields should only be reported for materials of demonstrated purity
- Experimental details and spectra in the SI are in the sequence that corresponds to the

manuscript

In addition to emphasizing safety hazards or risks associated with the reported work and how to mitigate them, the Editors encourage authors to mention the use of toxic and/or environmentally persistent reagents and solvents and provide a rationale on choice of these reagents and solvents. This acknowledgement is especially important in cases of “dual use” potential when the reported work could be directly misapplied by others to pose a threat to public health and safety. *Organic Letters* further encourages authors to consider the Principles of Green Chemistry in carrying out their research and consider reporting metrics such as atom economy, mass efficiency, E-factor, or others. For more information, please consult Research Tools provided by the ACS Green Chemistry Institute.

For each procedure, include the following details:

- Title containing the compound number and structure that corresponds to the manuscript
- For synthetic procedures, include: Reactant quantitiesDetailed purification techniquesProduct quantitesIsolated yieldsPhysical state/description of the compounds (i.e., color, solid, etc.)Characterization data Report ^{1}H chemical shift to two digits after the decimal pointReport ^{13}C chemical shifts to one digit after the decimal point

Chromatography

- When flash chromatography is used for product purification, the support should be identified and the solvent should be identified for each compound.
- HPLC analyses should be performed in two different solvent systems. The stationary phase, solvents (HPLC), detector type, and percentage of total chromatogram integration should be reported; alternatively, a copy of the chromatogram may be included as a figure in the Supporting Information.

Crystal Data

All Crystallographic Information Files (CIFs), structure factor tables, and CheckCIF reports must be submitted to the Cambridge Crystallographic Data Centre (CCDC) **prior to manuscript submission**. See Requirements for Depositing X-Ray Crystallographic Data [PDF] for complete details on submission of CIFs and a list of file types accommodated by CCDC.

- Before being submitted to CCDC, CIFs should be checked using the free checkCIF data-validation utility on the CIF Validation site.
- Any reported syntax errors should be corrected. Authors are required to correct/defend/or respond to any A-level alerts. Comments may be inserted into the CIF file using a Validation Response Form or uploaded as a separate document as Supporting Information for Review Only.
- checkCIF output files (combined into one PDF file) should be uploaded at submission as Supporting Information for Review Only.
- Any subsequent revisions to the CIFs or structure factor tables should be deposited directly with the CCDC before resubmitting the manuscript in ACS Paragon Plus.

Microwave Experiments

For reactions that require heating, identify the temperature and heat source (oil bath, heating

mantle, etc.) or the model and manufacturer number if a device is used, e.g. a microwave or sonicator. Reports of syntheses conducted in microwave reactors must indicate whether sealed or open reaction vessels were used, how the reaction temperature was monitored (external surface sensor or internal probe type), and the temperature reached or maintained in each experiment. Authors must comply with the requirement that at least one detailed complete method must be provided at the 1 mmol scale. *Organic Letters* does not publish reports of studies conducted with domestic (kitchen) microwave ovens in which yields or selectivities observed using microwave irradiation are compared with results obtained using conventional heating.

Compound Characterization

When manuscripts report the synthesis of compounds, submission of a Compound Characterization Checklist is recommended. The Checklist will be provided to Editors and reviewers to help them assess the thoroughness of the characterization of synthesized compounds. Compound characterization data provided should be sufficient to ensure that compounds being added to the chemical literature have been correctly identified and can be synthesized in known yield and purity by the reported preparation, isolation, and purification methods.

Note that authors are responsible for retaining their original data or having available original data from collaborators or from contractors who perform analyses on their behalf. Authors may be asked to provide copies of spectra or analytical reports if an editor or reviewer raises a question about reported results. Upon publication, authors are encouraged to link the manuscript to their data housed in a repository or other location, and to make their primary data freely available to others upon request.

New compounds: Evidence adequate to establish both identity and degree of purity (homogeneity) should be provided (see below).

Known compounds: Purity documentation must be provided for known compounds whose preparation by a new or improved method is reported (see below). Listings of IR absorptions and NMR resonances for known compounds should be presented only if they do not duplicate previously published data.

In addition, for noncommercial, known compounds used as starting materials, the method of preparation and the literature data used to confirm the materials' identity must be cited.

Authors are further encouraged to include additional data or revised data that was not reported in original references cited, and in doing so indicate which part of the data set is new information.

Identity – Compound Requirements

For all new compounds, a listing of ^{1}H and ^{13}C resonances, either HRMS or elemental analysis data and important IR absorptions should be included in the experimental details section. HPLC/LCMS can be substituted for biochemistry papers where the focus is not on compound synthesis. Hydrogen multiplicity (C, CH, CH_2, CH_3) information obtained from routine DEPT spectra should be included. If detailed peak assignments are made, the type of NOESY or COSY methods used to establish atom connectivities and spatial relationships should be identified in the Supporting Information.

If a required type of data is not obtainable, the reason for the absence of the data should be noted in the experimental section of the Supporting Information. For example:

- Compound is too insoluble to record a ^{13}C NMR spectrum
- Compound is too unstable to obtain a good elemental analysis

The following data should be included:

- **Spectral data**: Copies of ^{1}H and ^{13}C NMR spectra and/or relevant heteronuclei if appropriate should be provided for key transformations and final products.
- **HRMS/elemental analysis**: To support the molecular formula assignment, either the HRMS data accurate within 5 ppm, or combustion elemental analysis data accurate within 0.4%, *must* be reported for new compounds.

NOTE: in certain cases, a crystal structure may be an acceptable substitute for HRMS/elemental analysis (see Crystal Data for information on submitting CIF files to CCDC).

- **Melting point**: A melting point range should be reported for all crystalline compounds.*Melting points of noncrystalline amorphous compounds should not be reported.*
- **Specific Rotation.** Specific optical rotations should be reported for isolated natural products and enantioenriched compounds when sufficient sample is available. Specific rotations based on the equation [] = (100·)/(*l*·*c*) should be reported as unitless numbers as in the following example: $[]_D^{20}$ -25 (*c* 1.9, $CHCl_3$), where the concentration *c* is in g/l00 mL and the path length *l* is in decimeters. The units of the specific rotation, (deg·mL)/(g·dm), are implicit and are not included with the reported value. See also the section on Computational Data.

Experimental Electronic Circular Dichroism and Vibrational Circular Dichroism Spectra. When reported, experimental conditions of ECD and VCD spectra such as concentration, solvent, and optical path length should be indicated. Spectral intensities should be reported in units of molar absorptivity (, M^{-1} cm^{-1}). The method of baseline correction (subtraction of solvent or racemate spectrum) must be noted. The spectra should always be presented together with the corresponding unpolarized absorption spectra (UV/vis and IR) shown at the same scale. See also the section on Computational Data.

Oxygen Balance. Oxygen balance parameter gives potential of a compound or an explosive towards oxidation. Please report the oxygen balance in the following format including the complete formula used for calculation:

- Oxygen balance (OB, %) for CaHbNcOd: OB=1600×(d-2a-b/2)/Mw, Mw= molecular weight (based on carbon dioxide).

Purity – Compound Requirements

The types of evidence appropriate for demonstrating a compound's purity will necessarily depend on the method of preparation, the compound's air and thermal stability, the complexity of the structure, the nature of reasonably likely impurities, and the amount of sample available. For example, combustion analysis would not be a good choice for the product of an isomerization or rearrangement reaction; a "clean" NMR spectrum would need to be supplemented with other evidence when a reasonably likely impurity is NMR silent (e.g., an inorganic salt).

For all known compounds synthesized by a new or improved method, include one or more of the following characterization data:

- A well-resolved high field ^{1}H NMR spectrum showing at most only trace peaks not attributable to the assigned structure.
- A standard 1D proton-decoupled ^{13}C NMR spectrum.
- Combustion elemental analytical values for carbon and hydrogen (and nitrogen, if present)

agreeing with calculated values within 0.4%.
- Quantitative gas chromatographic analytical data for distilled or vacuum-transferred samples or quantitative HPLC analytical data for materials isolated by column chromatography or separation from a solid support.
- Electrophoretic analytical data obtained under conditions that permit observing impurities present at the 5% level.

Note: A typical example to report ^{1}H and ^{13}C NMR data to conform to ACS Guide format is (high to low): ^{1}H NMR (C_6D_6, 400 MHz): 6.00 (t, 1H, J = 4.0 Hz), 5.62 (t, 1H, J = 4.0 Hz), 1.95 (d, 1H, J = 4.0 Hz), 1.73 (s, 15H), 1.62 (s, 3H), 1.58 (s, 15H), 0.98 (s, 1H), 0.72 (d, 1H, J = 4.0 Hz), -0.53 (s, 1H). $^{13}C\{^{1}H\}$ NMR (C_6D_6, 125 MHz): 88.7, 88.0, 81.0, 80.8, 60.6, 54.2, 51.5, 38.3, 17.4, 10.6, 10.2.

Note: HRMS data may be used to support a molecular formula assignment but cannot be used as a criterion of purity.

Guidelines for Specific Compound Classes

Combinatorial libraries containing more than 20 compounds: complete characterization data must be provided for at least 20 diverse members.

Natural products whose structures are being proposed or revised: sufficient data should be provided to definitively establish molecular composition. Suggested analyses include: melting point of crystalline compounds, HRMS, IR spectra, ^{1}H and ^{13}C NMR spectra, 2D ^{1}H COSY, 2D $^{1}H/^{13}C$ HMQC, and 1D DEPT spectra as well as long-range ^{1}H COSY spectra and NOESY and/or NOE spectra (where NOE data is being used to assign a structure). An X-ray crystal structure can also be employed to establish the structure assignment. Specific optical rotations as []D values should be reported for isolated natural products and enantiopurecompounds.

Configurational Isomer Mixtures: For reporting the compositions, enantiomeror diastereomer ratios are preferred over enantiomeric or diastereomeric excess values.

Non-racemic chiral substances**:** Data to permit correlation ofabsolute configuration should be provided, preferably including []D values.

Biomacromolecules: The structures of biomacromolecules may be established by providing evidence about sequence and mass. Sequences may be inferred from the experimental order of amino acid, saccharide, or nucleotide coupling; from known sequences of templates in enzyme-mediated syntheses; or by standard sequencing techniques. Typically, a sequence will be accompanied by MS data that establish the molecular weight.

Spectra Standards. Spectra files should not be manipulated in any manner that could result in misinterpretation or misrepresentation of the original spectra. Nothing within an image such as spectral baselines or solvent/impurities should be enhanced, obscured, moved, removed, or introduced.

- Label each spectra with an image of the structure and a compound number
- Spectra should be legible and images are not faint or blurry
- Spectra should be at least a half page in size, preferably a full page Include magnified region(s) when necessary to show detail

- Display the NMR baseline and include the minimum chemical shift range: -1-9 ppm for ^{1}H spectra-10-190 ppm for ^{13}C spectraExtended range for functional groups that resonate from 9-14 ppm
- Integrate all peaks in the ^{1}H NMR arising from the compound
- Chemical shift values should be included for all peaks arising from the compound in the ^{1}H and ^{13}C spectra
- The largest peak in the ^{1}H NMR spectrum should normally be full scale and arise from the compound, not the solvent or impurities
- Field strength, solvent peak and nucleus being measured should be noted on each spectrum

Primary NMR Data Files

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is highly recommended. All original primary NMR data supporting a submission should be retained and provided if requested. For more information on packaging primary NMR data and metadata for submission, see the ACS Research Data Center.

When submitting FID files:

- One folder should be created for each compound
- Folder should be named clearly, using the compound number
- Include the FID files, acquisition data and processing parameters for each experiment
- Name each spectrum according to the type of nucleus measured: ^{1}H,^{13}C, DEPT, COSY, etc.
- NMR files should be compressed into zip file(s)
- Name the zipped file, "FID for Publication"

In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e., 300 MHz ^{1}H or 50 MHz ^{13}C). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

Electrochemistry Data. For reporting Voltammetry and Amperometry measurements, and for reporting Bulk Electrolysis procedures, please see the ACS Electrochemistry Guidelines.

Biological Data. For reporting information on specimens, techniques, and data, please see the ACS Biological Data Guidelines.

Computational Data. When computational results are included in a manuscript, complete details of computational methods and results, reported in sufficient detail to allow other researchers to repeat the computations, should be included either within the article or as Supporting Information. Graphics of computationally derived models that are not vital to the discussion should be placed in the Supporting Information. The level of theory, basis set, and relevant input parameters should be identified along with the specific program used. The data should include Z-matrices or Cartesian coordinates, grid size (for DFT calculations), and computed total energies of target or optimized structures. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states.

Description of specific programs and versions. If the author’s own or a modified version of a commercially available program is used, it is required that the program/code/modification be made

available to the scientific community (QCPE, publication in a computational journal, commercially, etc.). Policies in this regard are identical with those of several other ACS journals, as summarized in *J. Chem. Inf. Model.* 2006, *46*, 937. A clear exposition of any nonstandard equations and algorithms used and, where feasible, tests of the codes in various limiting cases should also be provided.

Details of the computations. The computed molecular model should be described clearly, possibly with a ChemDraw figure. If the model is based on an experimentally known complex/reaction, any modifications (such as truncations) should be clearly described and justified. Final optimized coordinates and keywords are to be provided. For DFT computations, the choice of functional must be justified, or the validation of the functional provided. The choice of basis sets must be explicitly discussed, including any deviation from standard basis sets. Convergence criteria, integration parameters, active space definition in multireference calculations, and, for open-shell systems, the way in which spin states are handled should be mentioned explicitly. The exact definition of any applied numerical or symmetry constraint should be indicated.

Details of the computational results. When relevant to the results of the study, data such as absolute energies, gross orbital populations, atomic spin densities, etc., should be supplied. Where feasible, critical checkpoint/restart files should be saved and made available upon request.

Cartesian Coordinates. Cartesian coordinates of all molecules, intermediates, transition states, etc. that are part of the manuscript must be uploaded in a single file that is formatted for convenient viewing with widely available molecular modeling packages. The .xyz and .mol formats are accepted at this time. The .xyz format is the most basic and easily prepared from computational output.

The first line of the .xyz format file denotes the number of atoms in the molecule.

The second line of the file is a comments line, and should begin with a descriptive name of the molecule/structure consistent with the designation in the manuscript, and any other pertinent information selected by the author, such as total energy.

Next follow lines for each element in the molecule. Each line contains the element symbol followed by the x, y, and z coordinates in angstroms (Å) separated by spaces in free-field format (i.e. precise formatting not required). More information on the .xyz file format is available at http://openbabel.sourceforge.net/wiki/XYZ.

Multiple structures are placed directly end-to-end in the file.

The file name should have the extension “.xyz”. A simple example with three molecules is shown below.

It is strongly recommended that authors view the structures in the file with a modeling program before uploading the file. The program Mercury (version 3.3 or later) is recommended for viewing and manipulating the multiple structures. The Cambridge Crystallographic Data Centre (CCDC) offers Mercury at no cost. Include the phrase “a text file of all computed molecule Cartesian coordinates in a format for convenient visualization” in the Supporting Information statement.

For additional guidance, see the ACS Simulations, Machine Learning, Computational Data guidelines.

When computational prediction of spectral properties is used to establish identity of new compounds, the following guidelines will apply:

- *General:* The level of theory, basis set, and relevant input parameters used for optimization and the prediction of spectral properties should be indicated in all cases. It must be noted/justified when geometry optimization and property calculations are carried out at different levels of theory.
- *Conformational search.* A thorough conformational search should be performed for all molecules, except those with no rotatable bonds. The methods and results of the conformational search should be reported in detail.
- *Optimized conformers.* The optimized geometries of all the conformers actually used to calculate a property should be reported, along with their energies and number of imaginary frequencies (if conformers are more than five, only significantly populated conformers, that is those with a calculated Boltzmann weight larger than 5%, can be reported).
- *^{1}H and/or ^{13}C NMR chemical shifts.* The scaling parameters used to calculate chemical shifts must be indicated. Calculated isotropic shielding values (before scaling to chemical shifts) for H and/or C atoms of all considered conformers should be reported. If possible, comparison with experimental chemical shifts should be accompanied by R^2, RMSD, or DP4+ values. Statistical methods can be used as well.
- *Electronic Circular Dichroism.* Parameters used to simulate the UV/Vis and ECD curves such as Gaussian band width and UV shift must be indicated. A qualitative comparison of the experimental and computed ECD spectra is generally sufficient. A comparison of the experimental and computed UV/Vis spectra should also be presented. Transition energies (or frequencies) and rotational strengths should be reported in tabular form for the significantly populated conformers. A figure with computed ECD curves of individual conformers is suggested, but not required. Any figure comparing the experimental and computed spectra should include both the UV and ECD spectra in the same figure; both sets of spectra should be shown in the same wavelength range.
- *Vibrational Circular Dichroism.* Parameters used to simulate the spectra such as the Lorentzian band width and the frequency scaling factor must be indicated. The presentation of the comparison of experimental and computed spectra should include both the IR and VCD spectra in the same figure; both sets of spectra should be shown in the same wavenumber range (e.g., 1800-900 cm^{-1}). A qualitative comparison between experimental and computed spectra is sufficient as long as convincing band correlations between major features in the experimental and computed spectra are indicated. Quantitative comparison can be made using similarity analysis algorithms which provide a degree of congruence between measured and calculated VCD spectra for the assigned enantiomer versus its opposite enantiomer. If VCD is used to distinguish diastereomers, a particular emphasis of the spectra comparison must be given to those signals that are used to differentiate the stereoisomers.
- *Optical rotation.* When computed optical rotation values are used to assign or to complement the assignment of an absolute configuration, it must be ensured that the experimental value is not solvent dependent (at least two experimental values in a polar and a non-polar solvent must be provided). Ideally, the optical rotation is also measured and computed at different wavelength.

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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

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Charts

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

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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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