December 15, 2018

SCOPE OF THE JOURNAL

ACS Combinatorial Science will publish original research describing the development and use of combinatorial, high-throughput, and related techniques in chemistry, materials science, analytical science, and biology. It welcomes submissions from a broad spectrum of scientific endeavor involving the discovery of functional molecules or systems using combinatorial techniques, molecular libraries, and evolving systems and the development of tools for speeding and understanding such discoveries. Examples include molecular synthesis and screening, biological and bio-inspired development of molecular function, molecular systems exhibiting feedback and evolution, combinatorial synthesis and testing of polymers and materials, parallel operations and engineering, robotics and automation, and analytical and computational methods, among many others.

The journal is dedicated to the proposition that combinatorial and evolutionary molecular science represents an emerging new discipline, while providing powerful tools for the further development of its contributing fields. Areas of interest include but are not limited to:

Chemistry

- Efficient synthetic techniques for application to combinatorial and diversity-oriented chemistry
- Hit-to-lead high throughput chemistry
- Techniques for the meaningful screening of combinatorial libraries for biological activity, including the development of signal-generating probes, in vitro and cell-based assays, and instrumentation
- Combinatorial development of catalysts
- Combinatorial chemistry of specialized molecular classes, including natural products, oligosaccharides, lipids, dyes, and inorganic and organometallic compounds
- Combinatorial methods as applied to green chemistry and sustainable synthesis
- Solid-phase synthesis, solid-supported reagents, and resin capture methodologies
- Theoretical and computational methods for designing and interpreting combinatorial experiments; methods of multivariate optimization
- Functional molecules to emerge from the above techniques

Materials Science

- Combinatorial methods for functional materials discovery, including synthesis and testing of polymers, resins, crosslinked materials, soft materials, inorganic and ceramic materials, self-assembled structures, and others
- Combinatorial engineering of surfaces and interfacial phenomena
- Combinatorial development of heterogeneous catalysts
- Combinatorial methods and techniques for biomaterial design and discovery
- Theoretical and computational methods for design and interpretation of combinatorial materials experiments
- Functional molecules to emerge from the above techniques, including applications of combinatorial materials synthesis to biology, biochemistry, chemistry, catalysis, and other fields. Examples include energy harvesting and storage, filtration, wound healing and tissue replacement, stem cell cultivation and differentiation, antimicrobial activity, biodegradability, selective binding interactions, catalytic activity and enantioselectivity, and many others.

Biological Molecules and Methods

- Application of combinatorial techniques to the synthesis and evaluation of small biomolecules, such as peptides, oligonucleotides, and oligosaccharides.
- Development and use of biomolecule arrays, such as with polynucleotides, proteins, and glycans.
- High-throughput methodologies in biomolecular screening and biosensors
- High-throughput methodologies, tools, and technologies relating to gene expression information including RNA interference, transcriptional and translational regulation, and epigenetic silencing and activation.
- Unnatural amino acids and nucleotide bases in discovery of molecular function

Directed Evolution of Molecular Function

- Phage display, ribosome display, and related techniques for in vitro evolution of peptides and proteins
- SELEX and related techniques for in vitro evolution of oligonucleotides and nucleic acids
- Two- and three-hybrid techniques and related methods for cell-based discovery of molecular function.
- Riboswitches and riboswitch-based methods for in vivo molecular evolution
- Organism-based evolution of molecular function, such as in bacterial colonies and virus populations

Robotics and Microfluidic Technologies

- Technologies for synthesis and screening on the micro and nano-scale
- Chemical and biological micro/nanoreactors and fluidic devices for chemical synthesis,
- Lab-on-chip and microarray-based technologies
- Robotics and other automation to enhance screening of libraries
- Technologies for high throughput purification and analysis

Theoretical and Computational Tools

- Molecular informatics as applied to library analysis
- Theoretical aspects of library creation and optimization

For more information, please visit "About the Journal".

MANUSCRIPT TYPES

ACS Combinatorial Science is a print and online publication that publishes Research Articles, Letters Reviews, Perspectives, Accounts, and Technology Notes. A description of each manuscript type and its key features follows, followed by a summary table.

Articles. Concise, yet comprehensive, original research presenting an advance of immediate, broad, and lasting impact. Articles are peer-reviewed and contain an unreferenced abstract of 250 words or fewer. Abstracts should be informative, as opposed to just indicative, and briefly state the purpose of the research, principal results, and major conclusions, without abbreviations or acronyms unless essential. A referenced introduction should set the work in context. Articles include the following headed sections: Introduction, combined Results and Discussion, Experimental Procedures, Author Information, Acknowledgments, Abbreviations and References. The first three may contain subheadings to promote

clarity. In general, Articles include up to 10 display items (figures/tables/schemes), embedded with the text for easier reading in the review process. Incisive referencing is important, and authors are encouraged to be complete without being excessive in their citations. Supporting Information may be included. Sufficient experimental details should be provided to allow others to reproduce the findings presented. Articles include a graphical Table of Contents entry/Abstract graphic consisting of a colorful figure representing the topic of the Article.

Letters. Short reports of original research focused on an individual finding of significance to the field. Letters are peer-reviewed and begin with an unreferenced abstract of 150 words or fewer. Abstracts should be informative, as opposed to just indicative, and briefly state the purpose of the research, principal results, and major conclusions, without abbreviations or acronyms unless essential. Letters include unheaded sections for the Introduction and combined Results and Discussion and headed sections for the Abstract, Experimental Procedures, Author Information, Acknowledgments, Abbreviations and References. It is recommended that most procedural details be placed in Supporting Information. Sufficient experimental details should be provided to allow others to reproduce the findings presented. Letters should be approximately 3500 words or less in length (4 journal), including the abstract, body text, methods, references, tables, graphics/artwork, and figure/scheme legends. Letters typically contain 4–6 display items (figures/tables/schemes), embedded with the text for easier reading in the review process, and no more than 30 references. Letters must be accompanied by a Table of Contents (TOC)/Abstract graphic consisting of a colorful figure representing the topic of the Letter.

Reviews. Comprehensive and critical summaries of published scientific papers describing work on a single research topic, either completely if new or infrequently reviewed, or covering a specific time range if the subject is more popular. Reviews are peer-reviewed and contain an unreferenced abstract of 250 words or less. 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. Extensive referencing is encouraged, as is the use of graphics to illustrate key concepts. All display items (figures, tables, schemes) should be embedded with the text for easier reading in the review process. A graphical Table of Contents entry/Abstract graphic consisting of a colorful figure representing the topic of the Review should also be included. Authors may choose to divide the review into headed sections for clarity. The journal recommends that authors define key words used in the review and key concepts in separate textboxes. Potential authors are strongly encouraged to seek the advice of the Editor prior to initiating work on a Review for the journal. We encourage authors to include an internal table of contents at the beginning of the Review.

Perspectives. Summaries of published scientific papers describing work on a single research subfield. Authors of Perspectives will choose published work felt to be of great importance and editorialize about the significance of each paper. Perspectives are meant to provide context for rapidly developing fields and encourage interest in new genres or disciplines. Because combinatorial science affects so many diverse areas, Perspectives can have a strong impact on our readership. Perspectives are peer-reviewed and start with an unreferenced abstract of 250 words or less. They should be approximately 5000 words or less in length (6 journal pages), including the abstract, body text, references, tables, graphics/artwork, and figure/scheme legends. All display items (figures, tables, schemes) should be embedded with the text for easier reading in the review process. However, prior to acceptance, you will be required to upload figures as individual high resolution images (see below for more details). Authors will have significant latitude in the organization of the manuscript to promote clarity. Potential authors are strongly encouraged to seek the advice of the Editor prior to initiating work on a Perspective for the

journal. Perspectives must be accompanied by a Table of Contents (TOC)/Abstract graphic consisting of a colorful figure representing the topic of the Perspective.

Accounts. Summaries of the work of a single Principal Investigator (or collaborating investigators) describing their work in one research area. Accounts are peer-reviewed and contain an unreferenced abstract of 250 words or less. A good account provides a more personal perspective and presents the most important motivations for, and lessons derived from, the body of work being described. Logical organization and liberal use of graphical material, both designed to make the material more easily accessible to non-experts, is required. All display items (figures, tables, schemes) should be embedded with the text for easier reading in the review process. While most references in an Account will be to the author's own published papers, authors are encouraged to include references to other key papers that help to place the work described into context. Include a graphical Table of Contents entry/Abstract graphic consisting of a colorful figure that represents the topic of the Account. Authors may choose to divide the account into sections preceded by headings. Potential authors are strongly encouraged to seek the advice of the Editor prior to initiating work on an Account for the journal.

Technology Notes. Short descriptive manuscripts outlining new or improved "toolbox" innovations in any of a wide variety of technologies that impact modern combinatorial science. These include high-throughput/high-content screening, robotics, microfluidics, structure- and fragment-based drug design, parallel synthesis, genomic manipulation and analysis, protein expression and analysis, parallel or evolutionary biological screening methods, cell sorting techniques, and many others. Comparisons of the reported advance to alternative known methods, techniques, or instrumentation are strongly encouraged. Technology Notes are peer-reviewed and begin with an unreferenced abstract of less than 150 words. Abstracts should briefly state the technological innovation and the major advancement over existing methods, without excessive abbreviations or acronyms. The format is identical to that of a Letter (see above). Supporting Information is encouraged and may contain technical details and experimental procedures. Technology Notes should be approximately 3500 words or less in length (no more than 6 journal pages), including the abstract, body text, methods, references, and figure/scheme legends. Technology Notes typically contain 4–6 display items (figures/tables/schemes), embedded with the text for easier reading in the review process, and no more than 30 references. Technology Notes must be accompanied by a Table of Contents/Abstract graphic as part of the manuscript.

Article Type	**Max. Length**	**Required Headings** [a]	**Max. # Display Items** [b]	**Max. # References**
Articles	none [c]	Ab, I, R&D, E, Ack, SI, R, TOC, KW	10	as needed [c]
Letters	3500 words	Ab, E, Ack, SI, R, TOC, KW	6	30
Reviews	none [c]	Ab, I, Ack, R, TOC, KW	as needed [c]	as needed [c]
Perspectives	5000 words	Ab, I, Ack, R, TOC, KW	as needed [c]	as needed [c]
Accounts	none [c]	Ab, I, Ack, R, TOC, KW	as needed [c]	as needed [c]

Technology Notes	3500 words	Ab, E, Ack, SI, R, TOC, KW	6	30

(a) Key: Ab = Abstract; I = Introduction; R&D = combined Results and Discussion; E = Experimental Procedures; Ack = Acknowledgments; SI = brief summary of the contents of Supporting Information, if used; R = References and Notes; TOC = graphical image used for Table of Contents and for the Abstract, KW = keywords
(b) Figures, Schemes, and Tables
(c) No formal guideline, but authors will be asked to condense excessively long manuscripts, and to trim the number of display items or references if necessary

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, 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.
- Sharing your research with the public through ACS Publications open access program

MANUSCRIPT PREPARATION

Review Ready Submission

All ACS journals have simplified their formatting requirements in favor of a streamlined and standardized review-ready 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.
- A two-column manuscript template is available and can be used for manuscripts submitted to any ACS journal. Templates are not required but may be useful to approximate how an article will compose. For manuscripts with word count limits, authors are not required to fit content into a page limit based on the template.
- References can be provided in any style, but they must be complete, including titles.
- Supporting Information should be submitted as a separate file(s).
- Author names and affiliations on the manuscript must match what is entered into ACS.

Document Templates and Format

General information on the preparation of manuscripts may also be found in The ACS Style Guide.

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 must contain clear and precise information about the submission, highlighting the significance of the work. The letter must contain the following elements:

- Manuscript title
- Name of the corresponding author, with contact information
- Paragraph explaining why the manuscript is appropriate for *ACS Combinatorial Science*
- Short lay summary (1 paragraph, ~150 words) describing the significance of the study and its interest for a broad audience
- Suggestions for possible reviewers, as well as sufficient justification for excluding potential reviewers that might have a conflict of interest, may be included in the cover letter. This information is also required to be entered separately in the ACS Paragon Plus manuscript submission process.

If your manuscript is accepted for publication, *ACS Combinatorial Science* may choose promote your research article through press communications and social media platforms.

Manuscript Text Components

Title. 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.

List of Author Names. All those who have made substantial contributions to the work should be included. To facilitate indexing and retrieval and for unique identification of an author, first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and surnames (e.g., J. Robert Smith) should be used. At least one author must be designated with an asterisk as the person to whom correspondence should be addressed. Please see the Author List section of this document for additional information.

Author Affiliations. This should include only the address or addresses at which the work was performed. Each address should be cross-referenced to the specific author unless all authors are affiliated with all addresses.

Abstract. All manuscripts must contain an abstract, which should provide a succinct, informative summation of the most important results and conclusions**.** The maximum length for the abstract of each manuscript type is shown above. Abbreviations should be used sparingly and spelled out when first used. The abstract should be written in complete sentences without the use of subheadings or specialized jargon. It should be accessible to a broad scientific audience, for example, by being easily understandable by a graduate student in the field. The TOC graphic will also be used as an Abstract graphic. Abstract graphics are required for all manuscript types except Additions & Corrections and Editorials.

Keywords. Authors should provide a list of up to six keywords to be displayed below the abstract of their publication. Keywords are required for all manuscript types except Additions & Corrections and Editorials.

Introduction. In this section, the purpose and significance of the research should be clearly stated and placed in the context of earlier work in the area. Extensive historical summaries are seldom warranted and a complete survey of the literature should not be made, but the most important and relevant prior work should be cited.

Results and Discussion. In Letters and Technology Notes, this section should be continuous with the Introduction and does not receive a heading; in Articles, it should be given a heading after the Introduction. Authors may choose to mix the presentation of data and interpretation, or present all of the data before the discussion, whichever provides the more clear and concise account. The same data should not be presented in more than one figure or in both a figure and a table, although summaries or tabulations of data presented in figures may be included in Supporting Information if this makes extraction of data easier for the reader. The purpose of the discussion is to interpret the results and to relate them to existing knowledge in the field.

Experimental Procedures. A clear, unambiguous description of materials, methods, and equipment should be provided in a format that permits repetition of the work elsewhere. Novel experimental procedures and characterization data for key compounds should be described in sufficient detail, but where pertinent, synthetic and bioassay protocols should refer to published procedures by literature citation of the original method and any later modifications used. Supporting Information can be useful for presenting experimental details while limiting the size of the main document. 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. Results from experiments involving humans or tissue samples must additionally include a statement that informed consent was obtained from the subject or from the next of kin. Authors must emphasize any unexpected, new, 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.

<u>Special notes for combinatorial libraries of synthetic small molecules</u>

1. Methods for library generation, including any procedures of molecular cloning, transformation, expression, selection, and the like that may occur in the generation of biomolecular libraries or systems, must be clearly described so as to allow replication by investigators trained in standard manipulations of the art. Because some readers of *ACS Combinatorial Science* will not be experts in these techniques, care should also be taken to clearly explain the experimental design and strategy, using as little jargon as possible.
2. Estimates of theoretical library sizes and library coverage should be given for cases in which these two values are unlikely to be the same, such as in the creation of a genetic library limited by transformation efficiency into host cells.

Author Information. The following information should be provided in these specific subheadings:

- Present Addresses: Current address for each author if different from the location(s) where the research was conducted.
- Author Contributions: *ACS Combinatorial Science* recommends that individual contributions of authors be listed.

    - Example:
        - *X.Z. and J.Y. conceived and designed the experiments, X.Z. performed the experiments, X.Z. and J.Y. co-wrote the manuscript and Supporting Information.*
- Funding Sources. Whenever possible, grant numbers should be included, as in: "This work was supported by the NIH (GM123456)."
- Conflict of Interest: If any conflicts exist, they should be described in this subheading. Please see the Conflict-of-Interest Disclosure section for more details.

Acknowledgments. Technical assistance, advice from colleagues, gifts, etc., should be included in this section.

Abbreviations. If nonstandard abbreviations (see *The ACS Style Guide*) are used within the manuscript, then a section should be added to identify the abbreviations. Such abbreviations should also be defined on first appearance in the manuscript text.

References. All references should be compiled together in a list at the end of the manuscript text. During the publication process, many of them will have links added to other Web resources, such as the corresponding abstracts in *Chemical Abstracts* and the full text on publisher Web sites. Because of this electronic linking and because the references are not checked in detail by Editors or reviewers, it is crucial that authors verify their accuracy.

See the descriptions of the types of manuscripts above for guidance concerning the number and suggested coverage of references expected in each. However, unnecessarily long lists of references should always be avoided. *Each reference should be listed as a separate citation, and each should be assigned a unique reference number*. Footnotes are not permitted. This information should be incorporated parenthetically within the body of the text or included in the reference list. Additional data and peripheral discussion should usually be placed in the Supporting Information. Supplementary references may be placed in the Supporting Information. Literature references must be numbered with Arabic numerals in the order of their first citation in the text, and the corresponding numbers must be inserted at the appropriate locations in the text. The following reference styles should be used.

For journals:
Rich, D. H.; Green, J.; Toth, M. V.; Marshall, G. R.; Kent, S. B. H. Hydroxyethylamine Analogues of the p17/ p24 Substrate Cleavage Site Are Tight-Binding Inhibitors of HIV Protease. *ACS Comb. Sci*. **2010**, *1*, 1285-1288.

For journal articles published online ahead of issue or online only, the DOI should be used as follows:
Liu, C.; Yang, S. Synthesis of Angstrom-Scale Anatase Titania Atomic Wires. *ACS Comb. Sci.*, published online March 23, 2009; DOI: 10.1021/nn900157r.

For monographs:
Casy, A. F.; Parfitt, R. T. *Opioid Analgesics*; Plenum Press: New York, 1986; pp 333-384.

For edited books:
Rall, T. W.; Schleifer, L. S. Drugs Effective in the Therapy of the Epilepsies. In *The Pharmacological Basis of Therapeutics*, 7th ed.; Gilman, A. G., Goodman, L. S., Rall, T. W., Murad, F., Eds.; Macmillan Publishing Co.: New York, 1985; pp 446-472.

Titles of journals should be abbreviated according to *Chemical Abstracts Service Source Index* (CASSI). Manuscripts accepted for publication should be cited as "in press"; the DOI should be given if the manuscript is published online. Manuscripts that are in preparation or have been submitted, but have not yet been accepted, should be cited as unpublished results or personal communications.

For work published online (*Just Accepted* Manuscripts or ASAP) and work submitted for publication (e.g., submitted; in press), the DOI should be furnished in addition to the standard bibliographic information. Authors are given instruction for citing work by DOI in an email communication when manuscript proofs are made available. A DOI is assigned to each manuscript and should be in the form http://dx.doi.org/10.1021/co000000a. DOI is an accepted form of citation before and after the article appears in an issue.

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 description of each file is required, and the paragraph and descriptions should be placed at the end of the manuscript before the list of references. The appropriate format is as follows:

Supporting Information. Brief descriptions in nonsentence format listing the contents of the files supplied as Supporting Information.

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.

Data Requirements

Nomenclature

Nonstandard abbreviations (see *The ACS Style Guide*) and acronyms should be used sparingly, and all usage should be defined at the first occurrence in the text. Whenever possible, systematic nomenclature as recommended by IUPAC and IUBMB for chemical compounds and biomolecules should be used. Names of organisms should comply with genetic conventions, with genus and species names written in italics and spelled out in full on first appearance. Gene symbols should conform to approved nomenclature and should be italicized, whereas corresponding protein products should start with a capital letter and should not be italicized. The available nomenclature databases (e.g., LocusLink) should be consulted for correct names and symbols. Enzyme names should be accompanied by their Enzyme Commission (EC) numbers (e.g., see http://www.expasy.ch/enzyme).

Known Compounds

For known compounds, the source or literature reference to the method of preparation and characterization should be provided. Authors are encouraged to ensure that these references actually provide such information, rather than directing the reader to other citations.

Characterization of Novel Matter

Library Compounds. For compounds prepared in a library format, a general experimental procedure should be provided, including full experimental details, with yields, for a representative selection of library members. The synthesis protocols and selected characterized compounds must reflect the reliability and scope of the reaction sequence. Complete characterization data for compounds comprising libraries need not be reported. However, the synthesis of mixtures without characterization of representative members having significant function does not constitute publishable research and therefore must be coupled with the identification and validation of active compounds. In other words, the synthesis and testing of mixtures may be reported, but library members responsible for observed activity should be identified and characterized, and their activity verified. (See discussion of Key Compounds, below.) Reviewer evaluation of the methods utilized for establishing overall library purity will be an integral part of the manuscript review process. The following guidelines will be used.

Authors must demonstrate the reliability of their reaction sequence and the purity of the compounds produced. In most instances, for the proposed chemistry to be considered successful and eligible to be judged significant, it is expected that at least 80% of the sampled members of an unpurified library will have chemical purities in excess of 80%. Of course, manuscripts describing higher standards should be considered to meet the significance criterion more readily. Sequences that meet lesser standards may be considered if their scope is clearly identified and they introduce strategies or concepts of significant novelty.

Spectroscopic analyses should be provided for a random sampling of all new libraries that are not composed of composite materials. In most cases, this shall mean that 5% or 20 members of a library (whichever is greater) shall be sampled for purity and identity using appropriate methods, such as high-performance liquid chromatography (HPLC), liquid chromatography-mass spectrometry (LC-MS), gas chromatography (GC and GC-MS), supercritical fluid chromatography (SFC and SFC-MS), NMR, or some combination for small molecules. Note, however, that ratios of peak areas in LC or GC analyses do not, in general, directly provide ratios of compound concentrations, and quantitative calibration must be performed in such situations. Similarly, chromatographic analyses in conjunction with gravimetric determinations are helpful in determining purity but are usually not definitive due to weaknesses in detecting the presence of residual solvent and inorganics. NMR against a known concentration of internal standard is an excellent technique, but significant errors can occur if tetramethylsilane (TMS) is used without consideration of its volatility. Hexamethyldisiloxane is an alternate internal standard of similar chemical shift (~0.2 ppm relative to TMS) and much lower volatility. As noted below, more stringent requirements for NMR data apply to key compounds, defined as those molecules exhibiting exemplary function, structure, or composition.

Techniques, such as HPLC, gel permeation chromatography (GPC), size-exclusion chromatography (SEC), and MS, can be employed for polymers, and gel electrophoresis and semi-quantitative sequencing techniques for proteins and polynucleotides. In some cases, less than 5% sampling may be acceptable if the reviewers are provided sufficient analytical data to convince them of the overall chemical integrity of the library.

The Editor also understands that some aspects of characterization may be extremely difficult, if not impossible, for certain types of compounds/materials. In such cases, a detailed explanation in a cover letter explaining the characterization conducted and why additional characterization is not possible is requested. Queries regarding the acceptability of a particular library characterization are welcomed.

Key Compounds. Complete data should be provided for key compounds, which are those compounds in a manuscript that receive extra attention beyond the primary or general screening that is applied to the entire set for structure–activity analysis. For example, key compounds are those that are subject to additional or follow-up studies for activity or function. The relevant characterization data for **key compounds** are as follows:

HRMS and Elemental Analysis. For novel key compounds (excluding biomacromolecules and crosslinked polymers or materials), elemental analysis data should be reported to support the molecular formula assignment. HRMS data, while less desirable, can serve as an alternative. The reported elemental analysis or HRMS data should include the molecular formulas on which the theoretical (calcd) values are based, including any added atoms (often H^+ or Na^+ for ionization in MS). Found values should be close enough to the calcd values, and have sufficiently small estimated uncertainties, to exclude alternative plausible formulas. For HRMS, the ionization method and the mass detector type should be reported. Elemental analysis values found for carbon, hydrogen, and nitrogen (if present) should be within 0.4% of the calcd values for the proposed formula. Complexed solvents, including water, should be confirmed by an additional analytical method, such as NMR for organic solvents and Karl Fischer titration for water, if possible.

NMR Spectral Data. ^{1}H NMR and ^{13}C NMR resonances should be provided for each key compound, according to the guidelines provided under the section below titled "Guidelines for Reporting and Stewardship of NMR Data" , and the solvent and instrument frequency should be identified. Authors are encouraged to place in the Supporting Information copies of well-resolved ^{1}H NMR and proton-decoupled ^{13}C NMR spectra for every new key compound, rather than providing only lists of peak positions and intensities. The structure and compound number should be clearly shown on each spectrum. ^{13}C NMR peak shifts should be rounded off to the nearest 0.1 ppm, except when greater precision is needed to distinguish between closely spaced peaks. If detailed peak assignments are made, the type of 2D NMR methods used to establish atom connectivities and spatial relationships should be identified in an Experimental Procedures paragraph in the Supporting Information. In cases where structure assignments of complex molecules depend heavily on NMR data interpretation, including isolated and synthesized natural products, copies of suitable 2D spectra should also be placed in the Supporting Information.

Melting Points. The reporting of melting points of key compounds isolated as pure solids is strongly encouraged; these values should be given as a *range*.

Isomers and Isomeric Mixtures. The composition of isomeric mixtures (regioisomers, diastereomers, and enantiomers) must be reported. Enantiomeric ratio (er) or diastereomeric ratio (dr) values are preferred over enantiomeric excess (ee) or diastereomeric excess (de) values. Specific optical rotations should be reported for enantiopure compounds, enantioenriched isomer mixtures, and isolated natural products, when a sufficient sample is available. Specific rotations based on the equation $[\alpha] = (100\cdot\alpha)/(l\cdot c)$ should be reported as unitless numbers as in the following example: $[\alpha]_D^{20}$ (*c* 1.9, MeOH), 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.

Three-Dimensional Structures. 3D structures will be allowed in the main manuscript only if they represent an essential component of the research described; otherwise, they should be placed in

Supporting Information. Manuscripts reporting new 3D structures of small molecules from crystallographic analysis should include a structural figure with probability ellipsoids and an electronic copy of the structural data in Crystallographic Information File (CIF) format. Authors are encouraged to check the quality of their CIF files through the checkCIF website of the International Union of Crystallography (http://checkcif.iucr.org). Those reporting NMR or X-ray crystal structures of macromolecules must include a table with relevant data collection and refinement statistics. For manuscripts reporting structures derived from electron microscopy experiments, authors must provide an image showing the distribution of particles being analyzed, the percentage of the particles being used in the reconstruction, and a correlation coefficient plot (or equivalent data) to indicate the resolution of the presented structure. Upon request from the Editor, the authors must provide sequence, structure data (including coordinate files and structure), and/or microarray data in a MIAME-compliant format to the Editors and reviewers for the purpose of evaluating the manuscript.

Power Diffraction Data. The presentation of X-ray powder diffraction data for new materials or for materials previously uncharacterized by this technique is encouraged. Data from X-ray powder measurements should be accompanied by details of the experimental technique: the radiation, its wavelength, filters or monochromators, camera diameter, the type of X-ray recording, and the technique for estimating intensities. In cases of an unindexed listing of the data, the *d* spacings of all observed lines should be listed in sequence, together with their relative intensities. In cases where filtered radiation is used, every effort should be made to identify residual β lines. Where resolution into α1–α2 doublets occurs, the identification of the *d* spacing for each line as *d*α1, *d*α2 gives a measure of the quality of the photograph. When an indexing of the data is offered, the observed and calculated 1/*d*2 values should be listed side by side along with the observed relative intensities (it is superfluous to give *d* spacings in this instance). All calculated 1/*d*2 values should be listed (exclusive of systematic absences), to the limit of the data quoted. If possible, the crystal system should be specified. Possible space groups may also be listed if the data warrant it. Relevant information about the specimen used should be included.

Peptides and Biomacromolecules. For peptide materials, it is necessary to provide an amino acid composition analysis. For biomacromolecules, structures 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 through standard sequencing techniques. Typically, a sequence will be accompanied by MS data that establish the molecular weight. Additional characterization and physical property data should be placed in the Supporting Information unless they are important to the main discussion.

QSAR/QSPR and Proprietary Data

General Guidelines. (1) Authors should explicitly state in the manuscript the novel features of the quantitative structure–activity relationships/quantitative structure–property relationships (QSAR/QSPR) study being reported. (2) All data and molecular structures used to carry out a QSAR/QSPR study should be reported in the manuscript or Supporting Information or must be readily available without infringements or restrictions. The use of proprietary data is generally not acceptable. (3) Standard QSAR/QSPR studies will only be considered if the predictions are experimentally tested and if the experimental data are novel and significant. Only QSAR/QSPR analyses that provide new insights into the mechanism of activity are encouraged.

Criteria for Establishing Significance in a Library Synthesis Project

Papers describing the syntheses of chemical libraries will be judged to be sufficiently significant by meeting one of two criteria: either (1) a fully characterized substance of novel, useful properties is identified or (2) evidence is provided that application of the methods described will very likely provide libraries in which there is high confidence that a large percentage of the library members consist of compounds of known structure in good homogeneity and in consistent amount. While synthetic methods leading to libraries of lower product confidence or purity may have value for the discovery of useful substances, applications of standard methods purely for the synthesis of libraries of acceptable purity are not in and of themselves sufficiently significant for publication. Submissions are also welcomed that describe methodology relevant to library synthesis, without reporting the synthesis of libraries, and their significance will be evaluated on a case-by-case basis.

Screening Data

Quantitative data are expected for manuscripts in which screening data are provided, unless unusual circumstances (e.g., compound instability) prohibit testing of specific substances. Test methods must be referenced or described in sufficient detail to permit the experiments to be repeated by others. Detailed descriptions of screening methods should be placed in the Experimental Section or Supporting Information (with a summary in the Experimental Section). Standard compounds should be tested in the same system for comparison. Data may be presented as numerical expressions or in graphical form; data for extensive series of compounds should be presented in tabular form. Tables consisting primarily of negative data will not usually be accepted; however, for purposes of documentation they may be submitted as Supporting Information.

In those cases where the major significance of a submission lies in the discovery of substances with novel properties, such members obtained from combinatorial syntheses should be resynthesized, purified if necessary, fully characterized (see “Key Compounds” section above), and retested to verify that the property of the pure substance conforms to the initial observation.

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. 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 data (usually a statement regarding inherent error, such as standard deviation, standard error of the mean, or the like) should be provided. References to statistical methods of calculation should be included. In vivo biological data should be accompanied by statistical limits (statistical significance). Concentrations and in vitro doses should be expressed as molar quantities (e.g., M, mM, μM, nM) whenever possible, rather than mass per volume, and in vivo doses as mass per unit animal weight.

Guidelines for Reporting and Stewardship of NMR Data

The following guidelines recommend a standard baseline for the submission of NMR data to ACS journals, and are intended in *ACS Combinatorial Science* to apply especially to “key compounds” in molecular libraries. These guidelines are intended to promote accuracy and consistency. Please also consult the ACS’ Ethical Guidelines to Publication of Chemical Research.

The guidelines are divided into three sections:

(1) NMR text, which outlines the preferred format for NMR data included in the Experimental Section

(2) NMR spectra, which outlines the preferred format for inclusion of hard copies of spectra in the Supporting Information
(3) Primary NMR data files, which outlines the procedure for submitting FID files, acquisition data and processing parameters to include in the Supporting Information

Authors are strongly encouraged to provide all three sets of data for all new and/or key compounds described in a manuscript submission. The benefits of providing a complete set of NMR data (text, spectra and primary data files) include:

For readers:
(a) Easy and direct data comparison
(b) Ability to evaluate compound purity
(c) Ability to zoom, integrate and manipulate spectra – NMR data is interactive

For Editors and reviewers, in addition to the benefits above, access to complete NMR datasets also provide:
(d) Consistent quality of NMR data across the ACS Portfolio
(e) Improved archiving for the long-term benefit of the scientific community

1. NMR Text (Experimental Section):

1.1 The compound must be clearly identified, for example in a header at the beginning of a) the synthetic procedure or b) the summary of spectroscopic data.
1.2 List the nucleus being measured, any nucleus being broad-band decoupled, the solvent used (formula preferred, e.g. C_6D_6 over benzene-d_6), the standard used, and the field strength.
1.2.1 Field strength should be noted for each spectrum, not as a comment in the general experimental section.
1.2.2 The standard(s) may be specified in the general experimental section; as an example, ^{1}H NMR data recorded in C_6D_6 listed as "residual internal C_6D_5H (δ 7.15)".
1.2.3 Indicate solvent or peak suppression protocols used in collecting data.
1.3 List the probe temperature when it is accurately known; ambient probe temperature is otherwise understood.
1.4 Give ^{1}H NMR chemical shifts to two digits after the decimal point. Include the number of protons represented by the signal, peak multiplicity, and coupling constants as needed (*J* italicized, reported with up to one digit after the decimal).
1.4.1 The number of bonds through which the coupling is operative, ^xJ, may be specified by the author if known with a high degree of certainty.
1.4.2 Accepted abbreviations for multiplicities and descriptors are:

s = singlet	dd = doublet of doublets
d = doublet	dt = doublet of triplets
t = triplet	td = triplet of doublets
q = quartet	br = broad signal
quint = quintet	
m = multiplet (denotes complex pattern)	

1.5 Chemical shifts should be listed consistently in a single article, starting either from downfield to upfield or vice-versa. Please consult the Author Guidelines for preferred formatting for each journal.

1.6 Assign peak identities under the following circumstances:

1.6.1 Non-decoupled or equivalent spectra have been collected (^{13}C, ^{31}P, etc).

1.6.1 2-D experiments have been performed.

1.6.2 Unambiguous assignment is possible without additional experiments, such as in the case of an organometallic metal-hydride ^{1}H signal, PF_6 vs. $MPPh_3$ ^{31}P signal, etc.

1.7 Give ^{13}C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks.

1.7.1 Include peak multiplicities for ^{1}H-coupled ^{13}C NMR spectra, or for signals in ^{1}H-decoupled spectra that are coupled to other magnetically active nuclei.

1.7.2 A ^{13}C NMR signal will be considered a singlet if the multiplicity is not assigned.

1.7.3 Only rarely is a true multiplet observed in a $^{13}C\{^{1}H\}$ NMR spectrum. However, a certain region may contain a group of unresolved peaks or signals.

1.8 Mention of unobserved resonances is encouraged.

Example 1 (no 2-D data collected):

(η^5-$C_5Me_5Co)_2$-μ-(η^4:η^4-C_9H_{10}) (**1**): ^{1}H NMR (C_6D_6, 400 MHz): δ -0.53 (s, 1H), 0.72 (d, 1H, *J* = 4.0 Hz), 0.98 (s, 1H), 1.58 (s, 15H), 1.62 (s, 3H), 1.73 (s, 15H), 1.95 (d, 1H, *J* = 4.0 Hz), 5.62 (t, 1H, *J* = 4.0 Hz), 6.00 (t, 1H, *J* = 4.0 Hz). $^{13}C\{^{1}H\}$ NMR (C_6D_6, 400 MHz): δ 10.2, 10.6, 17.4, 38.3, 51.5, 54.2, 60.6, 80.8, 81.0, 88.0, 88.7.

Example 2 (2-D data collected):

Silvestrol (**2**): ^{1}H NMR ($CDCl_3$ with 0.05% v/v TMS, 400 MHz): δ_H 7.10 (2H, d, *J* = 8.9 Hz, H2′ and H6′), 7.03-7.07 (3H, m, H3′′, H4′′ and H5′′), 6.83-6.85 (2H, m, H2′′ and H6′′), 6.66 (2H, d, *J* = 8.9 Hz, H3′ and H5′), 6.42 (1H, d, *J* = 1.8 Hz, H5), 6.26 (1H, d, *J* = 1.7 Hz, H7), 5.18 (1H, s, H1′′′), 5.01 (1H, d, *J* = 6.6 Hz, H1), 4.52 (1H, s, H2′′′), 4.27 (1H, d, *J* = 14.2 Hz, H3), 4.15 (1H, br d, *J* = 11.2 Hz, H4′′′), 4.05 (1H, t, *J* = 11.2 Hz, $H3_b$′′′), 3.88 (1H, *J* = 14.3, 6.8 Hz, H2), 3.86 (3H, s, $OCH_3$8), 3.69 (3H, s, $OCH_3$4′), 3.64 (3H, s, $COOCH_3$2), 3.49 (3H, br s, H5′′′ and H6′′′), 3.43-3.47 (1H, overlapped, $H3_a$′′′), 3.45 (3H, s, $OCH_3$2′′′). ^{13}C NMR ($CDCl_3$, 125 MHz): δ_C 170.6 (s, $\underline{CO}CH_3$2), 160.6 (s, C4a), 160.0 (s, C6), 158.8 (s, C4′), 157.1 (s, C8), 136.7 (s, C1′′), 129.0 (d, C2′ and C6′), 127.8 (d, C2′′, C3′′, C5′′ and C6′′), 126.6 (d, C4′′), 126.3 (s, C1′), 112.7 (d, C3′ and C5′), 109.6 (s, C8a), 101.9 (s, C3a), 95.2 (d, C2′′′), 94.0 (d, C1′′′), 93.9 (d, C7), 93.4 (s, C8b), 92.9 (d, C5), 79.7 (d, C1), 70.7 (d, C5′′′), 68.3 (d, C4′′′), 63.3 (t, C6′′′), 59.0 (t, C3′′′), 55.9 (q, $OCH_3$8), 55.1 (q, $OCH_3$4′), 55.0 (d, C3; q, $OCH_3$2′′′), 52.1 (q, $CO\underline{CH_3}$2), 50.3 (d, C2).

Note

Broad peaks between δ_H 1.5 to 3.0 ppm and at δ_H 3.79 ppm correspond to the protons of the OH groups on C-1, C-8, C-5′′′ and C-6′′′, which disappeared after D_2O exchange.

Example 3:

(*E,E*)-3,7,11-Trimethyl-2,6,10-dodecatrien-I-yl diphosphate (Farnesyl diphosphate, FPP, **3**): ^{1}H NMR (D_2O, 300 MHz): δ 1.61 (s, 6H), 1.68 (s, 3H), 1.72 (s, 3H), 2.17-1.99 (m, 8H), 4.45 (d of d, 2H, $J_{H,H}$ = 6 Hz, $J_{P,H}$ = 6 Hz), 5.23-5.15 (m, 2H), 5.46 (t, 1H, *J* = 6 Hz). ^{13}C NMR (D_2O, 75 MHz): δ 16.3, 16.6, 17.9, 25.9, 27.0, 27.2,

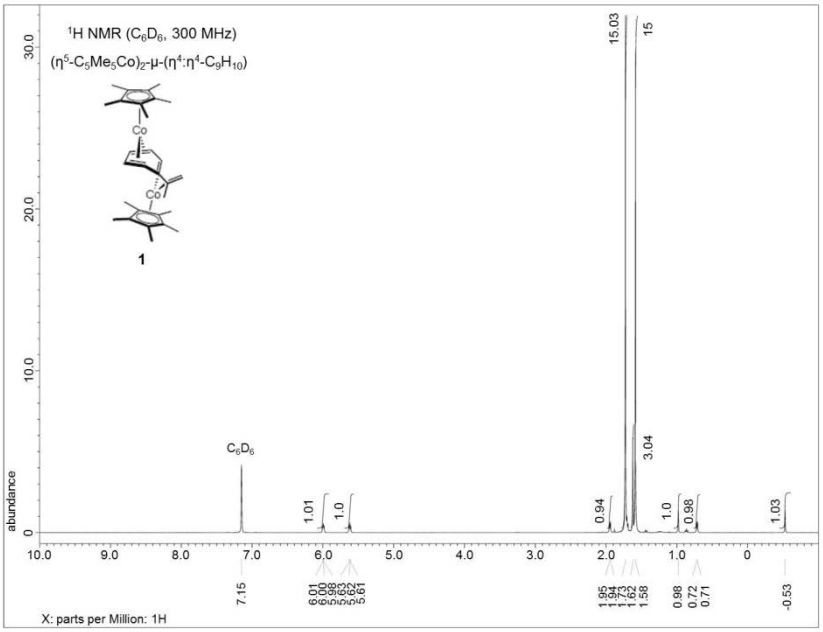
40.1, 40.2, 63.2, 120.5, 124.8, 125.1, 131.6, 135.9, 142.8. ^{31}P NMR (D_2O, 121.5 MHz): δ −6.56 (d, 1P, $J_{P,P}$ = 21.9 Hz), −9.89 (d, 1P, $J_{P,P}$ = 21.9 Hz).

2. NMR Spectra (Supporting Information):

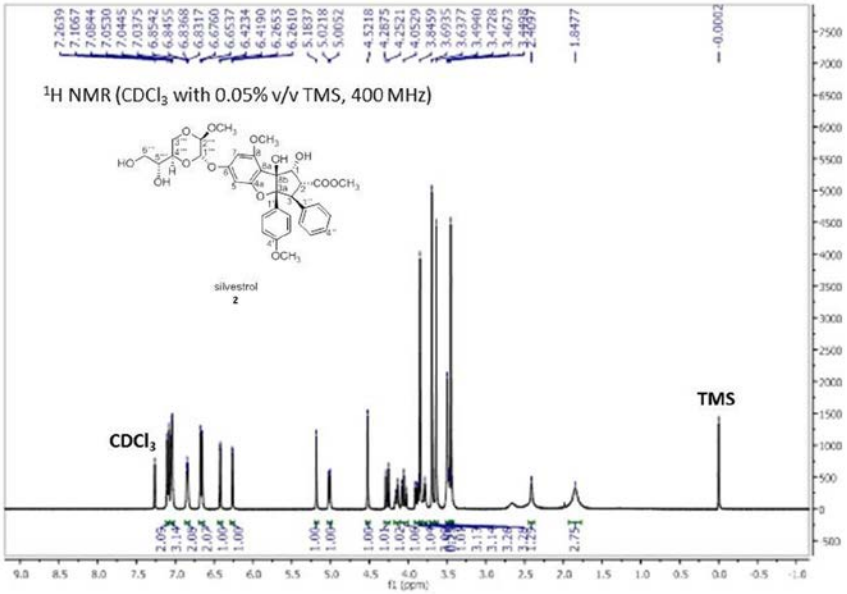
Submission of spectra (.doc, .docx, .txt, .pdf, .tif) is strongly recommended for all new and/or key compounds. When submitting spectra, please consider the following guidelines:

2.1 A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g. C_6D_6 over benzene-d_6) and the field strength.
2.2 A representation of the compound should be included on the spectrum – please use ChemDraw or a related program. The compound identifier used in the manuscript should be included.
2.3 The largest peak in the ^{1}H NMR spectrum should normally arise from the compound, not the solvent.
2.4 All peaks in the ^{1}H NMR spectrum should be integrated. Chemical shift values should be included.
2.5 The solvent peak should be clearly labeled on the spectrum.
2.6 All peaks should be visible on the spectrum. Insets are encouraged to show expanded regions. At minimum, the spectral window should be -1 ppm to 9 ppm for ^{1}H NMR and -10 ppm to 180 ppm for ^{13}C NMR.
2.7 Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

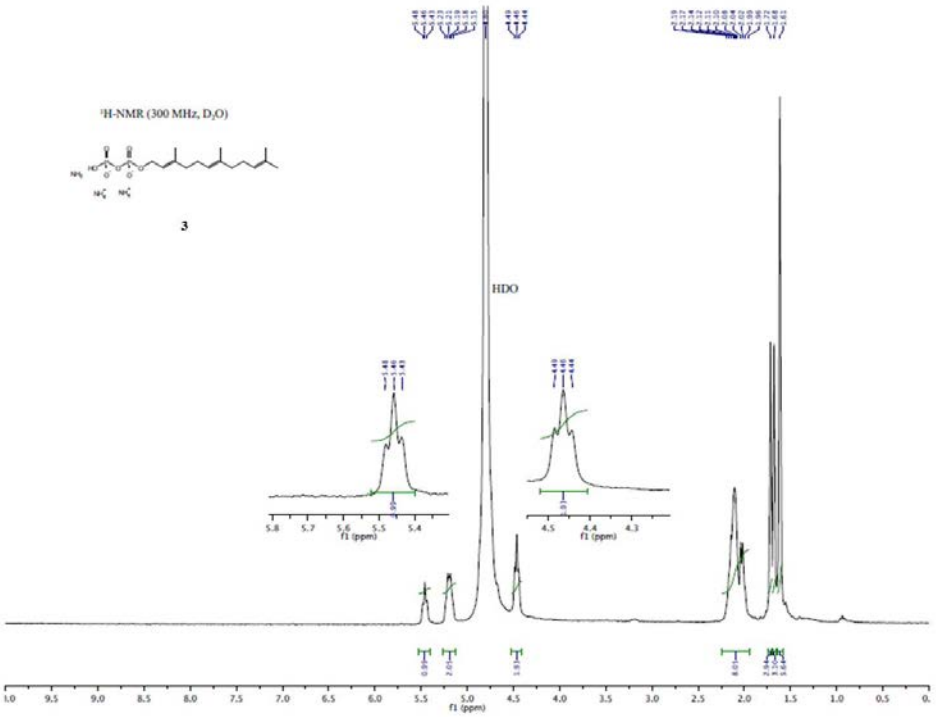
Example 1:

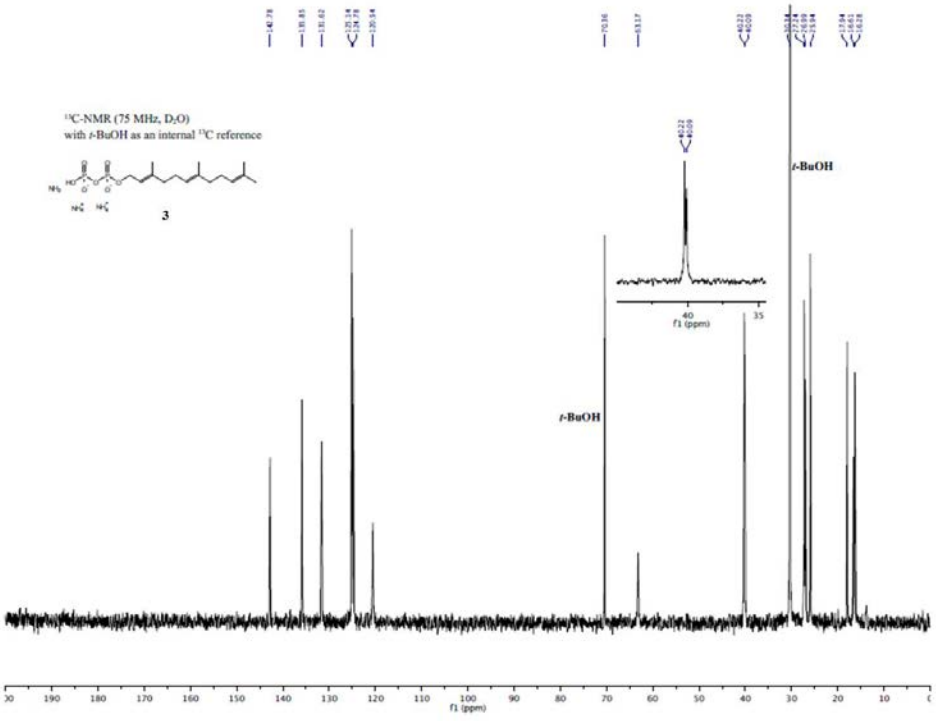


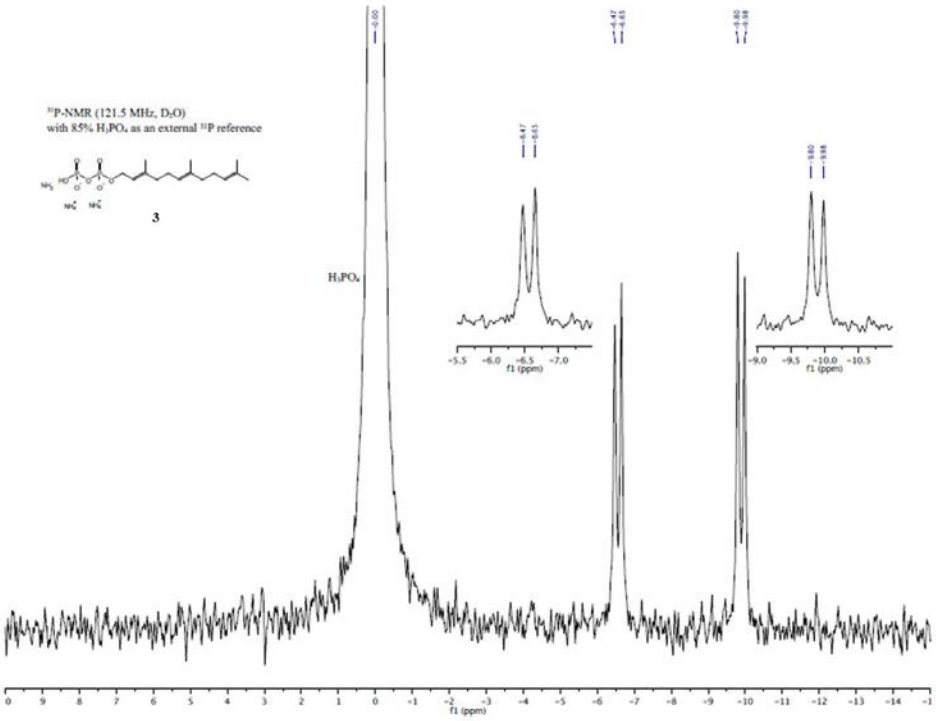
Example 2:



Example 3:


¹H-NMR (300 MHz, D₂O)
3
HDO
f1 (ppm)


¹³C-NMR (75 MHz, D₂O)
with t-BuOH as an internal ¹³C reference
3
t-BuOH
t-BuOH
f1 (ppm)



3. Primary NMR Data Files (Supporting Information)

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is encouraged for all new and/or key compounds. When submitting these files, please consider the following guidelines:

3.1 One folder should be created for each compound. The folder should be named clearly, using the compound name (if available) and compound identifier, as referenced in the Experimental Section or Supporting Information. Include the FID files, acquisition data and processing parameters for each experiment.

3.2 Name each spectrum according to the type of nucleus measured.

3.2.1 ^{1}H, ^{13}C, DEPT, COSY, etc

3.3 NMR files should be compressed into zip files -- please use multiple zip files if necessary. Files must be submitted in their native format.

3.4 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).

3.5 Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

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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 cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

Consult the Guidelines for Table of Contents/Abstract Graphics for specifications.

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 its contents

Tables

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter- relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

Schemes

Each scheme (sequences of reactions) may have a brief caption describing its contents.

Chemical Structures

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

Cover Art

Authors may submit their proposed cover art after manuscript acceptance by contacting the Managing Editor. Cover art should be colorful and interesting graphics with minimal text. It does not have to come from the manuscript. Images should be 8.438 inches wide x 7.375 inches high at 300 dpi. We are looking for high resolution, high-quality artwork. Acceptable formats are PSD, AI, TIF, PNG, EPS, JPG, PDF. We will also need a brief caption (20-30 words) describing the image.

Web Enhanced Objects (WEO)

The Web editions of ACS journals allow readers to view multimedia attachments such as animations and movies that complement understanding of the research being reported.

WEOs should be uploaded in ACS Paragon Plus with 'Web Enhanced Object' selected as the file designation. Consult the list of compatible WEO formats.