Information for Authors
(January 2017)

Contents (click on the topic)

Journal Scope

Types of Content


Additional Requirements – Nomenclature – Characterization of Novel Material – QSAR/QSPR and Proprietary Data – Criteria for Establishing Significance – Screening Data

Conditions of Acceptance


Guidelines for Reporting and Stewardship of NMR Data

Journal Scope

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

Types of Content

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 impacts 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.

**Additions and Corrections.** Additions and Corrections may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the ACS Paragon Plus environment by the corresponding author for publication in the “Addition/Correction” section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction, or provide evidence that such approval has been solicited. The Addition and Correction should include the original article title and author list, citation including DOI, and details of the correction. For proper formatting, see examples in a current issue of the Journal.

**Retractions.** Articles may be retracted for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. Retractions may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of Retraction will be published containing information about the original article title, author list, and the reason for the Retraction. Retracted articles will be accompanied by the related Retraction notice and will be marked as “Retracted”. The originally published article will remain on the web except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information see: [http://publicationethics.org/](http://publicationethics.org/).

The journal may also publish the *In This Issue* pieces, features devoted to highlighting research in the journal, and *Editorials* written by the editors or guest scientists.
## Summary of Guidelines for Manuscript Types

<table>
<thead>
<tr>
<th>Article Type</th>
<th>Max. Length</th>
<th>Required Headings</th>
<th>Max. # Display Items</th>
<th>Max. # References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Articles</td>
<td>none c</td>
<td>Ab, I, R&amp;D, E, Ack, SI, R, TOC, KW</td>
<td>10</td>
<td>as needed c</td>
</tr>
<tr>
<td>Letters</td>
<td>3500 words</td>
<td>Ab, E, Ack, SI, R, TOC, KW</td>
<td>6</td>
<td>30</td>
</tr>
<tr>
<td>Reviews</td>
<td>none c</td>
<td>Ab, I, Ack, R, TOC, KW</td>
<td>as needed c</td>
<td>as needed c</td>
</tr>
<tr>
<td>Perspectives</td>
<td>5000 words</td>
<td>Ab, I, Ack, R, TOC, KW</td>
<td>as needed c</td>
<td>as needed c</td>
</tr>
<tr>
<td>Accounts</td>
<td>none c</td>
<td>Ab, I, Ack, R, TOC, KW</td>
<td>as needed c</td>
<td>as needed c</td>
</tr>
<tr>
<td>Technology Notes</td>
<td>3500 words</td>
<td>Ab, E, Ack, SI, R, TOC, KW</td>
<td>6</td>
<td>30</td>
</tr>
<tr>
<td>Additions and Corrections</td>
<td>none c</td>
<td>as needed c</td>
<td>as needed c</td>
<td></td>
</tr>
<tr>
<td>Retractions</td>
<td>none c</td>
<td>as needed c</td>
<td>as needed c</td>
<td></td>
</tr>
</tbody>
</table>

(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

See the [Additional Requirements](#) section below for guidelines on acceptable methods for establishing the identity and purity of chemical compounds, materials, and biological structures reported in the journal.

## Editorial Process and Peer Review

Manuscripts are handled expeditiously, and full advantage is taken of web technology in the submission and review of manuscripts.

### Presubmission Inquiries

Presubmission inquiries can be made to the Editor-in-Chief by e-mail at [eic@combsci.acs.org](mailto:eic@combsci.acs.org).

### Review Process

The Editors evaluate submitted manuscripts, and only those judged to fall within the scope of the journal and to be of potential interest to our readers are sent to two or more reviewers for evaluation. Reviewers can suggest that a manuscript be published, revised, or rejected. Reviewers will evaluate the originality, technical quality (including appropriateness of compound characterization data), clarity of presentation, and significance to the field. The Editors evaluate the reviewers’ arguments in the context of the scope of the journal and make the final decision on each manuscript.

Editorial decisions are based on many factors. Reviewers’ concerns are considered very seriously. When reviewers suggest different decisions, additional information may be requested from the reviewers, other experts may be consulted, the authors may be asked to clarify questionable sections, or both. Reviewers may be asked to consider subsequent versions of the manuscript, especially if new data have been added to the manuscript, to evaluate whether the authors have sufficiently addressed
the scientific concerns. In such cases, blind copies of all previous reviewer comments may be sent to the reviewers. This practice allows the reviewers to obtain a clear understanding of the expectations of the Editors. The Editors will expedite any additional rounds of reviews to ensure timely publication.

**Anonymity**
The ACS strongly disapproves of any attempts by authors to determine the identity of reviewers or to confront potential reviewers. The editorial policy of this journal is to neither confirm nor deny any speculation about the identities of our reviewers. The journal will not release the identity of a reviewer to the authors or to other reviewers.

**Professional Ethics**
All parties—Editors, reviewers, and authors—are expected to adhere to the standards embodied in the American Chemical Society’s Ethical Guidelines to Publication of Chemical Research, which are available at [http://pubs.acs.org/ethics](http://pubs.acs.org/ethics). Authors are reminded of their obligation to obtain the consent of all coauthors before submitting a manuscript for publication. If any change in authorship is necessary after a manuscript has been submitted, the corresponding author must provide a signed letter (via e-mail with copy to all coauthors) to the Editor confirming that all of the original coauthors have been notified and have agreed to the change.

In publishing only original research, ACS is committed to deterring plagiarism, including self-plagiarism. ACS Publications uses CrossCheck’s iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process. Further information about plagiarism can be found in Part B of the [Ethical Guidelines to Publication of Chemical Research](http://pubs.acs.org/ethics).

**Submission Policies**

**Conflict-of-Interest Disclosure**
A statement describing any financial conflicts of interest or lack thereof is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors of the manuscript. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest (please see the [ACS Ethical Guidelines](http://pubs.acs.org/ethics)). The statement will be published in the final article. If no conflict of interest is declared, the following statement will be published in the article: “The authors declare no competing financial interest.”

**Funding Sources**
Authors are required to report ALL funding sources and grant/award numbers relevant to this manuscript. Enter all sources of funding for ALL authors relevant to this manuscript in BOTH the Open Funder Registry tool in ACS Paragon Plus and in the manuscript to meet this requirement. See [http://pubs.acs.org/page/4authors/funder_options.html](http://pubs.acs.org/page/4authors/funder_options.html) for complete instructions.

**Institution Identification**
Many Funders and Institutions require that institutional affiliations are identified for all authors listed in the work being submitted. ACS facilitates this requirement by collecting institution
information during manuscript submission under Step 2: Authors and Affiliations in ACS Paragon Plus.

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

**ORCID**
Authors submitting manuscript revisions are required to provide their own personal, validated ORCID iD before completing the submission, if an ORCID iD is not already associated with their ACS Paragon Plus user profiles. This iD may be provided during original manuscript submission or when submitting the manuscript revision. All authors are strongly encouraged to register for an ORCID iD, a unique researcher identifier. The ORCID iD will be displayed in the published article for any author on a manuscript who has a validated ORCID iD associated with ACS when the manuscript is accepted.

With an ORCID iD, you can create a profile of your research activities to distinguish yourself from other researchers with similar names, and make it easier for your colleagues to find your publications. If you do not yet have an ORCID iD, or wish to associate your existing ORCID iD with your ACS Paragon Plus account, you may do so by following the ORCID-related links in the Email/Name section of your ACS Paragon Plus account. Learn more at http://www.orcid.org.

**Publication Costs**
*ACS Combinatorial Science* does not impose submission or publication fees.

**Data Deposition**
Papers published in *ACS Combinatorial Science* will have complete experimental data and protocols available to readers in the primary journal publication, Supporting Information, or through deposition in a publicly used database such as those listed below. The hosting of such information on an author’s Web site is not an acceptable substitute. Authors should endeavor to make available to interested academic researchers research materials reported in their manuscript that are not otherwise reasonably obtainable. Any restrictions as to the availability of materials or information should be stated at the time of submission.

*Sequence Data.* Manuscripts reporting protein or nucleic acid sequences will not be published without an accession number to GenBank/EMBL/DDBJ, SWISS-PROT, or another appropriate database in the field that provides free access to the data for all scientists from the date of publication.
**Crystal and NMR Structures.** Small molecular crystallographic data should be submitted upon publication to the Cambridge Structural Database (www.ccdc.cam.ac.uk). For papers describing structures of biological macromolecules, the atomic coordinates and the related experimental data (structure factor amplitudes/intensities, NMR restraints, or both) must be deposited at a member site of the Worldwide Protein Data Bank (www.wwpdb.org): RCSB PDB (www.pdb.org), PDBe (www.ebi.ac.uk/pdbe), PDBj (www.pdbj.org), or BMRB (www.bmr.b.wisc.edu). These manuscripts must specifically state that the atomic coordinates have been deposited a member site of the Worldwide Protein Data Bank and must list the accession codes. The coordinates must be designated “for immediate release upon publication”. Authors are encouraged to release the atomic coordinates and experimental data when the associated article is published. Questions relating to depositions should be sent to deposit@wwpdb.org.

**Electron Microscopy Data.** No formal requirement exists for deposition of molecular envelope reconstruction from electron microscopy data, but the journal encourages authors to deposit relevant information in appropriate databases. Approved databases for deposition of electron microscopy data are the Worldwide Protein Data Bank (www.wwpdb.org), the Protein Data Bank Japan (www.pdbj.org), or the Macromolecular Structure Database–EMBL–European Bioinformatics Institute (MSD-EMBL-EBI, www.ebi.ac.uk/pdbe/).

**Microarray Data.** Data must be submitted to the GEO (www.ncbi.nlm.nih.gov/geo) or ArrayExpress (www.ebi.ac.uk/arrayexpress) databases, and the relevant accession numbers must be included in the published manuscript. Please reference the Microarray Gene Expression Data (MGED) open letter specifying microarray standards at https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1277123/.

**Genetically Modified Organisms and Mutants.** Established repositories such as the Jackson Laboratory, the Mutant Mouse Regional Resource Center, the American Type Culture Collection, the UK Stem Cell Bank, or another public storage area should be used whenever possible. Large data sets for which an approved database has not yet been established must be housed as online Supporting Information at ACS Combinatorial Science.

**Just Accepted Manuscripts**

*Just Accepted* manuscripts are peer-reviewed, accepted manuscripts that are posted on the ACS Publications website prior to technical editing, formatting for publication, and author proofing—usually within 30 minutes to 24 hours of acceptance by the editorial office. During the manuscript submission process, Authors can choose to have their manuscript posted online as a *Just Accepted* manuscript. To ensure rapid delivery of the accepted manuscript to the Web, Authors must adhere carefully to all requirements in the journal’s Information for Authors. For further information, please refer to the *Just Accepted* FAQ, accessible from http://help.acs.org. Note that publishing a manuscript as *Just Accepted* is not a means by which to comply with the NIH Public Access Mandate.

**Online Publication**

Authors should review proofs in detail to ensure that the text and figures are correct. ACS Combinatorial Science will publish manuscripts online within 1 to 4 days after the corrected proofs are returned. These ASAP (As Soon As Publishable) articles represent the final scientific articles of record. Published manuscripts are definitive and may be altered only through an Addition and Correction. All articles published receive a unique digital object identifier (DOI) number, which may be used for citation prior to compilation in a final issue of the journal.
Patent Activities and Intellectual Property Issues
Authors are responsible for ensuring that all patent activities and intellectual property issues are satisfactorily resolved prior to first publication (Just Accepted, ASAP, or in issue). Acceptance and publication will not be delayed for pending or unresolved issues of this nature.

Security Concerns
Certain manuscripts may represent a potential security risk to the public. Such manuscripts must be brought to the attention of the Editors of the journal. If necessary, outside reviewers with expertise in security matters will be consulted.

Submission Procedure
Manuscripts and all revisions must be submitted online via the ACS Paragon Plus Environment (http://paragonplus.acs.org/login). Complete instructions and an overview of the electronic online (Web) submission process are available through the secure ACS Paragon Plus Web site. The Web submission site employs state-of-the-art security mechanisms to ensure that all electronically submitted manuscripts are secure. These same security mechanisms are also utilized throughout the peer-review process, permitting access only to Editors and reviewers who are assigned to a particular manuscript. Submission is taken to imply that all coauthors have approved of the content and submission to ACS Combinatorial Science and that the corresponding author is authorized to represent all authors. The submission of the manuscript to ACS Combinatorial Science is done on an exclusive basis.

Writing Style and Language Usage
Scientists with a broad range of training and interests read ACS Combinatorial Science. Therefore, it is important for authors to make all manuscripts understandable to a wide scientific audience. The Editors will request that authors rewrite portions of the manuscript when this objective is not met. Clarity and conciseness are critical requirements for publications. Authors should consult The ACS Style Guide for guidance on style, word-usage conventions, nomenclature, physical quantity symbols and units, abbreviations, use of italics, and punctuation.

The ACS Style Guide also provides information about copyrights and insight on what Editors and reviewers look for in evaluating manuscripts. Spelling and the use of periods and commas in numbers should conform to U.S. usage. Any author who is not fully fluent in idiomatic English is urged to obtain assistance with manuscript preparation from a colleague whose native language is English. For more information, authors may visit the Language Editing Services listed under the Publishing Tools tab of the ACS Author & Reviewer Resource Center.

Manuscripts should be kept at minimum length. The rationale and objectives of the research should be stated in the introductory sentences of the manuscript. The background material should be brief and relevant to the research described. Detailed or lengthy descriptions of routine experimental procedures should be avoided in the introductory and discussion sections. Authors should state their conclusions or the significance of their findings following the discussion of results. Conclusions should also be summarized in the abstract in order to place the authors’ research in proper perspective.

Assistance with Improving Your Manuscript
Authors may want professional assistance with improving the English, figures, or formatting in their manuscript before submission. ACS ChemWorx Authoring Services can save you time and improve the communication of research in your manuscript. You can learn more about the services offered at http://es.acschemworx.acs.org.

Cover Letter
All manuscripts must be accompanied by a cover letter that contains 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 to modify, edit, and publish your lay summary in the *In This Issue* feature of the journal. The journal may also promote your research article through press communications.

Journal Publishing Agreement
A properly completed and signed Journal Publishing Agreement must be submitted for each manuscript. ACS Paragon Plus provides an electronic version of the Agreement that will be available on the My Authoring Activity tab of the Corresponding Author's Home page once the manuscript has been assigned to an Editor. A PDF version of the Agreement is also available, but Authors are strongly encouraged to use the electronic Journal Publishing Agreement. If the PDF version is used, all pages of the signed PDF Agreement must be submitted. If the Corresponding Author cannot or should not complete either the electronic or PDF version for any reason, another Author should complete and sign the PDF version of the form. Forms and complete instructions are available at http://pubs.acs.org/page/copyright/journals/index.html.

Acceptable File Formats and Graphics Specifications
*Graphical Table of Contents/Abstract Graphic.* Each manuscript must include a graphic for the Table of Contents, which will also be used as an Abstract graphic. This graphic should be designed to capture the readers’ attention and, in conjunction with the manuscript title, give readers a visual impression of the essence of the manuscript without providing specific results. The type size of labels, formulas, or numbers within the graphic must be legible at publication size. Tables or spectra are not acceptable. Color graphics are highly encouraged, with text kept to a minimum. At final published size, all text should be at least 6 points in size. These graphics should be approximate 1.5 inches high and 3.33 inches wide (3.81 x 8.46 cm).

*Text.* Please refer to the Manuscript Submission and Peer Review sections in the ACS Paragon Plus site (http://paragonplus.acs.org) for a complete listing of acceptable file formats.
Tables. Tables should be submitted within the body of the manuscript text file and have the following characteristics:

- Tables should be consecutively numbered and use Arabic numbers.
- A descriptive heading should be included that, together with the individual column headings, makes the table self-explanatory.
- Footnotes should be given letter designations and cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column.
- When a reference is cited, a lettered footnote should be inserted in the table and the reference number should be placed in a footnote.
- When columns are used, data should be arranged efficiently to save space.
- Tables may be created using a word processor’s text mode or table format feature. The table format feature is preferred. Ensure each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row.
- Crystallographic and NMR data tables should be placed last in a series of tables in a manuscript, because they are generally placed in the Experimental Procedures section. Where appropriate, these may also be moved to the Supporting Information section.

Graphics.

To facilitate the publication process, please submit manuscript graphics using the following guidelines:

- The preferred submission procedure is to embed graphic files in a Word document. It may help to print the manuscript on a laser printer to ensure all artwork is clear and legible.
- Additional acceptable file formats are: TIFF, PDF, EPS (vector artwork) or CDX (ChemDraw file). If submitting individual graphic files in addition to them being embedded in a Word document, ensure the files are named based on graphic function (i.e. Scheme 1, Figure 2, Chart 3), not the scientific name. Labeling of all figure parts should be present and the parts should be assembled into a single graphic.
  - EPS files: Ensure that all fonts are converted to outlines or embedded in the graphic file. The document settings should be in RGB mode. NOTE: While EPS files are accepted, the vector-based graphics will be rasterized for production. Please see below for TIFF file production resolutions.
  - TIFF files (either embedded in a Word doc or submitted as individual files) should have the following resolution requirements:
    - Black & White line art: 1200 dpi
    - Grayscale art (a monochromatic image containing shades of gray): 600 dpi
    - Color art (RGB color mode): 300 dpi
    - The RGB and resolution requirements are essential for producing high-quality graphics within the published manuscript. Graphics submitted in CMYK or at lower resolutions may be used, however, the colors may not be consistent and graphics of poor quality may not be able to be improved.
    - Most graphic programs provide an option for changing the resolution when you are saving the image. Best practice is to save the graphic file at the final resolution and size using the program used to create the graphic.
- Graphics should be sized at the final production size when possible. Single column graphics are preferred and can be sized up to 240 points wide (3.33 in.). Double column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). All graphics have a maximum depth
of 660 points (9.167 in.) including the caption (please allow 12 pts for each line of caption text).
  o Consistently sizing letters and labels in graphics throughout your manuscript will help ensure consistent graphic presentation for publication.
  o Arial font should be used for lettering within a graphic.
    ▪ Lettering should be ~6 points. If the submitted artwork must be reduced, larger lettering and thicker lines should be used so that, when reduced, the artwork meets the above-mentioned criteria.
    ▪ Lines should be no thinner than 0.5 point. Lettering and lines should be of uniform density.
    ▪ Text within a graphic should be initial-capped.
  • Panel labels should be bold, lowercase, and in the upper left-hand corner of the panel.
  • A rule should not be placed around the entire graphic.
  • Graphs containing similar information should be of similar size.
  • A graphic should be submitted for use as in the Table of Contents and Abstract. This graphic should give the reader a quick visual representation of the essence of the paper without providing specific details. The best images for these uses are simple, relatively free of text and technical characters, and make use of color for visual impact.
  • For more information, please visit http://pubs.acs.org/page/4authors/submission/index.html.

Organization of Manuscript

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.

**Special notes for combinatorial libraries of synthetic small molecules**

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.
Supporting Information. This information is made available to the reviewers during the peer-review process. For accepted papers, this information is made available free of charge to readers of the journal. The Supporting Information format of this journal can accommodate and make readily available almost any type of supplementary figures or data (e.g., reproductions of spectra, experimental procedures, tabulated data, or expanded discussion of peripheral findings). Supporting Information must be submitted at the same time as the manuscript and uploaded separately to the ACS Paragon Plus Environment. A list of acceptable file types is available on the Web. All Supporting Information files of the same type should be prepared as a single file (rather than submitting a series of files containing individual images or structures). For example, all Supporting Information available as PDF files should be contained in one PDF file.

If the manuscript is accompanied by any supporting information files for publication, a brief description of each file is required. The paragraph and descriptions should be placed at the end of the manuscript before the list of references. The appropriate format is:

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

Web-Enhanced Objects, Such as Movies. The use of multimedia attachments such as animations and movies is encouraged. These objects should complement a reader’s understanding of the research being reported. Authors should submit Web-enhanced objects via the ACS Paragon Plus Web site as part of their submissions and clearly indicate to the Editor that the material is Web-enhanced object content. Descriptions of Web-enhanced objects should be noted in the appropriate places within the graphic caption or text of the manuscript, noting the type of file and format. Example: “A 3D rotatable image in xyz format is available.” For acceptable file formats and specifications, please refer to the Specifications on Web Enhanced Objects (http://pubs.acs.org/page/4authors/submission/weo.html)

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:

  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:

- For edited books:

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.
Additional 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](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 tetrathelinsilane (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 calcld 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 calcld 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.** 1H NMR and 13C 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 1H NMR and proton-decoupled 13C 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. 13C 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: \([\alpha]_D^{20} (c \ 1.9, \text{MeOH})\), where the concentration \(c\) is in g/100 mL and the path length \(l\) is in decimeters. The units of the specific rotation, \((\text{deg} \cdot \text{mL})/(\text{g} \cdot \text{dm})\), 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 \(\beta\) lines. Where resolution into \(\alpha_1–\alpha_2\) doublets occurs, the identification of the \(d\) spacing for each line as \(da_1, da_2\) 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.

**Conditions of Acceptance**

When an article is accepted for publication in *ACS Combinatorial Science*, the authors will

- Honor any reasonable request from Editors, reviewers, and other scientists for materials, methods, or data necessary for verification of the conclusions reported in the article
- Have deposited protein and nucleic acid sequences, crystallographic structures, and microarray data in approved databases and provided accession numbers for inclusion in the published manuscript as described in the deposition policies described above
- Provide assurance that animals used in the study were cared for in accordance with institutional guidelines
- Verify that, in human studies, consent was obtained after the consequences of the studies were explained to the experimental subjects. All research on humans must have IRB approval
- Research involving animals must be performed in accordance with institutional guidelines as defined by Institutional Animal Care and Use Committee for US institutions or an equivalent regulatory committee in other countries. Authors from outside the US are requested to identify the institutional and/or licensing committee (that has approved the experiments) Research studies involving humans must have institutional review board approval. For research involving animals or humans, editors reserve the right to request additional information from authors
- Agree to disclose all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest
- Will not release to the press or the public the accepted manuscript prior to the stated embargo date

**Additional Information**

**Other Author Services and Policies**

For a list of free viewers for Supporting Information and more information on services and policies of the ACS, please refer to the following link: [http://paragonplus.acs.org](http://paragonplus.acs.org).

**Policy on Prior Publication**

*ACS Combinatorial Science* authors are allowed to deposit an initial draft of their manuscript in a preprint service, such as ChemRxiv, arXiv, or bioRxiv, or the applicable repository for their discipline prior to submission. Please note any use of a preprint server in the cover letter, and as appropriate,
state how the manuscript has been adjusted/updated between deposition and submission. All other prior/redundant publication is forbidden.

Upon publication in *ACS Combinatorial Science*, authors are requested to add a link from the preprint to the published paper via the Digital Object Identifier (DOI). For further details contact the Editorial Office.

**Manuscript Transfer Service**

If your submission is declined for publication by this journal, the editors might deem your work to be better suited for another ACS Publications journal and suggest that the authors consider transferring the submission. The Manuscript Transfer Service simplifies and shortens the process of submitting to another ACS journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied by ACS Paragon Plus to the new draft submission. Authors are free to accept or decline the transfer offer.

Once a transfer is accepted, authors will then complete the submission to the new journal in ACS Paragon Plus. During the submission process, they will have the opportunity to revise the manuscript and address comments received from editors or reviewers. Requirements of the new journal may be different, so authors should also check the Author Guidelines for the new journal and make any needed revisions in order to conform to those requirements. Please keep in mind that the reviews, reviewer identities, and decision letter will all be transferred to the new journal. Authors are encouraged to identify changes made to the manuscript in a cover letter for the new journal.

Note that transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor in the new journal. For complete details, see [http://pubs.acs.org/page/policy/manuscript_transfer/index.html](http://pubs.acs.org/page/policy/manuscript_transfer/index.html).

**ACS AuthorChoice Open Access**

*ACS AuthorChoice* options establish fee-based mechanisms for authors or their research funding agencies to sponsor the open availability of final published articles on the Web. *ACS AuthorChoice* offers authors a wide range of open access license options, such as Creative Commons licenses and provisions for immediate or 12-month embargoed open access, and includes *ACS Certified Deposit*. Authors will find useful information about compliance with open access policies available [here](http://pubs.acs.org) and FAQs [here](http://pubs.acs.org). Corresponding authors who published with ACS during 2014 may have access to *ACS Author Rewards*, a $60M stimulus program ACS provided to help authors transition to new open access publishing models.

Authors must sign the Journals Publishing Agreement. Forms and complete instructions are available [here](http://pubs.acs.org). After acceptance, authors will be presented with the opportunity to purchase an *ACS AuthorChoice* option, and authors who do so will be presented with the appropriate license at that time. For a review of all license options available, see [here](http://pubs.acs.org). For questions or further assistance with *ACS AuthorChoice*, please reach out to support@services.acs.org.

**Sharing Manuscripts**

Under the *ACS Articles on Request policy*, the Society will provide (free of charge) to all contributing authors a unique URL within the ACS Web site that they may e-mail to colleagues or post on external Web sites. These author-directed links are designed to facilitate distribution of an author’s published work to interested colleagues in lieu of direct distribution of the PDF file by the author. The ACS
Articles on Request policy allows 50 downloads within the first year after web publication and unlimited access via the same author-directed links 12 months after web publication. For additional details, please refer to the following link: http://pubs.acs.org/page/policy/articlesonrequest/index.html.

Proofs
Correction of the galley proofs is the responsibility of the corresponding (submitting) author(s). The corresponding author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via a secure Web site. Authors will access the secure site through ACS ChemWorx and will need an ACS ID. To obtain an ACS ID or to reset your password, go to http://www.acschemworx.org. Corrections other than composition errors should be avoided because they may cause a delay in publication. Substantive changes will require the approval of the Editor. Corrections exceeding one sentence and insertions should be submitted in a separate file, and their intended location should be noted on the galley proof. It is the responsibility of the corresponding author to ensure that all authors listed on the manuscript agree with the changes made on the proofs. Galley proofs should be returned in <48 h of receipt to ensure timely publication of the manuscript. Articles will be published on the ACS Combinatorial Science Web site within a few days of receipt of the galley proofs.

Corrections
If errors of consequence are found in the published paper, a correction of the error should be sent by the Corresponding Author to the Editor for publication in the “Additions and Corrections” section. As additional features become available, these instructions will be updated on the Journal’s website. Users can obtain up-to-date information on the submission of manuscripts at http://pubs.acs.org/page/acscce/submission/index.html.

Reprints
Hardcopy reprints must be ordered when the galley proof is received. A link to a website where you may order author reprints is included with the galley proof. You may also call Cierant Corporation – 866-305-0111 from 9AM to 5PM EST. Reprints will be shipped within two weeks after the issue publication date. Neither the Editors nor the Washington ACS Office keeps a supply of reprints; requests for single copies of papers should be addressed to the corresponding author of the paper concerned.

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

Guidelines for Reporting and Stewardship of NMR Data:

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. C₆D₆ over benzene-d₆), 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, ¹H NMR data recorded in C₆D₆ listed as “residual internal C₆D₅H (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 ¹H 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, ²J, may be specified by the author if known with a high degree of certainty.

      1.4.2 Accepted abbreviations for multiplicities and descriptors are:

      | Symbol | Description                  |
      |--------|------------------------------|
      | s      | singlet                      |
      | d      | doublet of doublets          |
      | t      | triplet                      |
      | q      | quartet                      |
      | 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):**

($\eta^5$-C$_5$Me$_5$Co)$_2$-$\mu$($\eta^4$-$\eta^4$-C$_9$H$_{10}$) (I): $^1$H NMR (CD$_6$D$_6$, 400 MHz): $\delta$ -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 (CD$_6$D$_6$, 400 MHz): $\delta$ 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): $\delta$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, H3b'''), 3.88 (1H, J = 14.3, 6.8 Hz, H2), 3.86 (3H, s, OCH$_3$), 3.69 (3H, s, OCH$_3$4'), 3.64 (3H, s, COOCH$_2$2), 3.49 (3H, br s, H5''' and H6'''''), 3.40-3.47 (1H, overlapped, H3a'''''), 3.45 (3H, s, OCH$_2$2'''''). $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$C 170.6 (s, COCH$_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$4'), 55.0 (d, C3; q, OCH$_2$2'''''), 52.1 (q, COCH$_3$2), 50.3 (d, C2).

**Note**

Broad peaks between $\delta$H 1.5 to 3.0 ppm and at $\delta$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$_2$O exchange.

**Example 3:**

($E,E$)-3,7,11-Trimethyl-2,6,10-dodecatrien-I-yl diphosphate (Farnesyl diphosphate, FPP, 3): $^1$H

---

25
NMR (D$_2$O, 300 MHz): $\delta$ 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$_2$O, 75 MHz): $\delta$ 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$_2$O, 121.5 MHz): $\delta$ –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$_6$D$_6$ 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:

$^1$H NMR (CD$_3$OD, 300 MHz)

Example 2:

$^1$H NMR (CDCl$_3$ with 0.05% v/v TMS, 400 MHz)
Example 3:
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.