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JOURNAL OF NATURAL PRODUCTS

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Scope of the Journal

The *Journal of Natural Products* invites and publishes papers that make substantial and scholarly contributions to the area of natural products research. Contributions may relate to the chemistry and/or biochemistry of naturally occurring compounds or the biology of living systems from which they are obtained. Specifically, they may be articles that describe secondary metabolites of microorganisms, including antibiotics and mycotoxins; physiologically active compounds from terrestrial and marine plants and animals; biochemical studies, including biosynthesis and microbiological transformations; fermentation and plant tissue culture; the isolation, structure elucidation, and chemical synthesis and semi-synthesis of novel compounds from nature; and the pharmacology of compounds of natural origin. When new compounds are reported, manuscripts describing their biological activity are much preferred. Manuscripts that focus on biological properties of chemically complex extracts, mixtures, or essential oils are outside of the scope of the journal.

Manuscript Types

Manuscripts may be submitted as Articles, Notes, Reviews, or Perspectives. Authors should indicate in a cover letter accompanying the manuscript which category they intend for their submission.

All manuscripts will be submitted to a review process. Manuscripts will be considered for publication on the understanding that they have not been published or submitted for publication elsewhere.

Articles. Articles are comprehensive, critical accounts of work in the areas outlined above.

Notes. Notes are abbreviated papers presented in the same general style as Articles. Generally, studies that are narrower in scope than published in Articles are reported as Notes. When only one or two new compounds are reported in a manuscript, these substances must be of significant structural, biogenetic, and/or biological interest. The publication of known compounds will be considered only if they have been demonstrated to possess potentially important bioactivity. Manuscripts solely reporting NMR assignments or X-ray crystallographic data of known compounds will not be considered. For known compounds, authors should submit full experimental details of the isolation and identification data for consideration by the referees but not for publication. Full details of the isolation and identification procedures for known compounds may be made available to the reader as Supporting Information. (See the subsequent section on Supporting Information.)

Authors investigating the chemistry of a single species should aim to publish their results in a single manuscript rather than in a series of manuscripts describing each new compound as it is found. Manuscripts that report fragmentary parts of a larger study will be returned to the authors at the Editors' discretion.

Reviews. Comprehensive reviews of topics within the scope of the journal and supported by significant literature should be submitted as reviews. Short reviews of recent literature that update

a topic are also considered. The information in Reviews should be presented objectively, not limited to the contributions of the authors, and written with the intent of familiarizing the general reader with the broad current state of knowledge of a topic of active interest. The length of reviews should be commensurate with the information available; there are no formal limitations on length. Reviews are considered upon invitation, or after approval of presubmission inquiries outlining a synopsis of the manuscript sent to eic@jnp.acs.org.

Perspectives. Perspectives are personal reviews of subject or a topic in natural products, which should be focused rather than comprehensive. Perspective authors should assess the current status of the selected subject or topic, with an emphasis toward identifying important advances being made or those advances that are needed. Perspective reviews should present a forward-thinking approach in discussing the selected topic to be covered. The Journal of Natural Products Perspective should address the recent literature, including key contributors, aiming primarily to inspire and provide new insights to direct future research efforts. Perspectives authors will be invited by the Editor, or presubmission inquiries outlining a synopsis of the manuscript can be sent to eic@jnp.acs.org. Perspectives should be no more than 9,000 words, including the abstract, main text, and figure captions

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

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

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

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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.

A statement should be included in the cover letter by the corresponding author that all persons named as co-authors have seen and approved the manuscript prior to submission. 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.

Manuscript Text Components

To assist with the subsequent editorial process, it is preferred that manuscripts submitted to the *Journal of Natural Products* be prepared in single columns per page, double-spaced, with font size 12. The template is available for on the Information for Authors page. Use of a template is encouraged but not mandatory. The template facilitates the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text.

Title Page

Manuscripts may be submitted as Articles, Notes, Reviews (by invitation of presubmission inquiry), Perspectives (by invitation or presubmission inquiry), and Editorials (by invitation) (see “Scope and Editorial Policy” document). The manuscript title should appear on a separate page and should be

followed by the author names and the institution name and address. The title, author name(s), and affiliations should all appear on their own respective line of text. Place an asterisk after the name of the author to whom enquiries regarding the paper should be directed and include that author's telephone and fax numbers and e-mail address. Author affiliations should be footnoted using sequential lower-case letters, numbers, or symbols. Subdivisions (e.g., departments) of an institution should be grouped on the same line or lines. In article titles, the words "new" or "novel" (with the latter referring specifically to a compound based on an unprecedented carbon skeleton) should not be included, and the number of new substances obtained should not be specified. The title page and the rest of the manuscript should be typed in font size 12.

Abstract

The abstract, detailing, in a single paragraph, the problem, experimental approach, major findings, and conclusions, should appear on the second page. It should be double spaced and should not exceed 200 words for Articles and Reviews or 100 words for Notes and Perspectives. Compounds mentioned in the abstract, and given as specific Arabic numerals that are bolded in the manuscript text, should also be accompanied in the abstract by the same bolded numerals. The abstract should be on a separate page and should be provided with the bolded and capitalized heading "ABSTRACT".

Introduction

The manuscript should include an untitled introductory section stating the purpose of the investigation and relating the manuscript to similar research.

Results and Discussion

The "Results and Discussion" should be presented as a coherent whole section, in which the results are presented concisely. The discussion should interpret the results and relate them to existing knowledge in the field in as clear and brief a fashion as possible. Tables and figures should be designed to maximize the presentation and comprehension of the experimental data. Authors submitting a manuscript as a Note should omit the heading "Results and Discussion." For Articles of unusual length, subheadings may be included within the "Results and Discussion" section. The major heading "Results and Discussion" should be bolded and capitalized, with the text starting on the line following. Subheadings are indented, followed by a period, and are a mix of uppercase and lowercase letters. The text follows on the same line as the subheading.

Bolded structural code numbers should only be used for new compounds and for those known compounds for which new biological data or spectroscopic values are being reported, and should be presented in the main text in ascending numerical order. Authors providing manuscripts focusing on the biological properties of two or fewer known natural products have the option of referring to the compound(s) concerned by name, rather than assigning each a bolded numerical code number. Other known compounds should be referred to in the text by name, wherever necessary. Sugar units in glycosides should not be inferred as D or L based solely on NMR data analysis, but should be determined by supporting experimental work such as measurement of their optical rotations following acid hydrolysis or by the preparation of chiral derivatives and comparison with standards using a chromatographic analytical method. If the aglycone of a glycoside is also a new compound, then it should be isolated and its physical constants and spectroscopic parameters stated. Authors are advised to use correctly the terms "relative and absolute configuration" instead of "relative and absolute stereochemistry". In, for example, a carbocyclic compound, only a stereogenic carbon or a stereogenic element, such as an axis,

possesses configuration. Substituents such as methyl groups are either alpha or beta oriented and are **not** alpha or beta configured. Care should be taken not to make erroneous configurational conclusions via NMR NOE associations from ring to side-chain protons of, for example, sterols and tetracyclic triterpenoids. The term “spectral” should be avoided in a structure elucidation discussion, when “spectroscopic” or “spectrometric” are meant instead. When describing mass spectrometric details, authors should not refer to the terms “pseudomolecular ion”, “quasimolecular ion”, or “protonated molecular ion" and should refer instead to, e.g., “a sodium adduct ion”, “a protonated molecule”, or a “deprotonated molecule” (see *Pure Appl. Chem*. **2013**, *85*, 1515–1609).

In manuscripts that present results of biological studies with tumor cell lines or animal-based tumor models, authors should pay special attention to the U.S. National Cancer Institute (NIH) guidelines for cancer drug discovery studies. Compounds that suppress the growth of, or kill, isolated tumor cell lines grown in culture should be referred to as either “cytostatic” or “cytotoxic”, as appropriate. Only compounds that inhibit the growth of tumors in animal-based models should be called “antitumor”. The term “anticancer” should be reserved for compounds that show specific activity in human-based clinical studies (see Suffness, M.; Douros, J. *J. Nat*. *Prod*. **1982**, *45*, 1–14). Some flexibility in this system is afforded in the description of compounds that show activity in molecular-targeted antitumor assays. Compounds should be compared against a suitable positive control substance and follow accepted guidelines when represented as “active”. For example, a cytotoxic pure substance when tested against a cancer cell line would exhibit an IC_{50} value of <10 M (or 4–5 g/mL).

Experimental Section

The presentation of specific details about instruments used, sources of specialized chemicals, and related experimental details should be incorporated into the text of the Experimental Section as a paragraph headed General Experimental Procedures. The general order for inclusion should be as follows: melting points; optical rotations; UV spectra; ECD and/or VCD spectra; IR spectra; NMR spectra; mass spectra; and chromatographic and other techniques.

In a separate paragraph, experimental biological material should be reported as authenticated if cultivated or from a natural habitat, and the herbarium deposit site and voucher number should be recorded. The month and year when the organisms were collected should be stated, and it is recommended that the exact collection location be provided using a GPS navigation tool. All microorganisms used experimentally should bear a strain designation number and the culture collection in which they are deposited. The scientific name (genus, species, authority citation, and family) should be presented when first mentioned in the body of the manuscript. Thereafter, the authority should be eliminated, and the generic name should be reduced (except in tables and figure legends) to the first capital letter of the name (but avoid ambiguity, if two or more generic names have the same first letter). If the biological material has not been identified as to species, the manuscript will not be considered for publication unless a special protocol has been followed. Thus, a voucher specimen of the organism should be deposited with a recognized taxonomist for the particular group of organisms in question. The taxonomist should then assign to the specimen an identifying number unique to the organism so that any additional collections of the same organism would bear this same number. The number will be retained until the organism is completely identified. The taxonomist should write a brief taxonomic description to be included in the manuscript, which should state how the organism in question relates morphologically to known species. Contributors should use DNA sequence analysis to assist with the taxonomic identification of unknown microorganisms, and to deposit these data in GenBank. Photographs of incompletely identified organisms may be included as Supporting Information. Authors should be aware of the fact that the large-scale collection of marine or terrestrial organisms may have

negative ecological effects. Therefore, authors describing an investigation derived from large-scale collections should thus include a statement in their manuscript (in the “Biological Material” paragraph of the Experimental Section) explaining why the collection had no significant adverse ecological effect or justifying such effect in terms of the benefit from the resulting work. When organisms are collected from a foreign country, the corresponding author must state in the cover letter with the submitted manuscript that formal collection permission was obtained. Authors who purchase dried “herbal remedies” or other materials from companies must make provision for their proper deposit in a herbarium or other permanent repository, for access by future workers. When a commercially available extract is obtained, the extraction procedure from the organism of origin must be specified. The identification of the extract should be supported by an HPLC trace of known secondary metabolite constituents of the organism, which should be included with the manuscript as Supporting Information.

When physical and spectroscopic data are presented in the body of the manuscript, the following general style must be used (with the various commonly used techniques presented in this same order):

Romucosine (1): colorless needles ($CHCl_3$); mp 152–153 °C; $[a]^{25}_D$ –110 (*c* 0.4, $CHCl_3$); UV (EtOH) $_{max}$ (log) 235 (4.23), 275 (4.18), 292 (sh) (3.52), 325 (3.41) nm; IR (Nujol) $_{max}$ 1680, 1040, 920 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) 8.11 (1H, d, *J* = 7.6 Hz, H-11), 7.54–7.28 (2H, m, H-9, H-10), 7.27 (1H, m, H-8), 6.59 (1H, s, H-3), 6.10, 5.97 (each 1H, d, *J* = 1.5 Hz, OC*H*$_2$O), 4.86 (1H, dd, *J* = 13.7, 4.4 Hz, H-6a), 4.44 (1H, m, H-5a), 3.77 (3H, s, NCOOC*H*$_3$), 3.06 (1H, m, H-7a), 2.99 (1H, m, H-5b), 2.91 (1H, m, H-7b), 2.82 (1H, m, H-4a), 2.61 (1H, m, H-4b); ^{13}C NMR ($CDCl_3$, 100 MHz) 155.8 (C, N*C*OOCH$_3$), 146.8 (C, C-2), 143.0 (C, C-1), 135.8 (C, C-7a), 130.7 (C, C-11a), 128.7 (CH, C-8), 127.79 (C, C-3a), 127.78 (CH, C-9), 127.2 (CH, C-10), 127.0 (CH, C-11), 125.6 (C, C-3b), 117.3 (C, C-1a), 107.6 (CH, C-3), 100.9 (CH2, OCH$_2$O), 52.7 (CH3, NCOO*C*H$_3$), 51.7 (CH, C-6a), 39.2 (CH2, C-5), 34.5 (CH2, C-7), 30.4 (CH2, C-4); EIMS *m*/*z* 323 $[M]^+$ (98), 308 (28), 292 (5), 262 (20), 248 (21), 236 (81), 235 (100), 206 (17), 178 (27), 88 (17); HREIMS *m*/*z* 323.1152 (calcd for $C_{19}H_{17}NO_4$, 323.1158).

The correct presentation of NMR spectroscopic data is shown in the table below.

Table 1. NMR Spectroscopic Data (400 MHz, C6D6) for Aurilides B (**1**) and C (**2**)

	aurilide B (**1**)			aurilide C (**2**)	
position	δ_C, type	δ_H (*J* in Hz)	HMBC[a]	δ_C	δ_H (*J* in Hz)
1	170.0, C			170.2	
2	58.9, CH	3.23, m	1, 3, 4, 5	59.6	3.08, m
3	13.8, CH_3	1.21, d (7.1)	1, 2	14.0	1.25, d (7.1)
4	36.1, CH_3	2.63, s	2, 5	36.8	2.55, s
5	172.1, C			172.1	
6	54.3, CH	5.12, dd (9.0, 7.4)	5, 7, 9	54.4	5.15, dd (9.0, 5.0)
7	31.0, CH	1.97, m		32.0	1.98, m
8	20.1, CH_3	1.15, d (7.0)	6, 7, 9	20.4	1.17, d (7.0)
9	17.3, CH_3	1.25, d (7.0)	6, 7, 8	17.5	1.28, d (7.0)
10	169.9, C			170.11	
11	51.8, CH_2	4.40, d (18.0) 3.80, d (18.0)	10, 12, 13	51.9	4.39, d (18.0) 3.80, d (18.0)
12	36.8, CH_3	3.23, s	11, 13	37.1	3.22, s
13	170.0, C			170.14	
14	58.6, CH	5.24, d (10.0)	13, 18, 19, 20	58.7	5.26, d (10.0)
15	33.9, CH	2.48, m	14, 16, 18	34.1	2.49, m
16	27.4, CH_2	1.86, 1.30, m	14, 15, 17	27.6	1.89, 1.30, m
17	12.1, CH_3	1.03, t (7.1)		12.2	1.03, t (6.9)
18	14.8, CH_3	0.85, d (7.0)	15, 16	15.1	0.86, d (7.0)
19	30.7, CH_3	2.88, s	20	30.6	2.85, s
20	173.1, C			173.2	
21	54.7, CH	4.78, dd (8.8, 8.8)	20, 22	54.9	4.75, dd (8.6, 7.5)
22	31.7, CH	1.98, m		31.0	1.95, m
23	18.1, CH_3	0.89, d (6.0)	21, 22, 24	18.9	0.88, d (6.0)
24	20.2, CH_3	0.90, d (6.0)	23	20.3	0.90, d (6.0)
25	170.3, C			170.3	
26	78.5, CH	4.90, d (6.1)	25, 27, 31	80.4	4.54, d (7.5)
27	37.2, CH	2.17, m	26, 30	30.5	2.36, m
28	26.1, CH_2	1.50, 1.14, m	29	18.7	1.00, d (7.0)
29	11.8, CH_3	0.83, t (7.7)	27, 28	18.4	0.88, d (7.0)
30	14.9, CH_3	1.03, d (6.0)	26, 27, 28	169.7	
31	169.3, C			128.3	
32	128.0, C			146.0	7.75, t (9.0)
33	145.3, CH	7.74, t (9.0)	31, 42	30.9	2.14, m
34	30.9, CH_2	2.19, m	32, 33, 42	71.2	3.98, m
35	71.0, CH	3.97, m	34	41.2	2.02, m
36	41.1, CH	2.07, m	43	82.6	5.17, d (11.2)
37	82.5, CH	5.18, d (11.2)	1, 36, 38, 44	132.1	
38	131.4, C			134.6	5.62, t (7.7)
39	134.2, CH	5.61, t (7.7)	37, 44	21.4	1.95, 1.92, m
40	21.4, CH_2	1.95, 1.92, m	38, 39, 41	14.3	0.89, t[b]
41	14.1, CH_3	0.89, t[b]	39, 40	12.8	1.95, s
42	12.7, CH_3	1.95, s	31, 32, 33	10.1	0.66, (7.0)
43	10.2, CH_3	0.64, d (7.0)	35, 36, 37	11.4	1.54, s
44	11.3, CH_3	1.54, s	37, 38, 39		
NH (1)		7.69 brd (9.1)	10		7.66 brd (9.1)
NH (2)		6.75 brd (8.8)	25		6.70 brd (8.8)

[a]HMBC correlations, optimized for 6 Hz, are from proton(s) stated to the indicated carbon.
[b]Signal partially obscured.

The correct format to present elemental analysis data is: anal. C 72.87, H 11.13%, calcd for $C_{37}H_{68}O_6$, C 73.02, H 11.18%. The structures of compounds are expected to be supported by high-resolution mass spectrometry (error limit 5 ppm or 0.003 *m*/*z* units) or elemental analysis. Melting point determinations should not be provided for compounds described as “amorphous solids.” The unit of concentration to be used for optical rotation measurements is grams per 100 mL. UV extinction coefficient data should be provided as log values, to two places of decimals. In reporting ^{1}H NMR data of diastereotopic methylene protons, the deshielded one should be listed as the “a” proton and the shielded one as the “b” proton, as in “H-10a” and “H-10b”, respectively. If two proton or carbon signals in an NMR spectrum appear at the same chemical shift but are still distinguishable, an additional decimal place (three for ^{1}H NMR data and two for ^{13}C NMR data) may be used to designate the resonance in question. Carbon-13 NMR data should be reported to the nearest 0.1 ppm with the number of attached protons designated using the C, CH, CH_2, and CH_3 notation.

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the Article, Note, or Rapid Communication.

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Author Information

A section may be included, as needed, entitled “Author Notes” to provide pertinent information on the authors, such as the names of authors who contributed equally to the article.

Acknowledgments

The Acknowledgments section should include credits [initial(s) and last name] for technical assistance, financial support, and other appropriate recognition. During manuscript submission, the submitting author is asked to select funding sources from the list of agencies included in the FundRef Registry.

References

The References section should provide both citations to the literature and all notes, regardless of their nature, which should be numbered in order of appearance in the manuscript and cited in the text with superscript numbers. Each reference may have its own citation number, or alternatively, references referring to the same topic may be grouped under a common number using alphabetical subdesignations (e.g., 1a, 1b, 1c). Each note should be assigned its own number. References and notes should follow the format shown:

1. Journal references can be provided in any style, as noted in the Review Ready Submission section, and titles must be included.
2. Linington, R. G.; Williams, P. G.; MacMillan, J. B. *Problems in Organic Structure Determination. A Practical Approach to NMR Spectroscopy*; CRC Press/Taylor and Francis Group: Boca Raton, FL, 2016.
3. Harada, N.; Nakanishi, K.; Berova, N. In *Comprehensive Chiroptical Spectroscopy, Vol. 2; Applications in Stereochemical Analysis of Synthetic Compounds, Natural Products, and Biomolecules*; Berova, N., Polavarapu, P. L., Nakanishi, K., Woody, R. W., Eds.; John Wiley & Sons: New York, 2012; pp 115–166.
4. Zheng, G.; Kakisawa, H. *Chin. Sci. Bull.* **1990**, *35*, 1406–1407; *Chem. Abstr.* **1991**, *114*, 43213*m*.
5. Imai, A. Pharmacognosy of the Aerial Parts of Black Cohosh (*Cimicifuga racemosa*). Ph.D. Dissertation, University of Illinois at Chicago, Chicago, IL, 2013.
6. Davis, R. U.S. Patent 5,708,591, 1998.
7. Partial data for plakinic acid M were reported in the Supporting Information of Ref 5a, but a more complete listing is given here for comparative purposes.
8. World Health Organization. Fact Sheet No. 94, 2015. http://www.who.int/mediacentre/factsheets/fs094/en/ (accessed October 1, 2015).

For additional information on the reference and note format to use, see *The ACS Style Guide*, 3rd ed. (2006) (https://pubs.acs.org/page/styleguide), available from Oxford University Press, Order Department, 2001 Evans Road, Cary, NC 27513 (http://www.oup.com).

The author is responsible for the accuracy and completeness of all references. In particular, authors must cite all of the references from their own work on a particular topic, such as all papers

published or submitted on the constituents of a given organism under consideration. In addition to the citation, it should be explicitly indicated in the text if this is a continuing work for the same group. Because subscribers to the Web edition are now able to click on the “CAS” tag following each reference to retrieve the corresponding CAS abstract, reference accuracy is critical. Journal abbreviations should be those used by *Chemical Abstracts* [see *Chemical Abstracts Service Source Index (CASSI) 1907–2004*]. A list of journal abbreviations in the *ACS Style Guide* can also be accessed.

The author should supply the Editor-in-Chief with copies of related manuscripts that are cited as “in press” or “submitted” for use by the editors and the reviewers in evaluating the manuscript under consideration.

Nomenclature

It is the responsibility of the authors to provide correct nomenclature. All nomenclature must be consistent and unambiguous and should conform with current American usage. Insofar as possible, authors should use systematic names similar to those used by Chemical Abstracts Service, the International Union of Pure and Applied Chemistry, and the International Union of Biochemistry and Molecular Biology. For new natural products that are closely related structurally to known compounds, it is much preferred to assign the new compound as a derivative of the known compound, rather than introduce a completely new trivial name into the literature.

Chemical Abstracts (*CA*) nomenclature rules are described in Appendix IV of the *Chemical Abstracts Index Guide*. A list of ring systems, including names and numbering systems, is found in the *Ring Systems Handbook*, American Chemical Society, Columbus, OH, 2003, and its latest cumulative supplement. For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334; tel: (614) 447- 3870; fax: (614) 447-3747; or e-mail: answers@cas.org.

For IUPAC rules, see:

- *Nomenclature of Inorganic Chemistry, Recommendations, 1990*; Blackwell Scientific Publications: Oxford, England, 1990.
- *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations, 1993*; Blackwell Scientific Publications: Oxford, England, 1993.
- *Nomenclature of Organic Chemistry, Sections A–F and H*; Pergamon Press: Elmsford, NY, 1979.
- *Compendium of Macromolecular Nomenclature*; Blackwell Scientific Publications: Oxford, England, 1991.
- *Biochemical Nomenclature and Related Documents*, 2nd ed.; Portland Press, Ltd.: London, England, 1992.
- Selected IUPAC recommendations can be found on the Web at http://www.chem.qmw.ac.uk/iupac/iupac.html.
- The ACS Web site has links to nomenclature recommendations: chemistry.org.

Abbreviations

Abbreviations are used without periods. Standard abbreviations should be used throughout the

manuscript. All nonstandard abbreviations should be kept to a minimum and must be defined in the text following their first use. The preferred forms of some of the more commonly used abbreviations are mp, bp, °C, K, s, min, h, mL, L, kg, g, mg, g, cm, mm, nm, mol, mmol, mol, ppm, TLC, GC, NMR, MS, UV, ECD/VCD, and IR. For further information, refer to *The ACS Style Guide* (2006).

Authors should not provide a separate list of abbreviations in a manuscript; additional abbreviations should be spelled out in full the first time they are mentioned. Authors are discouraged from using abbreviations for terms that are included in the manuscript in only a few instances.

Graphics

Figures, Schemes, and Charts are numbered with Arabic numerals. Blocks of chemical structures should not be designated as “Figures”. Each graphic must be identified outside the frame of the graphic. The quality of the illustrations depends on the quality of the originals provided. Graphics cannot be modified or enhanced by the journal production staff. The graphics must be submitted as part of the manuscript file and are used in the production of the Journal (material deposited as Supporting Information will not be published in the print edition). The preferred submission procedure is to embed graphics 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). Labeling of all figure parts should be present, and the parts should be assembled into a single graphic. (For EPS files, ensure all fonts are converted to outlines or embedded in the graphic file. The document settings should be in RGB mode.)

TIFF files should have the following minimum resolution requirements:

- Black and white line art: 1200 dpi
- Grayscale art: 600 dpi
- Color art (RGB mode): 300 dpi

Color graphics submitted in CMYK or at lower resolution may result in poor-quality images. Save graphic files at the final resolution and size using the program used to create the graphic. The inclusion of a color photograph is particularly recommended for manuscripts based on the constituents of organisms that are not identified beyond the genus level. Digital photographs are accepted. Photographs that are single or double column width so that they will not have to be reduced work best.

Layout. In preparing structures for publication, layout is critical. Figures, Schemes, Charts, and blocks of structures are presented in the Journal either in one-column or two-column format.

For efficient use of journal space, single-column illustrations are preferred.

- **Single-column (preferred)** Maximum width:240 pts (3.33 in.)Maximum depth: 660 pts (9.16 in.)
- **Double-column** Minimum width: 300 pts (4.16 in.)Maximum width: 504 pts (7 in.)Maximum depth: 660 pts (9.16 in.)

Authors are advised that structural material labeled as a “Figure” is placed at the top or bottom of

a page, as is all two-column material. All structural material that should immediately follow certain text must be designed to fit the one-column format, and its location in the text must be indicated in the manuscript. Structures, arrows, and compound designators should be arranged so as to make maximum use of the width afforded by the one-column or two-column format.

For best results, illustrations should be submitted in the actual size at which they should appear in the Journal. Consistently sized letters and labels in graphics throughout the manuscript will help ensure consistent graphic presentation for publication. Lettering should be no smaller than 4.5 points. (Helvetica or Arial type works well for lettering.) Lines should be no thinner than 0.5 point. Lettering and lines should be of uniform density. If artwork that should be reduced must be submitted, larger lettering and thicker lines should be used so that, when reduced, the artwork meets the above-mentioned parameters.

Complex textures and shading to achieve a three-dimensional effect should be avoided. To show a pattern, a simple cross-hatch design should be used.

Content. Abbreviations such as Me for CH_3, Et for C_2H_5, and Ph (but not) for C_6H_5 are acceptable. Make liberal use of “R and X groups” in equations, schemes, and structure blocks to avoid the repetition of similar structures. Do not repeat a structure; the number alone of an earlier structure can be used if a compound occurs several times. Within graphics, structures should be numbered with boldface Arabic numerals, consecutively from left to right, top to bottom, regardless of the order in which the compounds are discussed in the text. It is not necessary to give reagents and conditions in complete detail, since this detail is contained in the Experimental Section. Where needed, numbers such as NMR chemical shifts may be included directly on structural formulas.

Table of Contents/Abstract Graphic

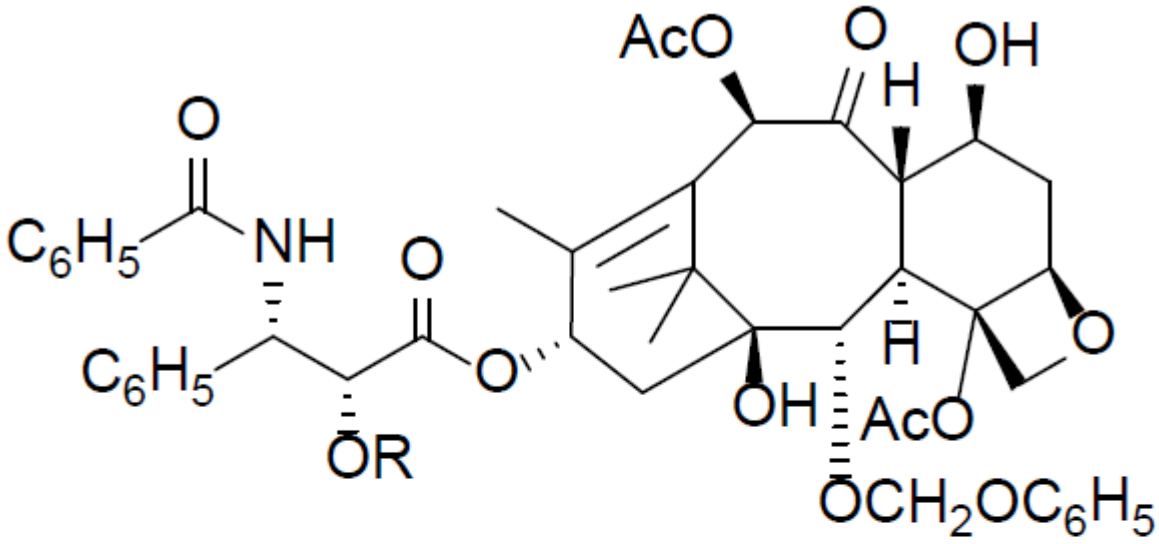
A graphic must be included with each manuscript that will be used for both the abstract and the Table of Contents (TOC) of the Web edition of the Journal issue in which the Article, Note, Perspective, or Review will appear. This graphic should capture the reader’s attention and, in conjunction with the manuscript’s title, should give the reader a quick visual impression of the type of chemistry described and/or the biological results obtained; however it should not be too complex. Structures in the TOC graphic should be constructed as specified in the “Chemical Structures” section below. The TOC graphic should be submitted at the actual size to be used and should be no larger than 3.25 in. (8.5 cm) wide and 1.75 in. (4.45 cm) tall. (See detailed instructions at http://pubs.acs.org/page/4authors/submission/howtosubmit.html.) Text should be limited to labels for compounds, reaction arrows, and figures. The use of color to enhance the scientific value is highly encouraged. The TOC graphic should be inserted on a separate page at the end of the manuscript file. The title and author list will be added during production.

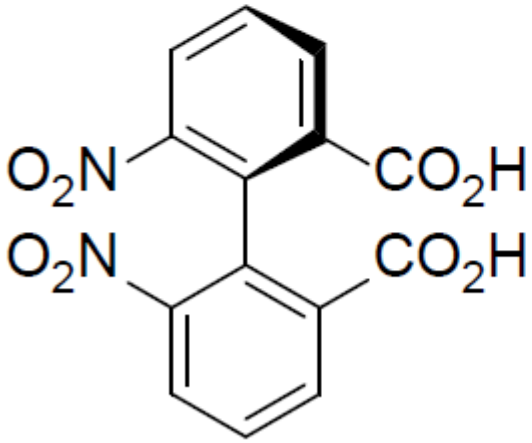
Chemical Structures

Structures should be produced with the use of a drawing program such as ChemDraw. Structure drawing requirements (preset in the ACS Stylesheet in ChemDraw) are as follows:

- (1) As drawing settings, select: chain angle, 120ºbond spacing, 18% of widthfixed length, 14.4 pt (0.508 cm, 0.2 in.)bold width, 2.0 pt (0.071 cm, 0.0278 in.)line width, 0.6 pt (0.021 cm, 0.0084 in.)margin width, 1.6 pt (0.056 cm, 0.0222 in.)hash spacing, 2.5 pt (0.088 cm, 0.0347 in.)
- (2) As text settings, select: font, Arial/Helveticasize, 10 pt
- (3) Under the preferences, choose: units, pointstolerances, 5 pixels

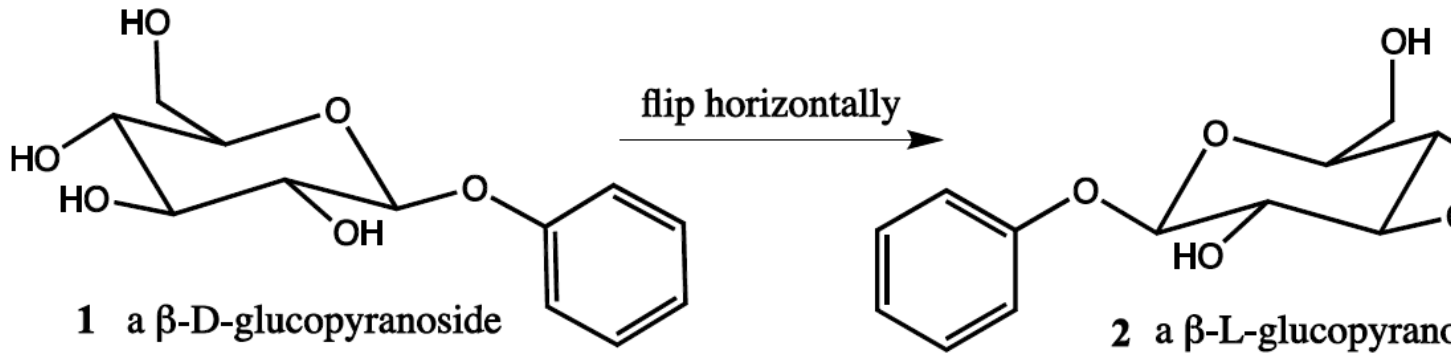
- (4) Under page setup, choose: paper, US Letterscale, 100%
- (5) Using the ChemDraw ruler or appropriate margin settings, create structure blocks, schemes, and equations having maximum widths of 11.3 cm (one-column format) or 23.6 cm (two-column format)
- (6) Embolden compound numbers, but not atom labels or captions.
- (7) Authors are urged to use only a single configurational descriptor when defining a stereocenter in a chemical structure. Atom numbering should be kept outside of rings wherever possible. Rather than rectangular solid and dashed lines, authors should use solid and dashed wedges to indicate configurations, as shown below. Dots at ring junctions intended to represent hydrogen atoms should not be used. Structures should be drawn in a neat manner ready for direct reproduction, and should not be cluttered or overlapping. Any arrows and numbering used for atoms in figures should not come into contact with bonds or ring systems. See an example of a prepared structure using ChemDraw with the specified preferences below. In molecules containing a chiral biphenyl axis, it is recommended that one of the aromatic rings be drawn in the plane of the paper and the second one be rotated out of the plane of the paper, to reflect the P or M conformation about the biphenyl bond (see below for example).





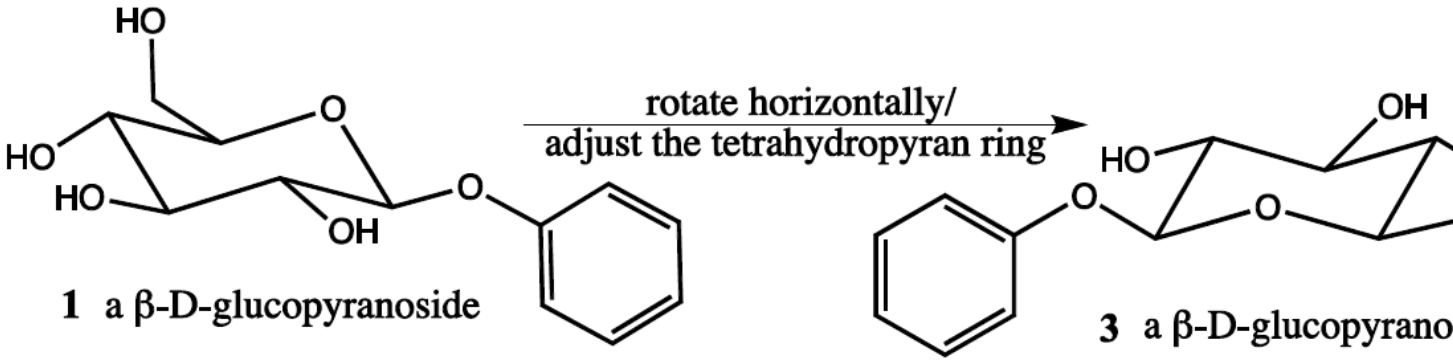
When the structure of a chiral compound is flipped horizontally, the stereodescriptors should be changed at **every** stereogenic carbon, otherwise the enantiomer of the relevant compound would be depicted. This is depicted below for the b-D-glucopyranoside of phenol. The **1** to **2** horizontal flip is **incorrect** since the depicted glucopyranosyl moiety belongs to the L-series of

glucopyranoses. The **1** to **3** horizontal rotation through 180°/adjustment of the tetrahydropyran ring is **correct** and shows the descriptor changes required to retain the D-configuration of the glucopyranose moiety. Alternatively, in the “planar” presentations the **4** to **5** horizontal flip is **incorrect** and the **4** to **6** horizontal rotation is correct, showing the proper descriptor changes. Please note that presentations **4** and **6** are InChI (International Chemical Identifier) compliant, while **1** and **3** are not.



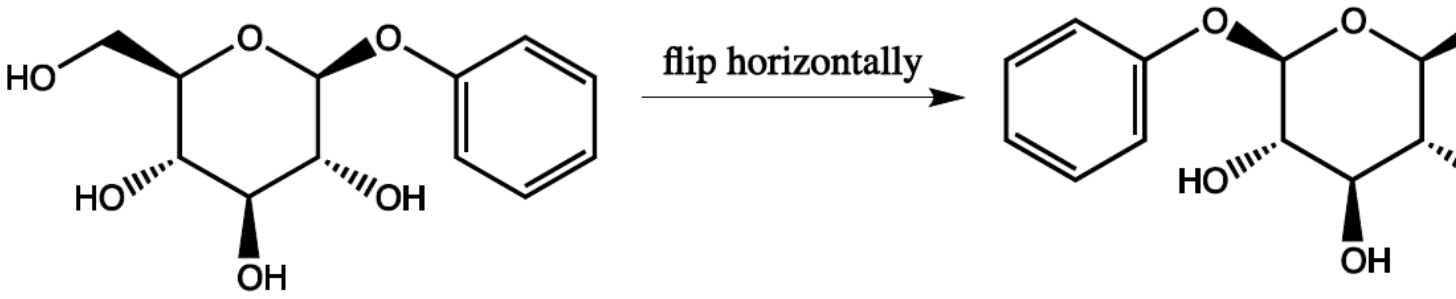
1 a β-D-glucopyranoside **2** a β-L-glucopyranc

INCORRECT



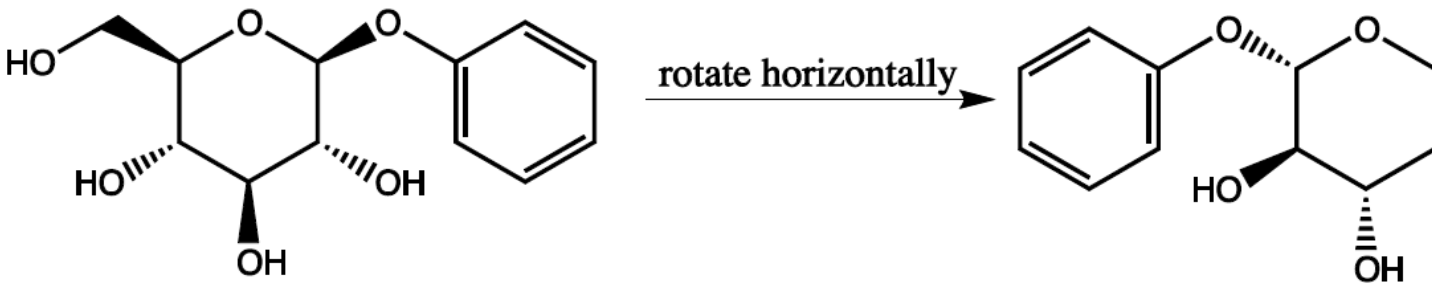
1 a β-D-glucopyranoside **3** a β-D-glucopyrano

CORRECT



4 a β-D-glucopyranoside **5** a β-L-glucopyra

INCORRECT



4 a β-D-glucopyranoside **6** a β-D-glucopyranosid

CORRECT

Authors using other drawing packages should, in as far as possible, modify their program's parameters so that they reflect the above guidelines.

Tables

These should be numbered consecutively with Arabic numerals and should be placed as they should appear in the paper. Footnotes in tables should be given lowercase letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column. If a footnote is cited both in the text and in a table, insert a lettered footnote in the table to refer to the numbered footnote in the text. Each table should be provided with a descriptive heading, which, together with the individual column headings, should make the table, as nearly as possible, self- explanatory. In setting up tabulations, authors are requested to keep in mind the type area of the journal page (17.8 × 25.4 cm) and the column width (8.5 cm), and to make tables conform to the limitations of these dimensions. Arrangements that leave many columns partially filled or that contain much blank space should be avoided.

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 to Publication of Chemical Research*). 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.”

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It is a mandatory requirement for authors to deposit copies of NMR spectra for all new compounds in the Supporting Information with at least the ^{1}H and ^{13}C NMR spectra included. A typical caption for a spectrum would be: “S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of the new compound **xx**”. Supporting Information pages should be consecutively numbered and a table of contents for the Supporting Information should be included.

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

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

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

Examples of insufficient descriptions: “Supporting Information: Figures S1-S3” or “Additional

figures as mentioned in the text”.

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

Research Data Policy

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

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

The ACS Research Data Policy provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

NMR Data Files

When submitting spectra, authors should adhere to the following guidelines:

A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g., $CDCl_3$), and the field strength. A representation of the compound should be included on the spectrum; please use ChemDraw or a related program. The bold compound number used in the manuscript should be included. The largest peak in the ^{1}H NMR spectrum should normally arise from the compound, not the solvent. All peaks in the ^{1}H NMR spectrum should be integrated. Chemical shift values should be included. The solvent peak should be clearly labeled on the spectrum. 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. The font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

For every new compound, a copy of a well-resolved 1D proton NMR spectrum and a copy of a proton- decoupled 1D carbon spectrum (conventional, DEPT, DEPTQ, or PENDANT), should be included 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 the 2D spectra are requested. All original primary NMR data supporting a submission should be retained and provided if requested. Additionally, authors are strongly encouraged to furnish a folder of the primary (“raw”) NMR data files (free induction decay (FID) and 2D serial files) as additional Supporting Information. Authors reporting compounds of complex, unusual, or unexpected structure are encouraged to provide FID data. The FID data should be mentioned in the Supporting Information availability statement in the manuscript file. The FID and serial file data can also be deposited in a public repository that provides a permanent link, such as a DOI.

When preparing raw NMR data (FIDs):

- One folder (root folder) should be created for each compound
- The root folder should be named clearly, including the compound number and/or a unique identifier

- Establish subfolders for each spectrum and name them according to the type of nucleus measured and experiment performed: 1H, 13C, DEPT, COSY, etc.
- Include in each subfolder the actual FID or serial files, acquisition data and processing parameters for each experiment; depending on the spectrometer used, this can be several files or a combination of further folders and files
- In a text document with the same name as the root folder, 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 operating frequency used to measure each nucleus (e.g. 300 MHz 1H or 75 MHz 13C)
- Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the strongly preferred format
- Compress the entire root folder into a single zip archive file

Recommendations for Crystal Structure Papers

Although the results of crystal structure determinations are frequently of interest to readers of the Journal, details of crystal structure experiments are generally not. Results appropriate for the Journal are not, however, sufficient to allow referees to assess the quality of an X-ray structure determination. Thus, it is recommended that manuscripts involving such determinations be accompanied by material provided for the benefit of the reviewers only. Authors should submit the following minimum materials, in tabular form where possible, for each compound for which X-ray crystallographic supplementary data are available.

Published Manuscript:

1. Crystal data, including chemical formula, formula weight, crystal system and space group, cell dimensions (with uncertainties), number of formulas per unit cell, calculated density, radiation used, and wavelength. When determined, the Flack and/or Hooft parameters should be included.
2. Final fractional atomic coordinates. Hydrogen atom coordinates should be included only if they have been experimentally determined or refined. Calculated coordinates should be provided as reviewer's material.
3. A *brief* outline of procedures used for data collection and refinement, including the method used for intensity measurement, 0 limits, portion of the full sphere collected, handling of absorption (if applicable), method of refinement, number of reflections used in the refinement and criteria for their choice, treatment of hydrogen atoms, and final *R* factor.
4. A perspective diagram (perhaps prepared by ORTEP, PLUTO, or similar programs) that gives the atom-numbering scheme if it is not unambiguous from the remainder of the paper. If the figure is a stereoview, it should be provided reduced to correct size, about 55–60 mm between images.

Besides a description of the structure, other information (important distances, torsion angles, results of best plane calculations, etc.) may be included if appropriate. A note should be cited at an appropriate place in the manuscript and included in the References and Notes Section: "Crystallographic data for the structure(s) reported in this paper have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-(0)1223-336033 or e-mail: deposit@ccdc.cam.ac.uk)."

Reviewer's Material:

1. Any calculated coordinate (e.g., hydrogen atoms).
2. A full list of bond distances (and their uncertainties).
3. A full list of bond angles (and their uncertainties).

All tables should be clearly legible, the contents nonredundant, and their interpretation immediately obvious. Authors must provide this information in the form of a Crystallographic Information File (CIF) for each compound for which X-ray crystallographic data are determined, with each CIF being separated from any other Supporting Information files.

Authors will deposit the tables of final fractional atomic coordinates and the full list of bond lengths and angles at the Cambridge Crystallographic Data Centre (CCDC) prior to the submission of their paper. The CCDC deposition number must be included in the submitted manuscript. A checklist of data items for deposition is available at www.ccdc.cam.ac.uk.

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

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Articles may be retracted for scientific or ethical reasons and may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. Articles that contain seriously flawed or erroneous data such that their findings and conclusions

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During the submission process, the Corresponding Author must provide a statement on behalf of all authors of the manuscript, describing all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest. If the manuscript is accepted, the statement will be published in the final article.

If the manuscript is accepted and no conflict of interest has been declared, the following statement will be published in the final article: "The authors declare no competing financial interest."

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Appendix 2: Preparing Graphics

Resolution

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

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

Size

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

Color

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

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

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

Our team of subject-matter experts and graphical designers can also help generate a compelling TOC graphic to convey your key findings. Learn more about our Graphical Abstract service.

Figures

A caption giving the figure number and a brief description must be included below each figure. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

Charts

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

Tables

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

Schemes

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

Chemical Structures

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

Cover Art

Journal of Natural Products authors are encouraged to submit images to be considered for use on the journal's front cover or Supplementary Covers at the time of the submission of their revised manuscript. If your article is accepted for publication, your suggestion may also be selected for use on one of the journal's covers. If your art is selected for front cover, ACS will send you information about how to request one complimentary 18" by 24" printed poster featuring your work. Images chosen for the front cover will be published at no cost to the author.

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Image files should be submitted as TIF, JPG, PNG, or EPS files (not PDF or PPT) with a resolution of at least 300 dpi for pixel-based images. Cover art should be 8.19 inches (20.8 cm) wide × 10 inches (25.4 cm) high at 300 ppi, and submission of “layered” artwork is encouraged. The journal’s logo will obscure the top 3 inches (7.62 cm) of the image. Authors should submit the cover image, along with a brief (<50-word) cover caption explaining the significance of the cover motif, inclusive of the citation of pertinent bibliography presented in the correct style for the journal. These items should be submitted as supplementary files to ACS Paragon Plus with the revised manuscript. Authors are responsible for providing signed permission forms as deemed necessary by the American Chemical Society.

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