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JOURNAL OF NATURAL PRODUCTS

Preparation and Submission of Manuscripts

(Revised Dec 2015)

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Title Page

The 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 must be footnoted using the following symbols in order (which should be used as superscripts): $^{\dagger, \ddagger, \S, \perp, \parallel, \nabla, \bigcirc}$. 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 one 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 Full Articles and Reviews or 100 words for Notes and Rapid Communications. Compounds mentioned in the abstract, and given as specific Arabic numerals that are bolded in the 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 introduction 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 Full 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. 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 μM (or 4–5 μg/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 (http://www.ncbi.nlm.nih.gov/). 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; $[\alpha]^{25}_D$ –110 (*c* 0.4, $CHCl_3$); UV (EtOH) λ_{max}(log ε) 235 (4.23), 275 (4.18), 292 (sh) (3.52), 325 (3.41) nm; IR (Nujol) ν_{max} 1680, 1040, 920 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 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) δ 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 (CH_2, OCH_2O), 52.7 (CH_3, NCOO*C*H$_3$), 51.7 (CH, C-6a), 39.2 (CH_2, C-5), 34.5 (CH_2, C-7), 30.4 (CH_2, 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, C_6D_6) 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 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 ε values, to two places of decimals. In reporting ^{1}H NMR data of diastereotopic methylene protons, the one at lower field should be listed as the "a" proton and that at the higher field 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.

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 http://www.crossref.org/fundref/.

References

References to the literature and all notes, regardless of their nature, 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, etc.). Each note should be assigned its own number. References and notes should follow the format shown:

(1) Dumdei, E.; Andersen, R. J. *J. Nat. Prod.* **1993**, *56*, 792–794.

(2) Cordell, G. A. *Introduction to Alkaloids: A Biogenetic Approach*; John Wiley & Sons: New York, 1981; p 43.

(3) Pelletier, S. W.; Mody, N. V. In *The Alkaloids*; Rodrigo, R. G. A., Ed.; Academic Press: New York, 1981; Vol. 18, Chapter 2, pp 100–216.

(4) Zheng, G.; Kakisawa, H. *Chin. Sci. Bull.* **1990**, *35*, 1406–1407; *Chem. Abstr*. **1991**, *114*, 43213*m*.

(5) Meyer, B. N. Brine Shrimp Toxicity: Certain Components of *Stapelia*, *Coryphantha*, *Lupinus*, and *Quinoa*. Ph.D. Thesis, Purdue University, West Lafayette, IN, 1983, p 35.

(6) Davis, R. U.S. Patent 5,708,591, 1998.

(7) The biogeographic zone comprising Madiera, the Canary Islands, the Cape Verde Islands, and the Azores.

For additional information on the reference and note format to use, see *The ACS Style Guide*, 3rd ed. (2006) (http://pubs.acs.org/books), 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. 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 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.

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: http://chemistry.org.

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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, μL, kg, g, mg, μg, cm, mm, nm, mol, mmol, μmol, ppm, TLC, GC, NMR, MS, UV, ECD/VCD, and IR. For further information, refer to *The ACS Style Guide* (2006).

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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.)

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Layout. In preparing structures for publication, layout is critical. Figuress, 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 (preferred)	double
width		
minimum		300 pts (4.16 in.)
maximum	240 pts (3.33 in.)	504 pts (7 in.)
maximum depth	660 pts (9.16 in.)	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 ϕ) 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.

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

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chain angle	120º
bond spacing	18% of width
fixed 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/Helvetica
size	10 pt

(3) Under the preferences choose:

units	points
tolerances	5 pixels

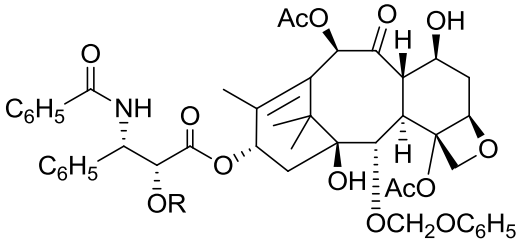
(4) Under page setup choose:

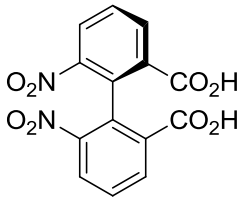
Paper	US Letter
Scale	100%

(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). Note: if the foregoing preferences are selected as cm values, the ChemDraw ruler is calibrated in cm. ChemDraw graphics will be reduced to 75% during production.

(6) Embolden compound numbers, but not atom labels or captions.

(7) Authors are urged to use only a single configurational descriptor (heavy line or dashed line, but not both) 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).





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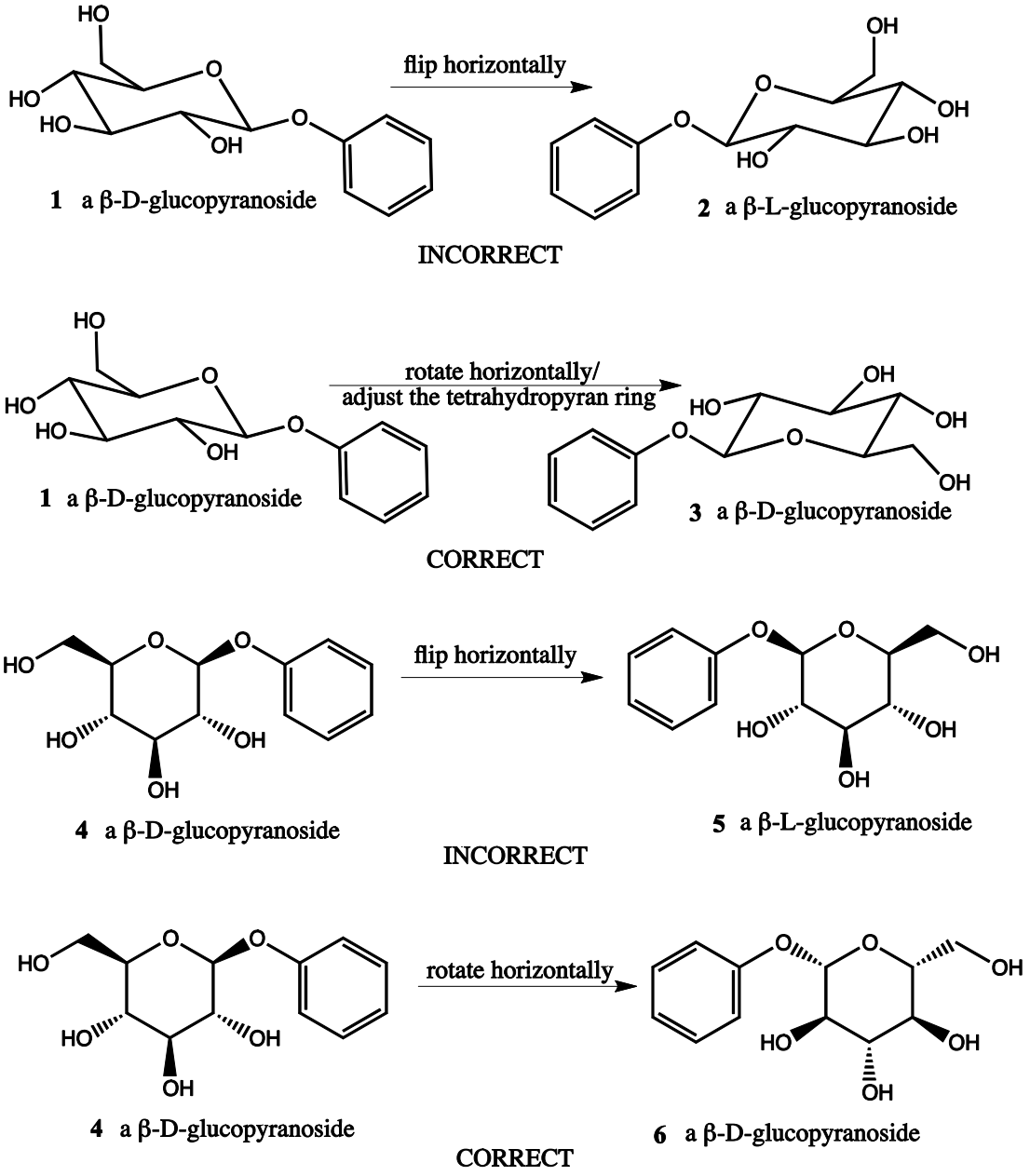

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