Marine Soft Corals of the Genus Pseudopterogorgia: A Resource for Novel Anti-inflammatory Diterpenoids

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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.

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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).

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- *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.
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(2) As text settings select:

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(3) Under the preferences choose:

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Paper	US Letter
Scale	100%

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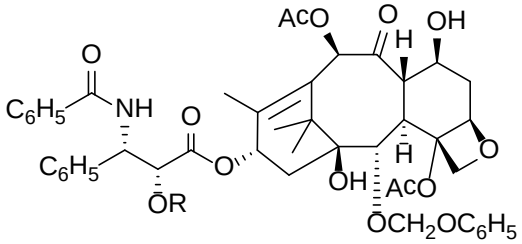

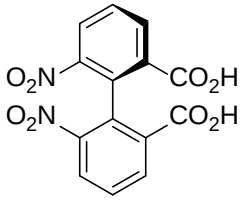

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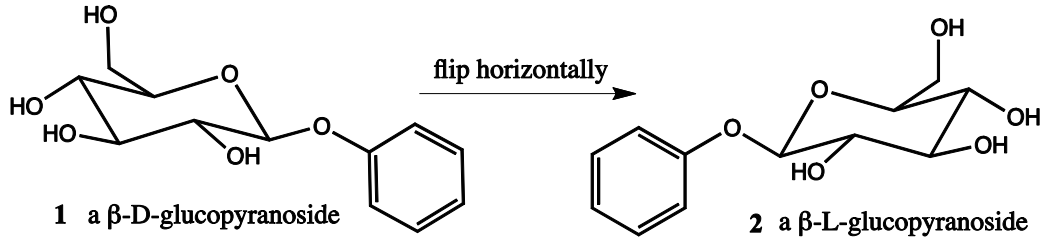
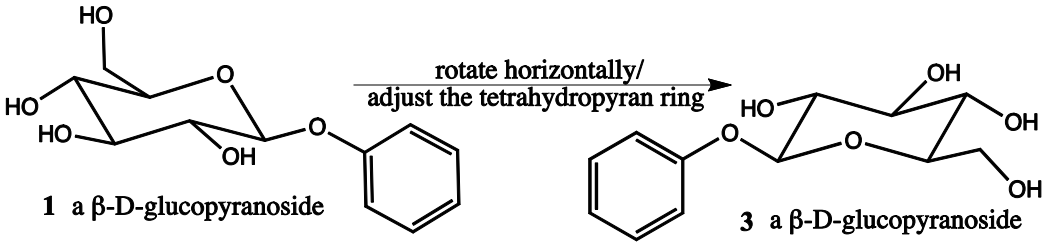


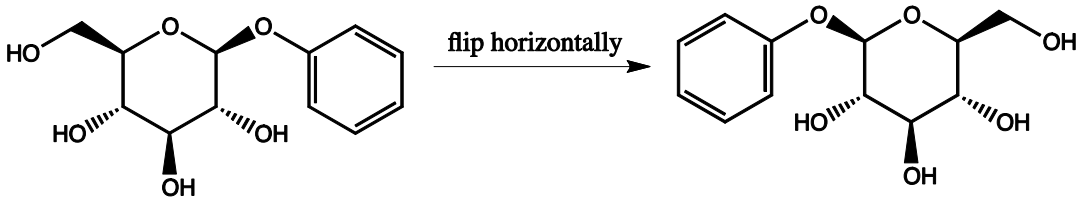
1 a β-D-glucopyranoside **2** a β-L-glucopyranoside

INCORRECT



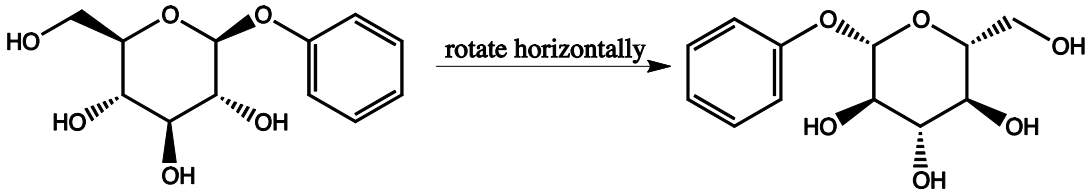
1 a β-D-glucopyranoside **3** a β-D-glucopyranoside

CORRECT



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

INCORRECT



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

CORRECT

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(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.

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