

9,11-SECO-24-HYDROXYDINOSTEROL FROM *PSEUDOPTEROGORGIA AMERICANA*

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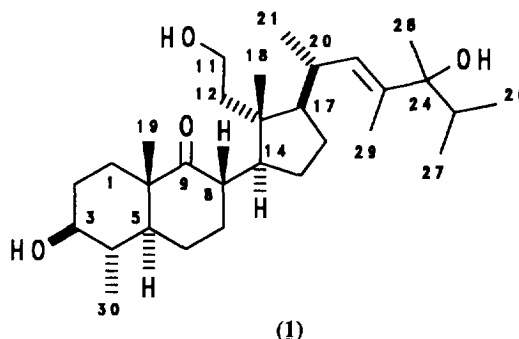
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Abstract: A new sterol with a 9,11-seco dinostane nucleus was isolated from *Pseudopterogorgia americana* and its structure determined by a combination of 2-D NMR experiments.

The number of marine sterols containing the 9,11-seco nucleus have been steadily increasing within recent years.¹⁻¹⁰ Without exception, the nucleus of these sterols is always derived from the cholestane system with varying levels of unsaturation, oxygenation, and alkylation. In continuation of our studies of Caribbean marine organisms,¹¹ we have investigated the extracts of a Barbadian specimen of *Pseudopterogorgia americana*. We report here the isolation and characterization of 9,11-seco-24-hydroxydinosterol (**1**) as a new metabolite from these extracts.

9,11-Seco-24-hydroxydinosterol (**1**) was isolated as a colorless gum, $[\alpha]_D -11.4^\circ$ (c 0.08, CHCl₃) and had infrared absorptions due to hydroxy (3440 cm⁻¹) and ketone (1700 cm⁻¹) functionalities. The positive ion FABMS had an (M+Na) at m/z 499 when NaCl was added to the matrix. The HREIMS did not give a molecular ion but had an M-H₂O at 458.3758 which indicated that (**1**) had the molecular formula C₃₀H₅₂O₄.

The ¹H NMR spectrum of (**1**) had signals due to eight methyls of which four were secondary, three were tertiary, and one was olefinic. The complete structure and the assignment of all proton and carbon resonances (Table 1) were achieved by a combination of 2-D NMR experiments, which included COSY, HETCOR, and FLOCK sequences. The stereochemistry at C-5, C-8, C-13, C-14, C-17, and C-20 were assigned by comparison of the ¹³C resonances with those of other 9,11-secosterols.^{4,6,8}



The isolation of 9,11-seco-24-hydroxydinosterol represents the first example of a secosterol possessing the dinostane

nucleus,^{12,13} while the only known example of a polyhydroxydinostane sterol was recently isolated from the related gorgonian, *P. acerosa*.¹⁴

Table 1. ¹³C and ¹H NMR Assignments of 9,11-Seco-24-hydroxydinosterol (**1**) in CDCl₃ at 400 MHz.

C#	δ _C	δ _H	C#	δ _C	δ _H
1	30.9	1.71, 1.59	16	24.5	1.81, 1.52
2	30.5	1.92, 1.49	17	50.2	1.73
3	75.7	3.07	18	17.7	0.63
4	33.1	2.45	19	16.7	1.18
5	51.9	1.08	20	38.9	1.47
6	24.8	1.67, 1.27	21	15.2	0.96
7	32.8	2.04, 1.10	22	128.6	5.40
8	44.4	2.81	23	136.8	-
9	218.0	-	24	77.4	-
10	49.0	-	25	34.0	1.87
11	59.3	3.80, 3.68	26	16.9	0.77
12	40.6	1.66, 1.37	27	16.9	0.84
13	45.3	-	28	13.2	1.59
14	42.3	2.52	29	23.9	1.18
15	23.9	1.51, 1.27	30	21.1	0.94

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