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**An Unusual Sesquiterpene Derivative from
the Caribbean Gorgonian
*Pseudopterogorgia rigida***

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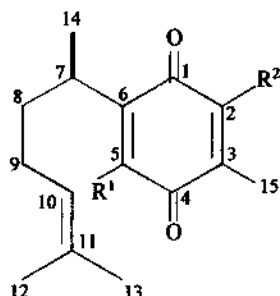
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A new sesquiterpene derivative named mochiquinone (**1**) was isolated from the Caribbean gorgonian coral *Pseudopterogorgia rigida* collected off northeastern Venezuela, along with the known compounds, α -curcumene, (–)-curcuphenol, (–)-curcuquinone, and (–)-curcuhydroquinone. The structure of the new compound was determined by spectroscopic analysis of its acetylated derivative and comparison with known compounds.

Earlier investigations of the gorgonian octocoral *Pseudopterogorgia rigida* Bielshowsky (order Gorgonacea, subclass Octocorallia, phylum Coelenterata), have yielded several bisabolane derivatives.^{1–3} As part of our continuing studies on Caribbean gorgonian corals, we have examined the EtOAc extract of this organism collected at Mochima Bay, Sucre, Venezuela. The MeOH-soluble fraction of the organism was further extracted with EtOAc. Si gel column chromatography followed by Si gel preparative TLC of this EtOAc extract of *P. rigida* afforded an unusual perezone (**3**)^{4,5} derivative, for which we propose the name mochiquinone (**1**), as well as four sesquiterpenoids previously reported:^{2,3} (–)-curcuquinone, (–)-curcuphenol, (–)-curcuhydroquinone, and the corresponding aromatic analogue α -curcumene. (–)-Curcuhydroquinone was fully characterized as its diacetate. These known compounds were characterized by comparison of their spectral data with those reported earlier for these sesquiterpenes.^{2,3,6,7}



- 1 $R^1 = \text{OH}, R^2 = \text{CH}_2\text{OH}$
 2 $R^1 = \text{OAc}, R^2 = \text{CH}_2\text{OAc}$
 3 $R^1 = \text{OH}, R^2 = \text{H}$

Mochiquinone (**1**) was isolated as a yellow oil. The IR spectrum showed a hydroxy absorption (3450 cm^{-1}) as well as the presence of a *p*-quinone system ($1650, 1630\text{ cm}^{-1}$). The ^1H NMR spectrum displayed a broad doublet at δ 4.55, which was consistent with an oxymethylene group attached to a quaternary carbon, a broad singlet at δ 2.70 and a singlet at δ 7.06 assignable to aliphatic and aromatic

hydroxyl groups. In addition, a triplet at δ 5.02 (vinylic proton), a multiplet at δ 3.06 (methine proton), two methylene signals (δ 1.69 and δ 1.94), two olefinic methyl group resonances at δ 1.55 and δ 1.68, an olefinic methyl at δ 2.13, and a fourth methyl signal as a doublet at δ 1.17 were present and comparable to proton signals of related compounds isolated earlier from *P. rigida*.^{1–3} In addition, the ^1H NMR spectrum of compound **1** appeared to be identical with the natural product perezone isolated from *Perezia* species,^{4,8} except that a proton in perezone is replaced by an oxymethylene group in **1**. Mochiquinone (**1**) was isolated as an unstable oil that gradually decomposed on standing. Consequently, this new metabolite was further characterized as its acetylated derivative. Upon acetylation, compound **1** yielded a diacetate (**2**) as a pale yellow oil. Its molecular formula $\text{C}_{20}\text{H}_{30}\text{O}_6$ was established by HREIMS (m/z 362.1720; calcd 362.1729) and was consistent with the ^1H and ^{13}C NMR spectral data (Table 1). 2D NMR techniques (COSY, HSQC, and HMBC) were used to establish the connectivities. An HSQC experiment showed the direct ^1H – ^{13}C correlations involving all protonated carbons, while an HMBC experiment allowed the assignment of the nonprotonated carbons. The ^1H NMR spectrum of **2** revealed an olefinic methyl singlet (δ 2.13), two acetyl methyl singlets (δ 2.07 and 2.34), a methine multiplet (δ 3.03), an olefinic triplet (δ 5.03), a methyl doublet (δ 1.2, $J = 7.0\text{ Hz}$), and two methyl singlets in the aliphatic region (δ 1.54 and 1.65). In addition, the oxymethylene protons of the *o*-acetoxymethylene group on the aromatic ring appeared at lower field (δ 5.02) compared with that in compound **1** (δ 4.55) and overlapped with the olefinic signal at δ 5.03.

The ^{13}C NMR spectrum of **2** confirmed the presence of four methyl, and one oxymethylene moieties, two methylenes, two methines, five quaternary carbons, two quinone carbonyls (δ 180.40 and 185.17), and two acetyl groups. In addition, the COSY spectrum of **2** established the proton relationships in which a methine multiplet (δ 3.03, H-7) in the side chain was coupled to a methyl doublet (δ 1.20, $J = 7.0\text{ Hz}$, H-14) and to the methylene protons (H-8). The vinylic proton at δ 5.03 (1H, t, $J = 7.0\text{ Hz}$) showed coupling with the protons of the olefinic methyl groups of the prenyl moiety. These cross-peaks confirmed the structure of the side chain. Also, the COSY data indicated that the oxymethylene protons were coupled to the aromatic methyl (H₃-15). The HMBC spectrum of **2** showed the expected correlations in support of this structure as illustrated in Figure 1. Mochiquinone (**1**) is a unique structure in that it

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320 (16), 260 (75), 191 (100), 178 (70); HREIMS m/z [M^+] 362.1720 (calcd for $C_{20}H_{26}O_6$, 362.1729).

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