

Aliphatic sulfates from the Brazilian ascidian *Botrylloides giganteum*

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Abstract

Two aliphatic sulfated compounds have been isolated from the Brazilian ascidian *Botrylloides giganteum*.

Introdução

As part of our research of Brazilian ascidians in search of marine natural active products, the species *Botrylloides giganteum* was selected for study, since there are few reports in the literature related to their chemical and biological activity.

The chemical investigation of BG extract afforded two known compounds: (3Z,6Z,9Z)-3,6,9-Dodecatrien-1-yl, 1-hydrogen sulfate (**1**) and (3Z)-4,8-dimethyl-,3-nonen-1-yl sulfate (**2**). Their structures were deduced from 1D, 2D spectral data, high resolution mass spectroscopy and by comparison with the literature.

Resultados e Discussão

The BG extract was cyclic loaded onto reversed-phase PSDVB beads with increasing amounts of Me₂CO in H₂O. The eluents were then concentrated to dryness to give 6 fractions (A-F). Combinations of normal phase (diol) and reversed-phase (C18) column chromatography and HPLC-ELSD of fraction C (40% Me₂CO) conducting the isolation of two aliphatic sulfated compounds **1** and **2**. The structures of **1** and **2** were determined on the basis of 1D and 2D NMR spectroscopy and by high-resolution mass spectrometry TOF-MS (-): *m/z* 259.1009 (C₁₂H₁₉O₄S) and *m/z* 249.1165 (C₁₁H₂₁O₄S), respectively. The signals of the pairs of olefinic carbons pairs at [δ (126.2; 131.4); (128.8; 129.5) and (128.2; 132.8)] in the ¹³C-NMR spectrum of **1** confirm the presence of three double bonds. In addition, the chemical shifts of the allylic methylene carbons (δ) 28.6 (C-2); 26.6 (C-5); 26.4 (C-8) and 21.5 (C-11)] support the Z-configurations of the three olefins. The ¹H-NMR spectrum of **2** showed a signal at δ 1.72 typical of methyl group linked to a sp² carbon. The signal at δ 0.89 (6H, d, 6.7 Hz) was related to the isopropyl group, and the chemical shift of the methylene signal at 68.9 in the ¹³C-NMR was

compatible with the presence of a Na⁺ (K⁺) sulfate group in this position.

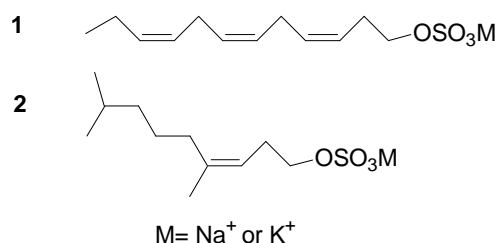


Figura 1. Chemical structures of compounds 1-2.

Compound **1** was previously isolated as a kairomone secreted by the crustacean *Daphnia magna* that induce morphological changes in a unicellular green alga *Scenedesmus gutwinski*¹. On the other hand, the compound **2** was obtained before from the Mediterranean ascidian *Microcosmus vulgaris* as an antiproliferative compound².

Conclusões

Sulfated alkanes/alcenes have been reported from marine organisms, however its ecological importance and biological potential needs further investigation.

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