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Polyoxygenated cembrane diterpenoids from the soft coral *Sarcophyton ehrenbergi*

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Five new polyoxygenated cembranoids, named (+)-1,15-epoxy-2-methoxy-12-methoxycarbonyl-11E-sarcophytoxide (1), (+)-2-*epi*-12-methoxycarbonyl-11E-sarcophine (2), 3,4-epoxyehrenberoxide A (3), ehrenbergol D (4) and ehrenbergol E (5), were obtained from the soft coral *Sarcophyton ehrenbergi*. The structures of 1-5 were established on the basis of comprehensive HRMS and NMR analyses and by comparison with reported data in literature. Compounds 4 and 5 showed moderate cytotoxicity against P-388 (mouse lymphocytic leukemia) cancer cell line with EC₅₀ values of 2.0 and 3.0 μM, respectively. Compound 2 exhibited slight antiviral activity against HCMV (human cytomegalovirus) with IC₅₀ values of 25.0 μg/mL.

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Characterization of 2,3-diaryl-xanthenes by electrospray mass spectrometry: Gas phase chemistry versus known antioxidant activity properties

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Xanthenes (XH) are a class of heterocyclic compounds widely distributed in nature holding numerous noteworthy biological and antioxidant activities. Therefore, it is important to achieve the utmost detailed structural information relevant to understand and predict their biological properties. In these studies we aimed to explore the potential relationship between radical-mediated xanthone chemistry in the gas phase and their antioxidant activities. The mass spectral fragmentation behavior of nine 2,3-diaryl-xanthenes bearing up to four hydroxyl groups at various sites on the two aryl rings was surveyed using electrospray ionization tandem mass spectrometry. Protonated XH were generated in the gas phase by electrospray ionization (ESI) and the main fragmentation pathways of the protonated XH formed due to collision-induced dissociation (CID) were investigated. In the CID-MS/MS spectra of [M+H]⁺ ions of six of the studied xanthenes, showing a most promising biological profile, the product ion produced with the highest relative abundance (RA) corresponded to the one formed through concomitant loss of H₂O plus CO. The product ion formed by loss of 64 Da (concomitant loss of two molecules of H₂O plus CO) is only observed for xanthenes containing a catechol unit. This product ion has the highest RA for the most potent scavenger of reactive oxygen and nitrogen species containing two catechol moieties. Through this studies a strong relationship between some of the biological activities of the studied 2,3-diaryl-xanthenes and their ESI-MS/MS fragmentation spectra was found. The multivariate statistical analysis results suggest that the selected MS features are related to the important biological features.

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