

Absolute configuration and corrected NMR assignment of 17-hydroxycyclooctatin, a fused 5-8-5 tricyclic diterpene.

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Abstract

The absolute configuration and corrected NMR assignment of 17-hydroxycyclooctatin isolated from *Streptomyces* sp. M56 recovered from a nest of South African *Macrotermes natalensis* termites are reported. 17-Hydroxycyclooctatin is a unique tricyclic diterpene (C₂₀) consisting of a fused 5-8-5 ring system, and in this study, its structure was unambiguously determined by a combination of HR-ESIMS and 1D and 2D NMR spectroscopic experiments to produce corrected NMR assignments. The absolute configuration of 17-hydroxycyclooctatin is reported for the first time in the current study using chemical reactions and quantum chemical ECD calculations. The corrected NMR assignments were verified using a gauge-including atomic orbital NMR chemical shifts calculation, followed by DP4 probability. To understand the pharmacological properties of 17-hydroxycyclooctatin, a network pharmacological approach and molecular docking analyses were used, which also predicted its effects on human breast cancer cell lines. Cytotoxicity and antiestrogenic activity of 17-hydroxycyclooctatin were determined, and it was found this compound may be an ER α antagonist.

Involved units

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