EC1000

A NEW CEMBRANOID DITERPENE FROM Sinularia flexibilis

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ABSTRACT

A new optically active cenbrane diterpene (m.p. 215 - 216 °C) was isolated by vacuum liquid chromatography from the dichloromethane extract of a Philippine soft coral Simularia Flexibilis. Microanalysis coupled with n.m.r. spectral data established a molecular formula of C_{20}H_{32}O_{7}.

A cenbrane-type skeleton was derived based on the IR, UV, and n.m.r. data and from other information obtained from the literature. The bicyclic variation of the cenbrane skeleton was necessary to satisfy the calculated index of hydrogen deficiency.

The $^{13}$C-n.m.r. spectrum revealed a ketone and a lactone carbonyl groups, and the aliphatic as well as the olefinic carbon atoms. The $^{1}$H-n.m.r. spectrum indicated aliphatic, olefinic as well as hydroxy protons. The ketone, lactone, hydroxy and olefinic functionalities were further indicated in the IR spectrum. One conjugated system was deduced from the UV spectrum.

A complete assignment of the $^{1}$H-n.m.r. and $^{13}$C-n.m.r. was made possible from the C-H correlation and COSY spectrum.