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NOTE

A New Sphingosine Derivative from a Soft Coral of *Nephthea* Species of the Andaman and Nicobar Coasts

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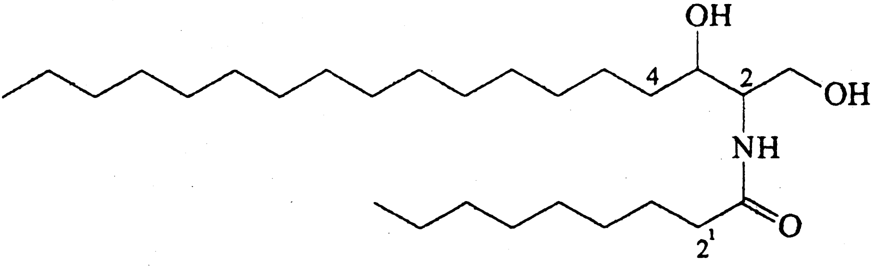
A new sphingosine derivative, 2-N-nonanoyl-4,5-dihydrosphingosine (1) was isolated from a soft coral of *Nephthea* species of the Indian Ocean. Structure elucidation of the compound is based on interpretation of the spectral data.

Key Words: Sphingolipid, *Nephthea* species, Soft coral, Indian Ocean.

Marine organisms have produced a wide variety of chemical compounds, *viz.*, terpenoids, steroids, sphingolipids, alkaloids etc. with various pharmacologically interesting activities. In our continuing search for bioactive secondary metabolites from marine organisms, we have investigated a soft coral of *Nephthea* species collected on the coasts of Andaman and Nicobar Islands of the Indian Ocean. The genus *Nephthea* is a rich source of many different classes of organic compounds. Earlier a variety of secondary metabolites like sesquiterpenes, diterpenes steroids[1–4] and aromatic compound[5] have been isolated from the genus *Nephthea*. In this paper, we are reporting the isolation and chracterization of a sphingosine derivative from the *Nephthea* species. This is the first report of a sphingosine derivative from the genus *Nephthea*.

General Experimental Procedures: Melting point was determined on a



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VEB analytic Dreader HMK hot plate and is uncorrected. IR spectrum was recorded on a Perkin-Elmer 281 double beam spectrophotometer, ^1H NMR spectra on a Bruker VM (400 MHz, FT) spectrometer and ^{13}C NMR spectra on a Jeol EX-90 spectrometer at 22.5 MHz. Opticai rotation was measured on a Jasco DIP-370 digital polarimeter. The mass spectrum was recorded on a Jeol D-300 (EI) spectrometer and elemental analysis was carried out on a Carlo-Erba EA 1108 instrument.

Collection and Isolation: The soft coral of *Nephthea* species (dry weight *ca.* 1.8 kg) was collected on the coasts of Andaman and Nicobar Islands (93°29'E, 70°57'N) during December 1986. It was identified by Dr. Phil Alderslade, Curator of Coelenterates, Northern Territory Museum of Arts and Sciences, Darwin, Australia. The soft coral was given voucher No. MF/CBR/28 and the specimens were deposited in the School of Chemistry, Andhra University, Visakhapatnam. The material was cleaned of the co-occurring organisms and thoroughly washed with water. It was then cut into thin slices, soaked in 95% ethanol at the site of collection and brought to the laboratory and extracted repeatedly with ethanol by percolation every 72 h (4 × 3 L). The combined concentrate was extracted with EtOAc and the soluble portion (18 g) was chromatographed over silica gel. Repeated silica gel chromatography of the high polar fractions (2% MeOH in $CHCl_3$) yielded compound **1** as a white solid which was purified by recrystallisation from chloroform-methanol as colourless crystals (160 mg).

2-N-Nonanoyl-4,5-dihydrosphingosine (**1**):. crystalline solid, m.p. 191–193°C (found: C, 73.06: H, 10.34; N, 3.15; $C_{27}H_{55}NO_3$ requires C, 73.24; H, 10.20; N, 3.17%); α_D^{27}: +26.0° (c, 0.35 in pyridine); IR (nujol): 3520, 3460, 2985, 1640 and 1025 cm^{-1}; ^1H NMR (d_5-pyridine): 0.88 (6H, t, J = 6 Hz), 1.26 (*ca.* 38H, m), 2.47 (2H, t, JT= 7 Hz), 4.28 (1H, dd, J = 7, 2 Hz), 4.39 (1H, dd, J = 7, 3 Hz), 4.49 (2H, m), 8.51 (NH, d, J = 10 Hz); ^{13}C NMR (d_5-pyridine): 14.3, 23.0, 29.9, 30.2, 32.1, 36.9, 48.6, 62.3, 67.9, 173.6; MS: m/z 441 (2%, M^+), 357 (22), 340 (24), 326 (18), 309 (19), 308 (27), 285 (100), 264 (8), 128 (14), 60 (82) and 43 (56).

Compound **1** was obtained as colourless crystals from chloroform-methanol with m.p. 191–193°C and analysed for $C_{27}H_{55}NO_3$ (M^+, m/z 441). The IR spectrum showed absorption bands for hydroxyl (3520 cm^{-1}), amide carbonyl (3460 and 1640 cm^{-1}) and aliphatic long chain (2985 cm^{-1}). The ^{13}C NMR spectrum in d_5-pyridine showed resonances for amide carbonyl carbon at δ 173.6 and two oxygenated carbons at δ 62.3, 67.0. It also showed a carbon resonance at δ 48.6, which is attributable to nitrogen bearing carbon atom.

The ^1H NMR spectrum (400 MHz, d_5-pyridine) showed a signal for two chain terminal methyls at δ 0.88 (6H, t, J = 6 Hz). The ^{13}C NMR and ^1H NMR spectral data further indicated the presence of a 2-N-acyl-1,3-dihydroxy chain in compound **1** [δ_H 4.28 (1H, dd, J = 7, 2 Hz, H_A-1), 4.39 (1H, dd, J = 7, 3 Hz, H_B-1), 4.49 (2H, m, H-2 and H-3), 8.51 (1H, d, J = 10 Hz, H-N, D_2O exchangeable) and δ_C 173.6 (s), 67.9 (d), 62.3 (t), 48.6 (d)]. The ^1H NMR spectrum also showed signals for long chain protons at δ 1.26 (38H, m) and carbonyl adjacent methylene protons at δ 2.47 (2H, t, J = 7 Hz, 2'-H).

The mass spectrum of the compound showed prominent fragment ions at m/z 441 (2%, M^+), 357 (22%) and 285 (100%). The fragment at m/z 357 was attributed to the loss of C_6H_{12} unit by a McLafferty rearrangement[6]. The base peak appearing at m/z 285 was due to the mass fragment $[M^+\text{-NHCO}(CH_2)_7CH_3]$[7] .From the foregoing spectral data of the compound, the structure could be assigned as 2-N-nonanoyl-4,5-dihydrosphingosine (**1**).

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