E2-03 A new contragestative sphingolipid from Sri Lankan marine red alga, *Gelidiella acerosa*

G A S Premakumara[1]*, L M V Tillekeratne[3], W D Ratnasooriya[1], A S Amarasekare [2], Att-ur-Rahman[4]
([1]*Dept of Zoology,* [2]*Dept of Chemistry, University of Colombo, Colombo 3,* [3]*Dept of Medicinal Chemistry, University of Toledo, Ohio, USA,* [4]*HEJ Research Institute of Chemistry, University of Karachi, Pakistan*)

In a programme of uncovering contraceptive agents from marine natural products a 1:1 CH_2Cl_2/MeOH extract of red alga *Gelidiella acerosa* was tested in pregnant rats and had highly potent contragestative activity (100% at 1000mg/kg/ml/day concentration), via an anti-progesterone mechanism. The active component, S-PC-1, was isolated through activity directed separation and S-PC-1 has been identified as a sphingosine derivative. In view of establishing the exact chemical structure, S-PC-1 was subjected to extensive spectroscopy: IR, ^{1}H & ^{13}C NMR, DEPT, COSY, HOHAHA, HMQC and HMBC. Mass fragmentations were studied using FDMS, EIMS and FAB+. A ^{1}H NMR for the acetylated product was also recorded. (***See p.276***)

IR spectrum had strong bifurcated band at 3350 cm^{-1} for OH and amide NH stretching and strong band at 1620 cm^{-1} for NH bond scissoring for hydroxyl and amide functionality. Presence of an amide functionality was supported with a peak at δ 175.57 in ^{13} C NMR ^{1}H NMR had 2 broad signals at δ 1.24 and 1.3 corresponding to 19 and 11 H respectively indicating 2 alkyl chains and 6H triplet at δ 0.84 for overlapping 2 terminal methyl groups. Range of protons were evident between δ 4.25 and 5.1 for protons attached to oxygenated carbons. ^{13}C NMR had signals between δ 61.84 and 76.57 for oxygenated carbons.

The spectral evidence presence of amide ester functionality, oxygenated carbons and long alkyl chains suggested S-PC-1 to be a sphingolipid derivative. With extensive analysis of mass fragmentation and other spectral data the structure of S-PC-1 was established as N-2'-hydroxy-lignoceroyl-2-amino-1,3,4-trihydroxy-octadecane(I).

No non-steroidal, anti-progesterone immediate post-implantation contragestative compound is available to date. As such, considering the absence of maternal or embryo toxicity S-PC-1 warranted further research in other animal models, sub-human primates followed by clinical trials to be evaluated for a potential once a month contraceptive pill for women.

Present address: Natural Products Development Group, Industrial Technology Institute (CISIR), Colombo 7

$[\alpha]_D^{28}$ = +2.7(c,5,C5H5N).

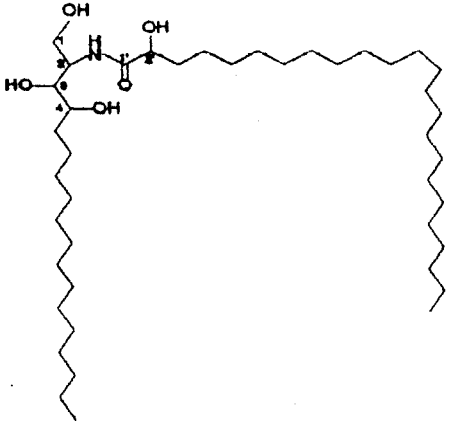
IR V_{max}^{KBr} cm^{-1}: 3350,3230,2900,2850,1620,1460.

FDMS (m/z): 684 $(M+H)^+$;

FAB^+ (m/z): 684$(M+H)^+$; EIMS (m/z): 683$(M)^+$, 665,647,357,339,308,280,265.

^{13}CNMR(δ)	14.07	25.62	26.44	29.92	31.94	33.94	35.50	52.81	61.84	72.32	72.85	76.67	175.57
DEPT (δ)	CH_3	CH_2	CH_2	CH_2	CH_2	CH_2	CH_2	CH	CH_2	CH	CH	CH	C=O
HMQC	0.84	1.67 1.45	1.76 1.35	1.24 1.29	1.90 2.23	1.90 2.23	2.20 2.03	5.10	4.40 4.47	4.33	4.25	4.50	
H-split(J+Hz)	2t(ol)	m(ol)	m(ol)	m(ol)	m(ol)	m(ol)	m(ol)	m(ol)	dd 4.65/10.85 4.98/10.85	dd 4.8/6.45	d/t 2.25/8.75	dd 3.7/7.7	

ol = overlap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