SUPPORTING INFORMATION

5-Bromo-8-methoxy-1-methyl-β-carboline, an Alkaloid from the New Zealand Marine Bryzoan *Pterocella vesiculosa*.

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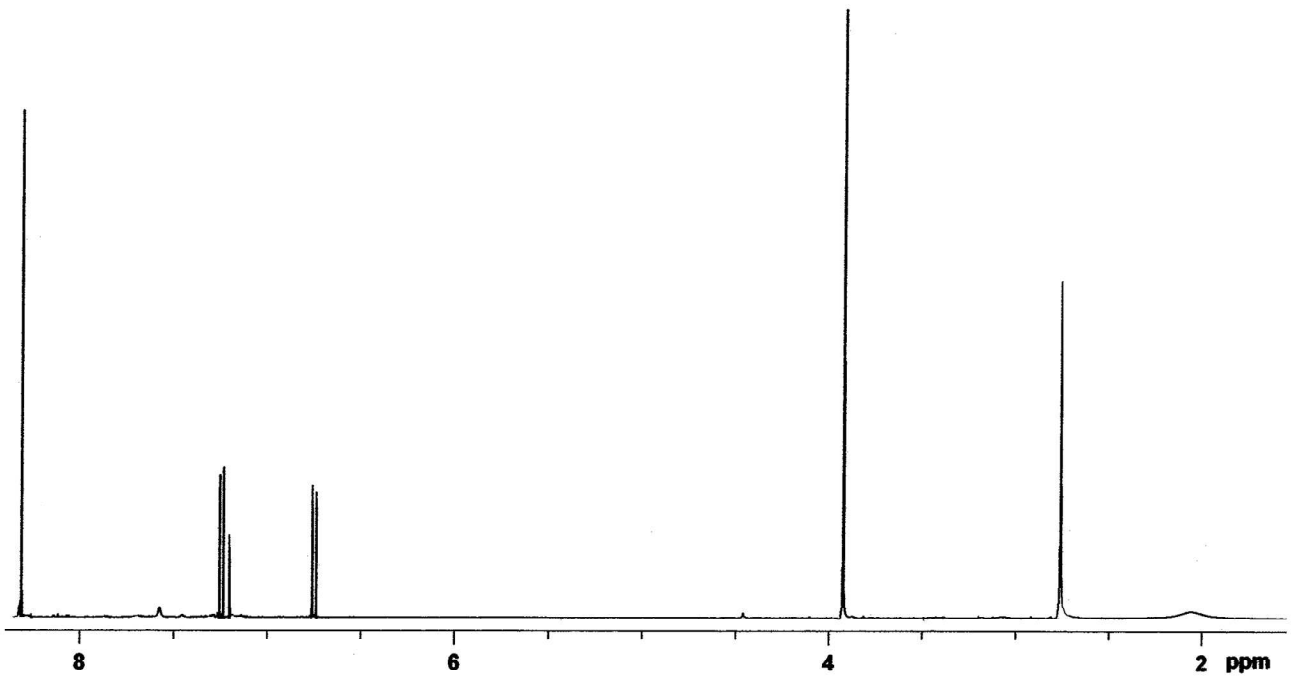

Figure S1: ^{1}H NMR spectrum of 5-bromo-8-methoxy-1-methyl-β-carboline (1) in $CDCl_3$ at 400 MHz

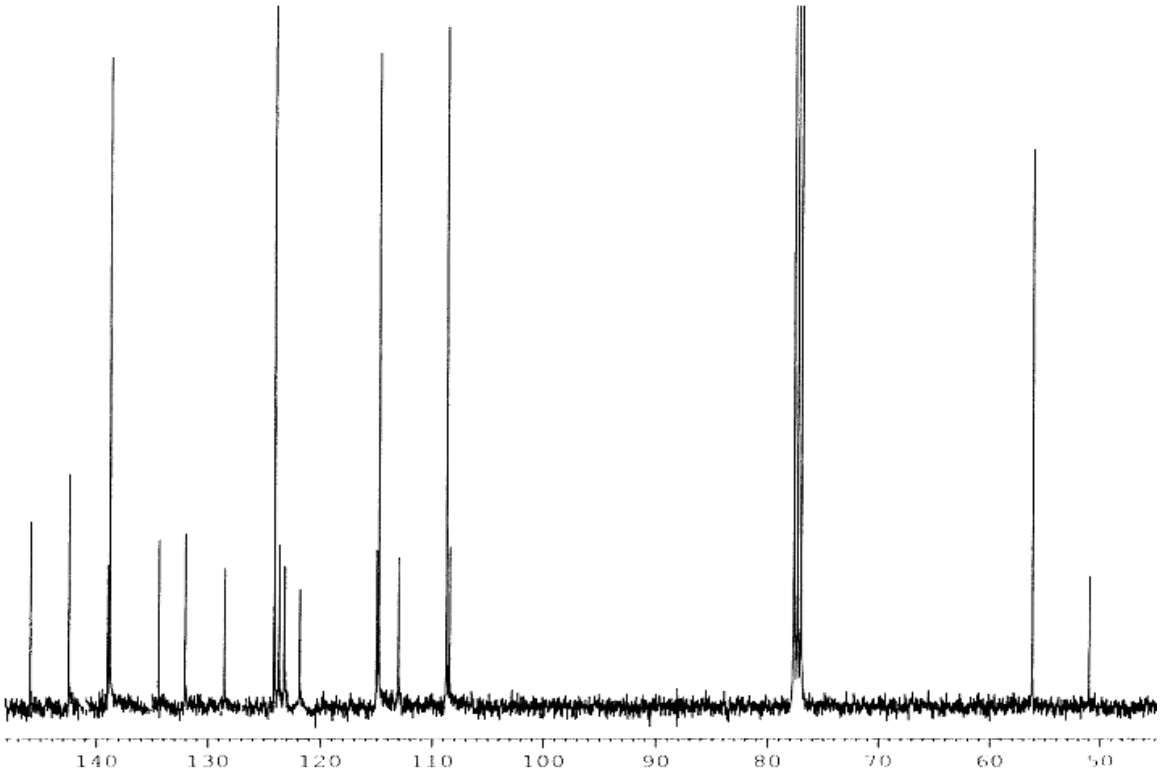

Figure S2: ^{13}C NMR spectrum of 5-bromo-8-methoxy-1-methyl-β-carboline (1) in $CDCl_3$ at 100 MHz

Table S1: Crystal Data and Structure Refinement for 5-bromo-8-methoxy-1-methyl-β-carboline (1) as the methanol solvate

Empirical formula	$C_{14}H_{15}BrN_2O_2$	
Formula weight	323.19	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P2(1)/c	
Unit cell dimensions	a = 9.6025(5) Å	alpha = 90°
	b = 10.9301(5) Å	beta = 107.645(2) °
	c = 13.3928(6) Å	gamma = 90°
Volume	1339.53(11) $Å^3$	
Z, Calculated density	4, 1.603 mg/m^3	
Absorption coefficient	3.068 mm^{-1}	
F(000)	656	
Crystal size	0.60 x 0.56 x 0.30 mm	
Theta range for data collection	2.90 < θ < 28.00°	
Limiting indices	-12 <= h <= 8, -13 <= k <= 14,	
	-15 <= l <= 17	
Reflections collected / unique	11505 / 3236 [R(int) = 0.0382]	
Completeness to θ = 28.00	99.9 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.4596 and 0.2604	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3236 / 0 / 199	
Goodness-of-fit on F^2	1.074	
Final R indices [I > 2sigma(I)]	R_1 = 0.0316, wR_2 = 0.0823	
R indices (all data)	R_1 = 0.0364, wR_2 = 0.0844	
Largest diff. peak and hole	1.211 and -0.447 e. $Å^{-3}$	

Table S2: Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (Å^2 x 10^3) for 5-bromo-8-methoxy-1-methyl-β-carboline (1). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Br(1)	7292(1)	983(1)	1311(1)	32(1)
O(1)	9883(2)	-3364(1)	-332(1)	23(1)
N(1)	11616(2)	-1691(2)	1139(1)	17(1)
N(2)	13724(2)	710(2)	2872(1)	22(1)
C(1)	13505(2)	-331(2)	2319(1)	20(1)
C(3)	12559(2)	1386(2)	2910(2)	24(1)
C(4)	11119(2)	1088(2)	2406(2)	21(1)
C(4a)	10853(2)	13(2)	1803(1)	17(1)
C(4b)	12076(2)	-690(2)	1776(1)	17(1)
C(5)	8070(2)	-396(2)	799(2)	21(1)
C(6)	7150(2)	-1175(2)	95(2)	23(1)
C(7)	7709(2)	-2198(2)	-302(2)	21(1)
C(8)	9195(2)	-2439(2)	11(1)	18(1)
C(9a)	10118(2)	-1642(2)	739(1)	16(1)
C(9b)	9581(2)	-604(2)	1137(1)	18(1)
C(10)	9001(2)	-4161(2)	-1121(2)	25(1)
C(1')	14797(2)	-1084(2)	2291(2)	27(1)
O(Methanol)	3521(2)	6457(1)	859(1)	27(1)
C(Methanol)	3419(3)	5987(2)	-148(2)	28(1)

Table S3. Bond lengths [Å] and angles [deg] for 5-bromo-8-methoxy-1-methyl-β-carboline (1) (methanol solvate).

Br(1)-C(5)	1.8998(19)
C(1)-C(1')	1.499(3)
C(1)-C(4b)	1.400(3)
C(3)-H(3)	0.980(2)
C(3)-C(4)	1.381(3)
C(4)-H(4)	0.930(2)
C(4)-C(4a)	1.405(3)
C(4a)-C(4b)	1.414(3)
C(4a)-C(9b)	1.443(3)
C(5)-C(6)	1.375(3)
C(6)-H(6)	0.920(3)
C(6)-C(7)	1.412(3)
C(7)-H(7)	1.000(2)
C(7)-C(8)	1.385(3)
C(8)-C(9a)	1.404(2)
C(9b)-C(5)	1.402(3)
C(9b)-C(9a)	1.415(3)
N(1)-H(1)	0.750(3)
N(1)-C(4b)	1.375(2)
N(1)-C(9a)	1.375(2)
N(2)-C(1)	1.339(2)
N(2)-C(3)	1.354(3)
O(1)-C(8)	1.361(2)
O(1)-C(10)	1.432(2)

C(1)-C(4b)-C(4a)	121.64(17)
C(1)-N(2)-C(3)	119.44(17)
C(3)-C(4)-H(4)	120.00(15)
C(3)-C(4)-C(4a)	117.32(19)
C(4)-C(3)-H(3)	119.00(13)
C(4)-C(4a)-C(4b)	117.54(17)

C(4)-C(4a)-C(9b)	135.98(18)
C(4a)-C(4)-H(4)	122.70(15)
C(4b)-C(1)-C(1')	121.40(17)
C(4b)-C(4a)-C(9b)	106.46(16)
C(4b)-N(1)-H(1)	129.00(2)
C(4b)-N(1)-C(9a)	108.22(16)
C(5)-C(6)-H(6)	120.30(16)
C(5)-C(6)-C(7)	120.64(18)
C(5)-C(9b)-C(4a)	136.34(17)
C(5)-C(9b)-C(9a)	117.87(17)
C(6)-C(5)-Br(1)	119.86(15)
C(6)-C(5)-C(9b)	120.57(18)
C(6)-C(7)-H(7)	118.60(13)
C(7)-C(6)-H(6)	119.10(16)
C(7)-C(8)-C(9a)	117.87(17)
C(8)-C(7)-C(6)	120.75(18)
C(8)-C(7)-H(7)	120.60(13)
C(8)-C(9a)-C(9b)	122.28(17)
C(8)-O(1)-C(10)	117.52(15)
C(9a)-C(9b)-C(4a)	105.74(16)
C(9a)-N(1)-H(1)	123.00(2)
C(9b)-C(5)-Br(1)	119.57(14)
N(1)-C(4b)-C(1)	128.74(17)
N(1)-C(4b)-C(4a)	109.59(16)
N(1)-C(9a)-C(8)	127.71(17)
N(1)-C(9a)-C(9b)	109.96(16)
N(2)-C(1)-C(1')	119.23(17)
N(2)-C(1)-C(4b)	119.37(18)
N(2)-C(3)-H(3)	116.30(13)
N(2)-C(3)-C(4)	124.67(18)

O(1)-C(8)-C(7)	126.86(17)
O(1)-C(8)-C(9a)	115.25(16)

Table S4: P388 Assay results for 5-bromo-8-methoxy-1-methyl-β-carboline (1) and selected 1-substituted β-carboline alkaloids

Compound	P388 IC_{50}[a]
1-Methyl-β-carboline (harman)	>12500[b]
5-Bromo-8-methoxy-1-methyl-β-carboline (1)	**5089**
1-Vinyl-β-carboline (pavettine)	100
8-Hydroxy-1-vinyl-β-carboline	100
8-Methoxy-1-vinyl-β-carboline	100
8-Acetoxy-1-vinyl-β-carboline	650
1-Ethyl-β-carboline	>12500
1-Ethyl-8-hydroxy-β-carboline	>12500
1-Ethyl-8-methoxy-β-carboline	>12500

Key: [a]The concentration of sample in ng/mL required to reduce the cell growth of the P388 leukemia cell line (ATCC CCL 46) by 50%.

[b]Values for all alkaloids except **1** taken from Prinsep, M. R.; Blunt, J. W.; Munro, M. H. G. *J. Nat. Prod.* **1991**, *54*, 1068-1076.

Table S5: Antimicrobial Assay results for 5-bromo-8-methoxy-1-methyl-β-carboline (1) and selected 1-substituted β-carboline alkaloids

	Organism		
Compound	**Bs**[a]	**Ca**	**Tm**
1-Methyl-β-carboline (harman)	7.5-15[b,c]	1.9-3.8	3.7-7.5
5-Bromo-8-methoxy-1-methyl-β-carboline (1)	**2-4**	**7.5-15**	**7.5-15**
1-Ethyl-β-carboline	7.5-15	1.9-3.8	1.9-3.8
1-Ethyl-8-hydroxy-β-carboline	30-60	30-60	30-60
1-Ethyl-8-methoxy-β-carboline	>60	7.5-15	7.5-15
1-Vinyl-β-carboline (pavettine)	1.9-3.8	1.9-3.8	0.1-0.2
8-Hydroxy-1-vinyl-β-carboline	7.5-15	15-30	0.45-0.9
8-Methoxy-1-vinyl-β-carboline	7.5-15	15-30	0.45-0.9

[a]Bs = *Bacillus subtilis*, Ca = *Candida albicans*, Tm = *Trichophyton mentagrophytes*. (All strains developed and held in Department of Plant and Microbial Sciences, University of Canterbury, 1984).

[b]Activities expressed as minimum inhibitory doses in μg/disc.

[c]Values for all alkaloids except **1** taken from Prinsep, M. R.; Blunt, J. W.; Munro, M. H. G. *J. Nat. Prod*. **1991**, *54*, 1068-1076.