

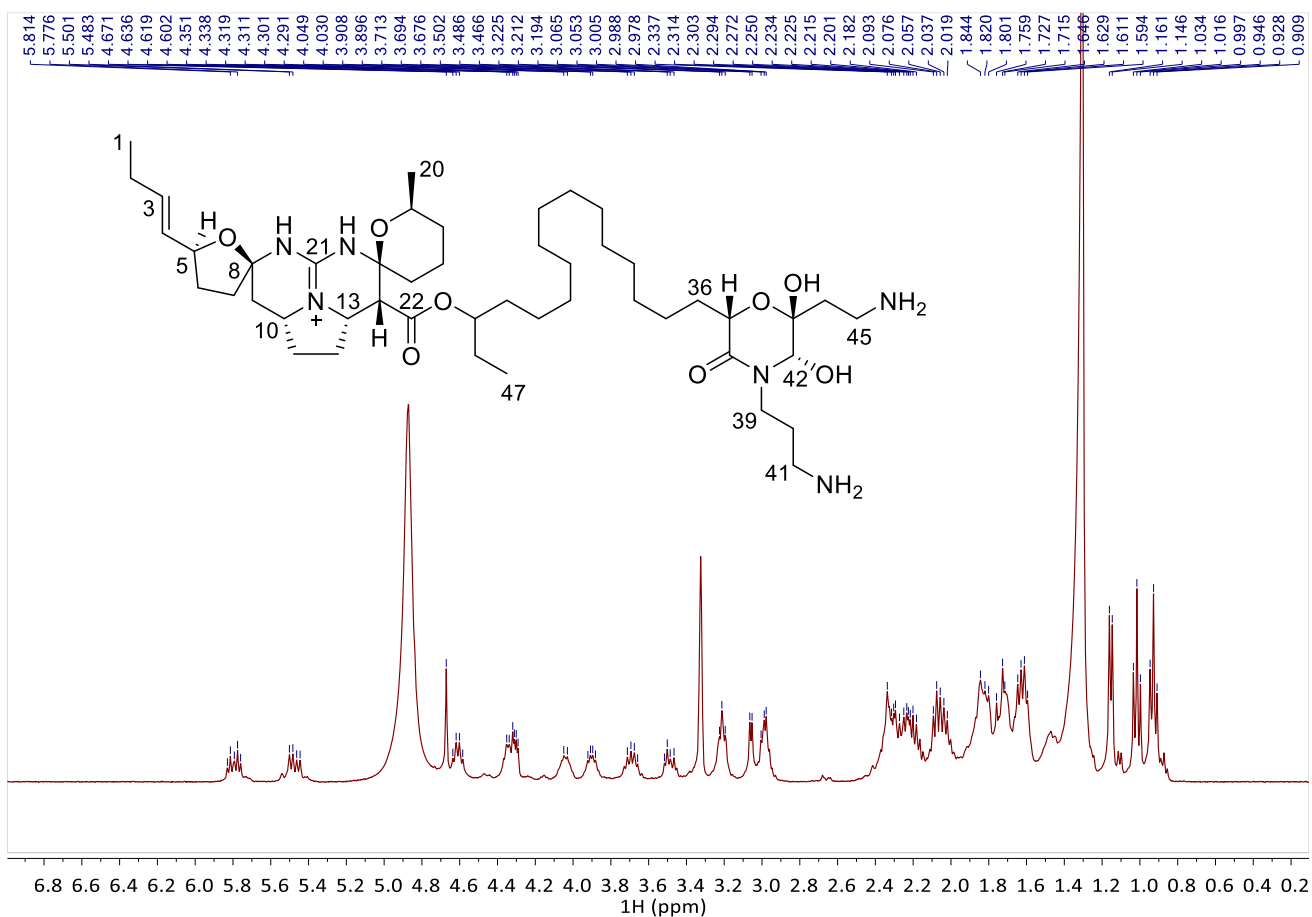
Supplementary Material

SI Table 1. ^1H and ^{13}C NMR Data for Compound 1.

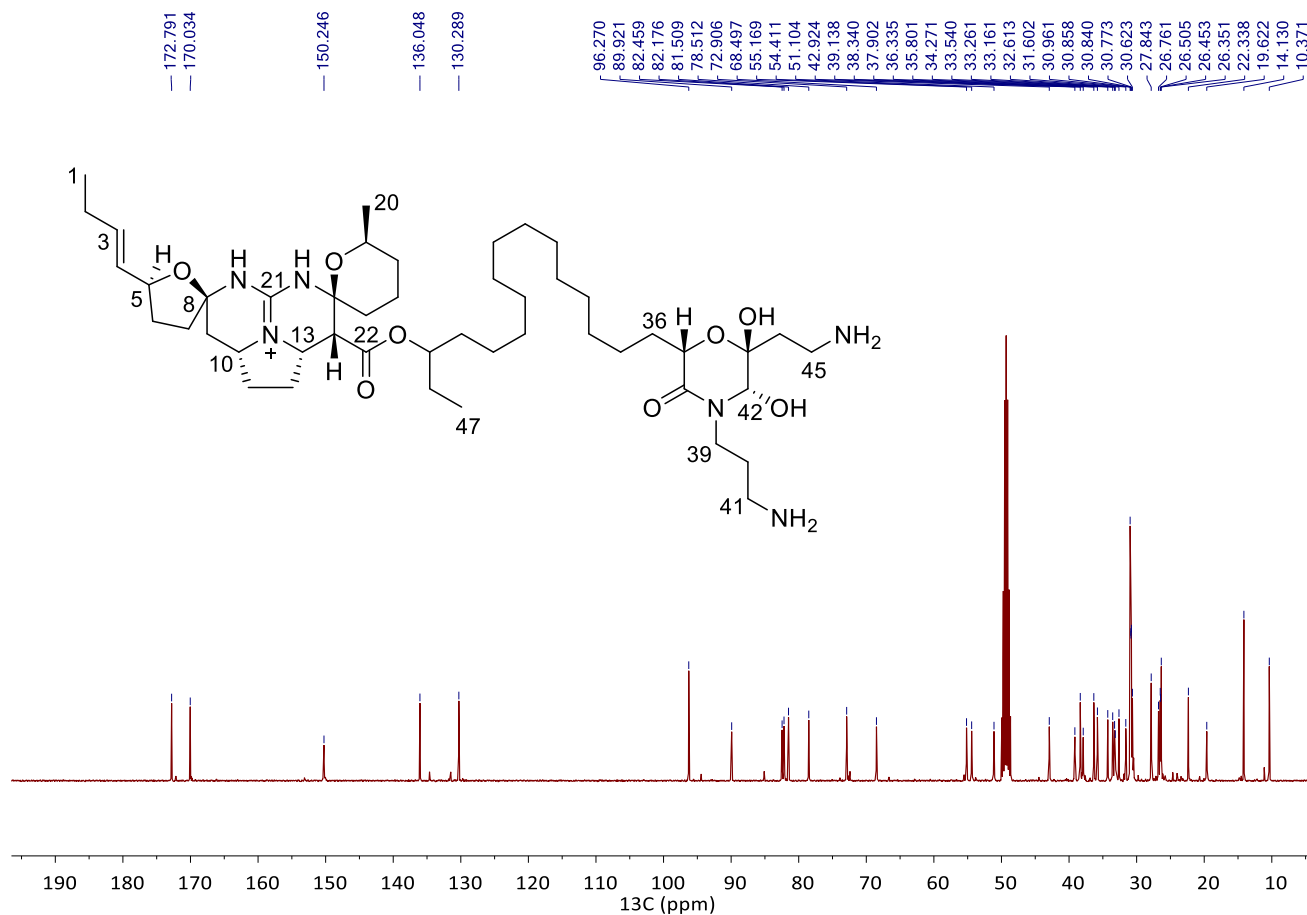
Position	Experimental CD_3OD		Published CD_3OD^1		
	δ_{H} (mult)	δ_{C}	δ_{H} (mult)	δ_{C} (DEPT)	COSY
1	1.02 (t)	14.1 CH_3	0.99 (t)	14.3 CH_3	H2
2	2.06 (m)	26.5 CH_2	2.05 (m)	26.8 CH_2	H1, H3
3	5.79 (dt)	136.0 CH	5.77 (dt)	136.9 CH	H2, H4
4	5.44-5.50 (m)	130.3 CH	5.45 (ddt)	130.7 CH	H3, H5
5	4.62 (dt)	81.5 CH	4.57 (br. q)	82.4 CH	H4, H6a, H6b
6		33.3 CH_2	1.78 (m), 2.22 (m)	33.5 CH_2	H5, H6b, H7
					H5, H6a
7		37.9 CH_2		38.4	H6a
8		89.9 C		90.6	
9	1.73 (m)	39.1 CH_2	1.69 (m), 2.27 (dd)	39.9	H9b, H10
					H9a, H10
10	4.04 (m)	55.2 CH	4.02 (m)	55.4	H9a, H9b
11		27.8 CH_2	1.64 (m), 2.29 (m)		H10, H11b
					H10, H11a
12		26.5 CH_2	1.77 (m), 2.29 (m)	28.2	H12b, H13
					H12a, H13
13	4.29-4.35 (m)	54.4 CH	4.32 (m)	55.3	H14
14	3.06 (d)	51.1 CH	3.04 (d)	51.5	H13
15		82.2 C		83.2	
16	1.73 (m)	33.2	1.69 (m)	33.2	
17	1.82 (m)	19.6 CH_2	1.82 (m)	20.0	H16, H18a
18		33.2 CH_2	1.27 (m), 2.24 (m)	33.2	
					H18a, H19
19	3.90 (dd)	68.5 CH	3.86 (m)	69.2	H18, H20
20	1.15 (d)	22.3 CH_3	1.13 (d)	22.5	H19
21		150.2 C		151.1	
22		170.0 C		170.8	
23		78.5 CH	4.82 (m)	79.2	H46
24		34.3	1.58	34.8	H23
25-34		31.6-30.6			
35		26.8 CH_2	1.45 (m)	27.0	
36		33.5 CH_2	1.79 (m), 1.86 (m)	34.0	H37
37	4.29-4.35 (m)	72.9 CH	4.27 (dd)	73.5	H36
38		172.8 C		173.6	
39	3.49 (dd)	42.9 CH_2	3.46 (dt)	43.3	H39b, H40
	3.69 (dd)		3.66 (m)		H39a, H40

40		26.5 CH ₂	1.98 (m)	27.4	H39a, H39b, H41
41	2.99 (m)	38.3 CH ₂	2.95 (m)	38.6	H40, NH ₂ 41
42	4.62 (dt)	82.5 CH	4.59 (br.s)	83.3	OH42
43		96.3 C		96.7	
44		35.8 CH ₂	2.12 (m), 2.22 (m)	36.5	H45
45	3.21 (m)	36.3 CH ₂	3.18 (m)	36.7	H44a, H44b, NH ₂ 45
46	1.62 (m)	27.8 CH ₂	1.60 (m)	28.3	H23, H47
47	0.93 (t)	10.4 CH ₃	0.90 (t)	10.6	H46

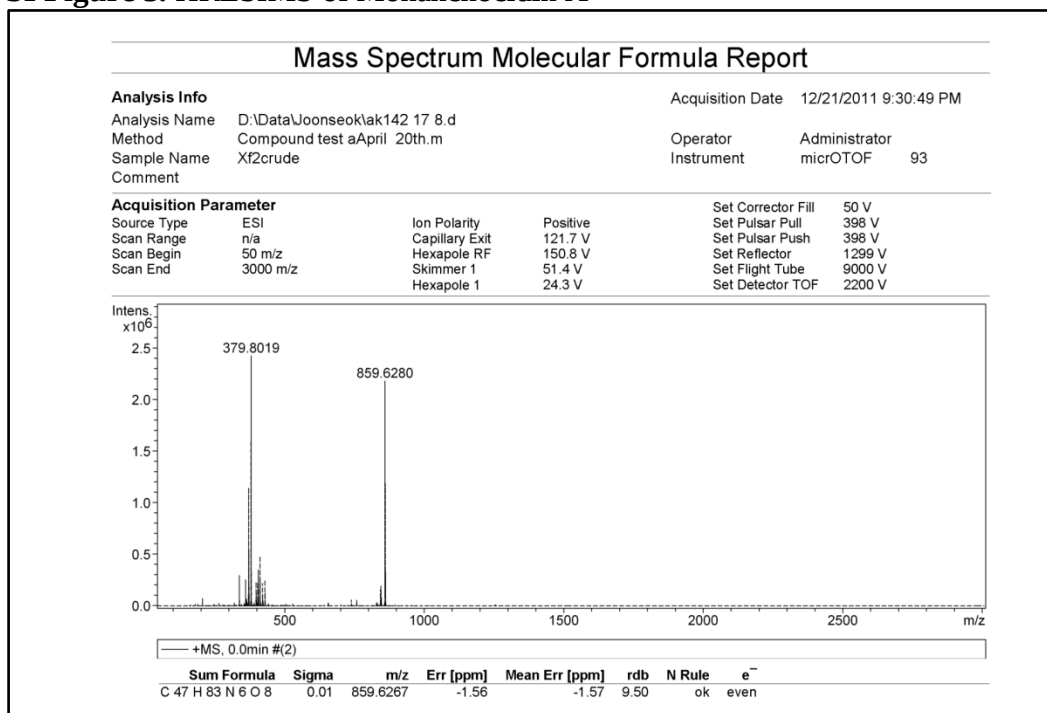
SI Figure 1. ¹H NMR Spectrum of Monanchocidin A in CD₃OD

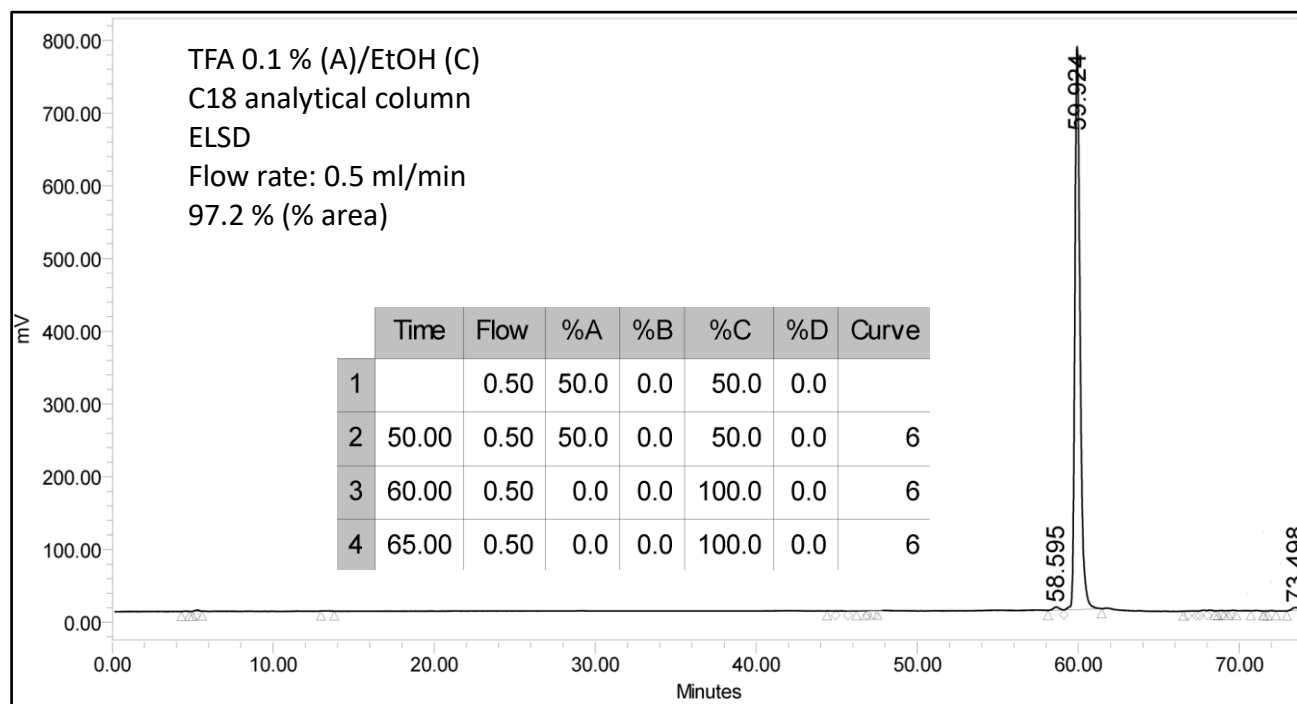


SI Figure 2. ^{13}C NMR Spectrum of Monanchocidin A in CD_3OD



SI Figure 3. HRESIMS of Monanchocidin A



SI Figure 4. LC-MS Chromatogram of Monanchocidin A

References.

1. Guzii, A. G., Makarieva, T. N., Denisenko, V. A., Dmitrenok, P. S., Kuzmich, A. S., Dyshlovoy, S.A., et al. (2010). Monanchocidin: a new apoptosis-inducing polycyclic guanidine alkaloid from the marine sponge *Monanchora pulchra*. *Org. Lett.* 12, 4292–4295. doi: 10.1021/ol101716x.