Supplementary Materials: Ergosterols from Culture Broth of a Marine Derived *Streptomyces* sp. H41-59

Yang-Mei Zhang, Hong-Yu Li, Chen Hu, Hui-Fan Sheng, Ying Zhang, Bi-Run Lin and Guang-Xiong Zhou

Compound 1

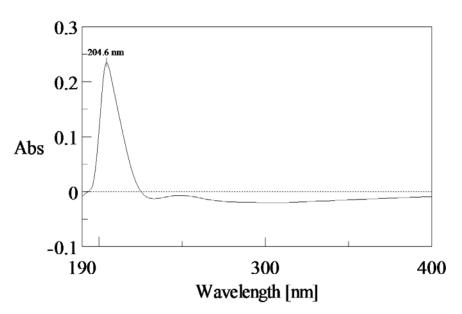


Figure S1. UV spectrum of compound 1 in MeOH.

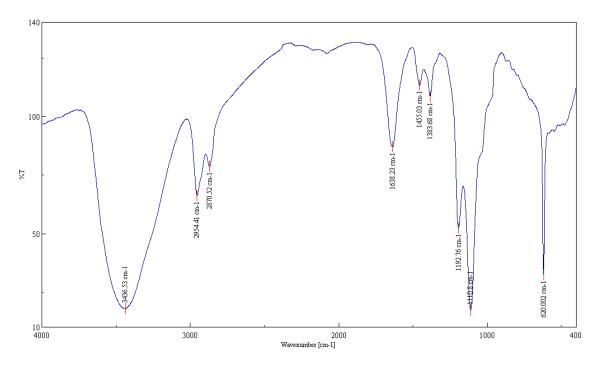


Figure S2. IR spectrum of compound 1.

	- A	lon	Formula	Abundance											
m/z	69.3293	(M+Na)+	C28 H46 Na O4	Abundance 10910.9											
Be		Formula (M)	Ion Formula	Calc m/z	Score V	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DB
	st 🔽	C28 H46 O4	C28 H46 Na D4	469.3288	79.43	C1022.20016	446.3401	446.3396	-1,18			49.69	98.72	469.3293	UB
	-								1.10	1.10	12.00	43.03	30.12	403.3233	
Isc	kope 1	Abund% 100	Calc Abund% 100	Calc Abund Sum% 76.36	m/z 469.3293	Calc m/z 469.3288	Diff (ppm) -1.1	Abund Sum% 75.73							
	2	32.04	30.97	23.64	465.5255	463.3200	-1.7	24.27							
_	4	32.04	30.37	23.04	470.333	470.3322	.1.7	24.27							
2															
						-									
	lator (A)	Chromatogram Re	sults 📲 MS For	nula Results: + Sce	un (0.427 min)										
carcu															
Spec	trun Res	ults													
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SSpec ↔ ‡	trun Res Q. 🚺	ults १४/४४/ <mark>▲</mark> ▲		• 🕕 🚴 % 🗞											
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S Spec + +ES - +ES 	trun Res Q. 🚺	ults १४/४४/ <mark>▲</mark> ▲		 ■ ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ●											
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Figure S3. HR-TOF-MS of compound 1.

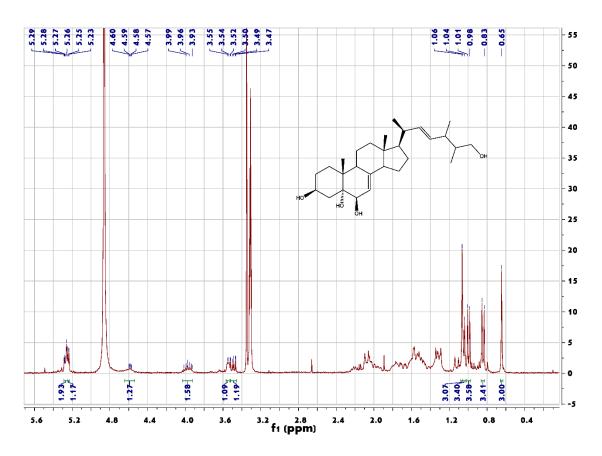


Figure S4. ¹H-NMR spectrum of compound 1 (300 MHz in MeOH).



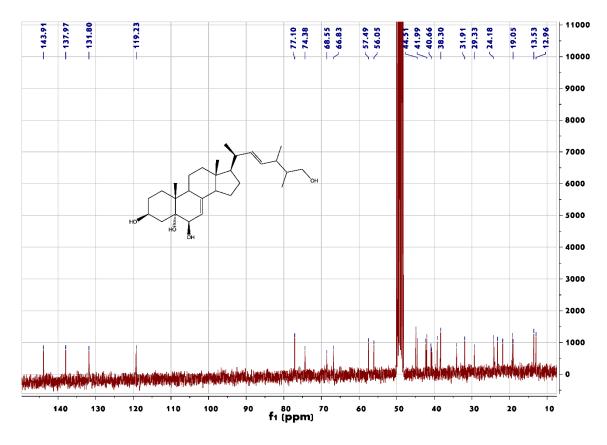


Figure S5. ¹³C-NMR spectrum of compound 1 (75 MHz in MeOH).

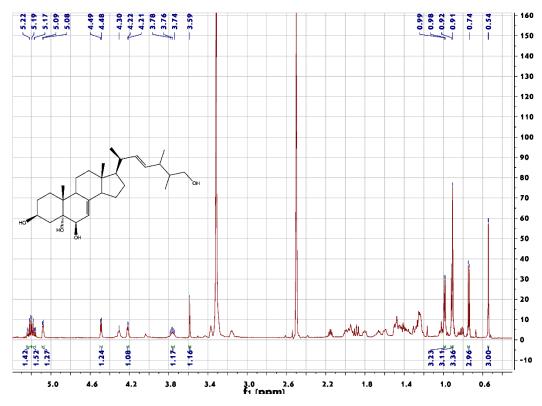


Figure S6. ¹H-NMR spectrum of compound 1 (300 MHz in DMSO-d6).

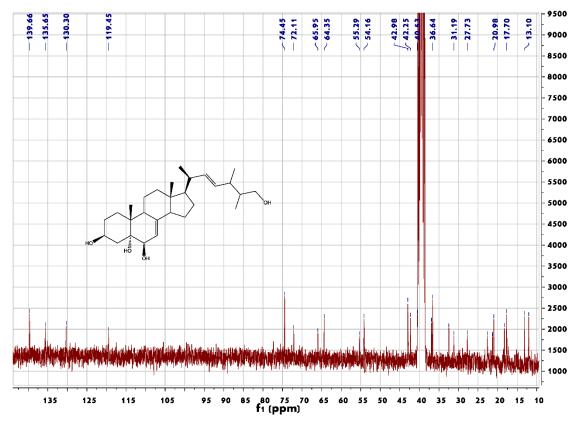


Figure S7. ¹³C-NMR spectrum of compound 1 (75 MHz in DMSO-d6).

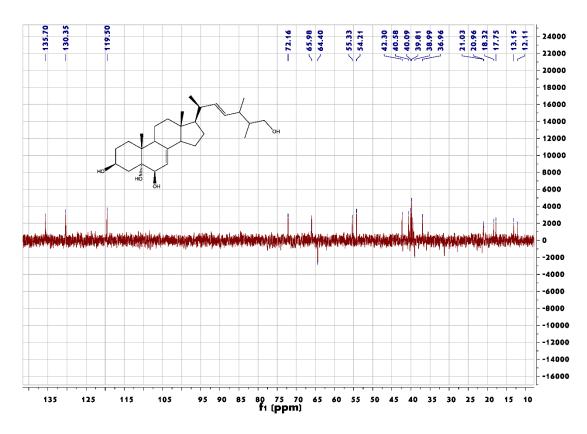


Figure S8. DEPT spectrum of compound 1 (75 MHz in DMSO-d6).

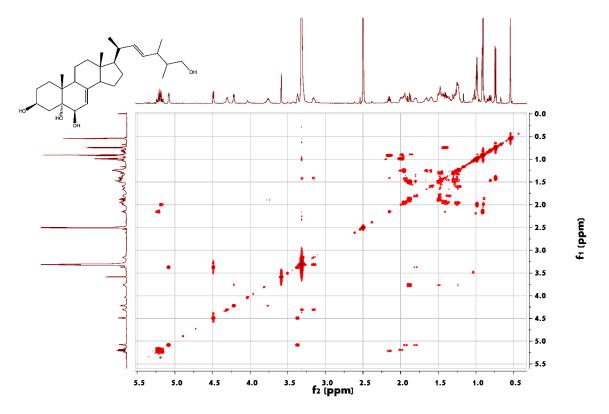


Figure S9. COSY spectrum of compound 1 (600 MHz in DMSO-*d*6).

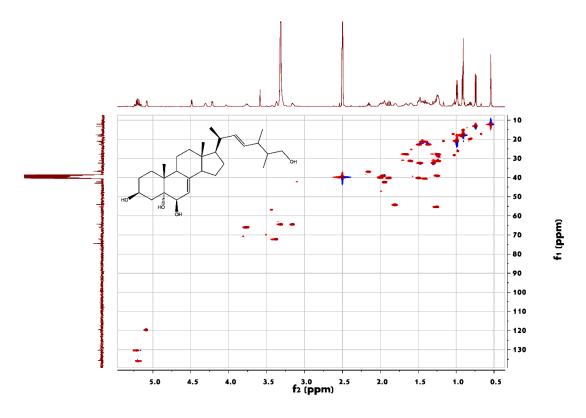


Figure S10. HMQC spectrum of compound 1 (600 MHz in DMSO-d6).

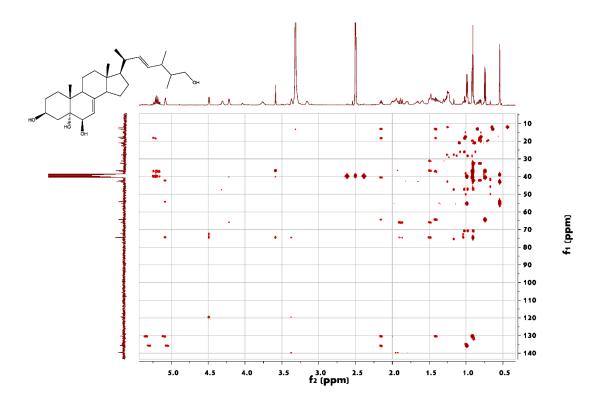


Figure S11. HMBC spectrum of compound 1 (600 MHz in DMSO-*d*6).

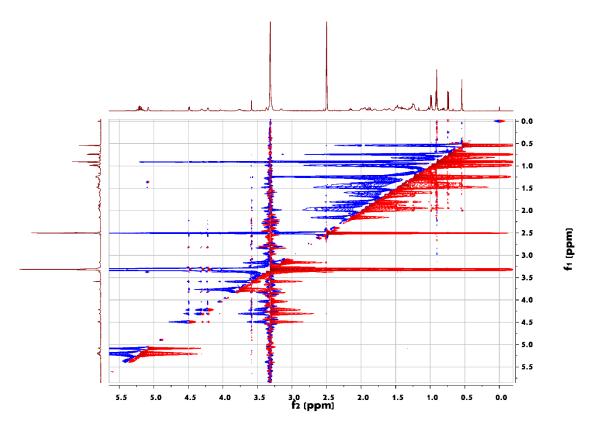


Figure S12. NOESY spectrum of compound 1 (600 MHz in DMSO-d6).

Compound 2

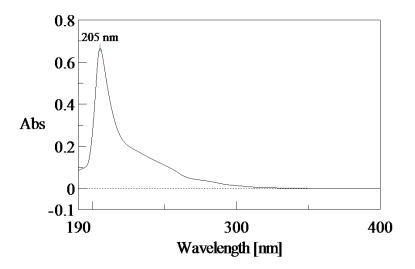


Figure S13. UV spectrum of compound 2 in MeOH.

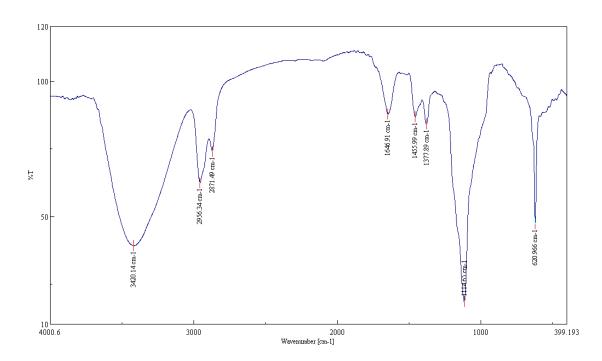


Figure S14. IR spectrum of compound 2.

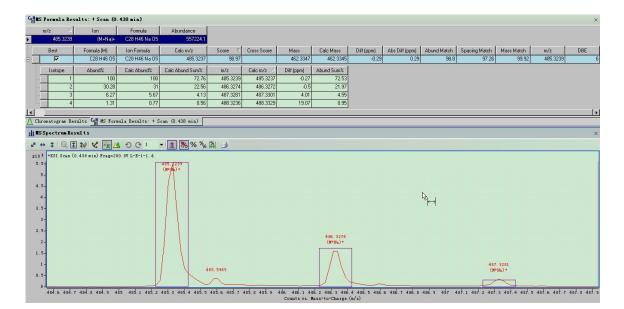


Figure S15. HR-MS of compound 2.

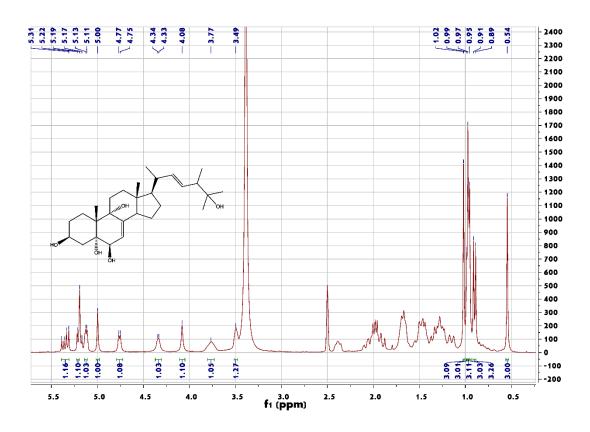


Figure S16. ¹H-NMR spectrum of compound 2 (300 MHz in DMSO-*d*6).

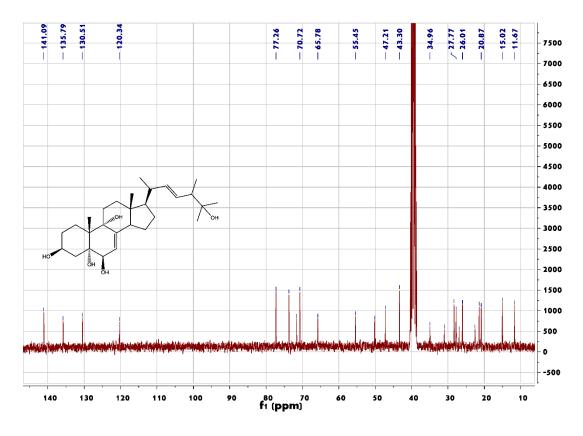


Figure S17. ¹³C-NMR spectrum of compound 2 (75 MHz in DMSO-d6).

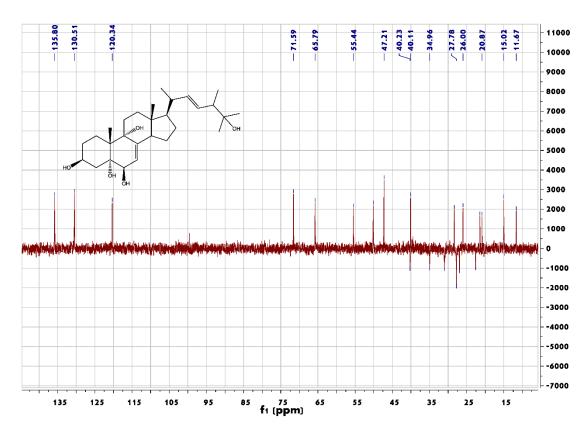


Figure S18. DEPT spectrum of compound 2 (75 MHz in DMSO-d6).

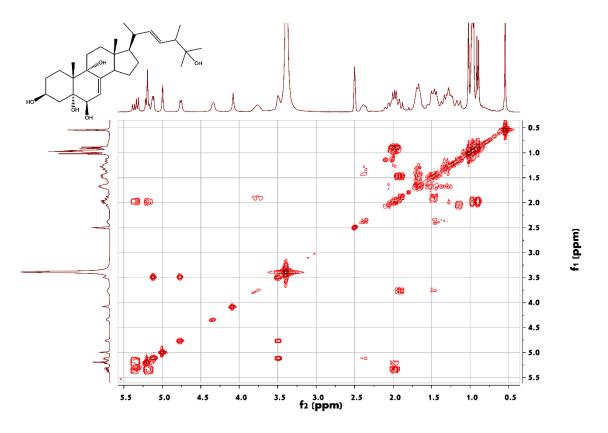


Figure S19. COSY spectrum of compound 2 (300 MHz in DMSO-*d*6).

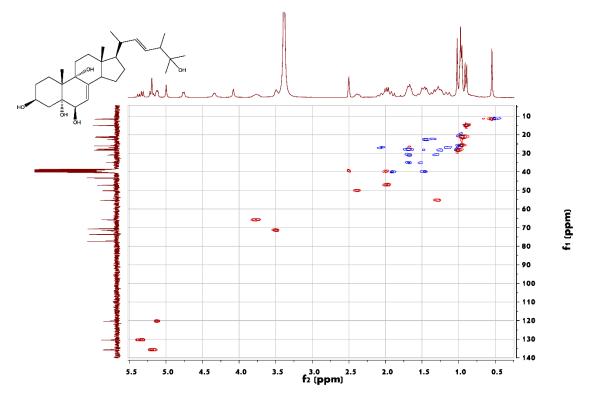


Figure S20. HMQC spectrum of compound 2 (300 MHz in DMSO-*d*6).

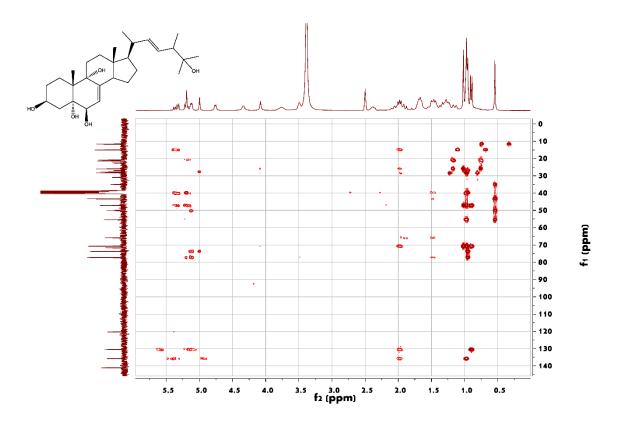


Figure S21. HMBC spectrum of compound 2 (300 MHz in DMSO-d6).

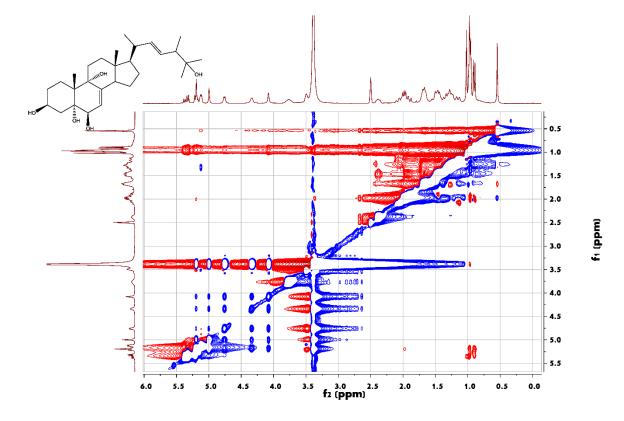


Figure S22. NOESY spectrum of compound 2 (300 MHz in DMSO-d6).

Compound 3

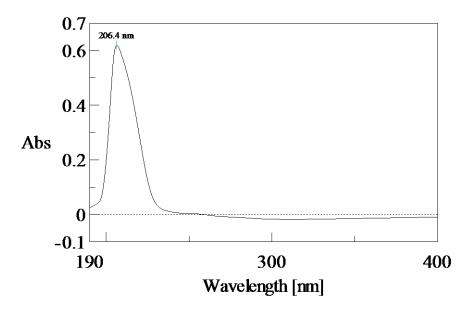


Figure S23. UV spectrum of compound 3 in MeOH.

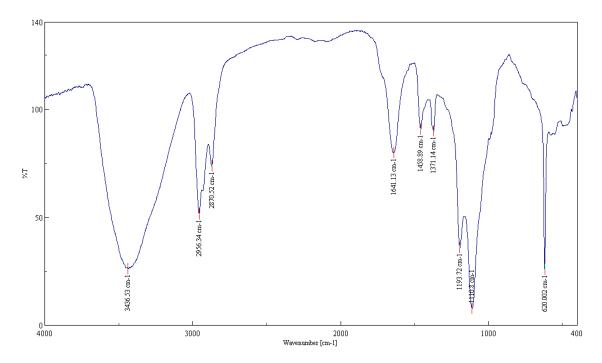


Figure S24. IR spectrum of compound 3.

	v/z ∆	lon	Formula	Abundance											
	451.3218	(M+Na)+	C28 H44 Na O3	63327.2											
	Best	Formula (M)	Ion Formula	Calc m/z	Score V	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DB
	N	C28 H44 O3	C28 H44 Na O3	451.3183	71.65		428.3326	428.329	-8.24	8.24	77.26	99.31	54.46	451.3218	
	Isotope	Abund%	Calc Abund%	Calc Abund Sum%	m/z	Calc m/z 🗠	Diff (ppm)	Abund Sum%							
	1	100	100		451.3218	451.3183	-7.8	73.74							
	2	26.21	30.9		452.3256	452.3217	-8.62	19.32							
	3	7.55	5.23		453.3287	453.3248	-8.54	5.57							
	4	1.85	0.63	0.46	454.3386	454.3277	-23.88	1.37							
U8															
	al colletor 10	\ Chronatogram Re	sults 📲 MS For	mula Results: + Sca	a (1.078 min)	1									
		-													
	pectrum Res														
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ss ⇔	pectrum Res]* V 🛧 🛛		• <u>1</u> % % %	× 3										
ss ⇔	pectrum Res]* V 🛧 🛛		• 🕕 🎘 % %	<u> </u>		451, 3218								
SS ↔ 3 ⁴ 8- 7-	pectrum Res]* V 🛧 🛛		• 🕕 🧞 % %	<u>a 3</u>		451.3218 (N*Na)+								
SS ↔ 4 8- 7-	pectrum Res]* V 🛧 🛛		• 🏦 🚴 % 🐁	<u>a s</u>		451. 3218 (#*Na)+								
SS ↔ 4 8- 7-	pectrum Res]* V 🛧 🛛		• 🕕 🚴 % 🗞	¥ 3		451.3218 (#*Ns)+								
SS ↔ 4 8- 7-	pectrum Res]* V 🛧 🛛		• 🕕 🚴 % 🍾	N 3		451, 3218 ()(+)(a) +								
ss ⇔	pectrum Res]* V 🛧 🛛		• 🕕 🧏 % 🗞	X 3		451. 3218 ()(+%)+								
SS ↔ 8- 7-	pectrum Res]* V 🛧 🛛		• 🕕 🎘 % 🐁	料 3		451. 3218 (te1%a)+								
SS ↔ 8- 7-	pectrum Res]* V 🛧 🛛		• <u>I</u> & % %	料 3		451.3218 ((te)%a)+	Γ							
SS ↔ 4 8- 7-	pectrum Res]* V 🛧 🛛		• 1 8% % %	A 3		451.3218 (X*Xs)+		Λ						

Figure S25. HR-MS of compound 3.

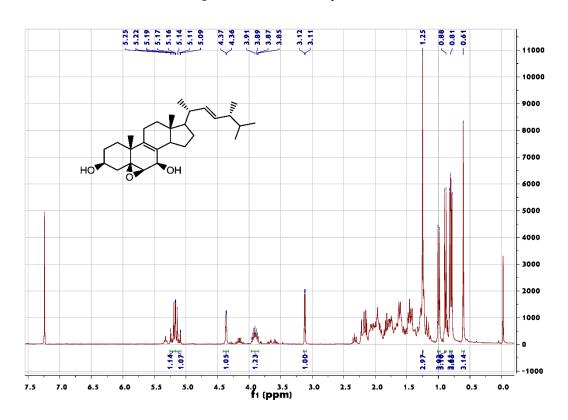


Figure S26. ¹H-NMR spectrum of compound 3 (300 MHz in CDCl3).

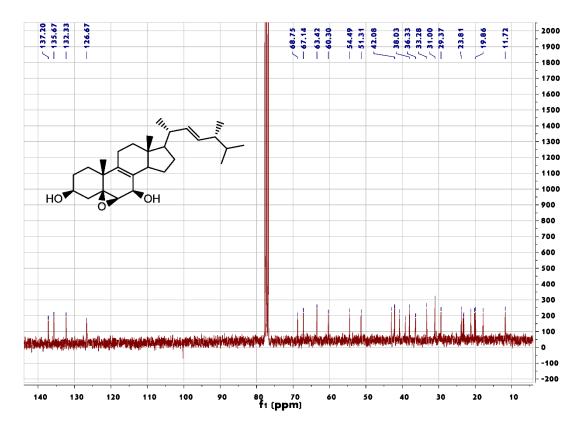


Figure S27. ¹³C-NMR spectrum of compound 3 (75 MHz in CDCl3).

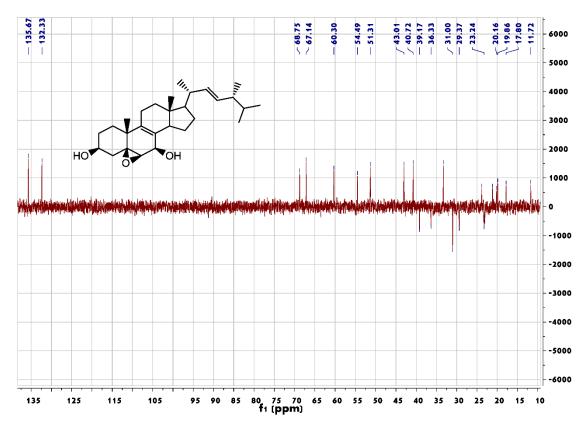


Figure S28. DEPT spectrum of compound 3 (75 MHz in CDCl3).

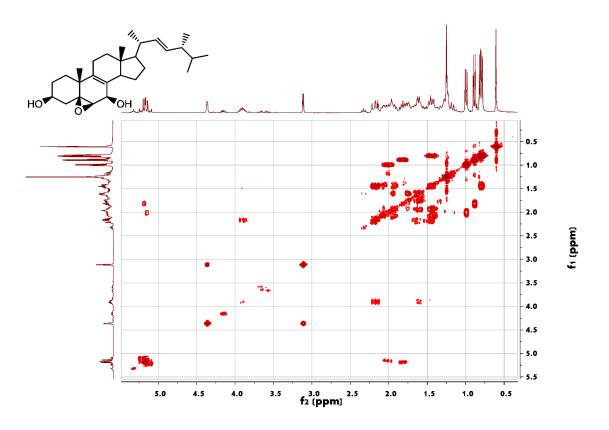


Figure S29. COSY spectrum of compound 3 (300 MHz in CDCl3).

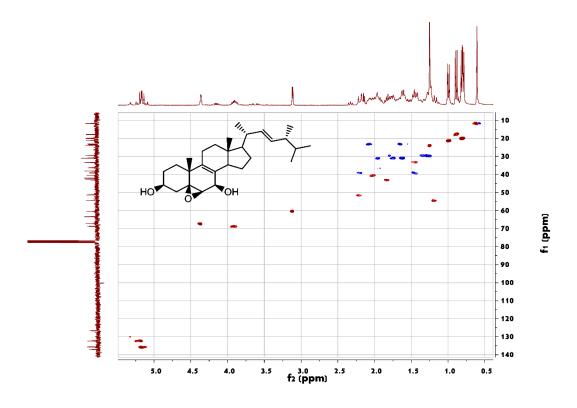


Figure S30. HMQC spectrum of compound 3 (300 MHz in CDCl3).

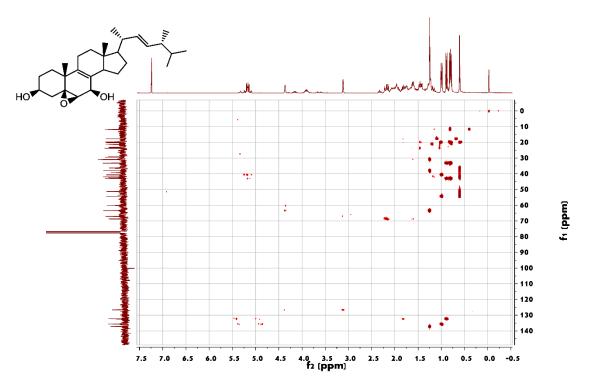


Figure S31. HMBC spectrum of compound 3 (300 MHz in CDCl3).

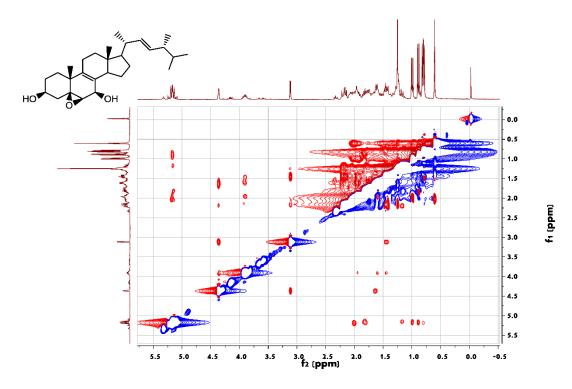


Figure S32. NOESY spectrum of compound 3 (300 MHz in CDCl3).

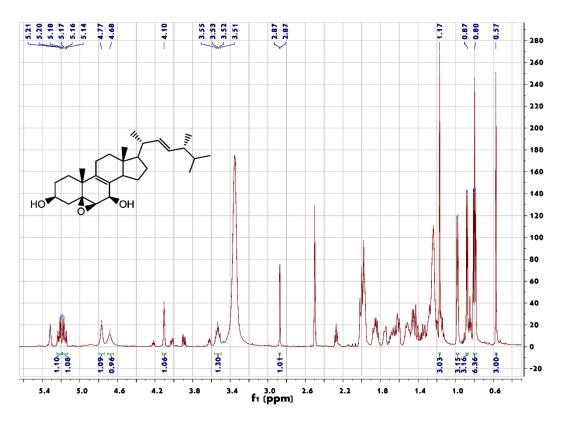


Figure S33. 1H-NMR spectrum of compound 3 (600 MHz in DMSO-d6).

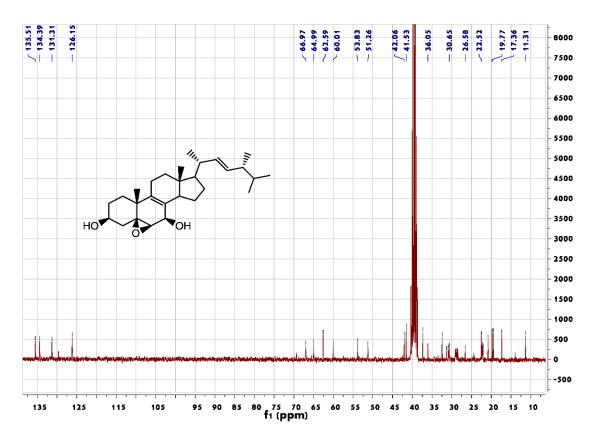


Figure S34. ¹³C-NMR spectrum of compound 3 (150 MHz in DMSO-d6).

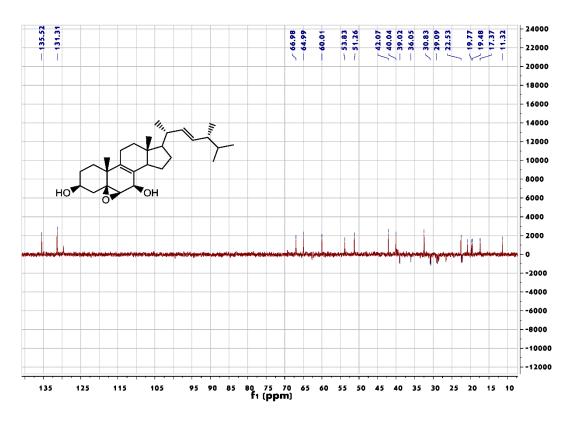


Figure S35. DEPT spectrum of compound 3 (150 MHz in DMSO-d6).

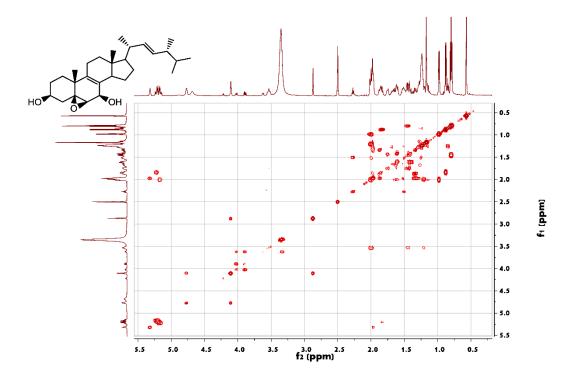


Figure S36. COSY spectrum of compound 3 (600 MHz in DMSO-d6).



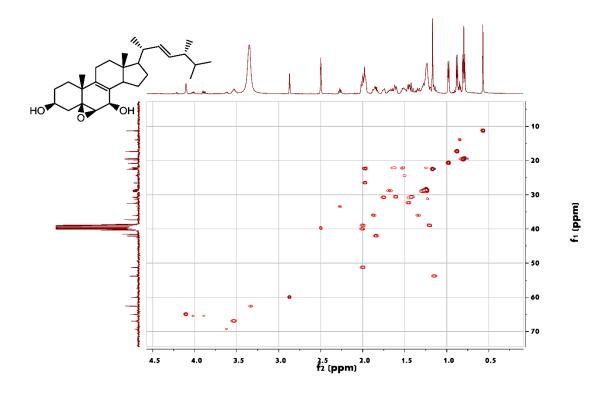


Figure S37. HMQC spectrum of compound 3 (600 MHz in DMSO-d6).

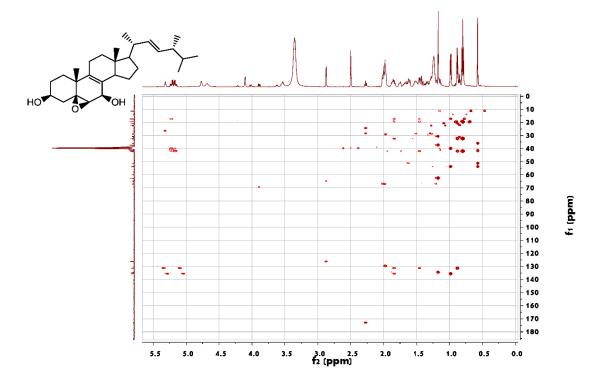


Figure S38. HMBC spectrum of compound 3 (600 MHz in DMSO-d6).

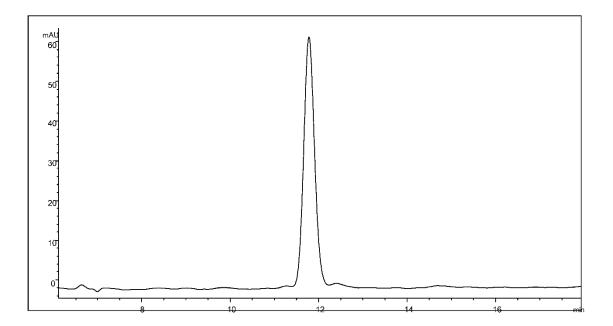


Figure S39. HPLC profile of compound $\,1\,(80\%$ MeOH at 210 nm).

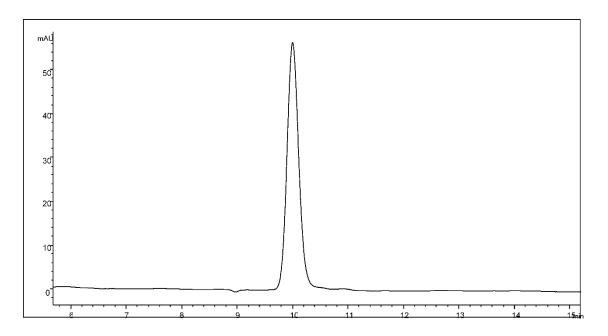


Figure S40. HPLC profile of compound 2 (75% MeOH at 210 nm).

mAU

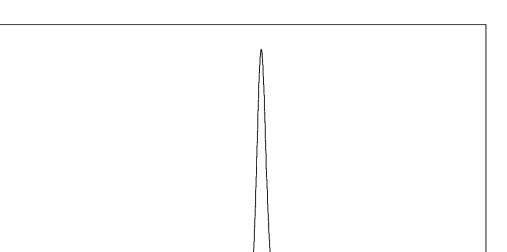


Figure S41. HPLC profile of compound $\ 3$ (90% MeOH at 210 nm).

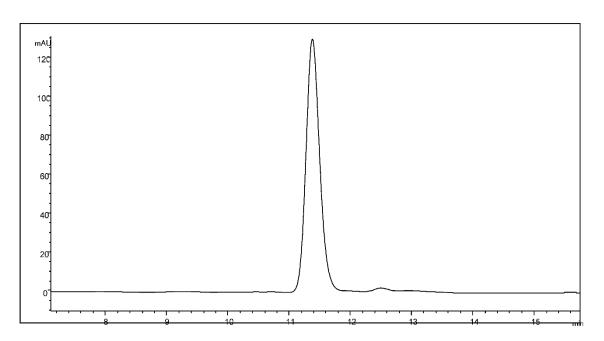


Figure S42. HPLC profile of compound 4 (80% MeOH at 210 nm).

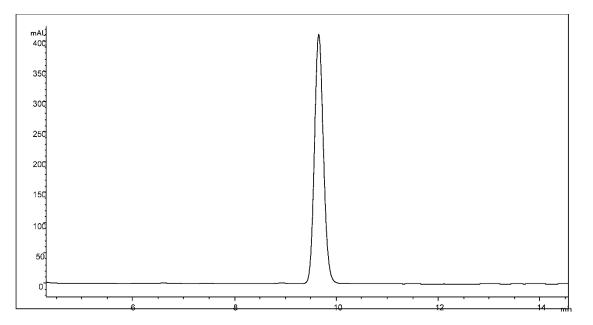


Figure S43. HPLC profile of compound 5 (95% MeOH at 210 nm).

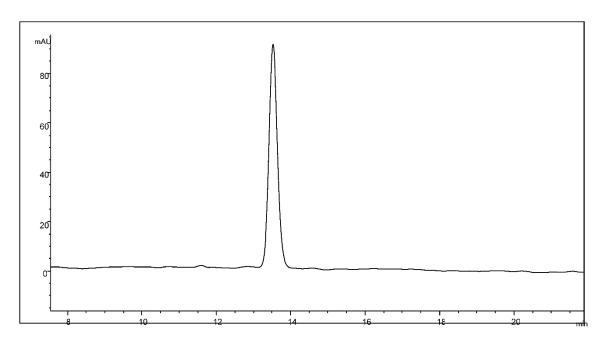


Figure S44. HPLC profile of compound 6 (95% MeOH at 210 nm).

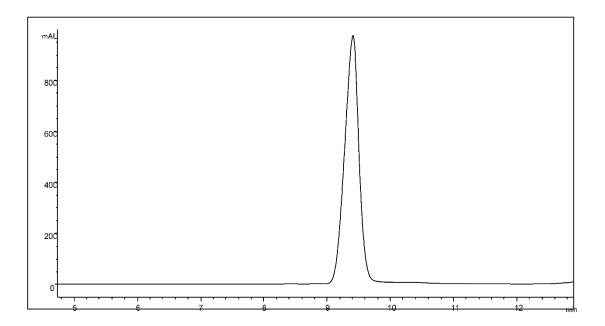


Figure S45. HPLC profile of compound 7 (90% MeOH at 210 nm).

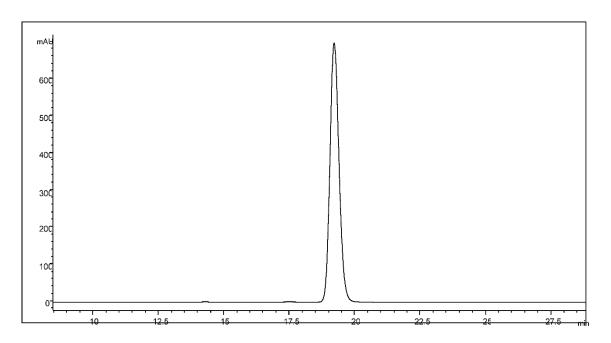


Figure S46. HPLC profile of compound 8 (80% MeOH at 210 nm).

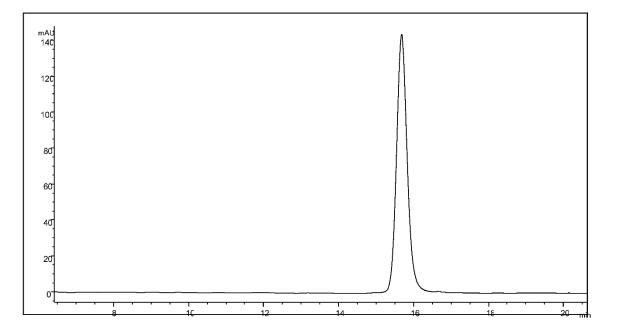


Figure S47. HPLC profile of compound $\,11$ (90% MeOH at 210 nm).

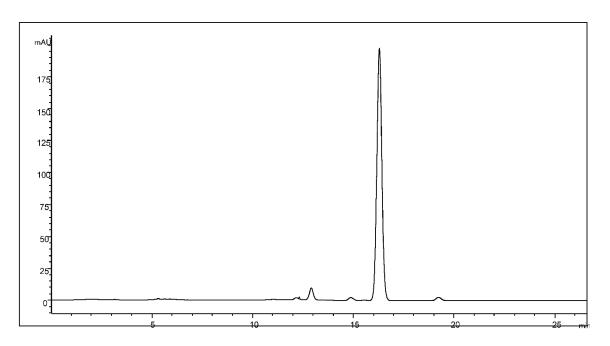


Figure S48. HPLC profile of compound 12 (100% MeOH at 280 nm).



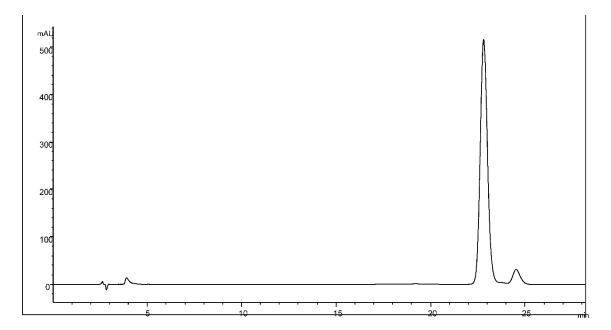


Figure S49. HPLC profile of compound 13 (90% MeOH at 210nm).

Compounds	Retention Time (min)	Purity	Wavelength
1	11.773	97.60%	210
2	10.004	98.97%	210
3	19.003	99.00%	210
4	11.376	96.805%	210
5	9.657	99.09%	210
6	13.524	99.12%	210
7	9.406	93.57%	210
8	19.227	98.87%	210
11	15.686	98.07%	210
12	15.803	97.893	280
13	22.797	93.774	210

				01.01		(0) 01 1 10	, (10 IVII IZ)			
No.	4 a	5 a	6 a,*	7 ^a	8 ^b	9ь	10 a,*	11 a,*	12 ^b	13 ^b
1	31.2	31.2	31.4	26.9	30.4	31.1	30.7	31.7	38.6	31.4
2	32.5	32.5	30.9	31.0	31.0	32.2	31.0	31	32.0	33.2
3	65.9	66.0	65.6	65.8	68.8	68.7	65.1	65.1	70.7	68.9
4	40.2	40.0	39.2	40.2	39.3	39.6	40.5	40.9	41.0	39.5
5	74.5	74.5	74.5	73.7	65.9	67.8	74.5	76.3	140.0	65.1
6	72.1	72.2	69.1	71.6	62.8	61.3	77.9	76.0	116.5	60.5
7	119.5	119.5	120.6	120.3	67.0	65.1	71.6	71.6	119.8	63.9
8	139.7	139.7	139.7	141.1	127.1	125.2	127.2	127.0	141.6	126.9
9	42.3	42.3	42.6	77.3	134.7	38.7	136.2	36.4	46.3	39.8
10	36.7	36.6	38.1	40.0	38.2	35.8	40.2	39.8	37.2	34.9
11	27.7	21.3	20.6	26.9	23.6	19.0	23.0	18.8	21.3	19.5
12	39.0	38.9	38.9	35.0	35.9	36.6	35.9	36.6	39.3	37.3
13	43.0	43.0	43.1	43.3	42.3	42.9	41.3	42.4	43.0	43.8
14	54.2	54.2	54.2	50.1	49.8	152.5	49.4	147.6	54.6	151.9
15	22.6	22.6	22.4	22.6	24.1	24.9	28.6	24.7	23.2	26.1
16	27.7	27.8	27.9	27.8	29.2	27.2	22.7	27.2	28.5	28.2
17	55.3	55.3	55.2	55.4	53.8	56.8	53.9	56.0	55.8	55.6
18	12.1	12.0	12.0	11.7	11.5	17.6	11.2	18.0	12.3	17.9
19	17.7	17.7	17.4	21.4	23.0	16.5	22.9	17.5	16.5	17.1
20	40.1	40.0	39.8	39.8	40.6	39.3	40.0	38.5	42.9	40.6
21	20.9	21	21	21.0	21.2	21.2	20.9	21.2	21.3	21.3
22	135.7	135.4	135.4	135.5	135.8	135.3	135.5	135.5	135.8	135.4
23	130.5	131.4	131.4	131.4	132.2	132.2	131.3	131.5	132.2	132.5
24	47.2	42.0	41.9	42.1	43.0	42.8	42.1	42.1	40.4	43.1
25	70.7	32.5	32.5	32.5	33.3	33.1	32.5	32.5	33.3	33.3
26	26.0	19.5	19.5	19.5	19.9	19.7	19.5	19.5	19.9	19.9
27	28.3	19.8	19.8	19.8	20.2	20.0	19.8	19.8	20.2	20.2
28	15.0	17.3	17.3	17.4	17.9	18.1	17.4	17.4	17.8	17.9

Table S2. 13 C-NMR data (δ) of 4–13 (75 MHz).

^a Measured in DMSO-d6; ^b Measured in CDCl3; * Measured in solvent different from literature.