SUPPORTING INFORMATION

Calabanones A–H, chromanone derivatives from the stem bark of *Calophyllum calaba* and their cytotoxic activities against cancer cells

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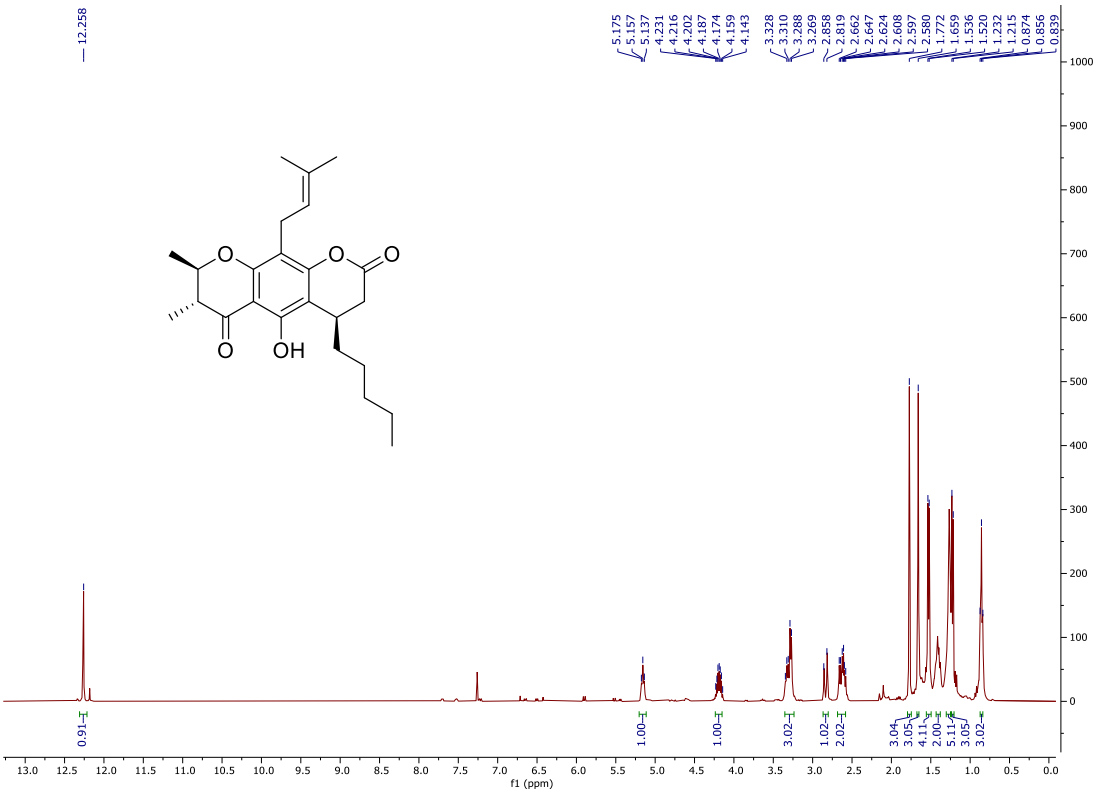

Figure S1. ^{1}H NMR spectrum of compound **1** in $CDCl_3$

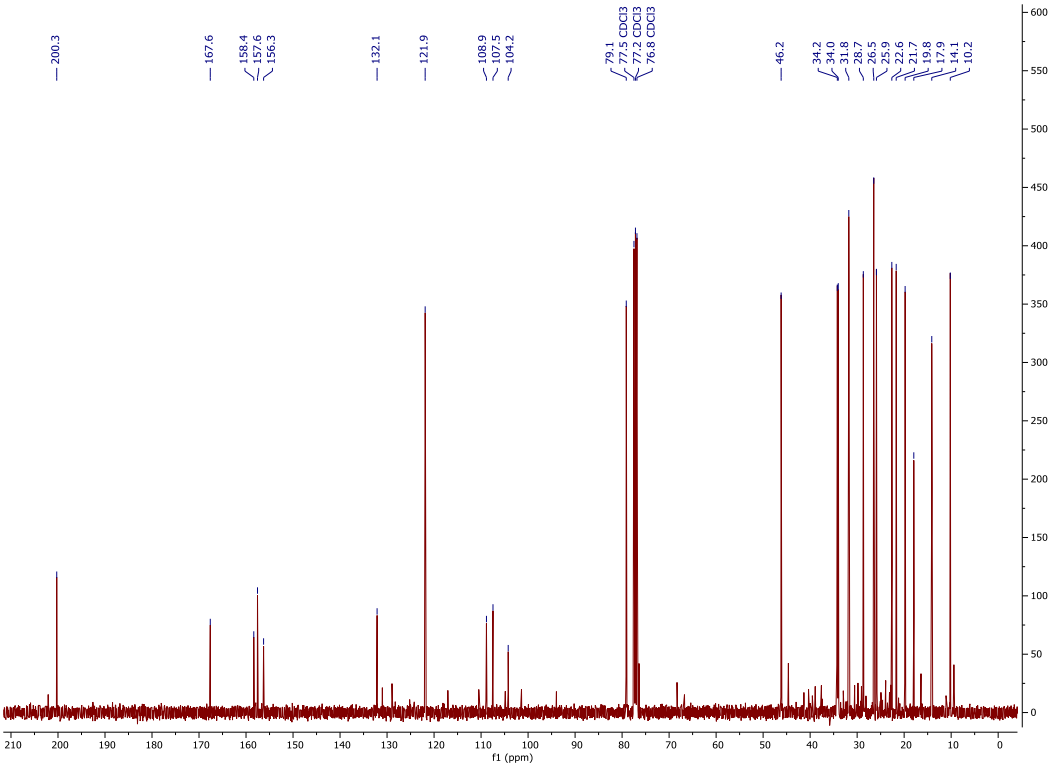

Figure S2. ^{13}C NMR spectrum of compound **1** in $CDCl_3$

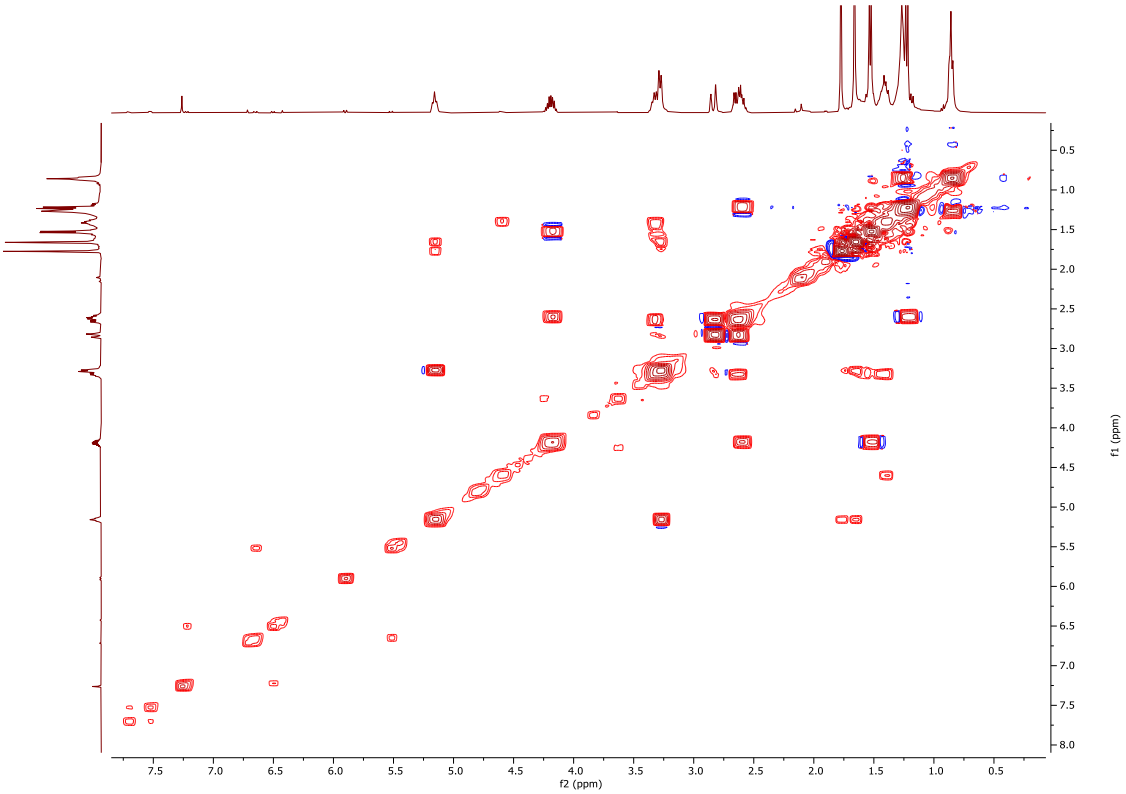

Figure S3. COSY spectrum of compound **1** in $CDCl_3$

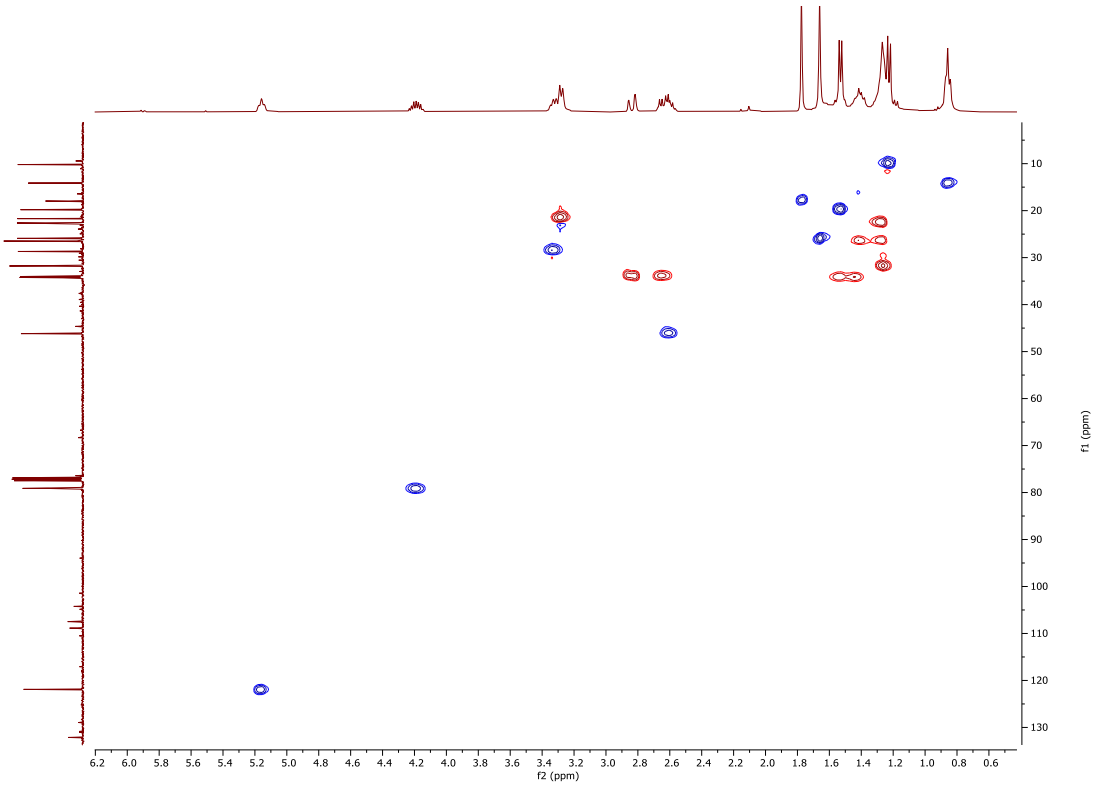

Figure S4. HSQC spectrum of compound **1** in $CDCl_3$

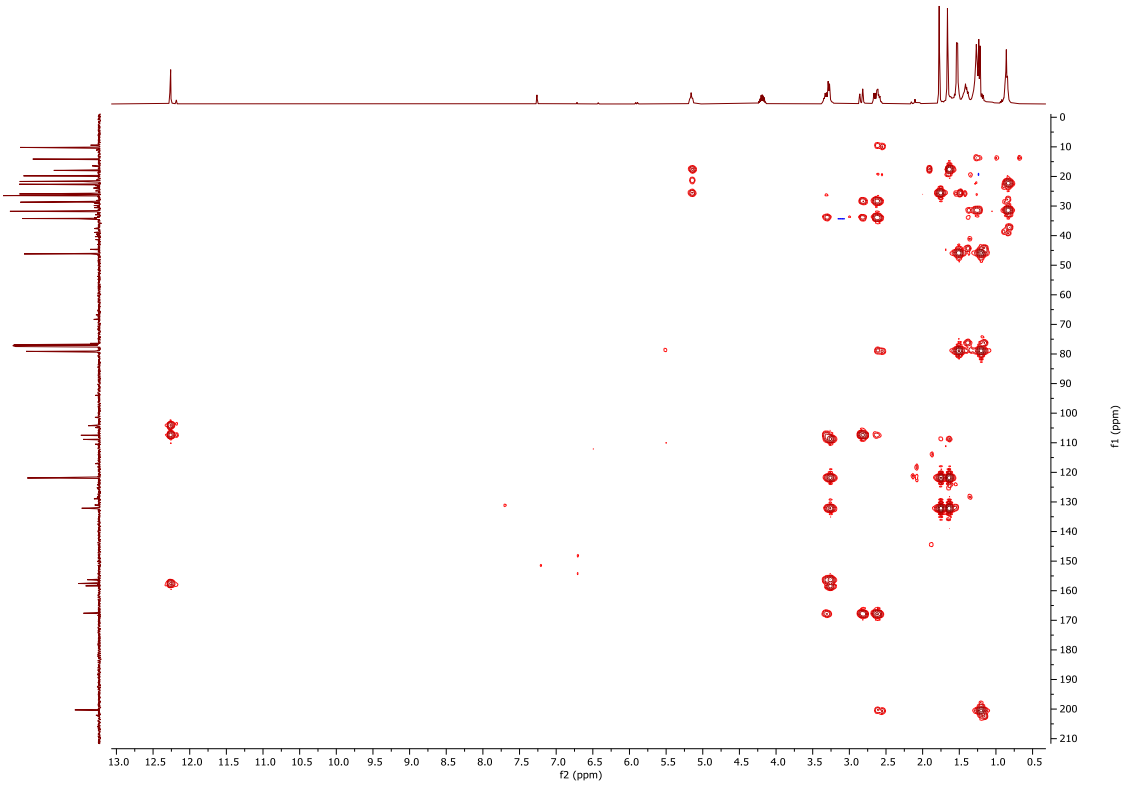

Figure S5. HMBC spectrum of compound **1** in $CDCl_3$

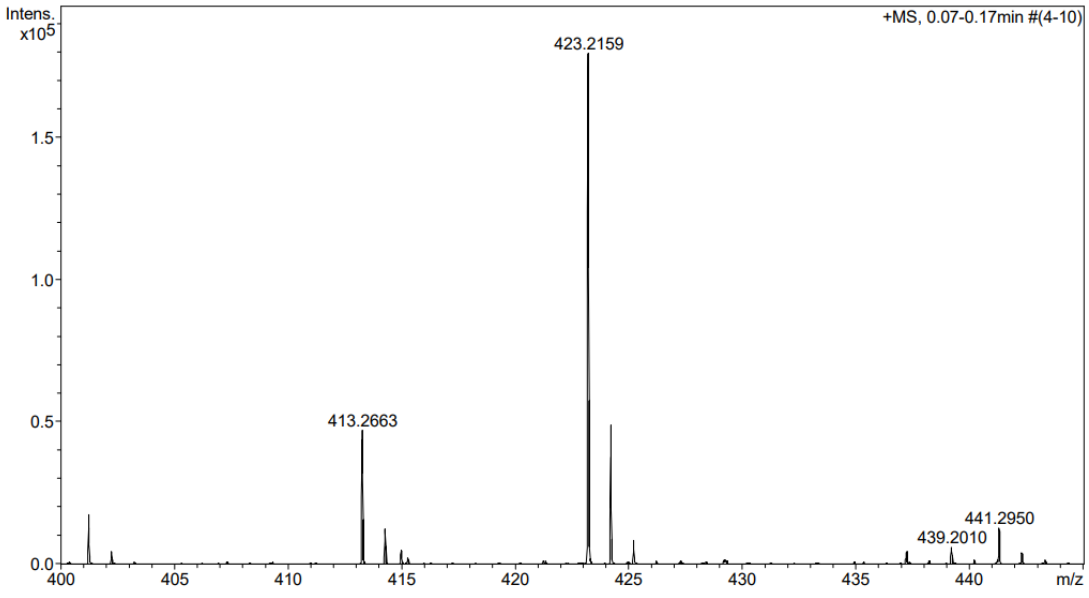

Figure S6. HRESIMS spectrum of compound **1** in MeCN

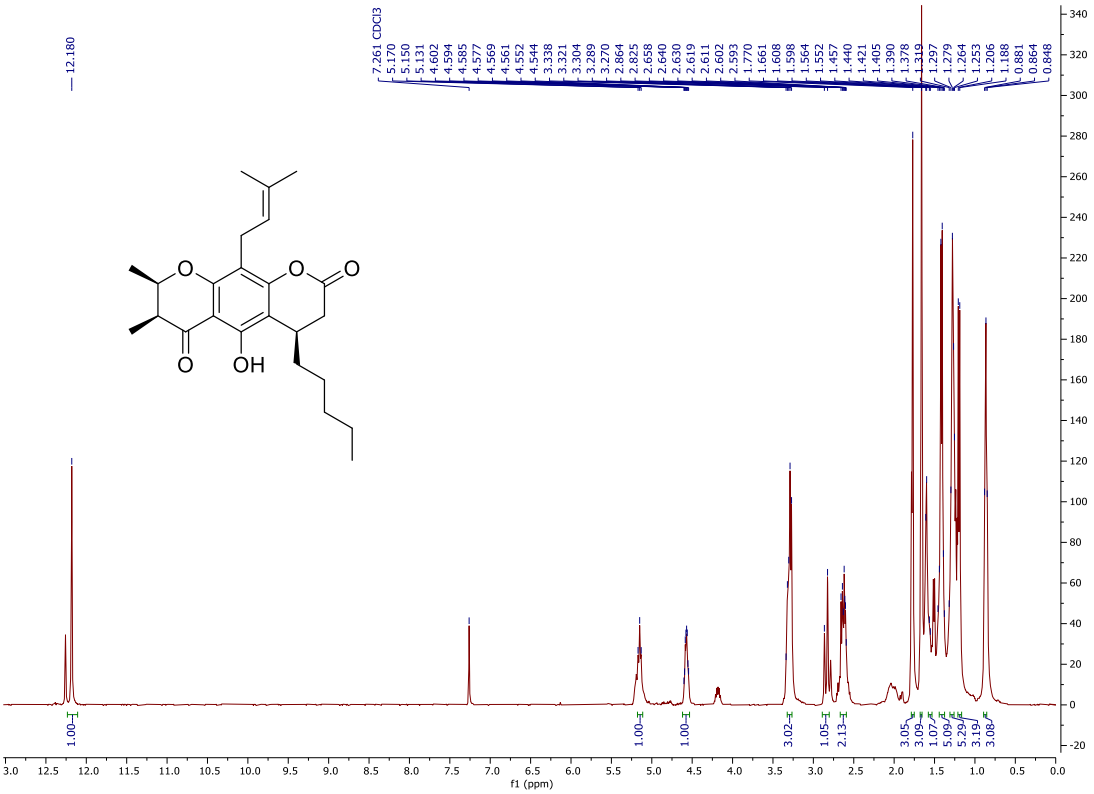

Figure S7. ^{1}H NMR spectrum of compound **2** in $CDCl_3$

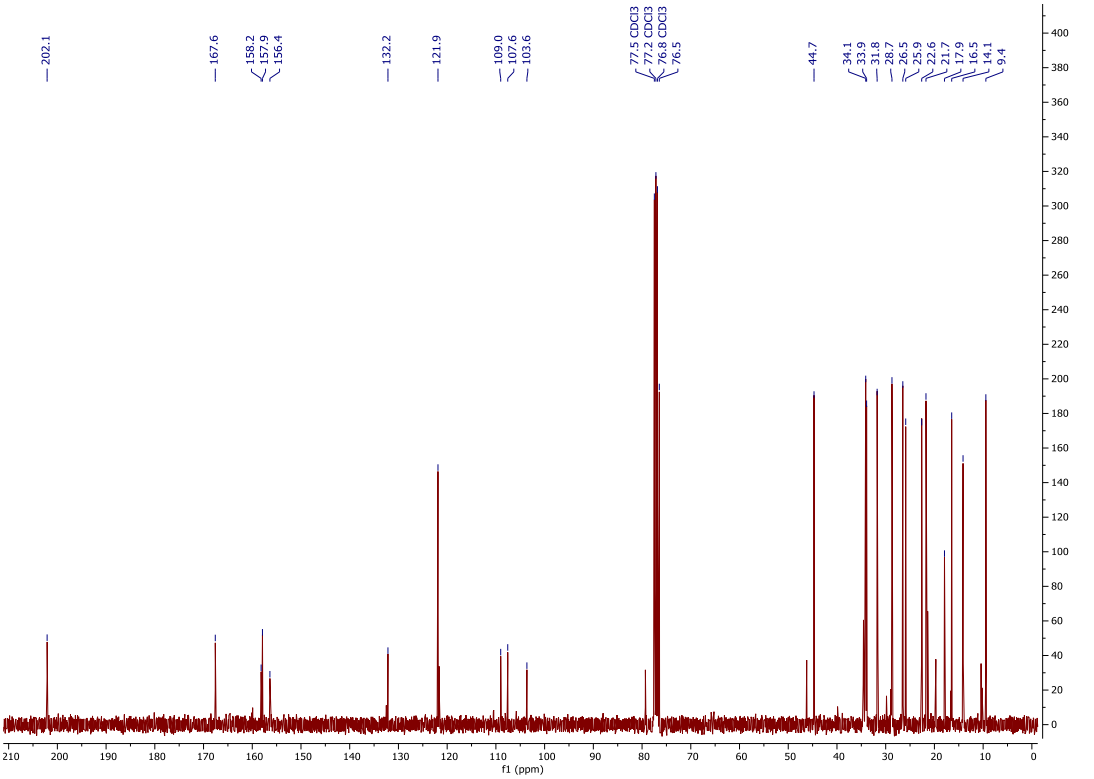

Figure S8. ^{13}C NMR spectrum of compound **2** in $CDCl_3$

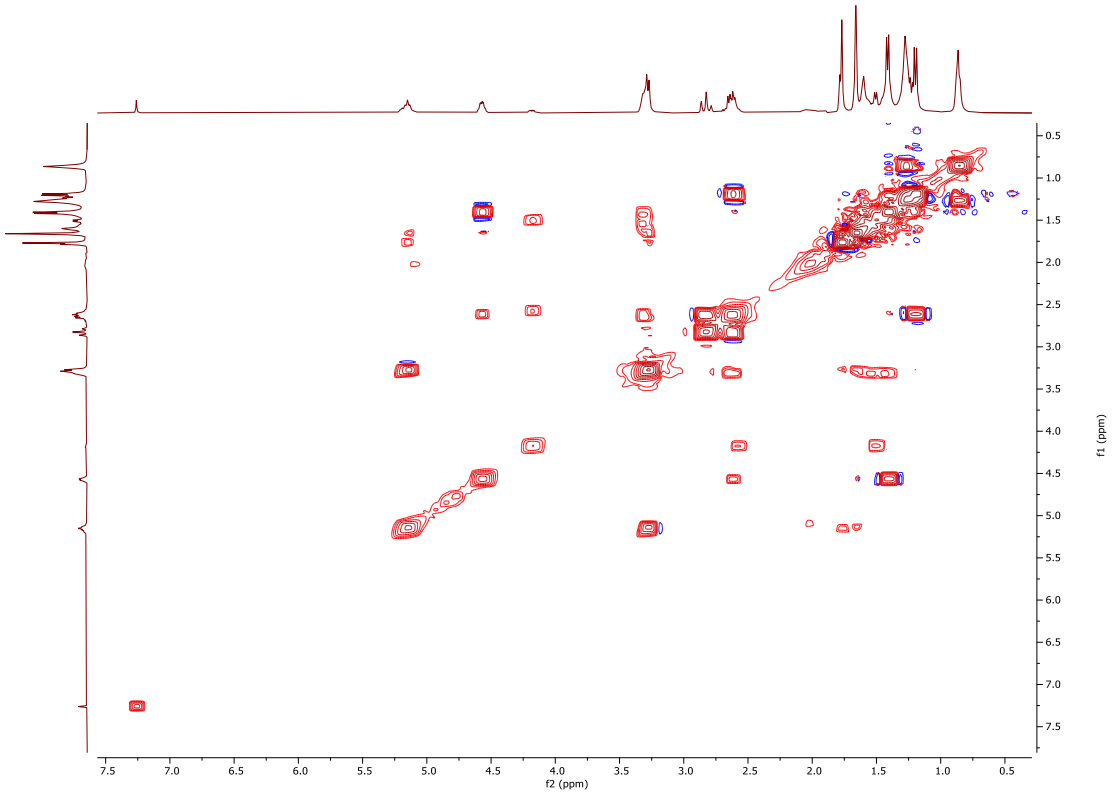

Figure S9. COSY spectrum of compound **2** in $CDCl_3$

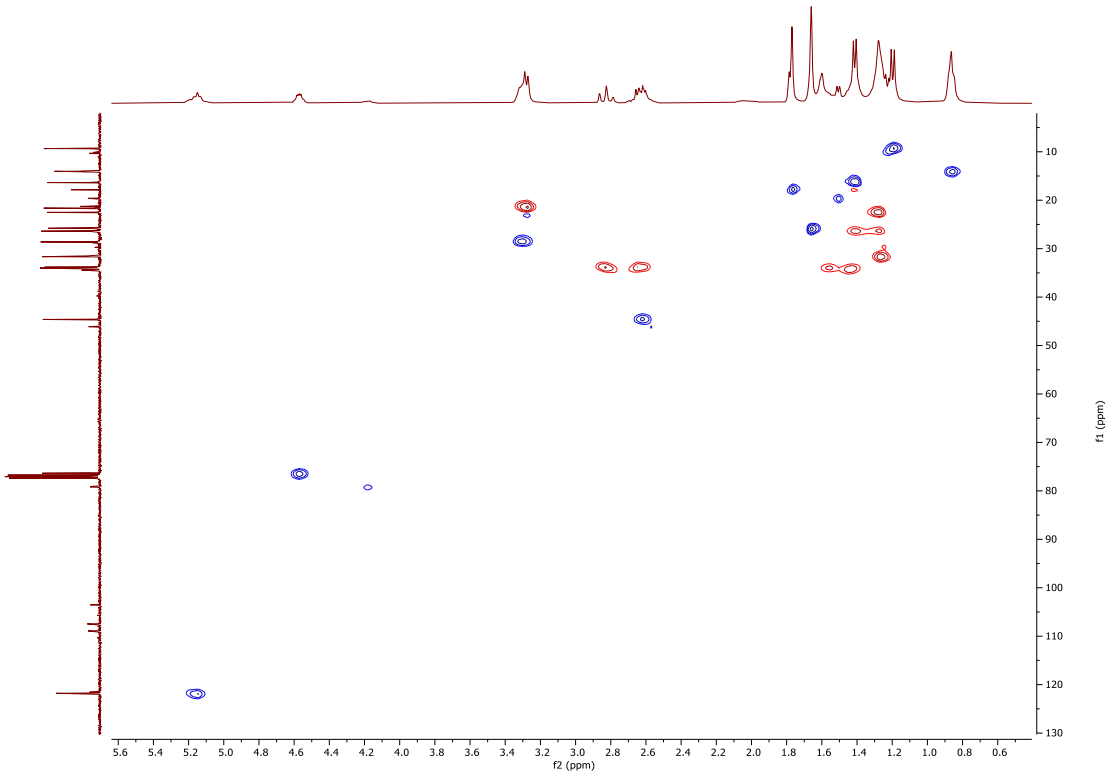

Figure S10. HSQC spectrum of compound **2** in $CDCl_3$

Figure S11. HMBC spectrum of compound **2** in $CDCl_3$

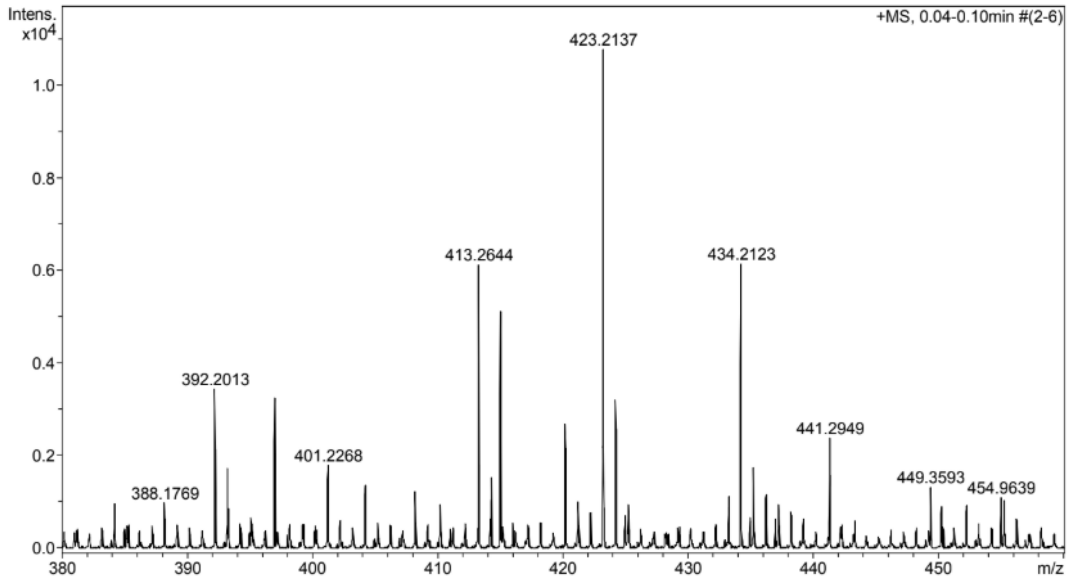

Figure S12. HRESIMS spectrum of compound **2** in MeCN

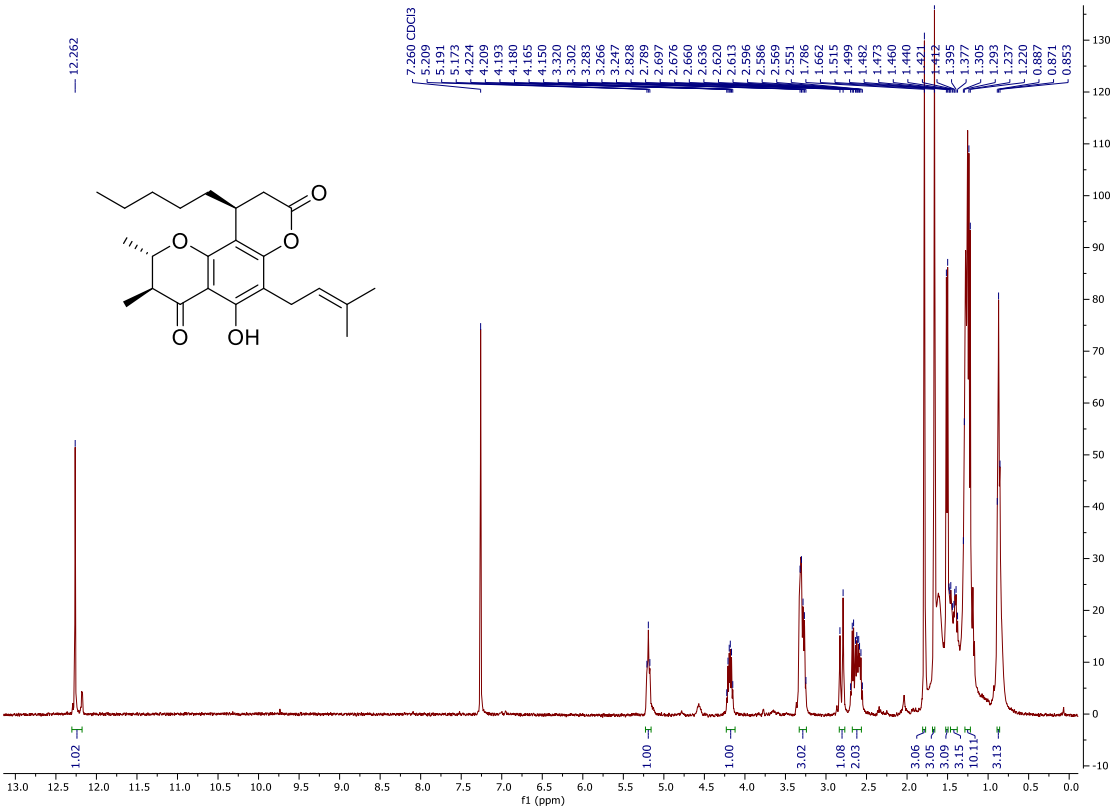

Figure S13. ^{1}H NMR spectrum of compound **3** in $CDCl_3$

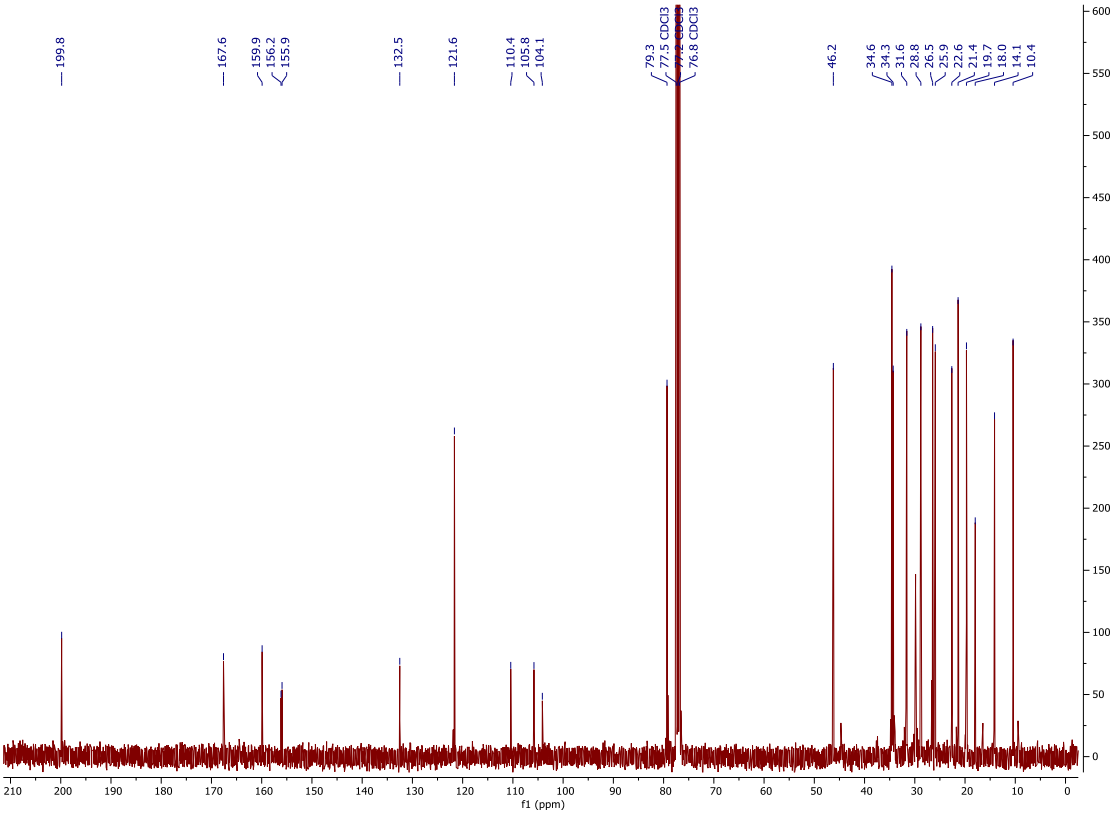

Figure S14. ^{13}C NMR spectrum of compound **3** in CDCl3

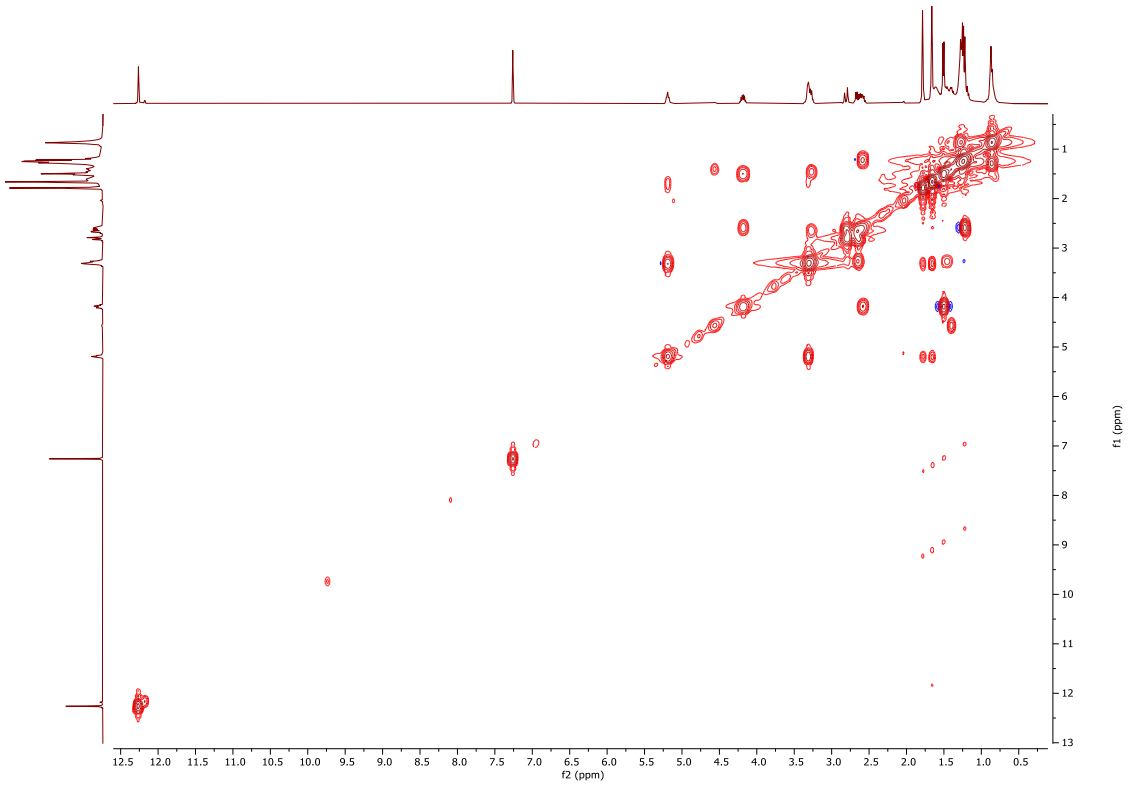

Figure S15. COSY spectrum of compound **3** in $CDCl_3$

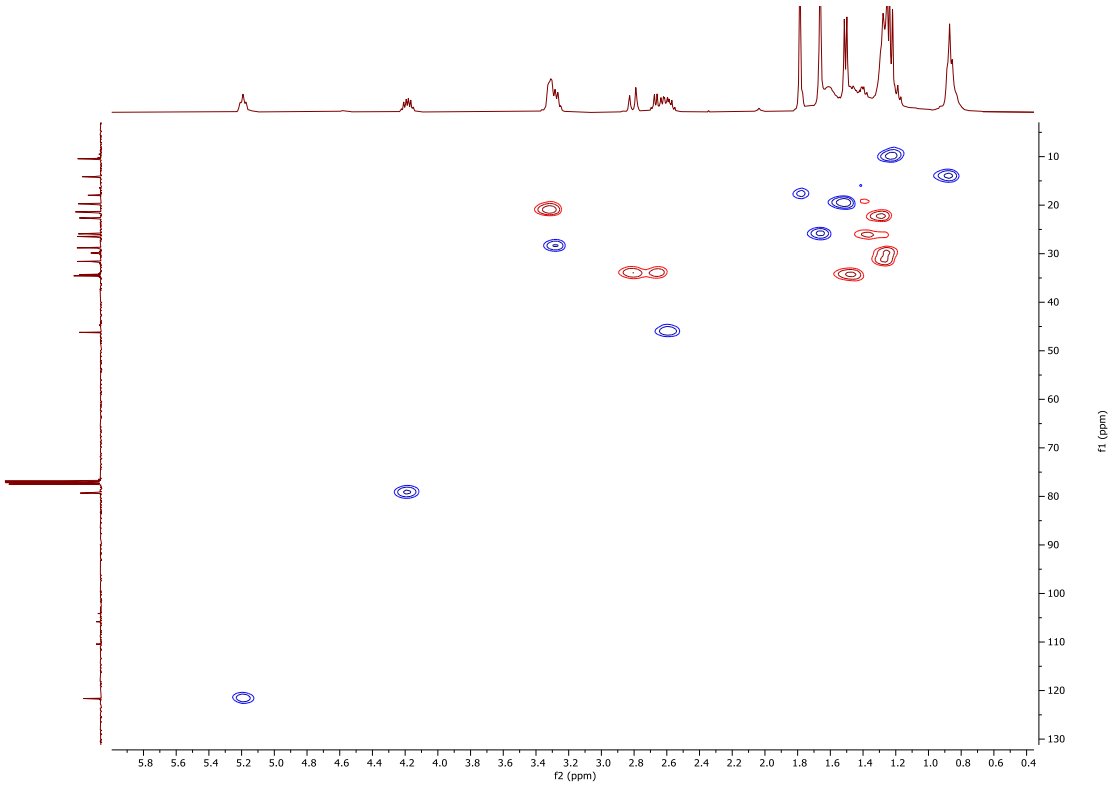

Figure S16. HSQC spectrum of compound **3** in $CDCl_3$

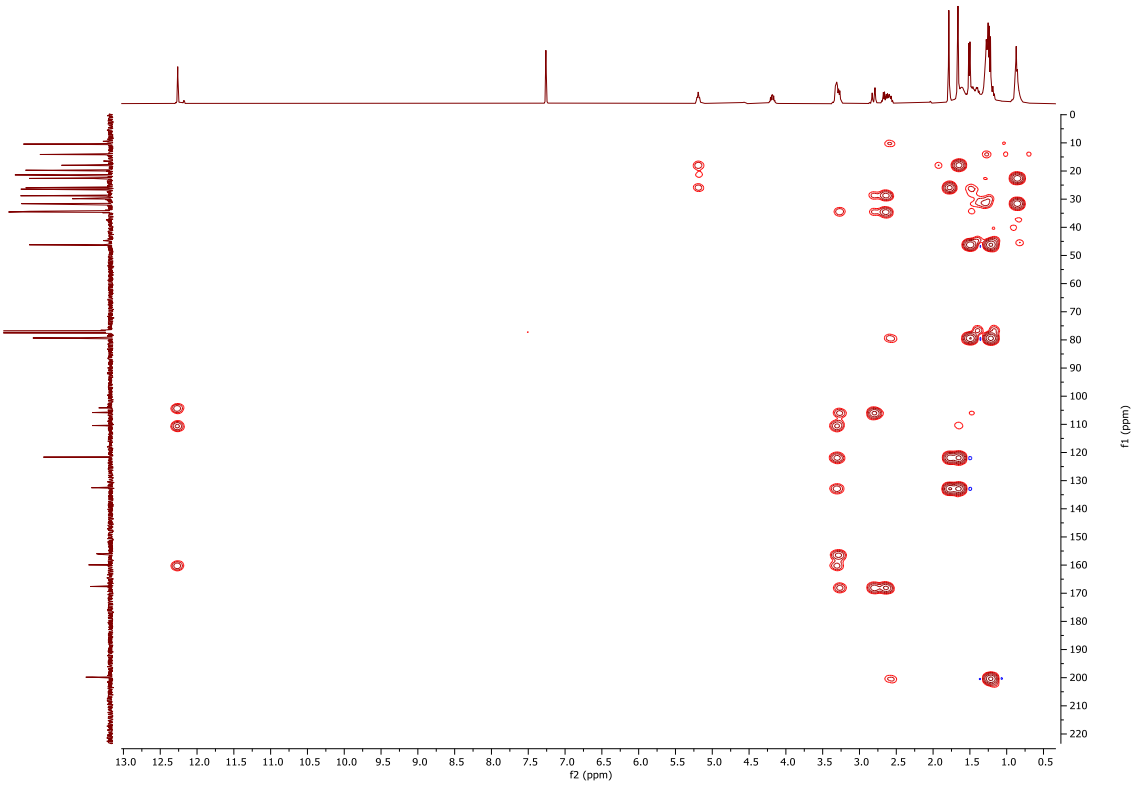

Figure S17. HMBC spectrum of compound **3** in $CDCl_3$

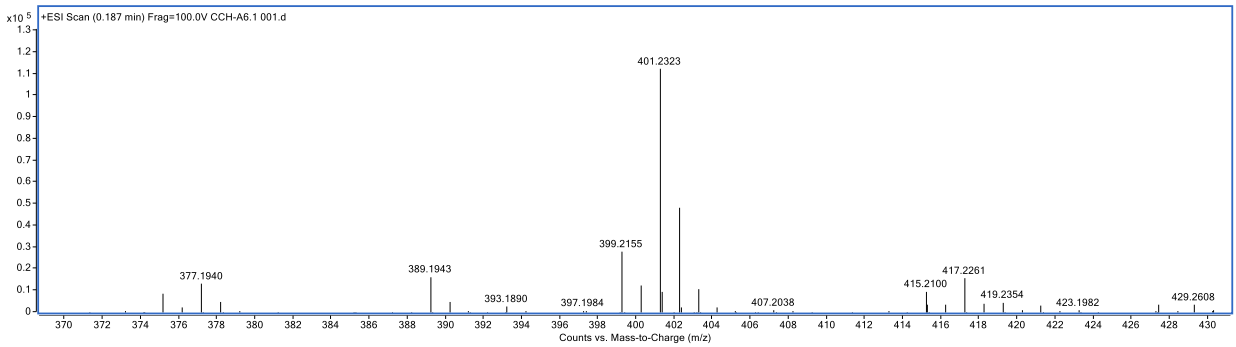

Figure S18. HRESIMS spectrum of compound **3** in MeCN

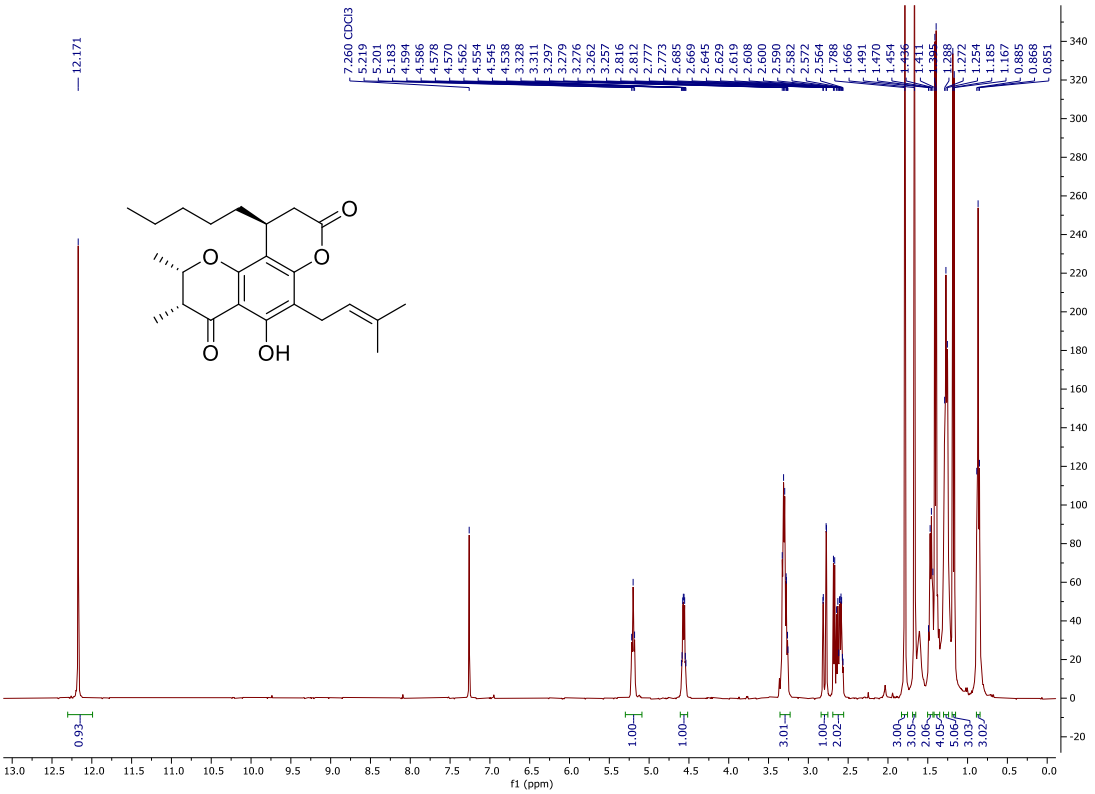

Figure S19. ^{1}H NMR spectrum of compound **4** in $CDCl_3$

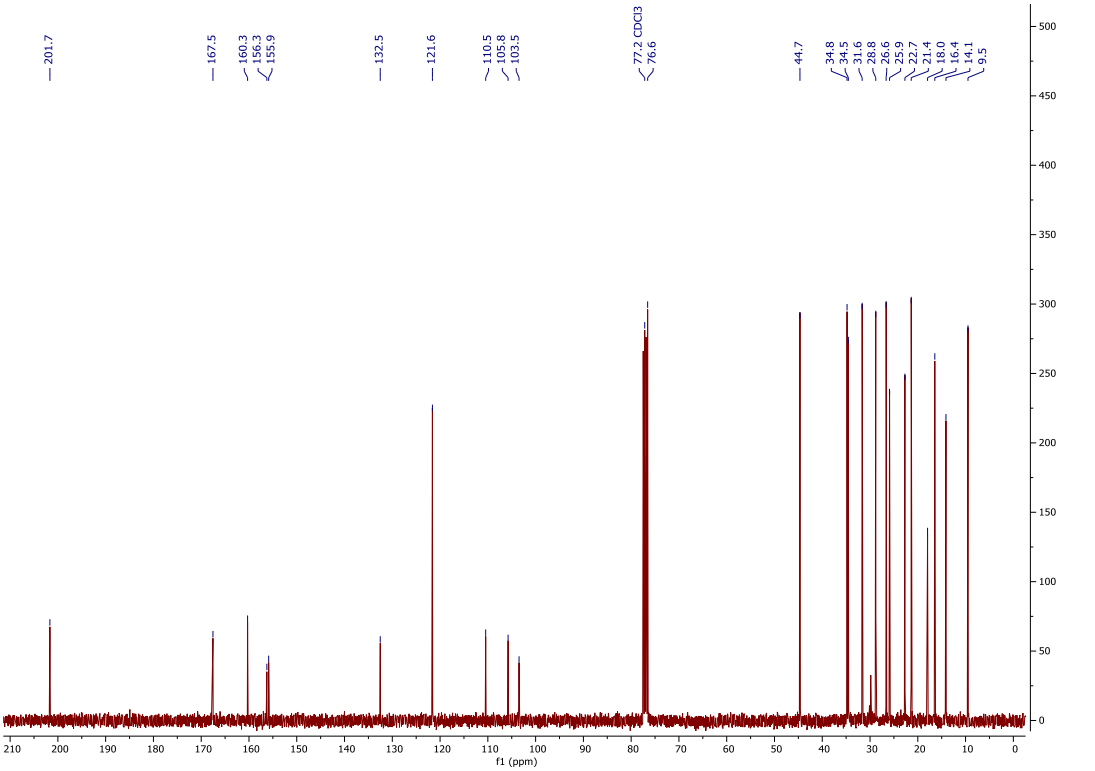

Figure S20. ^{13}C NMR spectrum of compound **4** in $CDCl_3$

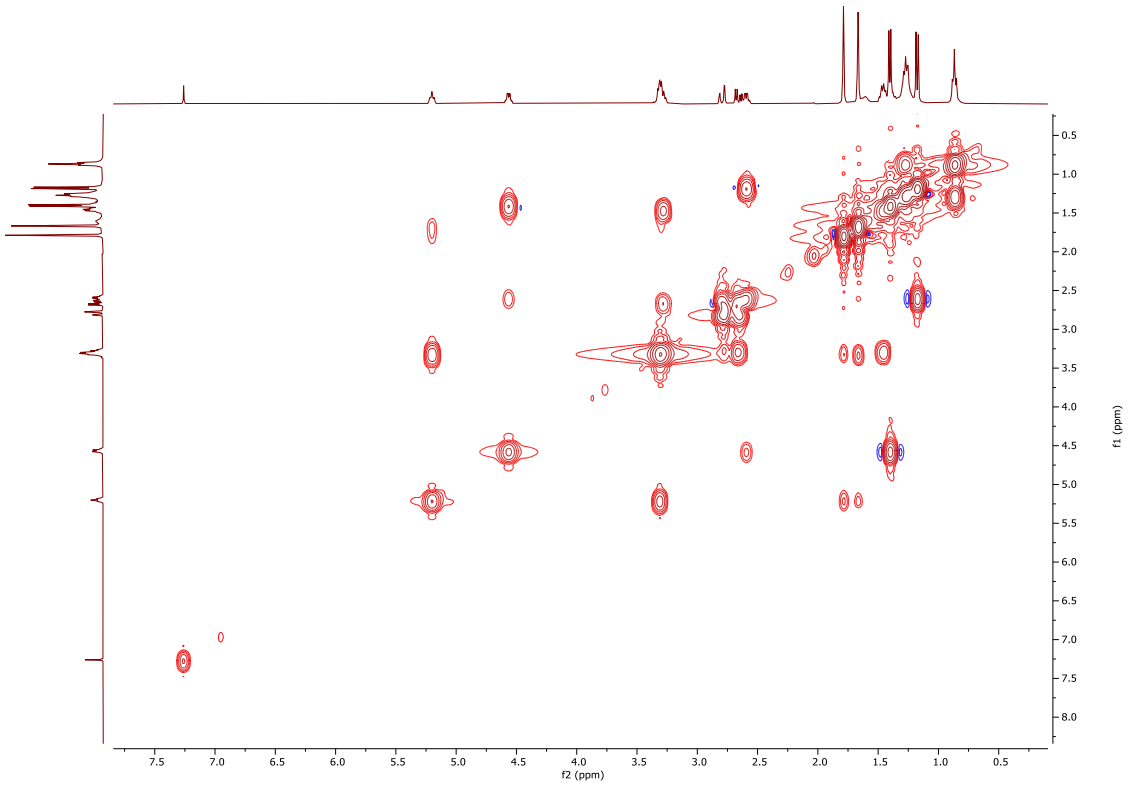

Figure S21. COSY spectrum of compound **4** in $CDCl_3$

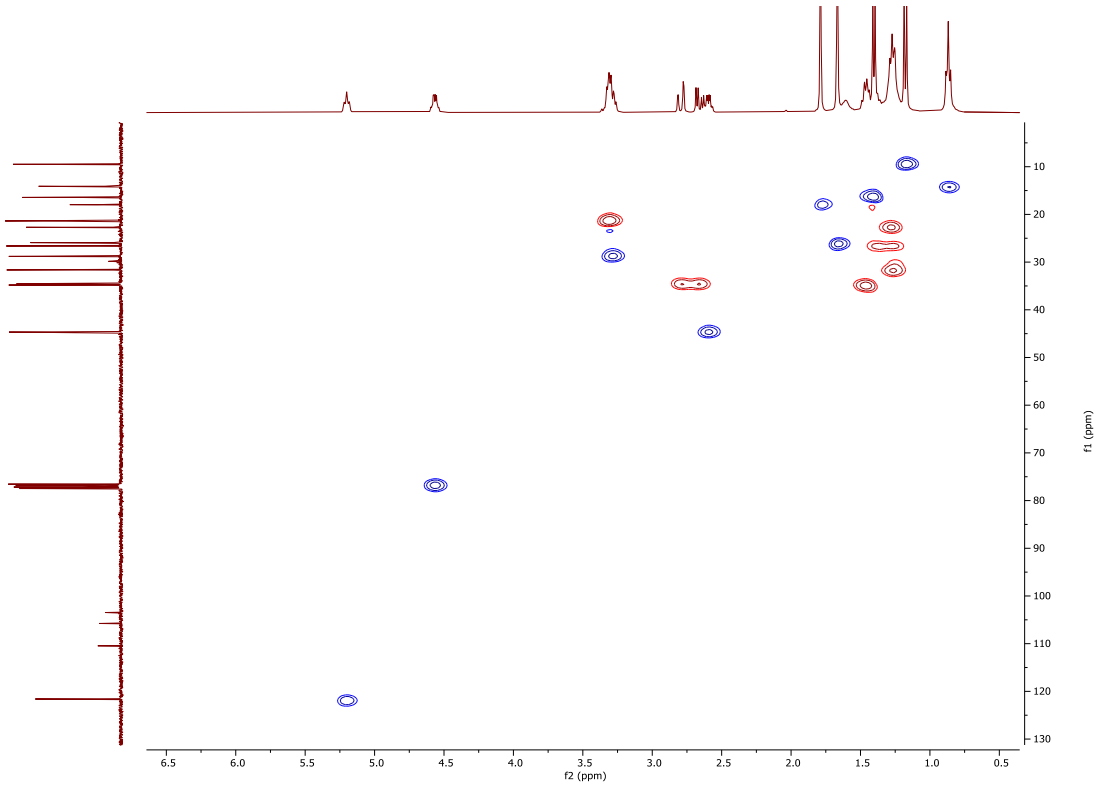

Figure S22. HSQC spectrum of compound **4** in $CDCl_3$

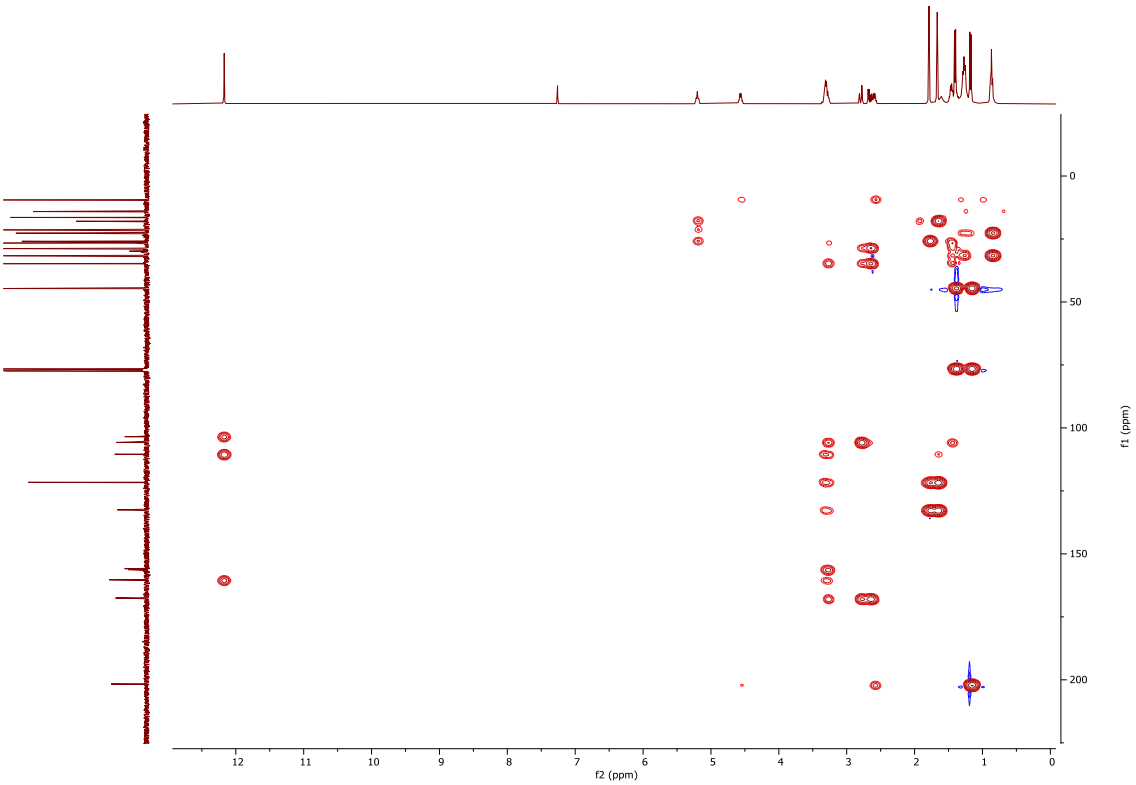

Figure S23. HMBC spectrum of compound **4** in $CDCl_3$

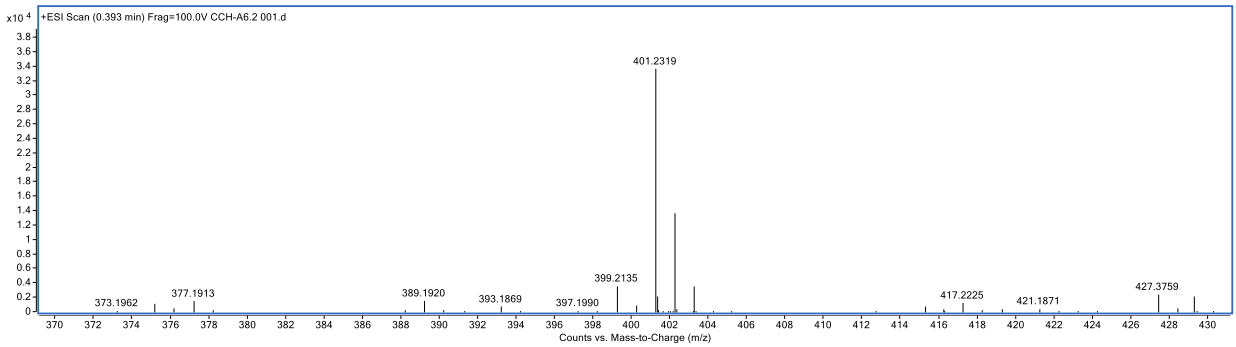

Figure S24. HRESIMS spectrum of compound **4** in MeCN

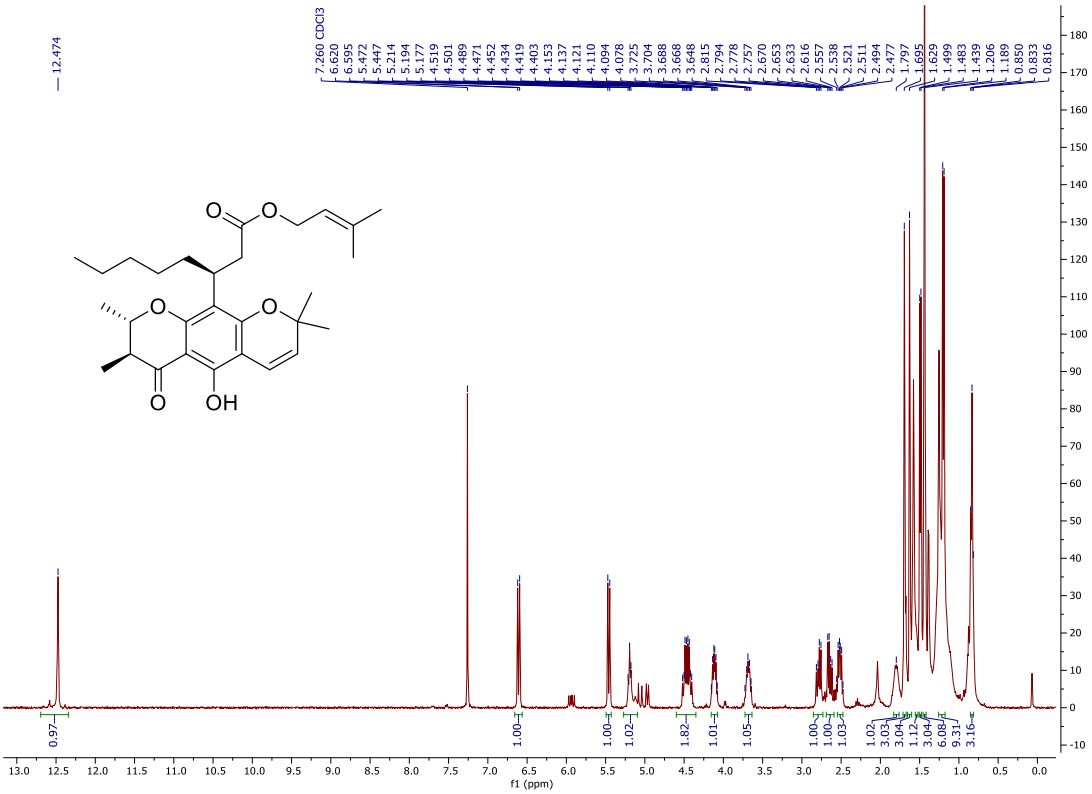

Figure S25. ^{1}H NMR spectrum of compound **5** in $CDCl_3$

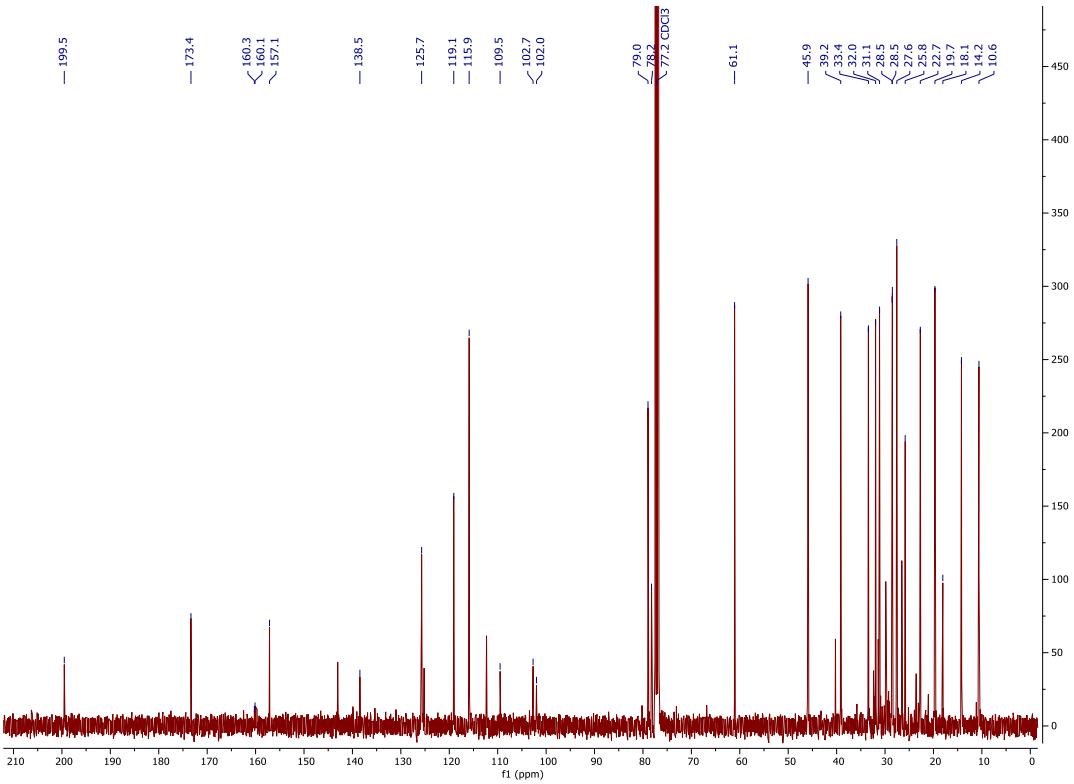

Figure S26. ^{13}C NMR spectrum of compound **5** in $CDCl_3$

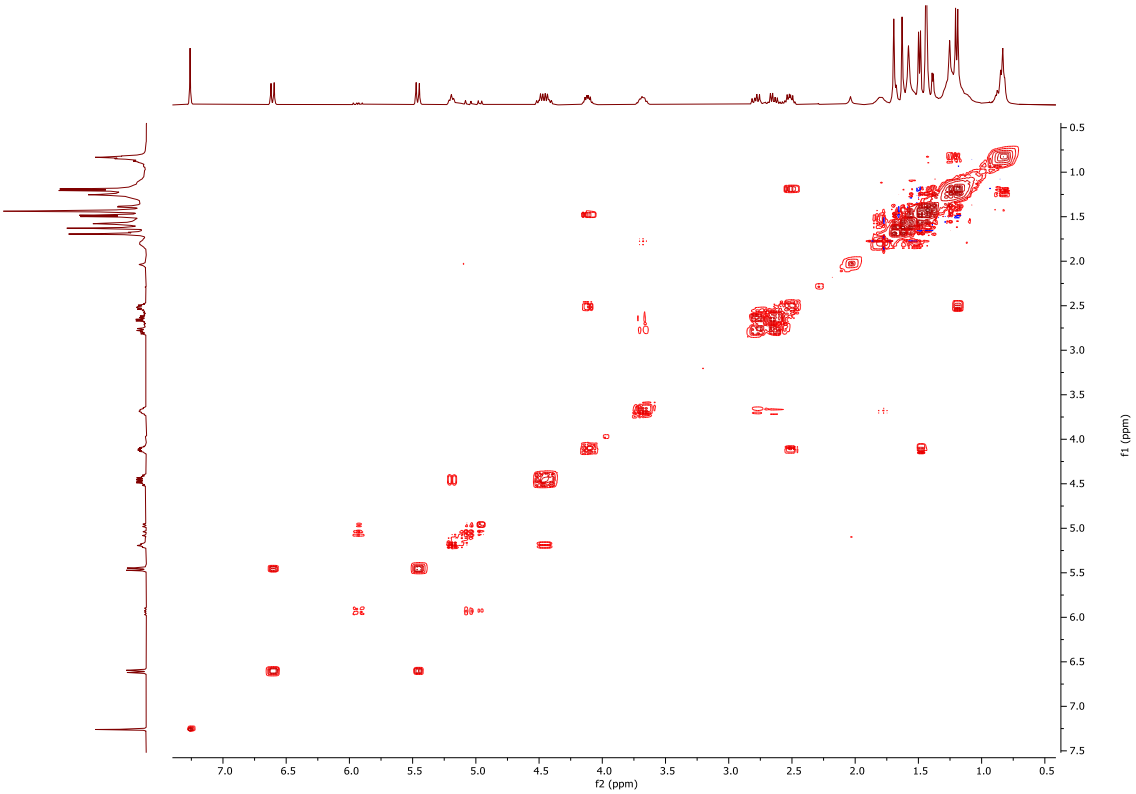

Figure S27. COSY spectrum of compound **5** in $CDCl_3$

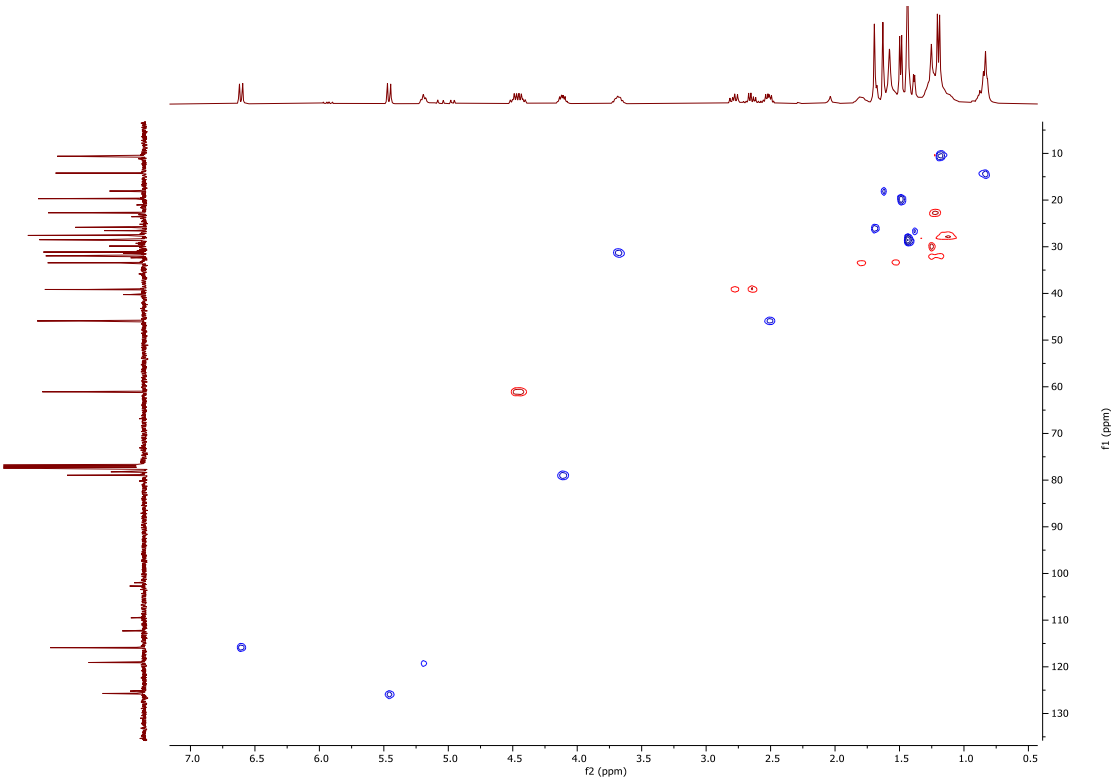

Figure S28. HSQC spectrum of compound **5** in $CDCl_3$

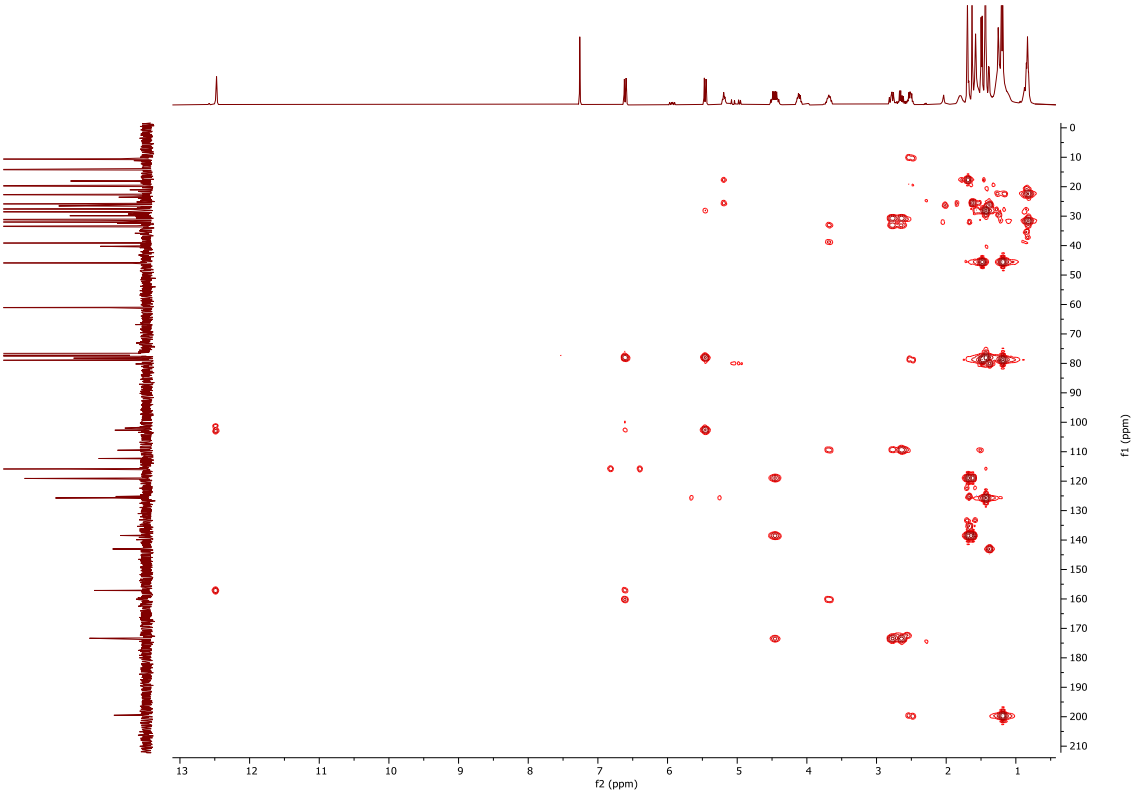

Figure S29. HMBC spectrum of compound **5** in $CDCl_3$

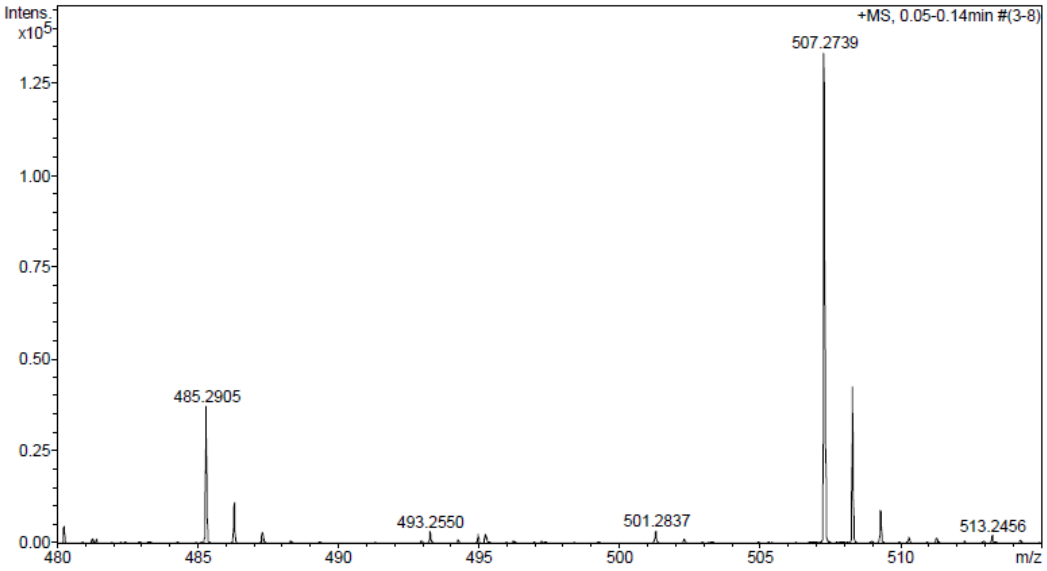

Figure S30. HRESIMS spectrum of compound **5** in MeCN

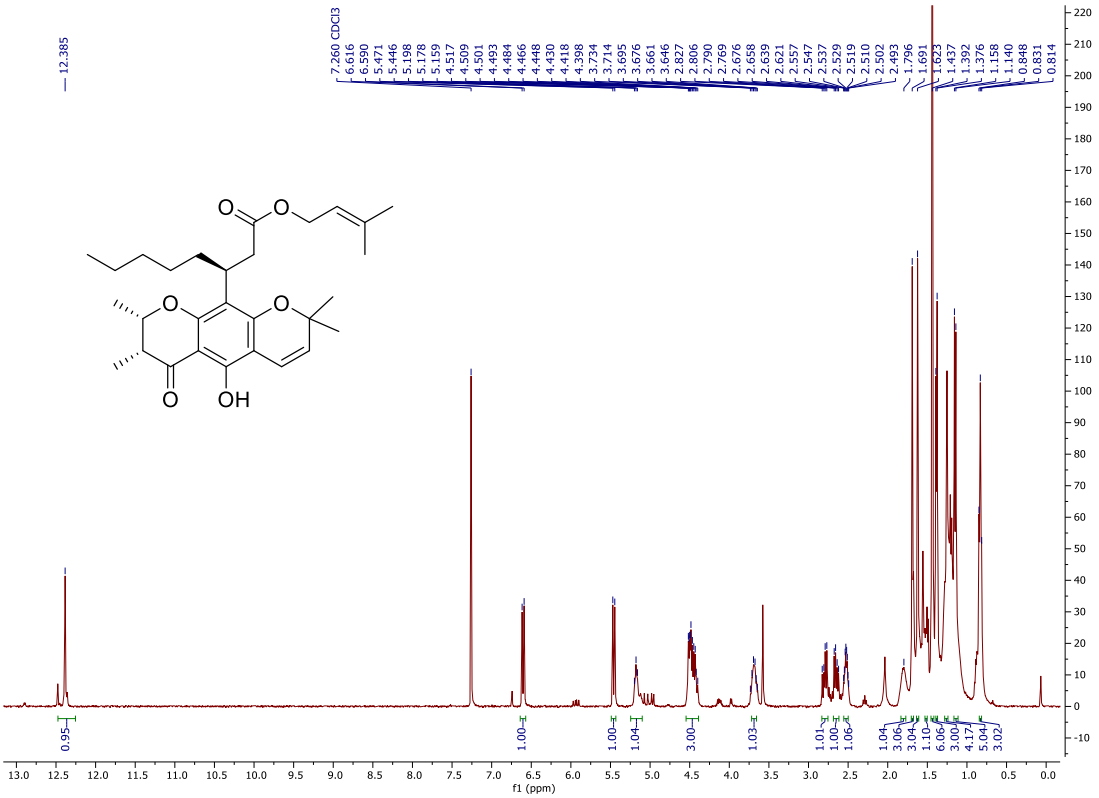

Figure S31. ^{1}H NMR spectrum of compound **6** in $CDCl_3$

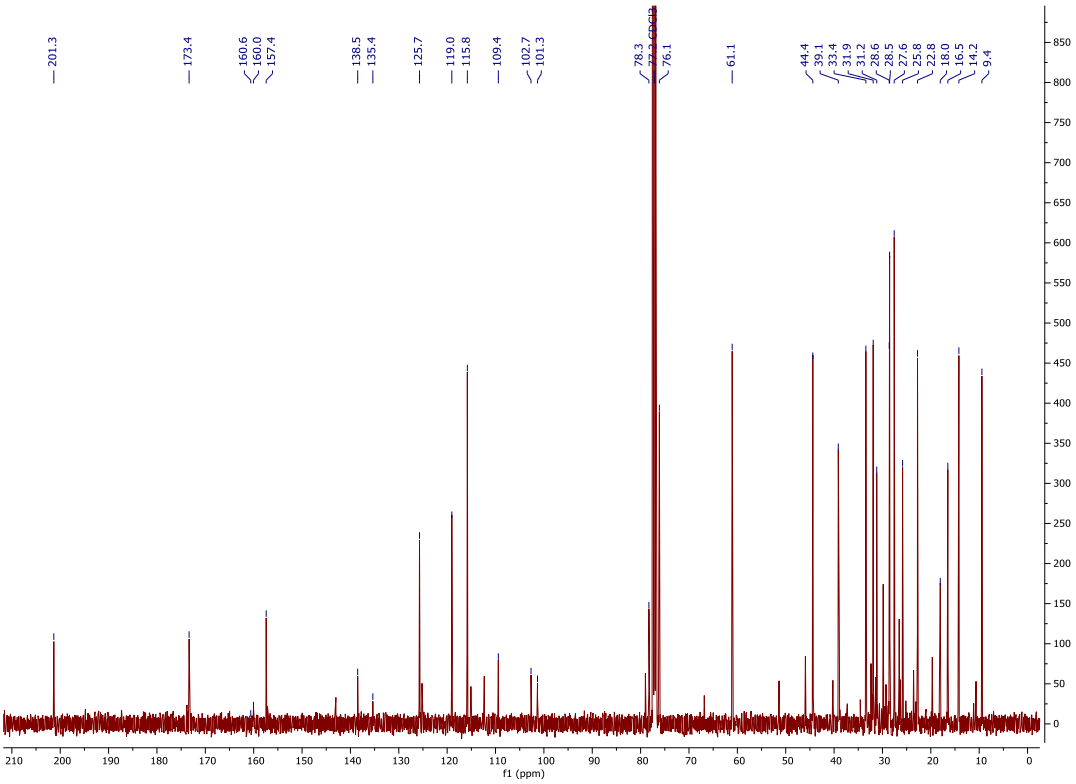

Figure S32. ^{13}C NMR spectrum of compound **6** in $CDCl_3$

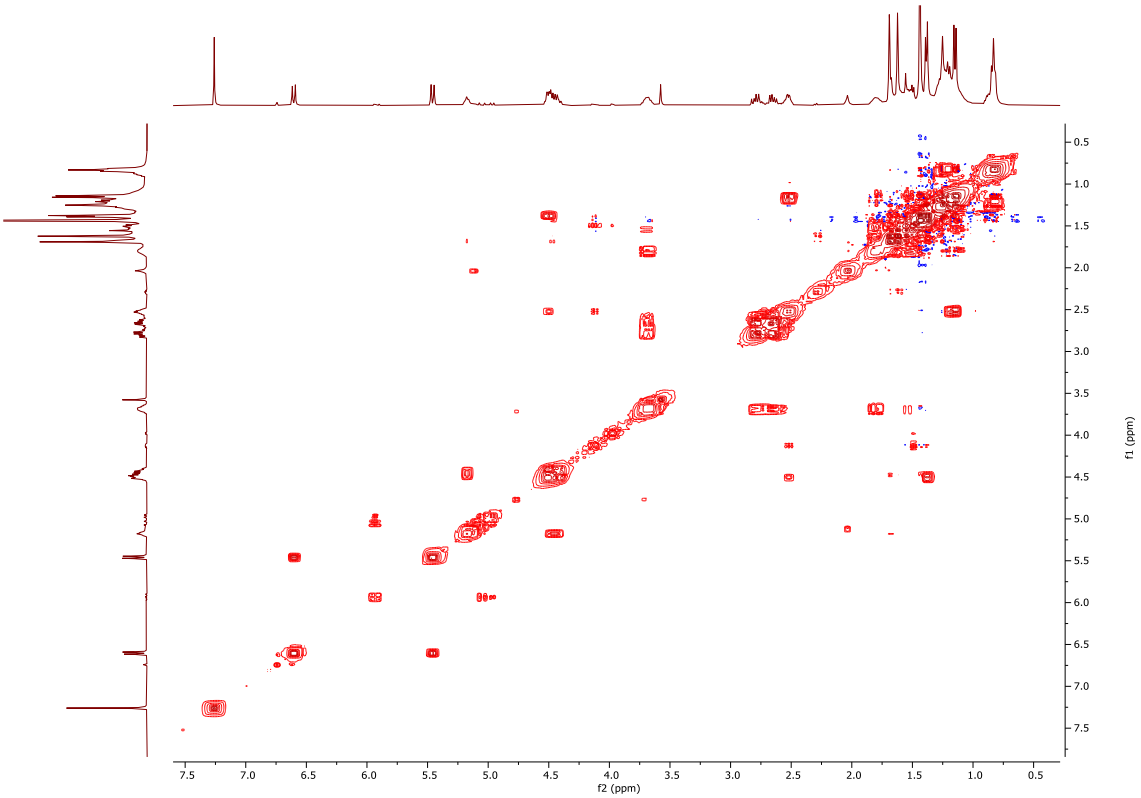

Figure S33. COSY spectrum of compound **6** in $CDCl_3$

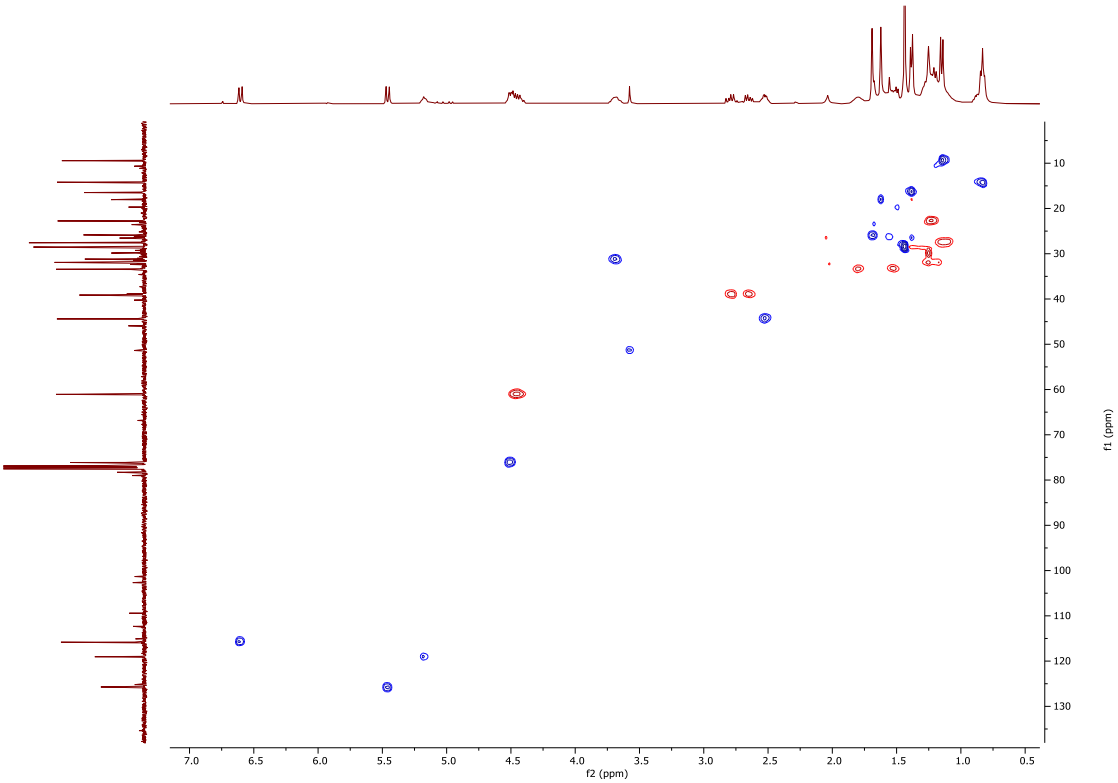

Figure S34. HSQC spectrum of compound **6** in $CDCl_3$

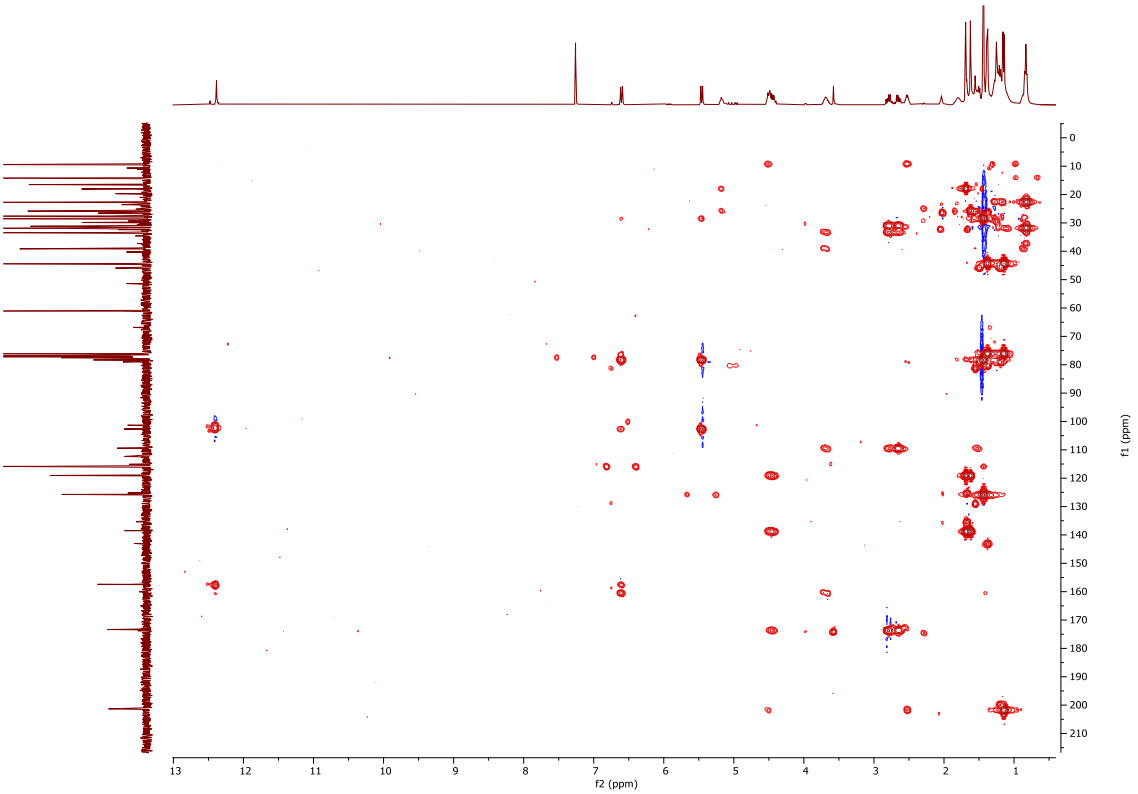

Figure S35. HMBC spectrum of compound **6** in $CDCl_3$

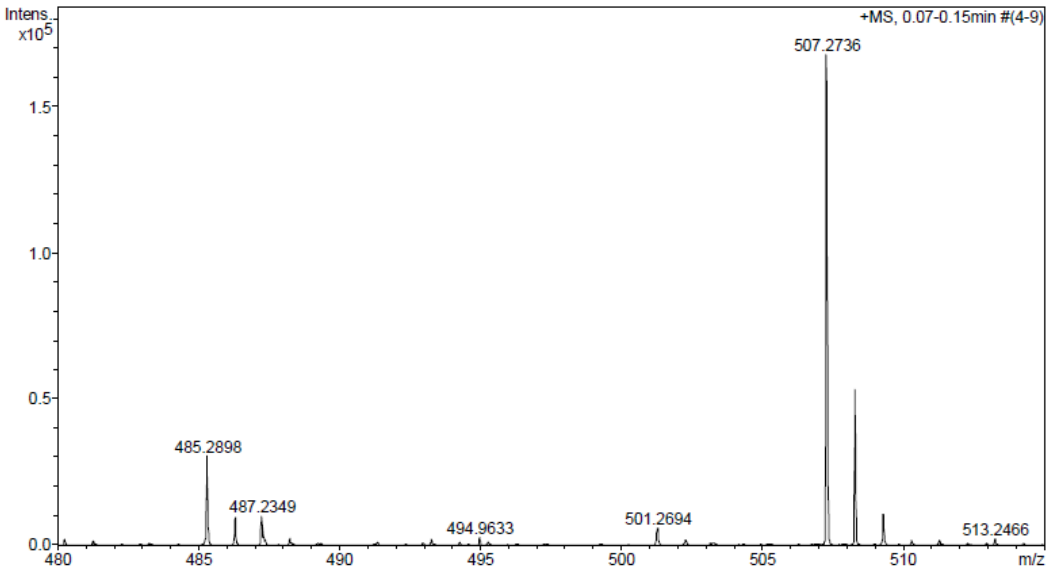

Figure S36. HRESIMS spectrum of compound **6** in MeCN

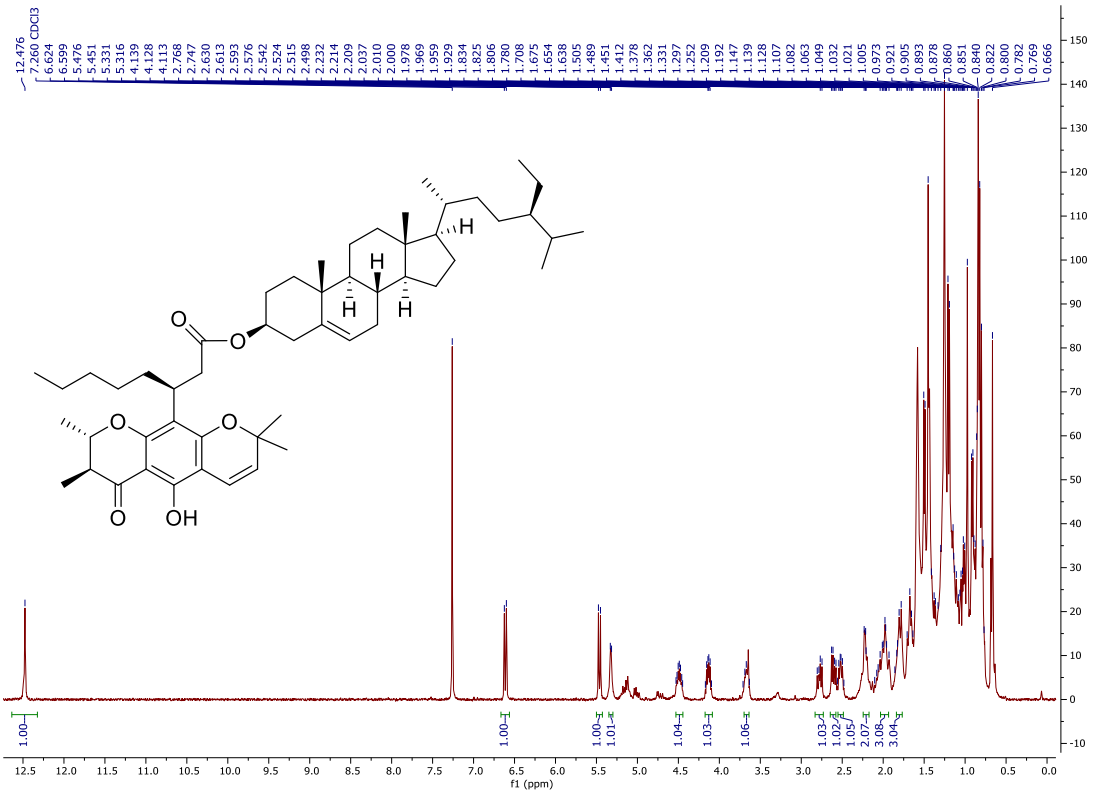

Figure S37. ^{1}H NMR spectrum of compound **7** in $CDCl_3$

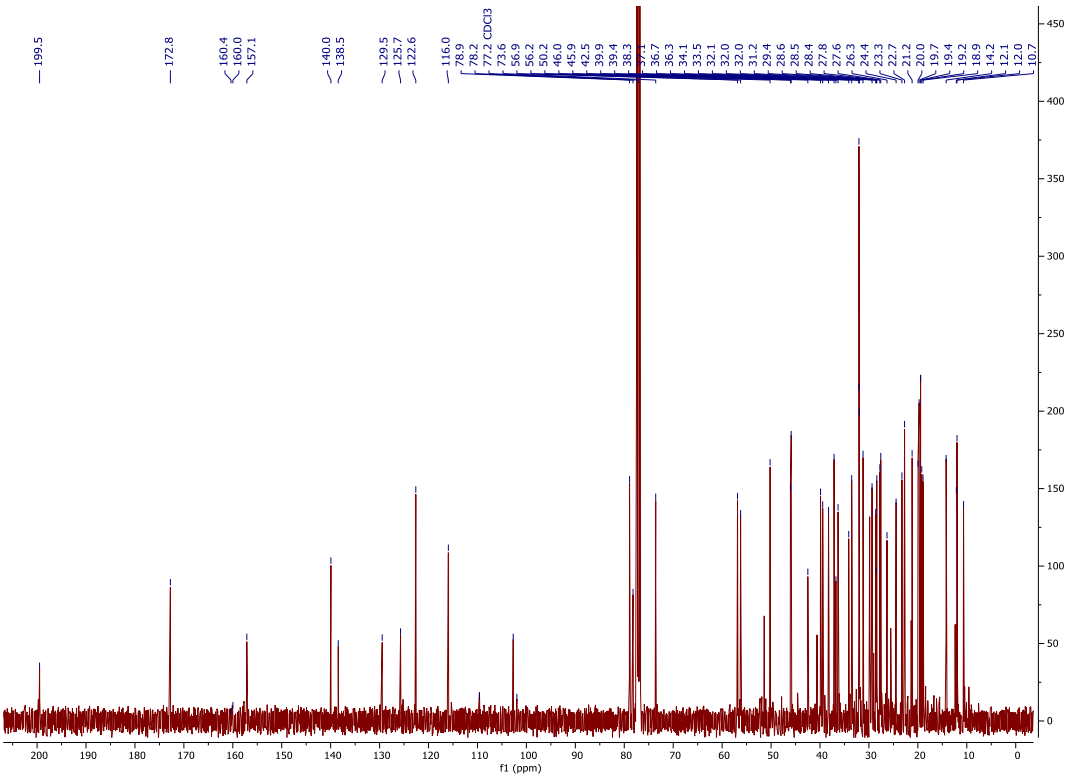

Figure S38. ^{13}C NMR spectrum of compound **7** in $CDCl_3$

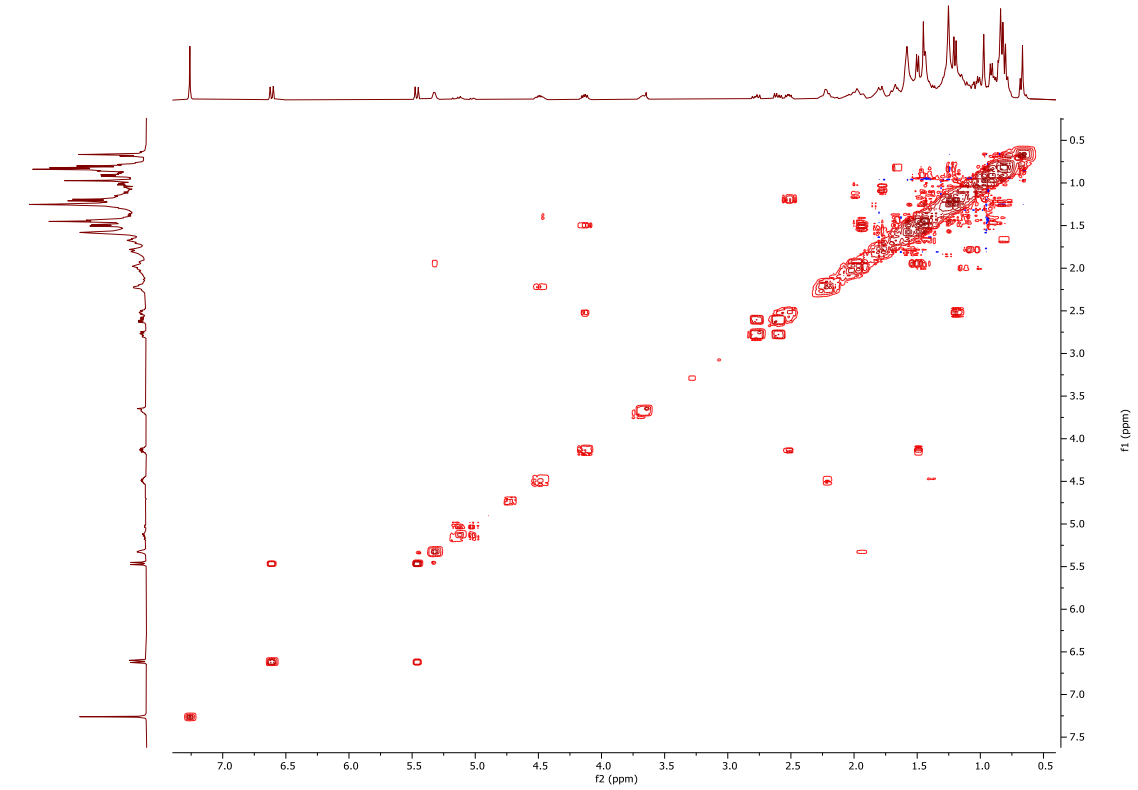

Figure S39. COSY spectrum of compound **7** in $CDCl_3$

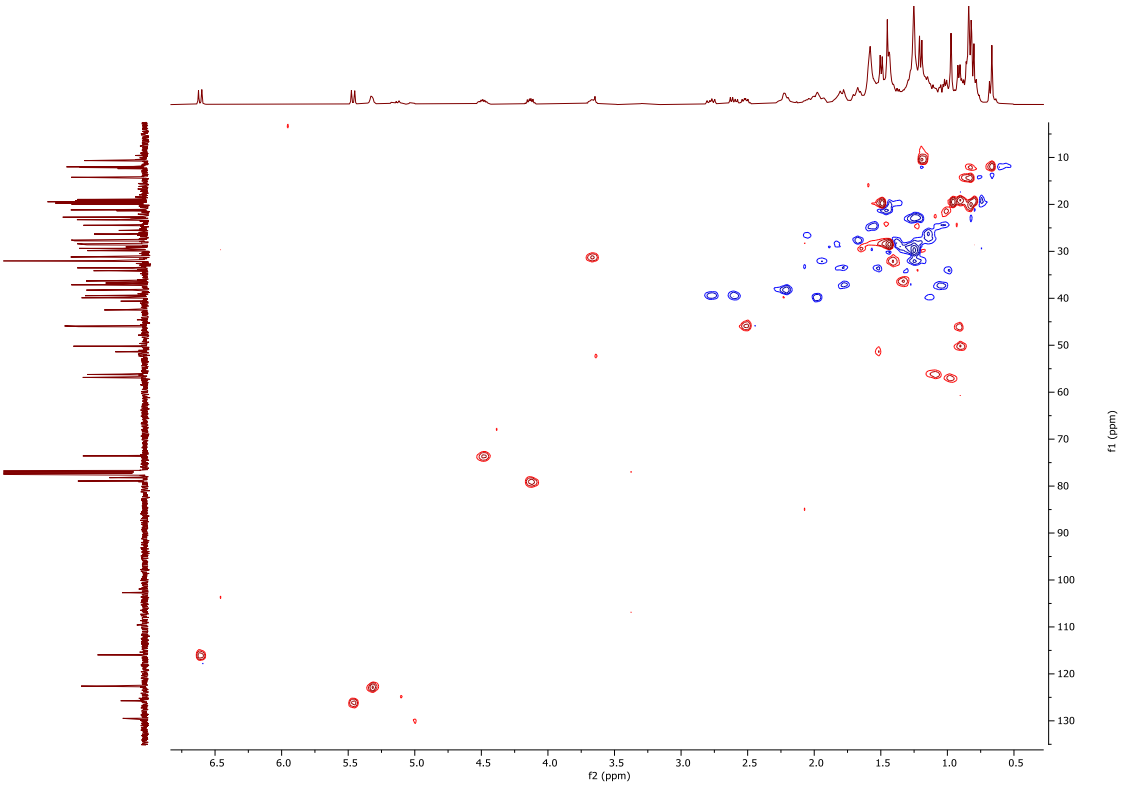

Figure S40. HSQC spectrum of compound **7** in $CDCl_3$

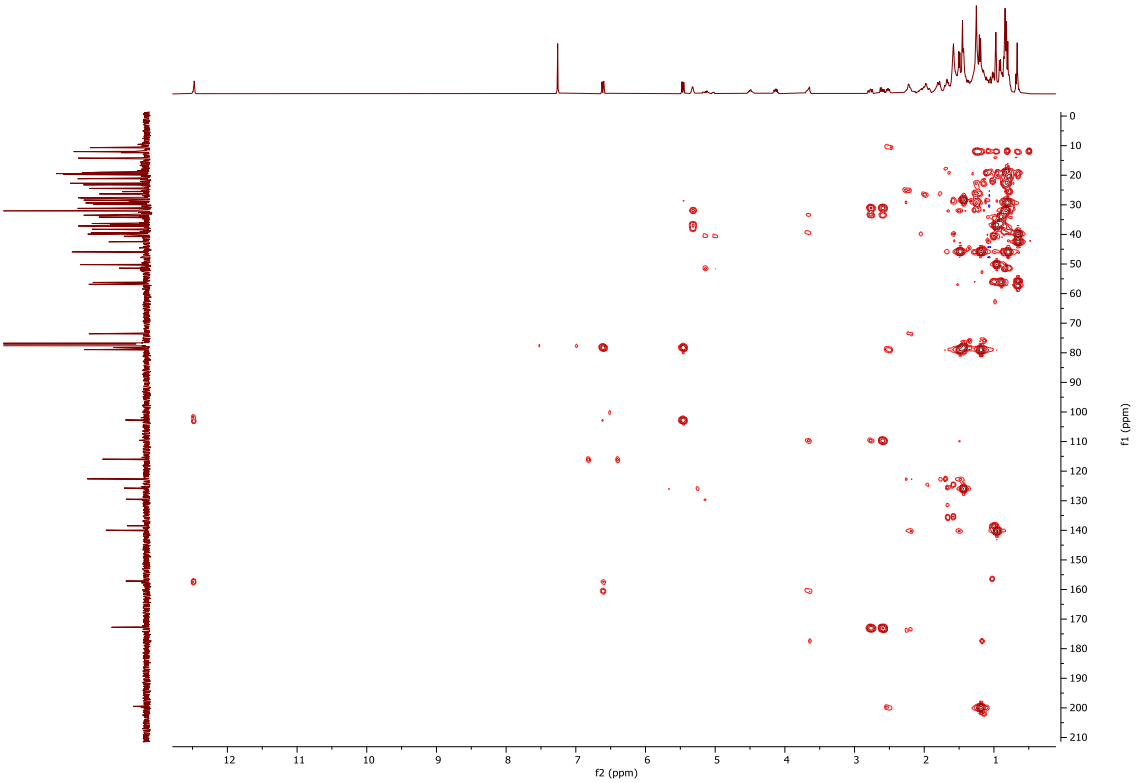

Figure S41. HMBC spectrum of compound **7** in $CDCl_3$

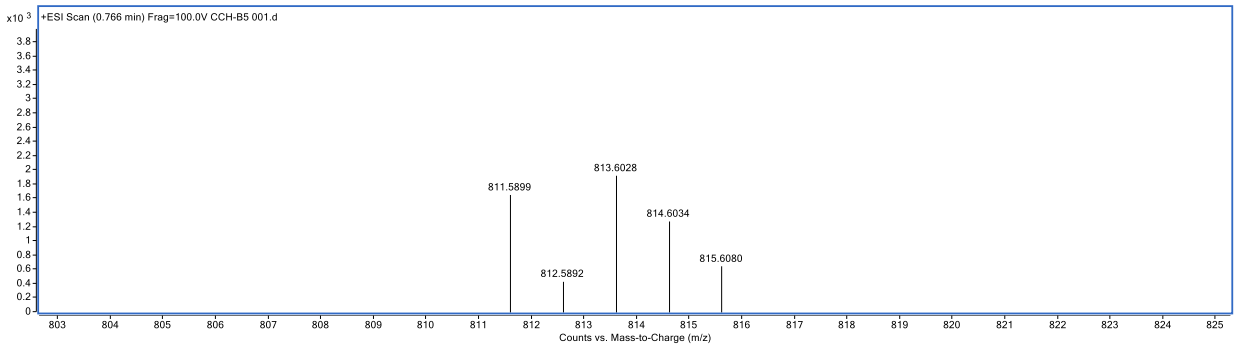

Figure S42. HRESIMS spectrum of compound **7** in MeCN

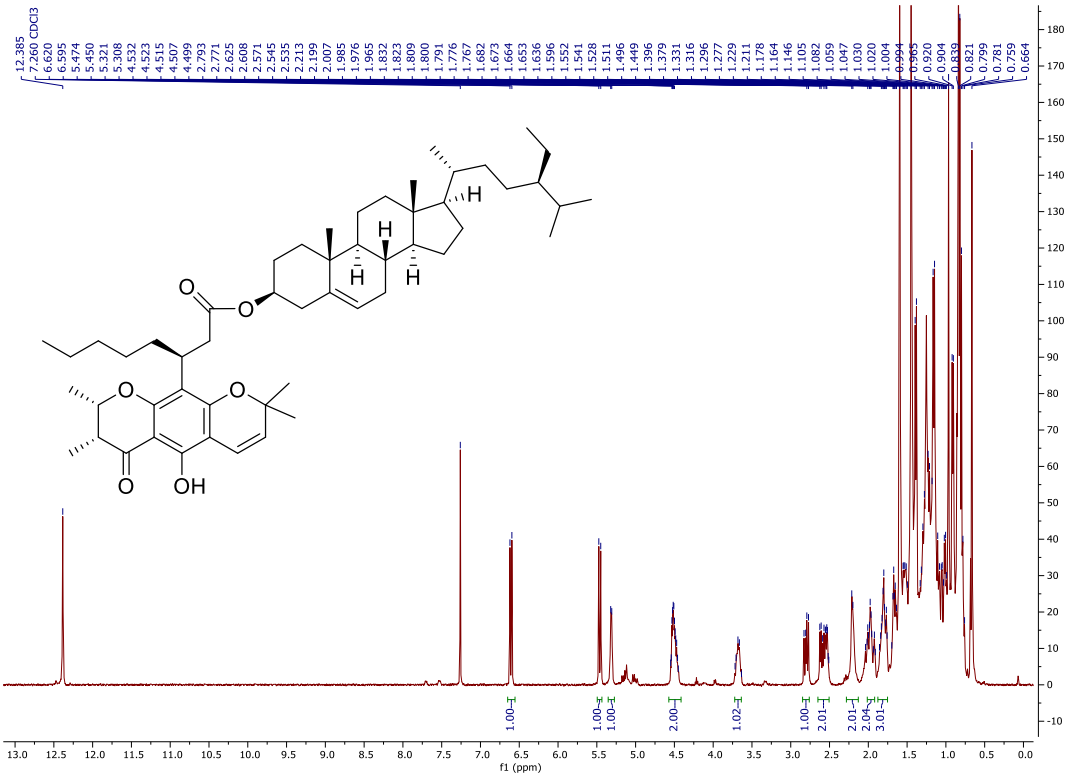

Figure S43. ^{1}H NMR spectrum of compound **8** in $CDCl_3$

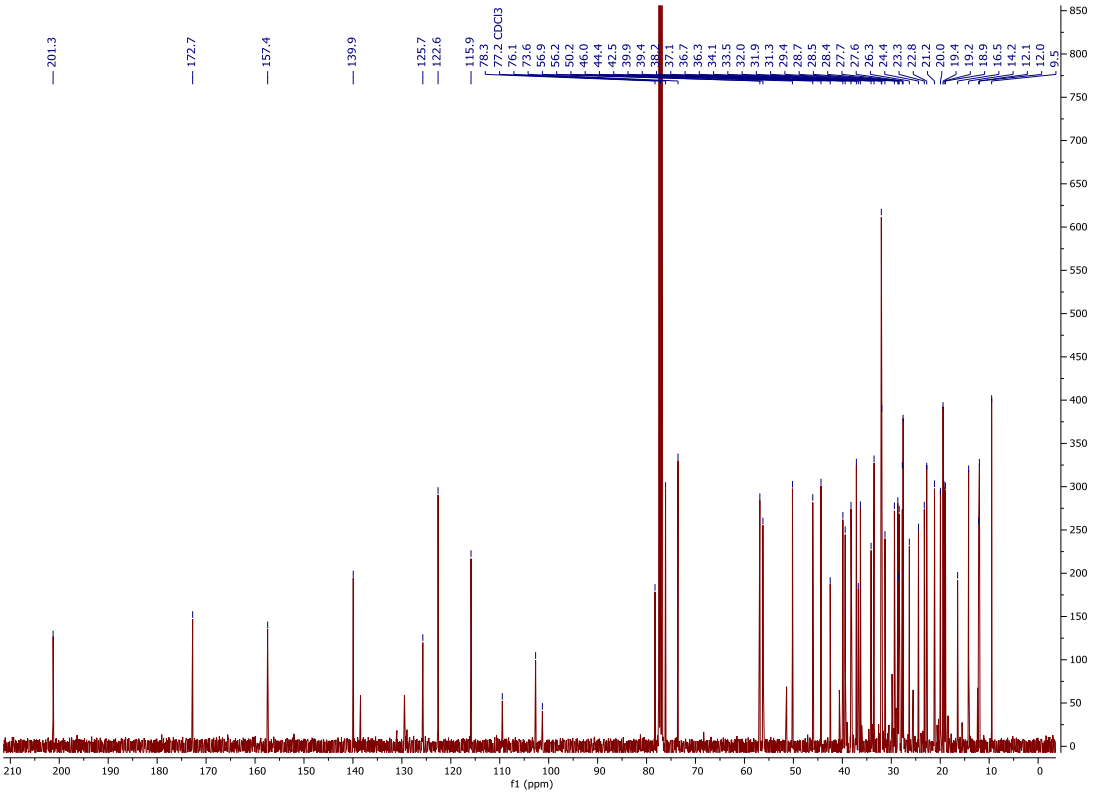

Figure S44. ^{13}C NMR spectrum of compound **8** in $CDCl_3$

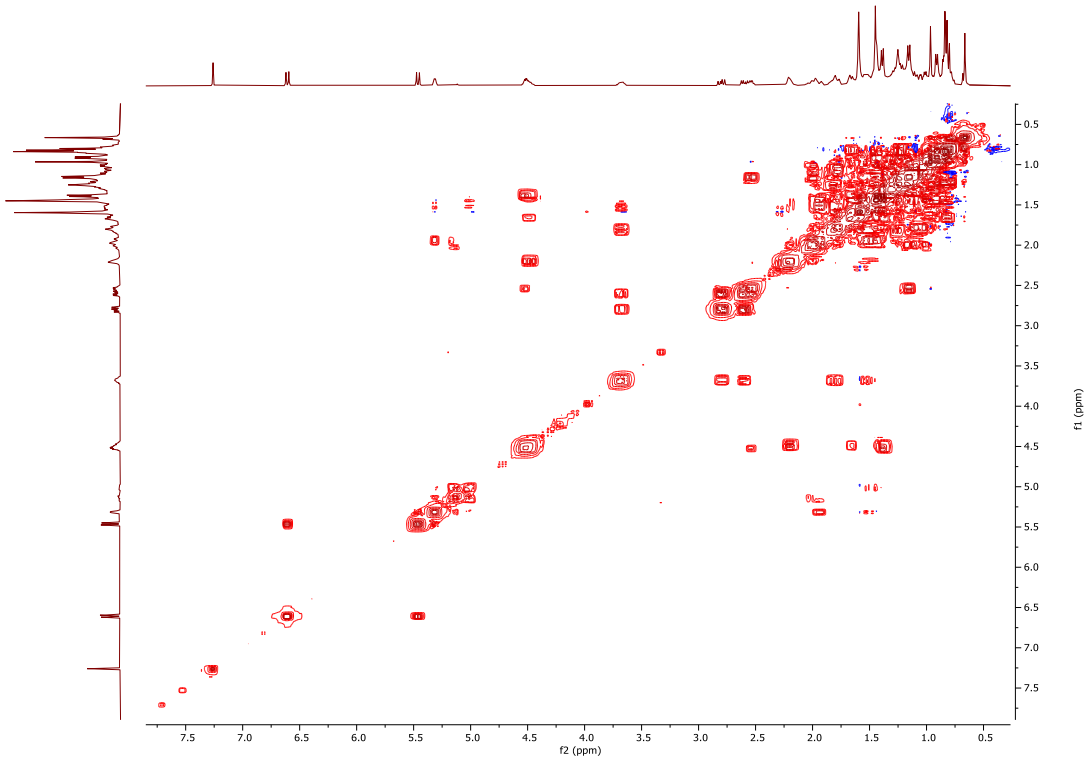

Figure S45. COSY spectrum of compound **8** in $CDCl_3$

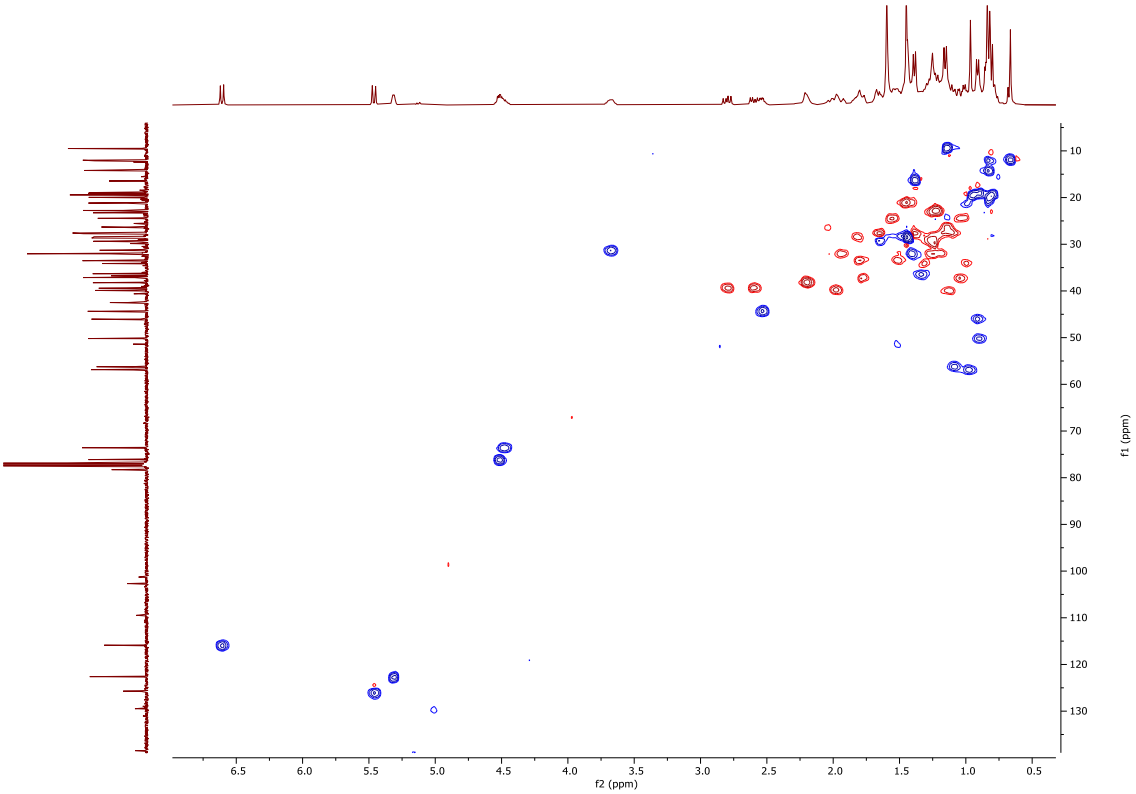

Figure S46. HSQC spectrum of compound **8** in $CDCl_3$

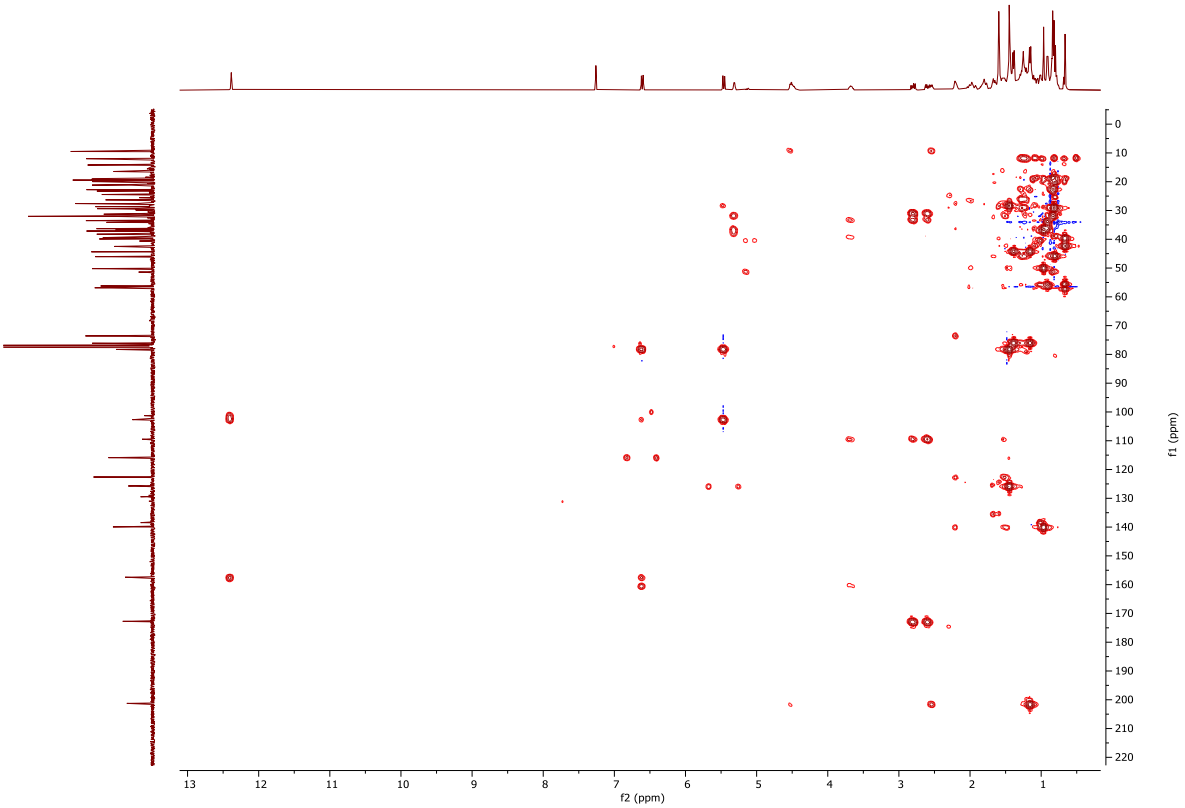

Figure S47. HMBC spectrum of compound **8** in $CDCl_3$

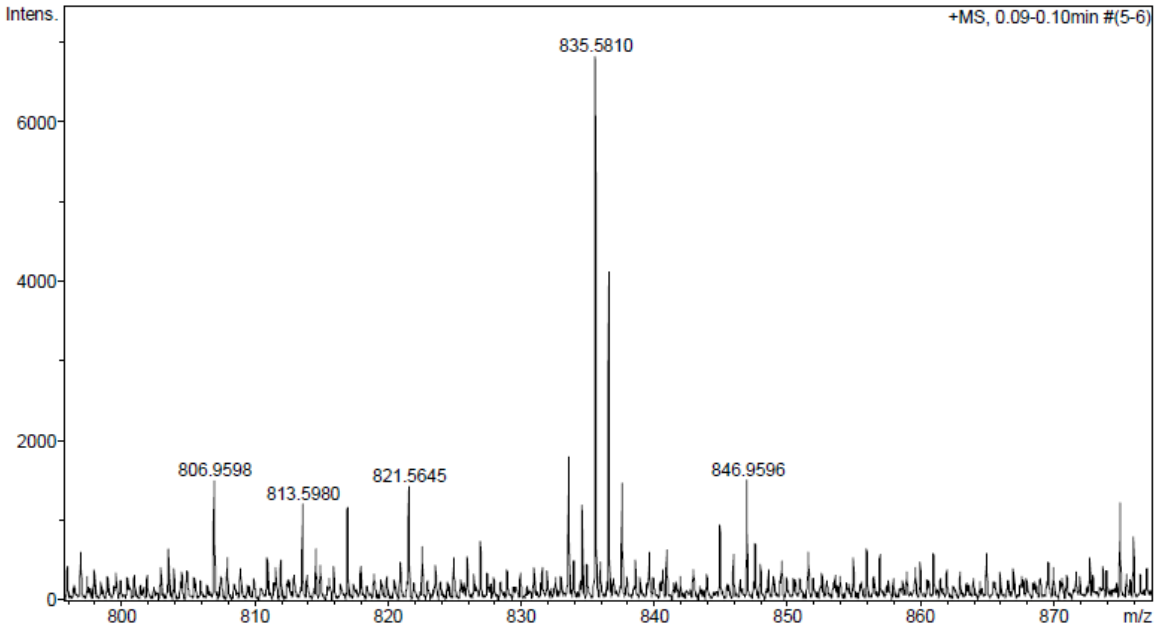

Figure S48. HRESIMS spectrum of compound **8** in MeCN

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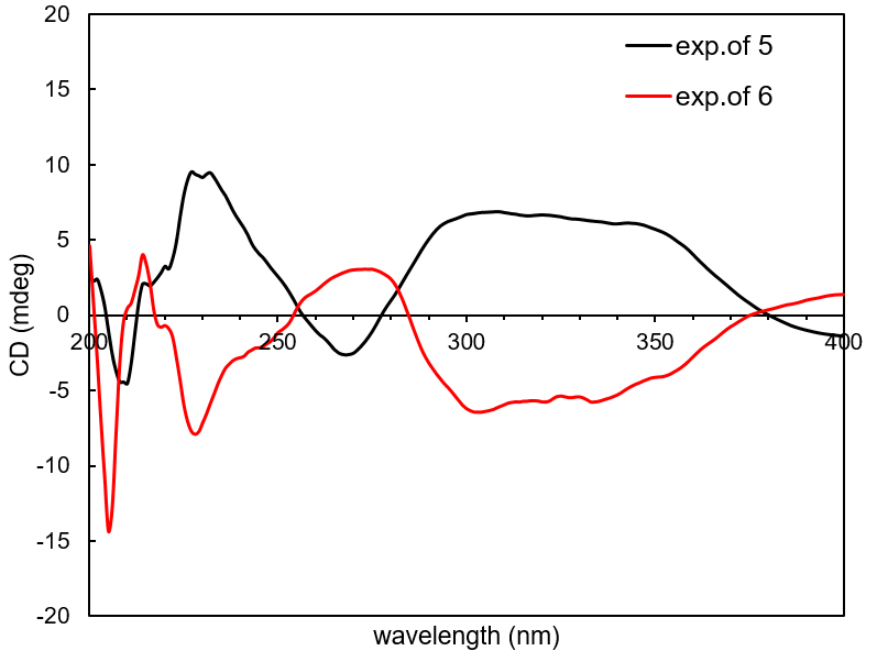

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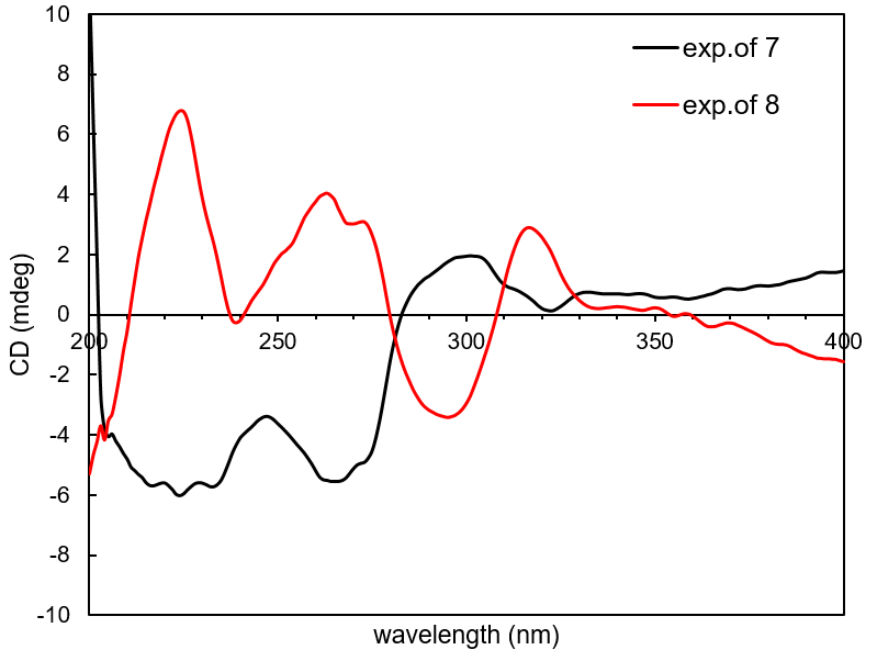


Figure S49. Experimental ECD spectra for (a) compounds **5** and **6**, (b) compounds **7** and **8**

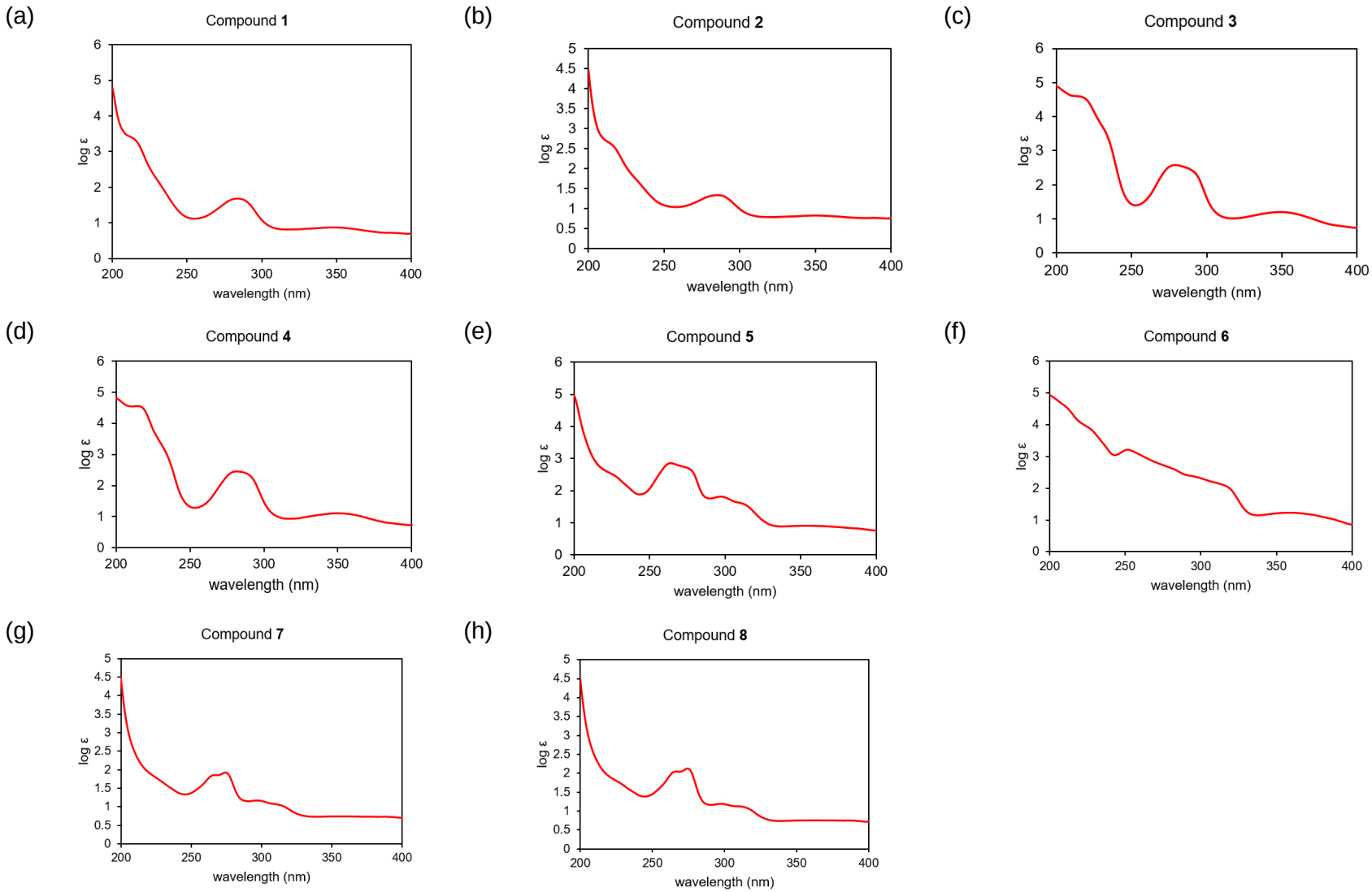


Figure S50. UV spectra for compounds **1–8** in MeOH.

Esterification reaction

A solution of (–)-calomembranone P (6.7 mg) and β-sitosterol (7.0 mg) in anhydrous MeOH (1 mL) and conc. H_2SO_4 or CH_3COOH (20 μL) was stirrred under reflux overnight. The reaction was neutralized with aqueous $NaHCO_3$ and cocentrated under vacuum. The reaction was extracted with EtOAc and the organic layer wa dried over anhydrous Na_2SO_4 to give crude products [1].

Reference

[1] Mersal KI, Abdel-Maksoud MS, Ali EMH, Ammar UM, Zaraei SO, Kim JM, Kim SY, Lee KT, Lee KH, Kim SW, Park HM, Ji MJ, Oh CH. Design, synthesis, in vitro determination and molecular docking studies of 4-(1-(tert-butyl)-3-phenyl-1H-pyrazol-4-yl) pyridine derivatives with terminal sulfonamide derivatives in LPS-induced RAW264.7 macrophage cells. Med. Chem. Res. 2021, 30: 1925–1942. https://doi.org/10.1007/s00044-021-02784-9

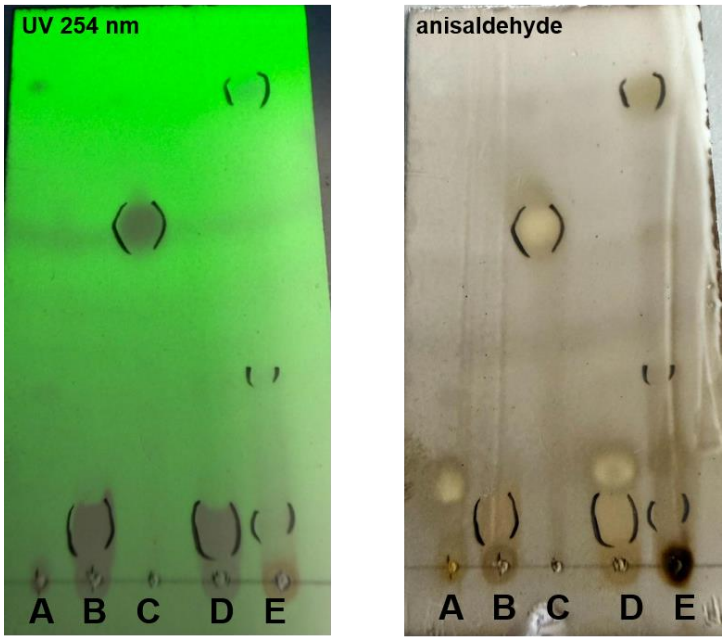
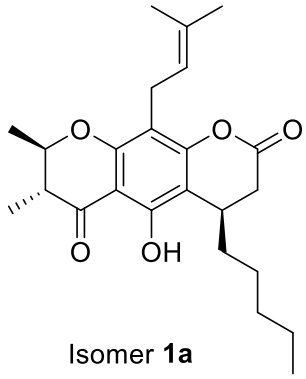
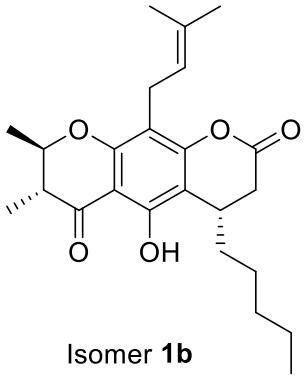


Figure S51. TLC profile under UV 254 nm and after stained using anisaldehyde reagent of (A) β-sitosterol; (B) (–)-calomembranone P (**10**); (C) calabanone H (**8**); (D) crude product using catalyst conc. acetic acid; and (E) crude product using conc. H_2SO_4

Table S1. DP4+ probability analysis of possible isomers 2*R*,3*R*,16*R*-**1a** and 2*R*,3*R*,16*S*-**1b**



Isomer **1a**



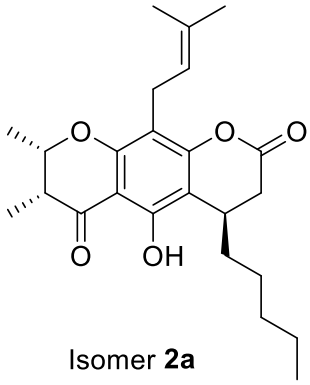
Isomer **1b**

Functional	Solvent?		Basis Set		Type of Data	
B3LYP	PCM		6-31+G(d,p)		Shielding Tensors	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	95.50%	4.50%	-	-	-	-
sDP4+ (C data)	66.28%	33.72%	-	-	-	-
sDP4+ (all data)	97.66%	2.34%	-	-	-	-
uDP4+ (H data)	96.32%	3.68%	-	-	-	-
uDP4+ (C data)	51.30%	48.70%	-	-	-	-
uDP4+ (all data)	96.50%	3.50%	-	-	-	-
DP4+ (H data)	99.82%	0.18%	-	-	-	-
DP4+ (C data)	67.44%	32.56%	-	-	-	-
DP4+ (all data)	99.91%	0.09%	-	-	-	-

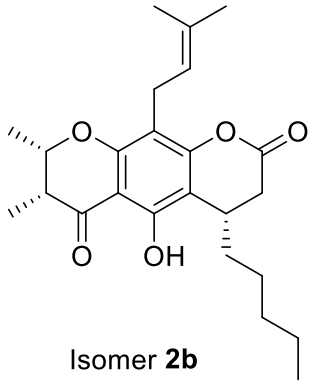
Table S2.Comparison of the experimental (exp.) and calculated (calcd.) NMR chemical shifts for compound **1**

Position	Compound **1** (exp.)		Isomer **1a** (calcd.)		Isomer **1b** (calcd.)	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
2	4.19	79.1	3.91	78.2	3.92	78.4
3	2.59	46.2	2.29	45.0	2.57	45.1
4		200.3		201.3		201.4
4a		104.2		107.6		107.5
5		157.6		160.4		160.5
6		107.5		110.5		110.6
7		156.3		159.2		159.1
8		108.9		112.3		112.2
8a		158.4		160.8		160.5
9	1.53	19.8	1.12	17.0	1.13	17.0
10	1.22	10.2	0.77	6.8	0.78	6.9
11	3.28	21.7	3.00	21.8	3.02	22.0
12	5.16	121.9	4.87	124.6	4.94	124.4
13		132.1		137.5		137.8
14	1.66	25.9	1.29	23.0	1.29	22.9
15	1.77	17.9	1.38	14.7	1.48	14.6
16	3.33	28.7	2.88	30.7	2.91	30.7
17	2.83	34.0	2.36	33.2	2.36	33.1
	2.64		2.15		2.15	
18		167.6		171.0		171.0
19	1.54	34.2	1.14	35.2	1.14	35.3
	1.44		0.91		0.91	
20	1.41	26.5	1.12	28.8	1.13	28.8
	1.28		0.74		0.75	
21	1.26	31.8	0.76	33.0	0.77	33.0
22	1.28	22.6	0.90	24.0	0.91	24.0
23	0.86	14.1	0.49	12.3	0.50	12.3
OH-5	12.26		12.65		12.66	

Table S3. DP4+ probability analysis of possible isomers 2*S*,3*R*,16*R*-**2a** and 2*S*,3*R*,16*S*-**2b**



Isomer **2a**



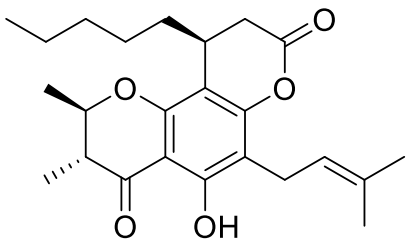
Isomer **2b**

Functional	Solvent?	Basis Set	Type of Data			
B3LYP	PCM	6-31+G(d,p)	Shielding Tensors			
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	44.50%	55.50%	-	-	-	-
sDP4+ (C data)	44.77%	55.23%	-	-	-	-
sDP4+ (all data)	39.39%	60.61%	-	-	-	-
uDP4+ (H data)	10.59%	89.41%	-	-	-	-
uDP4+ (C data)	43.74%	56.26%	-	-	-	-
uDP4+ (all data)	8.43%	91.57%	-	-	-	-
DP4+ (H data)	8.67%	91.33%	-	-	-	-
DP4+ (C data)	38.66%	61.34%	-	-	-	-
DP4+ (all data)	5.65%	94.35%	-	-	-	-

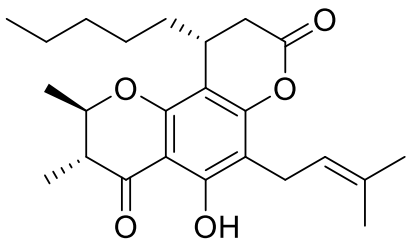
Table S4.Comparison of the experimental (exp.) and calculated (calcd.) NMR chemical shifts for compound **2**

Position	Compound **2** (exp.)		Isomer **2a** (calcd.)		Isomer **2b** (calcd.)	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
2	4.57	76.5	4.27	76.4	4.16	76.1
3	2.60	44.7	2.00	44.6	1.93	44.5
4		202.1		205.2		205.3
4a		103.6		107.4		107.4
5		157.9		161.3		161.1
6		107.6		110.2		109.9
7		156.4		159.4		159.3
8		109.0		112.4		112.5
8a		158.2		161.0		161.1
9	1.41	16.5	1.08	14.4	1.04	14.5
10	1.20	9.4	0.86	8.0	0.82	8.0
11	3.28	21.7	3.06	22.1	3.04	22.0
12	5.15	121.9	4.89	124.7	4.79	124.9
13		132.2		138.1		137.8
14	1.66	25.9	1.30	23.0	1.30	23.0
15	1.77	17.9	1.47	14.6	1.47	14.7
16	3.30	28.7	2.90	30.1	2.91	30.4
17	2.82	33.9	2.26	34.2	2.37	34.4
	2.63		2.13		2.20	
18		167.6		172.4		172.4
19	1.55	34.1	1.13	36.2	1.15	36.3
	1.44		0.92		0.96	
20	1.40	26.5	1.09	29.1	1.09	29.2
	1.28		0.73		0.71	
21	1.26	31.8	0.73	33.2	0.73	33.2
22	1.28	22.6	0.88	24.0	0.87	24.0
23	0.86	14.1	0.48	12.4	0.48	12.4
OH-5	12.18		12.76		12.75	

Table S5. DP4+ probability analysis of possible isomers 2*R*,3*R*,16*S*-**3a** and 2*R*,3*R*,16*R*-**3b**



Isomer **3a**



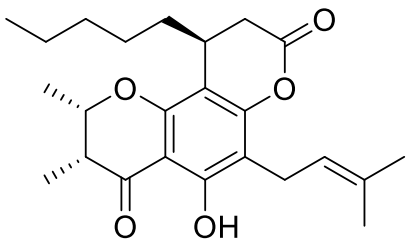
Isomer **3b**

	Functional	Solvent?		Basis Set		Type of Data	
	B3LYP	PCM		6-31+G(d,p)		Shielding Tensors	
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		22.42%	77.58%	-	-	-	-
sDP4+ (C data)		7.05%	92.95%	-	-	-	-
sDP4+ (all data)		2.15%	97.85%	-	-	-	-
uDP4+ (H data)		56.30%	43.70%	-	-	-	-
uDP4+ (C data)		16.21%	83.79%	-	-	-	-
uDP4+ (all data)		19.95%	80.05%	-	-	-	-
DP4+ (H data)		27.12%	72.88%	-	-	-	-
DP4+ (C data)		1.45%	98.55%	-	-	-	-
DP4+ (all data)		0.54%	99.46%	-	-	-	-

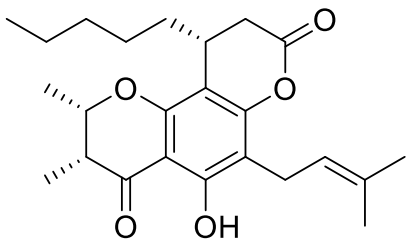
Table S6.Comparison of the experimental (exp.) and calculated (calcd.) NMR chemical shifts for compound **3**

Position	Compound **3** (exp.)		Isomer **3a** (calcd.)		Isomer **3b** (calcd.)	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
2	4.19	79.3	3.91	79.1	3.92	78.6
3	2.60	46.2	2.33	45.0	2.32	44.9
4		199.8		202.2		202.0
4a		104.1		107.8		107.9
5		159.9		162.7		162.7
6		110.4		113.6		113.6
7		156.0		159.0		159.1
8		105.8		108.9		108.8
8a		156.2		159.2		159.2
9	1.51	19.7	1.09	16.8	1.08	16.7
10	1.23	10.4	0.78	6.8	0.77	6.8
11	3.32	21.4	3.08	21.5	3.07	21.6
12	5.19	121.6	4.89	124.7	4.88	124.7
13		132.5		137.8		137.7
14	1.79	18.0	1.28	23.0	1.28	23.0
15	1.66	25.9	1.46	14.5	1.47	14.5
16	3.27	28.8	2.83	30.7	2.86	30.5
17	2.81	34.3	2.24	34.4	2.27	34.4
	2.67		2.12		2.13	
18		167.6		172.5		172.5
19	1.48	36.6	1.02	36.1	0.99	35.8
20	1.40	26.5	1.04	29.1	1.07	28.6
	1.29		0.73		0.67	
21	1.27	31.6	0.74	33.3	0.74	33.2
22	1.29	22.6	0.89	24.0	0.89	24.1
23	0.87	14.1	0.49	12.4	0.49	12.4
OH-5	12.26		12.99		12.98	

Table S7. DP4+ probability analysis of possible isomers 2*S*,3*R*,16*S*-**4a** and 2*S*,3*R*,16*R*-**4b**



Isomer **4a**



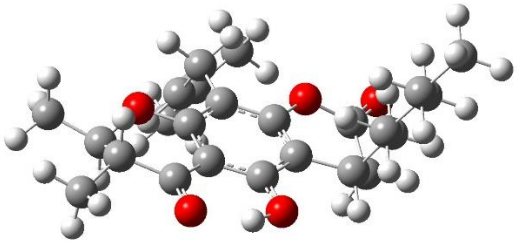
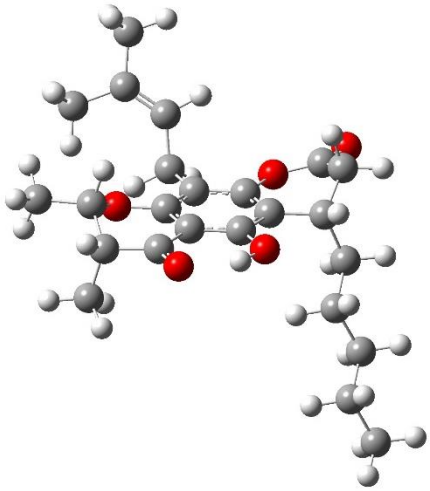
Isomer **4b**

Functional	Solvent?		Basis Set		Type of Data	
B3LYP	PCM		6-31+G(d,p)		Shielding Tensors	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	77.71%	22.29%	-	-	-	-
sDP4+ (C data)	77.74%	22.26%	-	-	-	-
sDP4+ (all data)	92.41%	7.59%	-	-	-	-
uDP4+ (H data)	73.21%	26.79%	-	-	-	-
uDP4+ (C data)	77.27%	22.73%	-	-	-	-
uDP4+ (all data)	90.28%	9.72%	-	-	-	-
DP4+ (H data)	90.50%	9.50%	-	-	-	-
DP4+ (C data)	92.23%	7.77%	-	-	-	-
DP4+ (all data)	99.12%	0.88%	-	-	-	-

Table S8.Comparison of the experimental (exp.) and calculated (calcd.) NMR chemical shifts for compound **4**

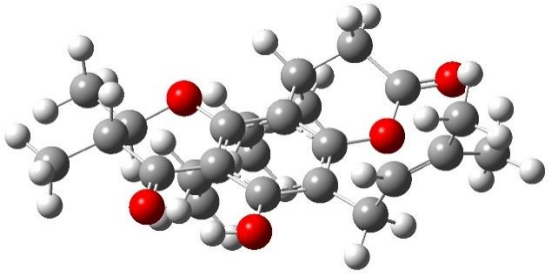
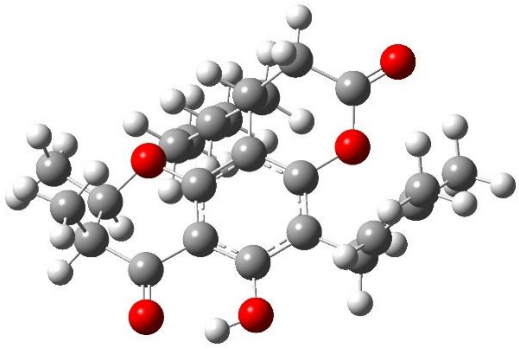
Position	Compound **4** (exp.)		Isomer **4a** (calcd.)		Isomer **4b** (calcd.)	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
2	4.57	76.6	4.36	76.9	4.36	77.5
3	2.60	44.7	2.46	43.7	2.46	43.5
4		201.7		203.3		203.3
4a		103.5		107.6		107.7
5		160.3		162.7		162.6
6		110.5		113.4		113.3
7		155.9		159.2		159.4
8		105.8		109.2		109.2
8a		156.3		158.2		158.3
9	1.40	16.4	0.93	12.1	0.95	12.0
10	1.18	9.5	0.78	7.9	0.78	7.8
11	3.32	21.4	3.07	21.5	3.07	21.5
12	5.20	121.6	4.89	124.7	4.87	124.7
13		132.5		137.8		137.8
14	1.67	25.9	1.29	23.0	1.29	23.0
15	1.79	18.0	1.47	14.5	1.47	14.5
16	3.28	28.8	2.83	30.6	2.83	30.6
17	2.79	34.5	2.26	34.4	2.24	34.5
	2.66		2.13		2.12	
18		167.5		172.4		172.5
19	1.46	34.8	1.00	35.9	1.02	35.9
20	1.37	26.6	0.90	28.8	1.07	29.2
	1.27		0.85		0.77	
21	1.26	31.6	0.73	33.2	0.75	33.4
22	1.28	22.7	0.89	24.0	0.91	24.1
23	0.87	14.1	0.49	12.4	0.50	12.4
OH-5	12.17		12.85		12.83	

Table S9. DFT-optimized structures, total molecular energies, and Cartesian Coordinates of the dominant conformers 2*R*,3*R*,16*R*-**1a** and 2*S*,3*R*,16*S*-**2b** at the B3LYP/6-31G(d,p) level of theory.

							
2*R*,3*R*,16*R*-**1a**				2*S*,3*R*,16*S*-**2b**			
Etot= –1309.962030 Hartree				Etot= –1309.948680 Hartree			
Coordinates (Angstroms)				Coordinates (Angstroms)			
Atomic	X	Y	Z	Atomic	X	Y	Z
C	2.722896	2.962112	0.315667	C	2.925866	2.376561	0.203434
C	1.492164	3.870232	0.181712	C	1.847259	3.449309	0.360088
C	0.402565	3.128588	-0.589546	C	0.648716	2.781422	0.990351
C	0.36077	1.685023	-0.450881	C	0.411871	1.356039	0.670455
C	1.328694	1.008961	0.334507	C	1.336648	0.688721	-0.144283
O	2.356062	1.693064	0.908942	O	2.464058	1.305403	-0.63012
C	-0.696215	0.930421	-1.037672	C	-0.73088	0.692575	1.139856
C	-0.796064	-0.447925	-0.820095	C	-0.970086	-0.639057	0.787554
C	0.200055	-1.047835	-0.039222	C	-0.034955	-1.286642	-0.02785
C	1.270702	-0.367308	0.56567	C	1.11406	-0.645145	-0.525149
C	-1.889961	-1.30842	-1.415854	C	-2.190668	-1.399439	1.243023
C	-1.246726	-2.658599	-1.787464	C	-1.755328	-2.83806	1.517847
C	-0.544271	-3.281179	-0.604487	C	-1.114711	-3.460141	0.306889
O	0.163269	-2.410871	0.203334	O	-0.237295	-2.639929	-0.38852
O	-0.432949	3.752865	-1.270521	O	-0.146062	3.387337	1.708058
O	-1.622835	1.53362	-1.802061	O	-1.648911	1.309643	1.949076
C	2.328149	-1.091481	1.380057	C	2.103505	-1.388574	-1.397351
C	3.483344	-1.573731	0.529024	C	3.093976	-2.181037	-0.584701
C	3.940578	-2.829376	0.383039	C	4.426338	-2.003813	-0.481719
C	5.127417	-3.11449	-0.509241	C	5.255059	-2.924389	0.376485
C	3.365178	-4.048655	1.061716	C	5.218281	-0.926732	-1.167365
O	-0.536408	-4.450607	-0.315246	O	-1.297896	-4.629736	-0.016319
C	3.83615	3.521201	1.187218	H	3.188221	1.959019	1.187202
C	1.807201	5.234168	-0.443714	C	1.413178	4.123692	-0.937948
C	-3.103633	-1.518116	-0.474968	C	-3.346423	-1.356415	0.216609
C	-3.885431	-0.247269	-0.121535	C	-3.985996	0.028162	0.067883

C	-5.10704	-0.530079	0.763468	C	-5.198438	-0.018634	-0.865769
C	-5.900125	0.730707	1.132844	C	-5.832741	1.363512	-1.021076
C	-7.121189	0.441859	2.013573	C	-7.037574	1.321976	-1.947841
H	3.111934	2.744895	-0.692204	C	4.208472	2.919194	-0.417946
H	1.085227	4.023879	1.194901	H	2.209581	4.210078	1.061898
H	-2.247434	-0.829143	-2.332928	H	-2.552784	-0.993806	2.196572
H	-0.494996	-2.508875	-2.574243	H	-2.620955	-3.44462	1.805726
H	-1.975268	-3.384382	-2.154986	H	-1.030012	-2.885461	2.339581
H	-1.403937	2.50438	-1.809235	H	-1.366849	2.242592	2.089379
H	2.708598	-0.395036	2.13547	H	1.56254	-2.082431	-2.054669
H	1.861335	-1.921247	1.912353	H	2.587003	-0.695797	-2.091624
H	3.994924	-0.783094	-0.021101	H	2.646147	-3.012574	-0.040214
H	4.857978	-3.820459	-1.306337	H	6.014407	-3.427571	-0.231123
H	5.51719	-2.205	-0.976026	H	5.759561	-2.356085	1.164619
H	5.942366	-3.582844	0.058986	H	4.651096	-3.698883	0.860718
H	3.09262	-4.808095	0.317938	H	5.750381	-0.322951	-0.424626
H	4.114397	-4.508962	1.719986	H	5.958261	-1.374071	-1.839062
H	2.474191	-3.838716	1.654348	H	4.608576	-0.244119	-1.762147
H	4.625808	2.774058	1.304446	H	4.58734	3.781829	0.138552
H	4.273285	4.413233	0.731702	H	4.060718	3.204993	-1.464743
H	3.457039	3.78271	2.180672	H	4.983291	2.145345	-0.420765
H	0.88085	5.774502	-0.646258	H	1.080942	3.39608	-1.68671
H	2.336775	5.117026	-1.39621	H	2.23005	4.710201	-1.37082
H	2.426247	5.839514	0.223012	H	0.576262	4.80725	-0.757181
H	-3.782066	-2.231514	-0.963925	H	-4.123784	-2.062137	0.536428
H	-2.76664	-2.003798	0.452064	H	-3.001585	-1.694179	-0.76809
H	-3.224018	0.462496	0.391309	H	-3.255597	0.737919	-0.335555
H	-4.207579	0.251885	-1.044854	H	-4.29743	0.398363	1.052465
H	-5.774367	-1.237856	0.249847	H	-5.941841	-0.72082	-0.468702
H	-4.781228	-1.034335	1.685176	H	-4.890691	-0.395207	-1.848671
H	-5.235291	1.436796	1.64935	H	-5.095089	2.068275	-1.422179
H	-6.223938	1.23599	0.21246	H	-6.145362	1.742441	-0.041123
H	-7.664044	1.361109	2.25919	H	-6.752837	0.976994	-2.947161
H	-7.8224	-0.233962	1.509528	H	-7.475242	2.319893	-2.045384
H	-6.825926	-0.03256	2.957093	H	-7.80805	0.649182	-1.558846

Table S10. DFT-optimized structures, total molecular energies, and Cartesian Coordinates of the dominant conformers 2*R*,3*R*,16*R*-**3b** and 2*S*,3*R*,16*S*-**4a** at the B3LYP/6-31G(d,p) level of theory.

							
2*R*,3*R*,16*R*-**3b**				2*S*,3*R*,16*S*-**4a**			
Etot= –1309.948983 Hartree				Etot= –1309.948991 Hartree			
Coordinates (Angstroms)				Coordinates (Angstroms)			
Atomic	X	Y	Z	Atomic	X	Y	Z
C	-2.736269	1.911659	-0.712214	C	2.652369	2.149313	0.460032
C	-2.063476	3.284561	-0.756481	C	1.907612	3.483148	0.402052
C	-0.830825	3.205314	0.123805	C	0.662649	3.261039	-0.423853
C	-0.117629	1.909309	0.170162	C	0.038708	1.919365	-0.375787
C	-0.660571	0.8263	-0.527498	C	0.660996	0.921743	0.385178
O	-1.835344	0.91533	-1.227605	O	1.835203	1.134469	1.061413
C	1.093224	1.767657	0.868241	C	-1.167933	1.654207	-1.042701
C	1.7808	0.545422	0.867085	C	-1.773307	0.392811	-0.950933
C	1.22795	-0.513132	0.127834	C	-1.142709	-0.577372	-0.153471
C	0.01562	-0.399035	-0.564456	C	0.066425	-0.339308	0.512614
O	-0.376592	4.162377	0.747963	O	0.138483	4.156101	-1.084267
C	-3.992865	1.830289	-1.573713	C	3.947097	2.224485	1.26211
C	-2.978365	4.416132	-0.294114	C	1.506404	4.057727	1.759205
O	1.65232	2.81284	1.56013	O	-1.802112	2.614129	-1.790617
O	1.933742	-1.738531	0.111774	O	-1.76546	-1.842015	-0.046456
C	1.697356	-2.707574	-0.852397	C	-1.45539	-2.728059	0.975391
C	0.69992	-2.326716	-1.912596	C	-0.476416	-2.213116	1.993831
C	-0.505834	-1.601644	-1.313923	C	0.672811	-1.452581	1.332418
O	2.304046	-3.774033	-0.860288	O	-1.989776	-3.828778	1.060621
C	-1.340839	-2.551381	-0.42532	C	1.561935	-2.40286	0.496997
C	3.10568	0.386776	1.581602	C	-3.092526	0.101351	-1.633572
C	4.272924	0.707751	0.685205	C	-4.266582	0.404585	-0.740595
C	5.222334	-0.123323	0.21184	C	-5.154667	-0.453409	-0.198904
C	6.317891	0.399317	-0.680398	C	-6.271927	0.054668	0.675453
C	5.307285	-1.598946	0.486834	C	-5.144878	-1.946905	-0.376734
C	-2.685096	-1.958027	0.012167	C	2.859223	-1.752768	0.003767
C	-3.525267	-2.984209	0.775688	C	3.759584	-2.770853	-0.698901
C	-4.860865	-2.386845	1.216331	C	5.049323	-2.118318	-1.196934
C	-5.70156	-3.401155	1.975081	C	5.94896	-3.12401	-1.895493
H	-3.009324	1.633925	0.315863	H	2.915301	1.821749	-0.556519
H	-1.705009	3.502642	-1.77136	H	2.533366	4.210911	-0.129443

H	-3.777779	2.119495	-2.608789	H	3.753286	2.397998	2.325945
H	-4.793339	2.467811	-1.189212	H	4.481086	1.269165	1.201866
H	-4.365852	0.800309	-1.606974	H	4.605867	3.011744	0.884081
H	-2.438636	5.369597	-0.262086	H	0.911892	3.34826	2.343976
H	-3.367904	4.224462	0.711934	H	2.387438	4.333292	2.346793
H	-3.824948	4.549281	-0.973756	H	0.899437	4.961693	1.631941
H	1.071244	3.60151	1.462515	H	-1.279112	3.445825	-1.747391
H	1.218338	-1.698823	-2.648013	H	-1.028473	-1.573306	2.693444
H	0.37342	-3.236583	-2.428758	H	-0.085149	-3.063661	2.563217
H	-1.124677	-1.275502	-2.159152	H	1.277747	-1.030627	2.145782
H	-1.538692	-3.473186	-0.987421	H	1.824884	-3.270181	1.117714
H	-0.77556	-2.844125	0.468657	H	1.008424	-2.791415	-0.366665
H	3.145156	1.052244	2.454217	H	-3.18618	0.703727	-2.545318
H	3.170067	-0.615432	2.015309	H	-3.095078	-0.930165	-1.999133
H	4.327368	1.762774	0.413845	H	-4.387725	1.469234	-0.5367
H	6.225784	1.474611	-0.86761	H	-7.242053	-0.212652	0.24393
H	7.296444	0.22541	-0.221028	H	-6.201437	-0.386943	1.674527
H	6.292602	-0.109076	-1.649533	H	-6.247598	1.143477	0.79149
H	4.532306	-1.964983	1.163456	H	-4.357779	-2.305345	-1.041973
H	5.217473	-2.161186	-0.449493	H	-5.00756	-2.439444	0.591575
H	6.273784	-1.841084	0.942065	H	-6.09979	-2.280132	-0.79905
H	-2.518005	-1.088411	0.657785	H	2.628878	-0.94255	-0.695971
H	-3.240128	-1.614923	-0.868705	H	3.398331	-1.315273	0.851861
H	-3.705852	-3.859193	0.138737	H	4.003652	-3.586202	-0.007307
H	-2.969275	-3.333186	1.654417	H	3.22158	-3.21484	-1.546201
H	-4.685783	-1.513891	1.856381	H	4.811123	-1.305195	-1.892218
H	-5.420298	-2.039099	0.340367	H	5.592106	-1.675215	-0.353428
H	-5.182407	-3.744768	2.875813	H	5.447851	-3.562772	-2.76397
H	-6.651951	-2.952663	2.281287	H	6.86572	-2.636009	-2.242924
H	-5.923084	-4.27283	1.350861	H	6.232693	-3.935693	-1.21648