

Supporting Information

Scalemic Caged Xanthoness Isolated from the Stem Bark Extract of *Garcinia propinqua*

Teerayut Sriyatep,[†] Raymond J. Andersen,[‡] Brian O. Patrick,[‡] Stephen G. Pyne,[§] Chatchai Muanprasat,[⊥] Sawinee Seemakhan,[⊥] Suparek Borwornpinyo,[⊥] and Surat Laphookhieo^{*,†}

[†]Natural Products Research Laboratory, School of Science, Mae Fah Luang University, Chiang Rai 57100, Thailand.

[‡]Departments of Chemistry and Earth, Ocean & Atmospheric Sciences, University of British Columbia, 2036 Main Mall, Vancouver, BC, Canada V6T 1Z1.

[§]School of Chemistry, University of Wollongong, Wollongong, New South Wales, 2522, Australia

[⊥]Department of Physiology, Faculty of Science, Mahidol University, Rajathevi, Bangkok 10400, Thailand

[⊥]Excellent Center of Drug Discovery, Faculty of Science, Mahidol University, Rajathevi, Bangkok 10400, Thailand

*Corresponding author. Tel: +66-5391-6238; Fax: +66-5391-6776.

E-mail address: surat.lap@mfu.ac.th

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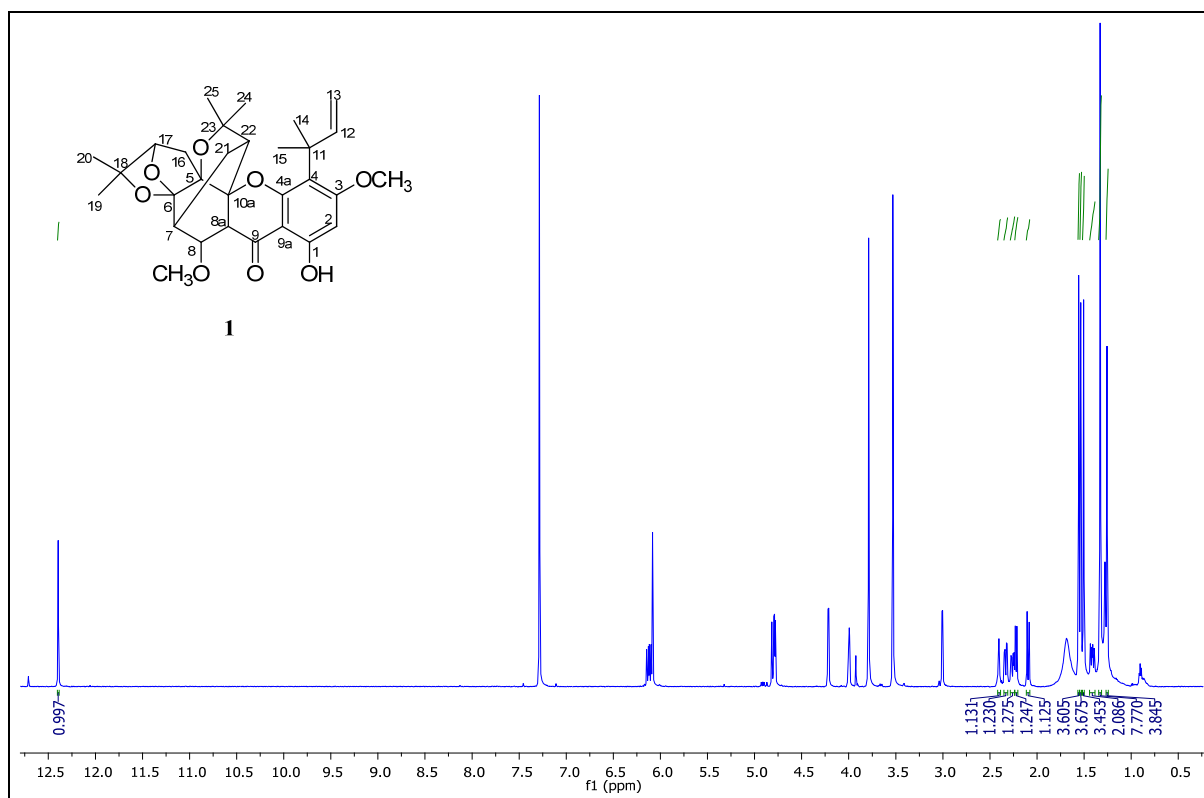


Figure S1. ¹H NMR spectrum of compound **1** in CDCl₃ (600 MHz).

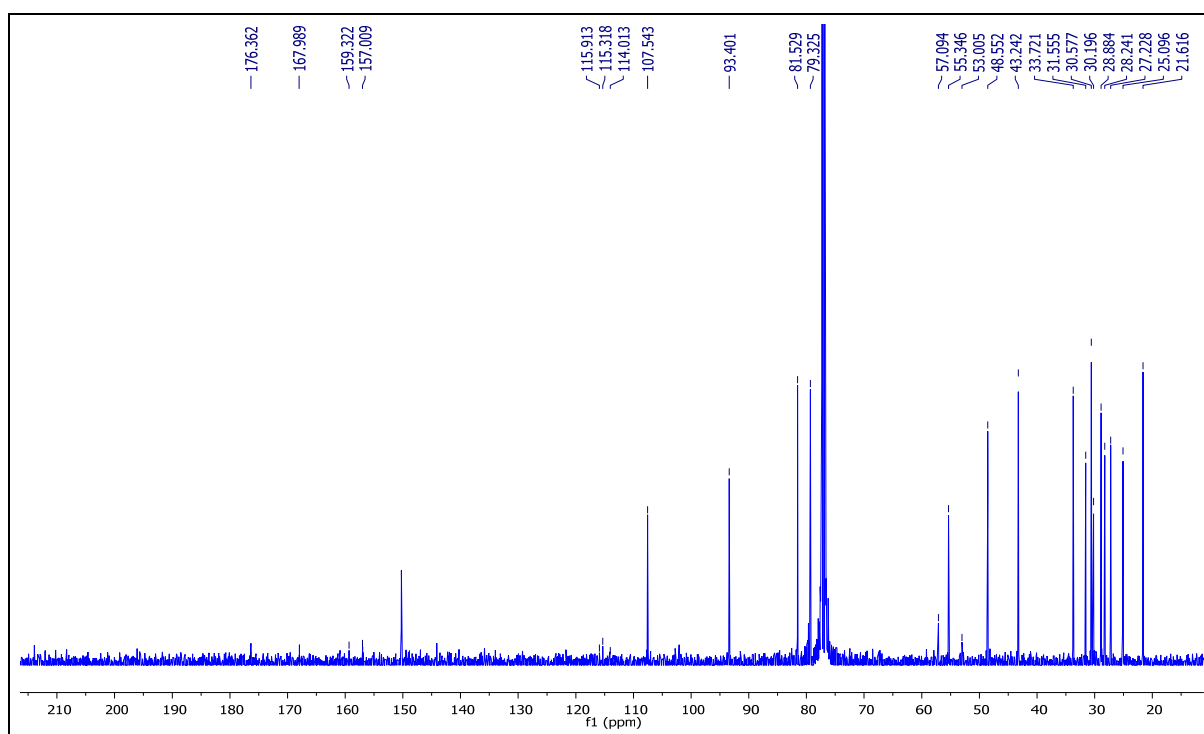


Figure S2. ¹³C NMR spectrum of compound **1** in CDCl₃ (150 MHz).

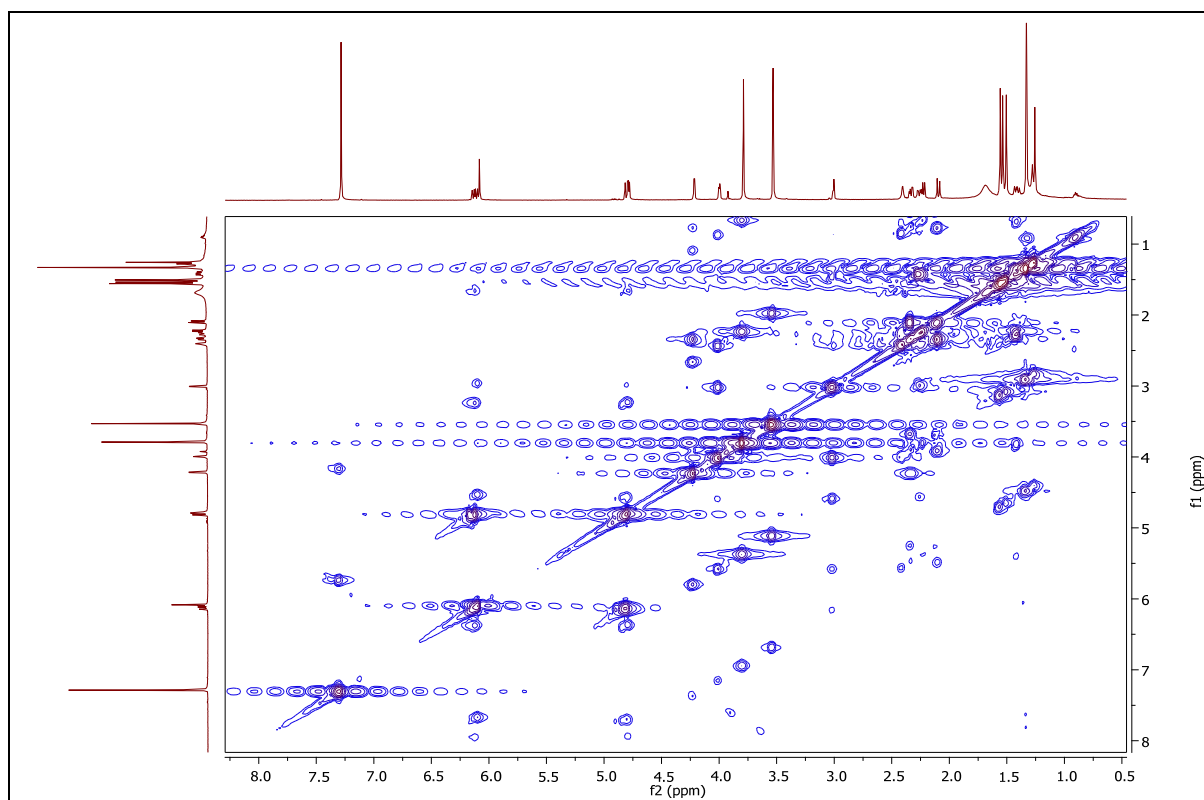


Figure S3. COSY spectrum of compound **1** in CDCl₃ (600 MHz).

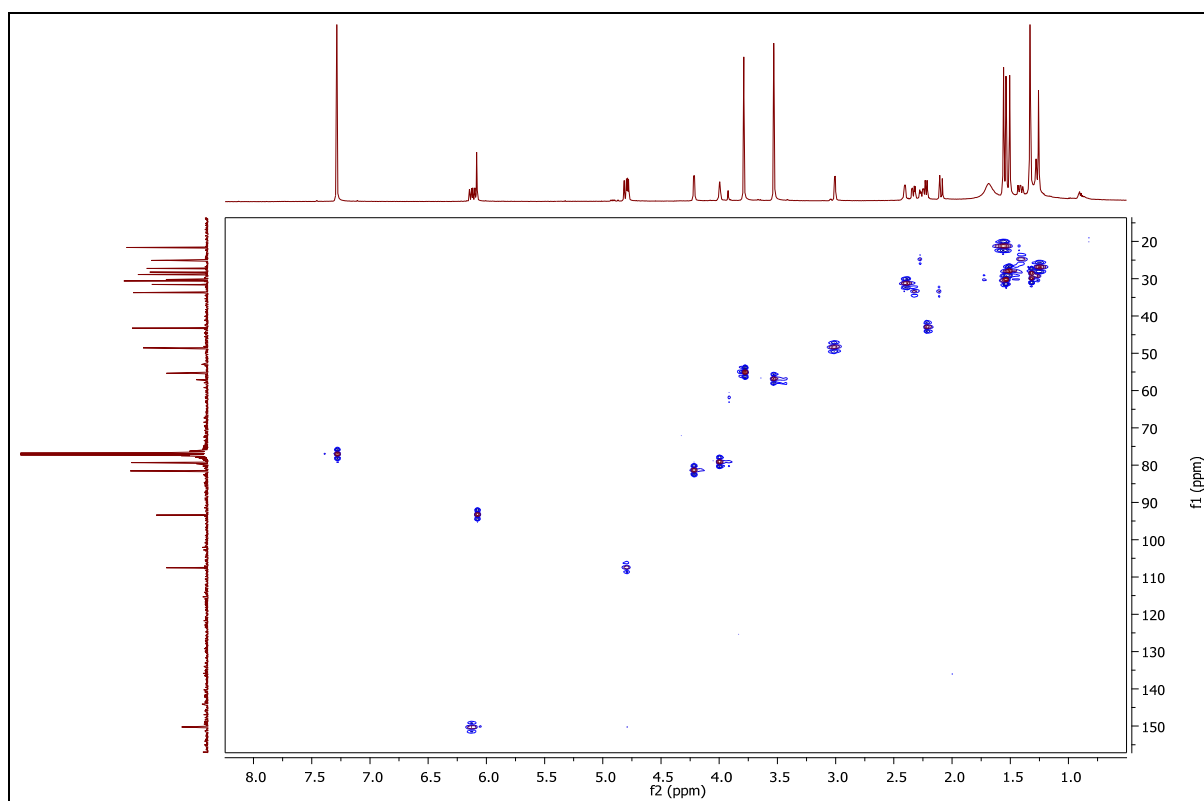


Figure S4. HSQC spectrum of compound **1** in CDCl₃ (600 MHz).

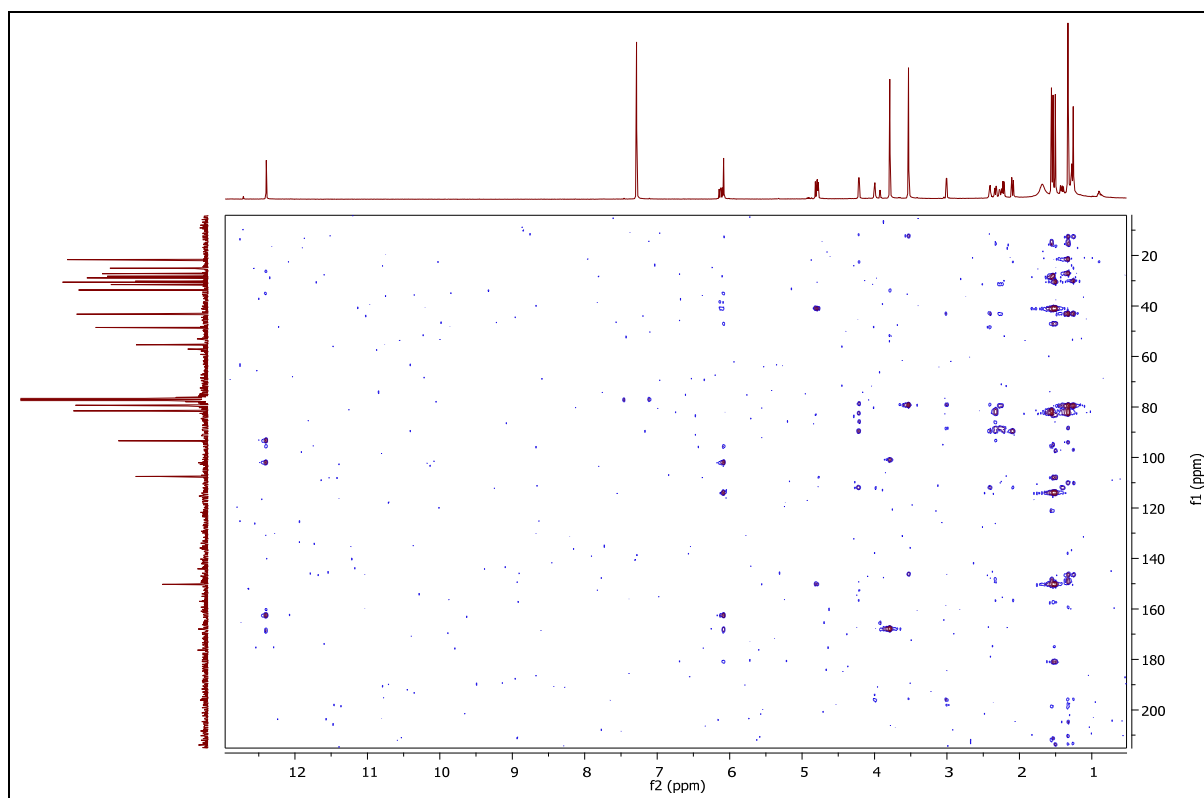


Figure S5. HMBC spectrum of compound **1** in CDCl₃ (600 MHz).

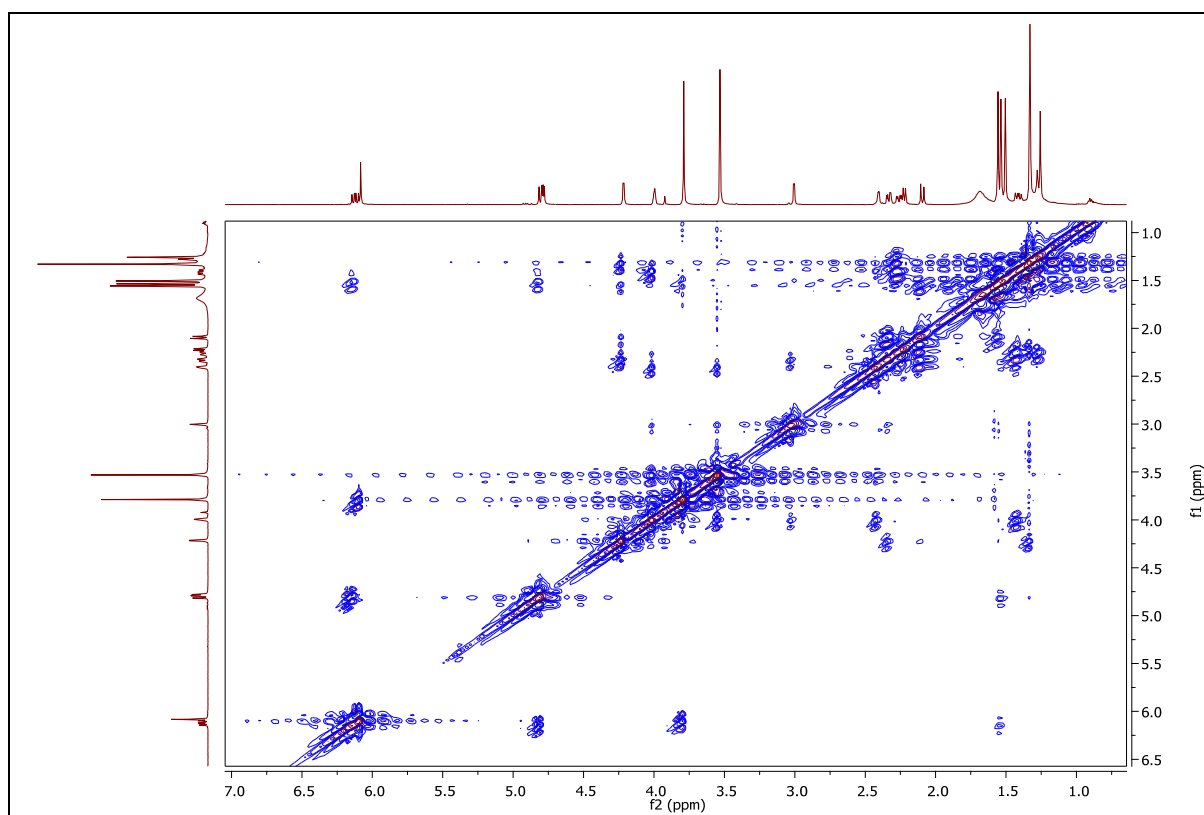


Figure S6. NOESY spectrum of compound (+)-**1** in CDCl₃ (600 MHz).

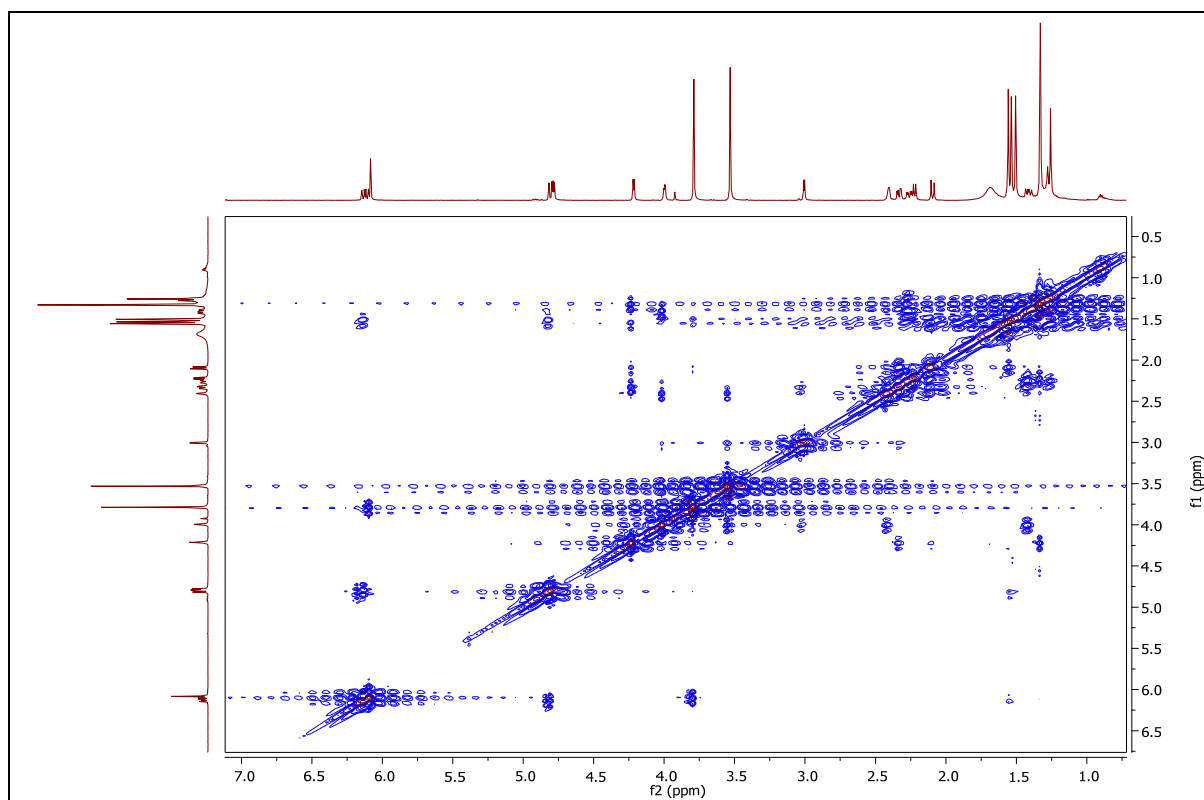


Figure S7. NOESY spectrum of compound (–)-1 in CDCl₃ (600 MHz).

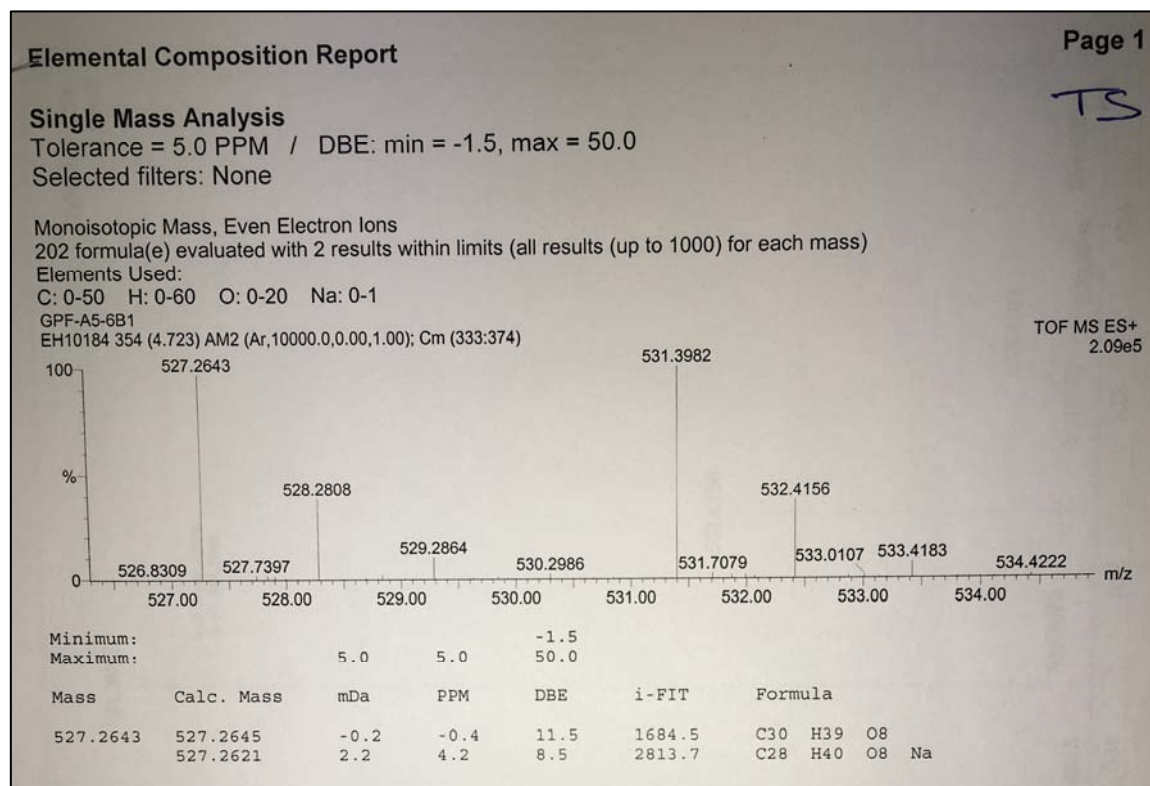


Figure S8. ESI-TOF-MS of compound 1.

Table S1. ^1H , ^{13}C and HMBC Spectroscopic Data of **1** in CDCl_3 .

Position	1			HMBC
	δ_{C} , type		δ_{H} , (J in Hz)	
1	162.5	C	-	
2	93.4	CH	6.08, s	1,3,4,9a
3	168.0	C	-	
4	114.0	C	-	
4a	157.0	C	-	
5	89.5	C	-	
6	115.3	C	-	
7	31.6	CH	2.41, m	5,6,8,8a,22
8	79.3	CH	4.00, dd (4.4, 2.6)	9
8a	48.6	CH	3.01, d (4.4)	8,9,10a,22
9	196.1	C	-	
9a	102.1	C	-	
10a	88.5	C	-	
11	41.2	C	-	
12	150.3	CH	6.12, dd (17.4, 10.8)	4,11
13	107.5	CH ₂	4.80, dd (17.4, 1.2) 4.79, dd (10.8, 1.2)	11,12
14	30.6	CH ₃	1.54, s	4,11,12,13,15
15	28.2	CH ₃	1.51, s	4,11,12,13,14
16	33.7	CH ₂	2.33, dd (13.4, 4.7) 2.09, d (13.4)	5,10a,17,18 5,6
17	81.5	CH	4.21, d (4.7)	5,6,18
18	85.8	C	-	
19	21.6	CH ₃	1.56, s	17,20
20	28.9	CH ₃	1.33, s	17,19
21	25.1	CH ₂	2.26, dd (15.2, 5.2) 1.41, dd (15.2, 10.2)	6,7,8,10a,22 6
22	43.2	CH	2.22, d (10.2)	5,10a,24
23	79.5	C	-	
24	27.2	CH ₃	1.26, s	22,23,25
25	30.2	CH ₃	1.33, s	22,23,24
OH-1	-		12.39, s	1,2,9a
OMe-3	55.4	OCH ₃	3.79, s	3
OMe-8	57.1	OCH ₃	3.53, s	8

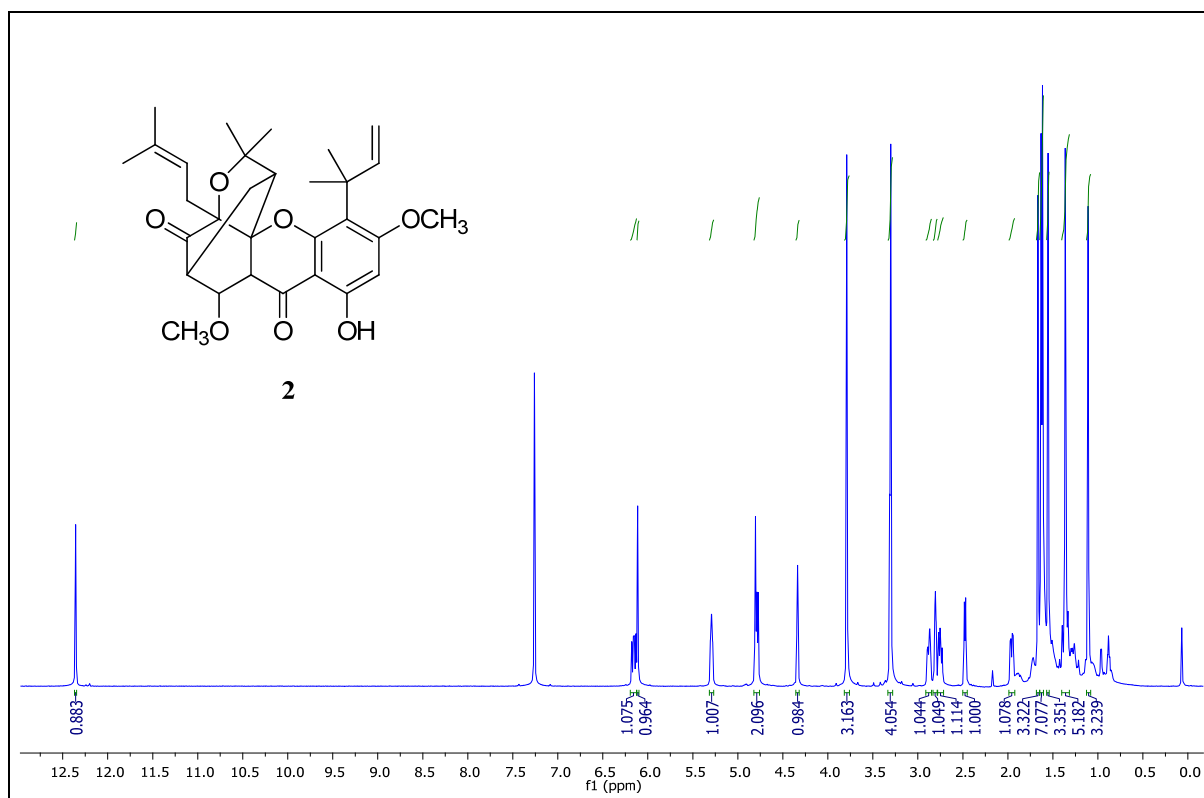


Figure S9. ^1H NMR spectrum of compound **2** in CDCl_3 (600 MHz).

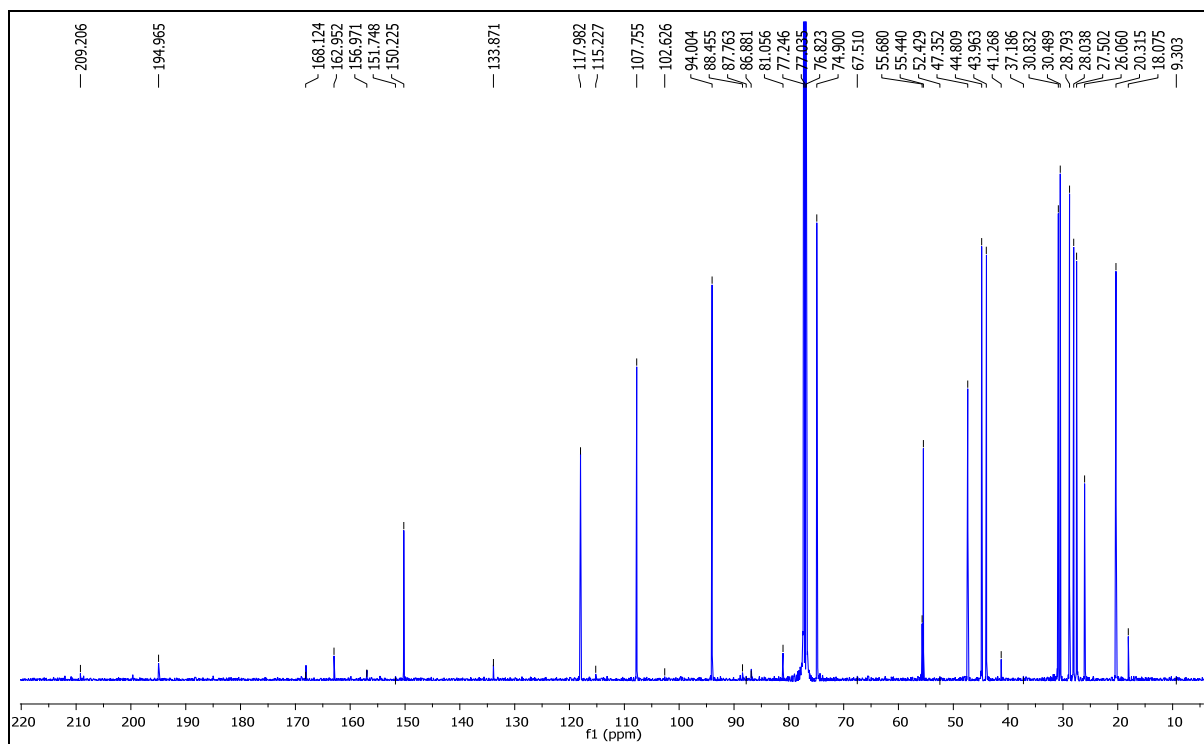


Figure S10. ^{13}C NMR spectrum of compound **2** in CDCl_3 (150 MHz).

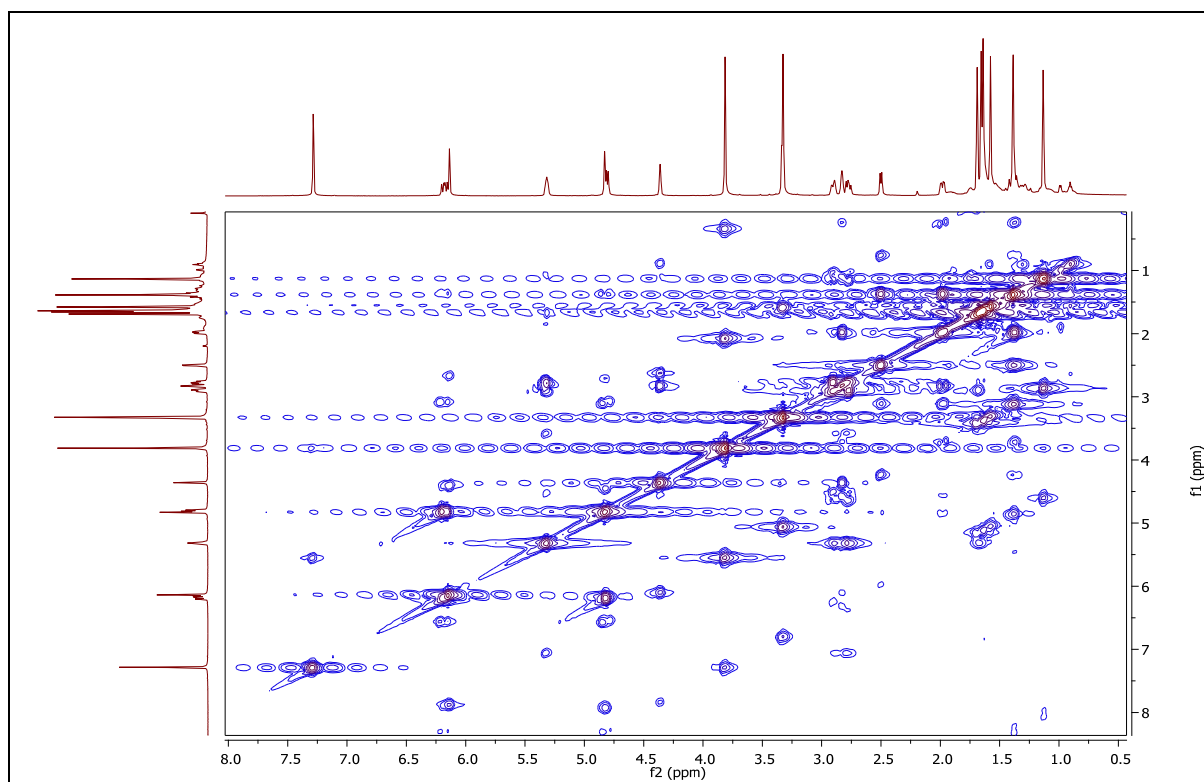


Figure S11. COSY spectrum of compound **2** in CDCl₃ (600 MHz).

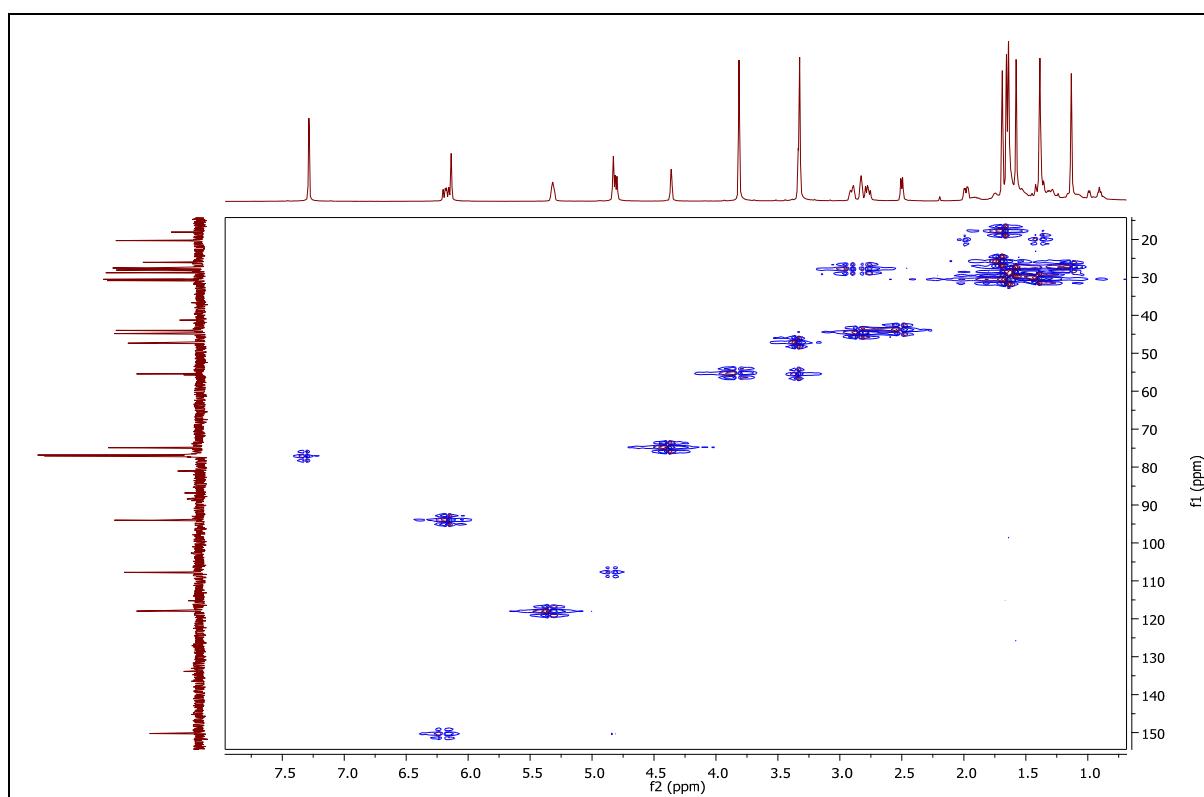


Figure S12. HSQC spectrum of compound **2** in CDCl₃ (600 MHz).

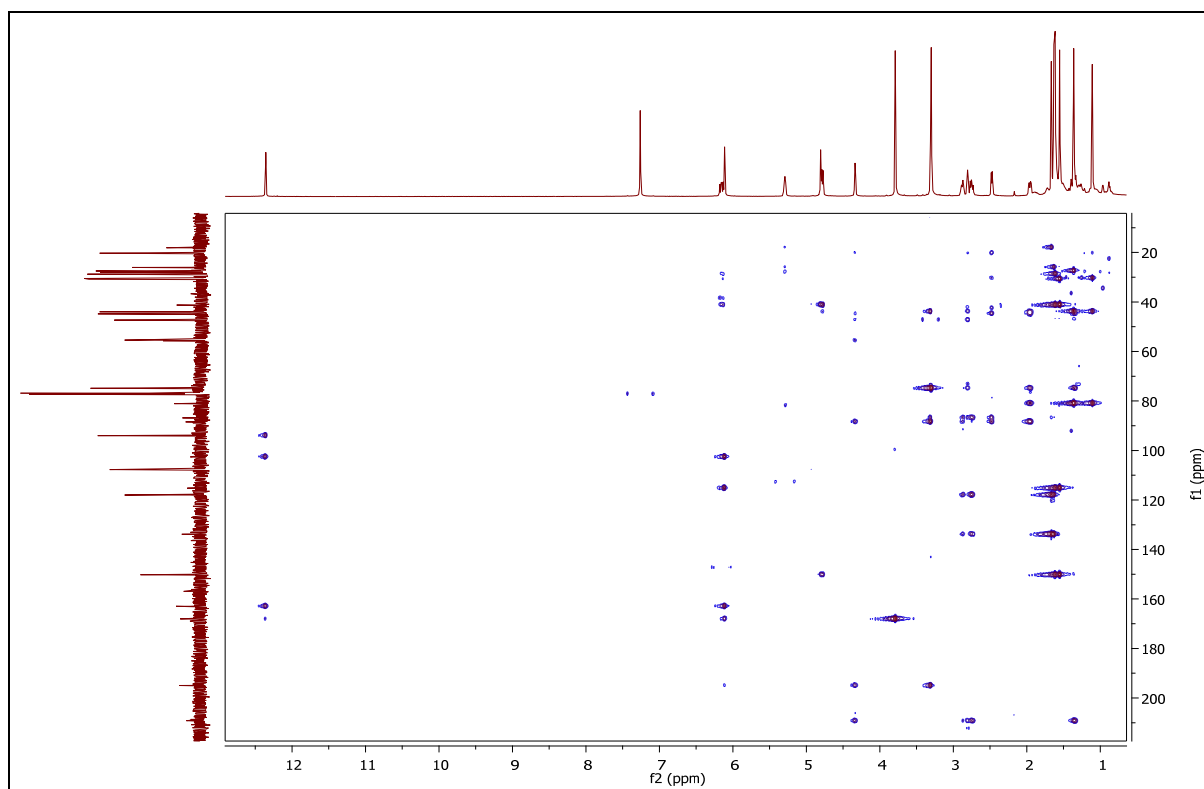


Figure S13. HMBC spectrum of compound **2** in CDCl₃ (600 MHz).

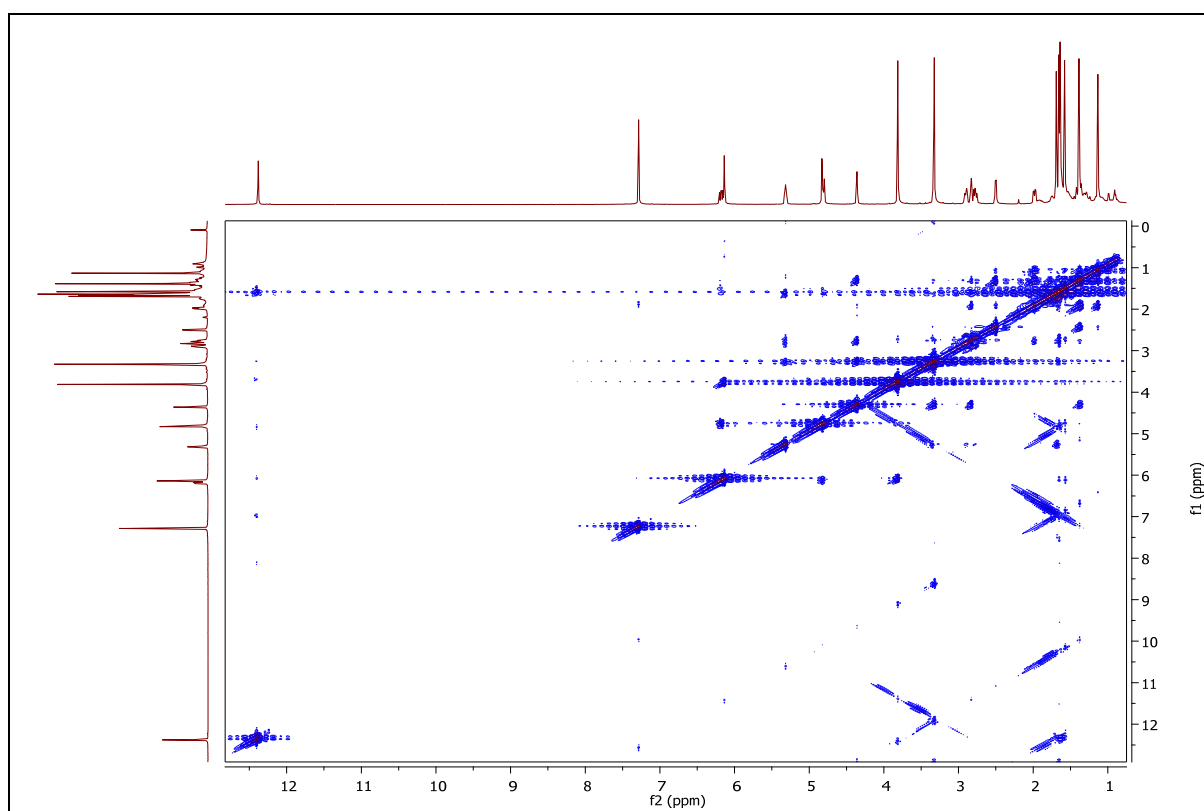


Figure S14. NOESY spectrum of compound (+)-**2** in CDCl₃ (600 MHz).

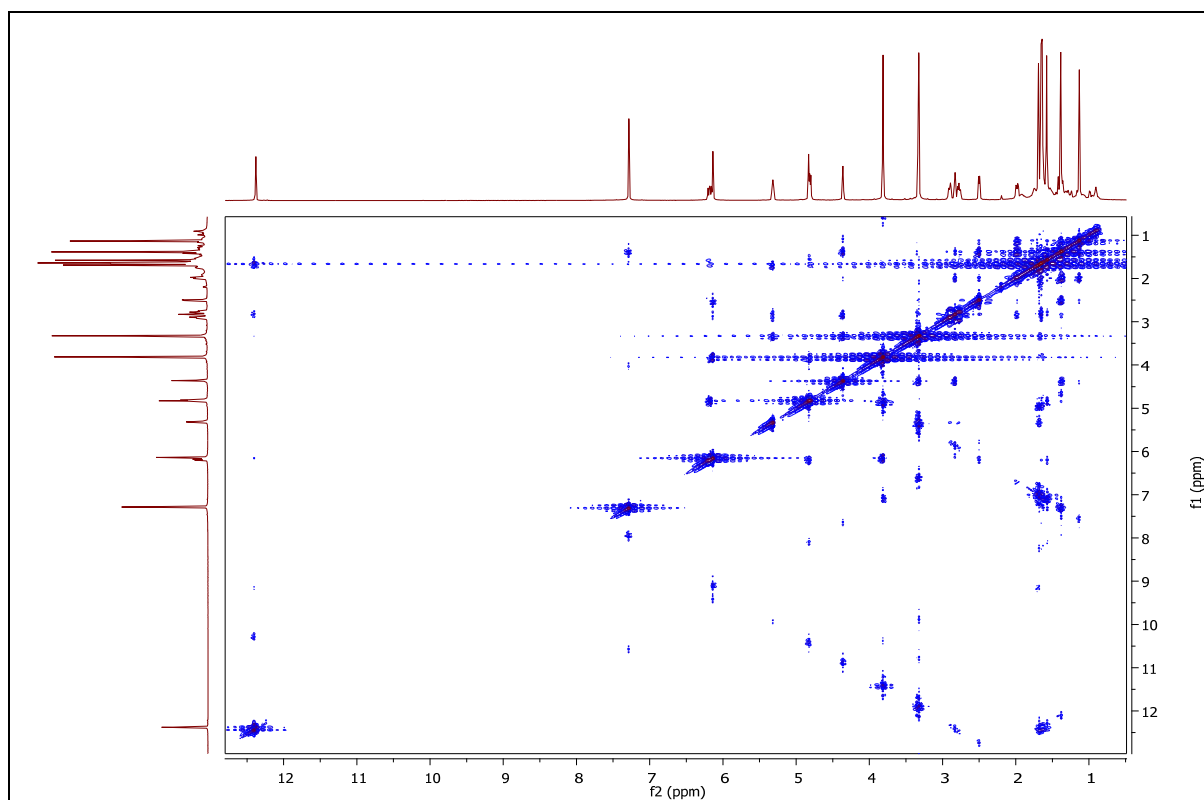


Figure S15. NOESY spectrum of compound (-)-2 in CDCl₃ (600 MHz).

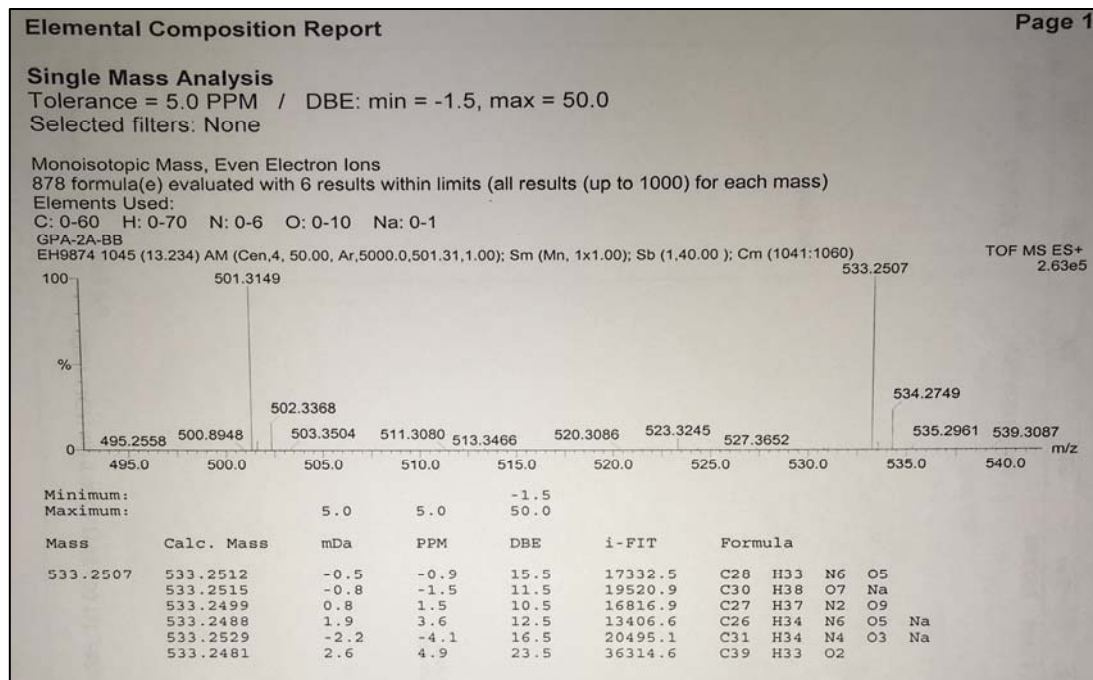


Figure S16. ESI-TOF-MS of compound 2.

Table S2. ^1H , ^{13}C and HMBC Spectroscopic Data of **2** in CDCl_3 .

Position	2			HMBC
	δ_{C} , type		δ_{H} , (J in Hz)	
1	163.0	C	-	
2	94.0	CH	6.11, s	1,3,4,9a
3	168.1	C	-	
4	115.2	C	-	
4a	157.0	C	-	
5	86.9	C	-	
6	209.2	C	-	
7	44.8	CH	2.81, m	5,6,8,8a,21,22
8	74.9	CH	4.34, m	6,7,8a,9,10a,21
8a	47.4	CH	3.31, m	5,8,9,10a,22
9	195.0	C	-	
9a	102.6	C	-	
10a	88.5	C	-	
11	41.3	C	-	
12	150.2	C	6.16, dd (17.2, 10.8)	4,11,14,15
13	107.8	CH ₂	4.80, d (17.2) 4.78, d (10.8)	11,12
14	30.8	CH ₃	1.55, s	4,11,12,15
15	28.8	CH ₃	1.62, s	4,11,12,14
16	28.0	CH ₂	2.88, m 2.75, dd (14.0, 9.5)	5,6,10a,17,18
17	118.0	CH	5.29, t (7.8)	16, 19, 20
18	133.9	C	-	
19	18.1	CH ₃	1.63, s	17,18,20
20	26.1	CH ₃	1.67, s	17,18,19
21	20.3	CH ₂	1.96, dd (14.4, 5.4) 1.39, m	6,8,10a,22,23 6,7,8,22,23
22	44.0	CH	2.48, d (8.5)	5,7,10a,21,24
23	81.1	C	-	
24	27.5	CH ₃	1.11, s	22,23,25
25	30.5	CH ₃	1.36, s	22,23,24
OH-1	-	-	12.36, s	1,2,9a
OMe-3	55.4	OCH ₃	3.79, s	3
OMe-8	55.7	OCH ₃	3.30, s	8

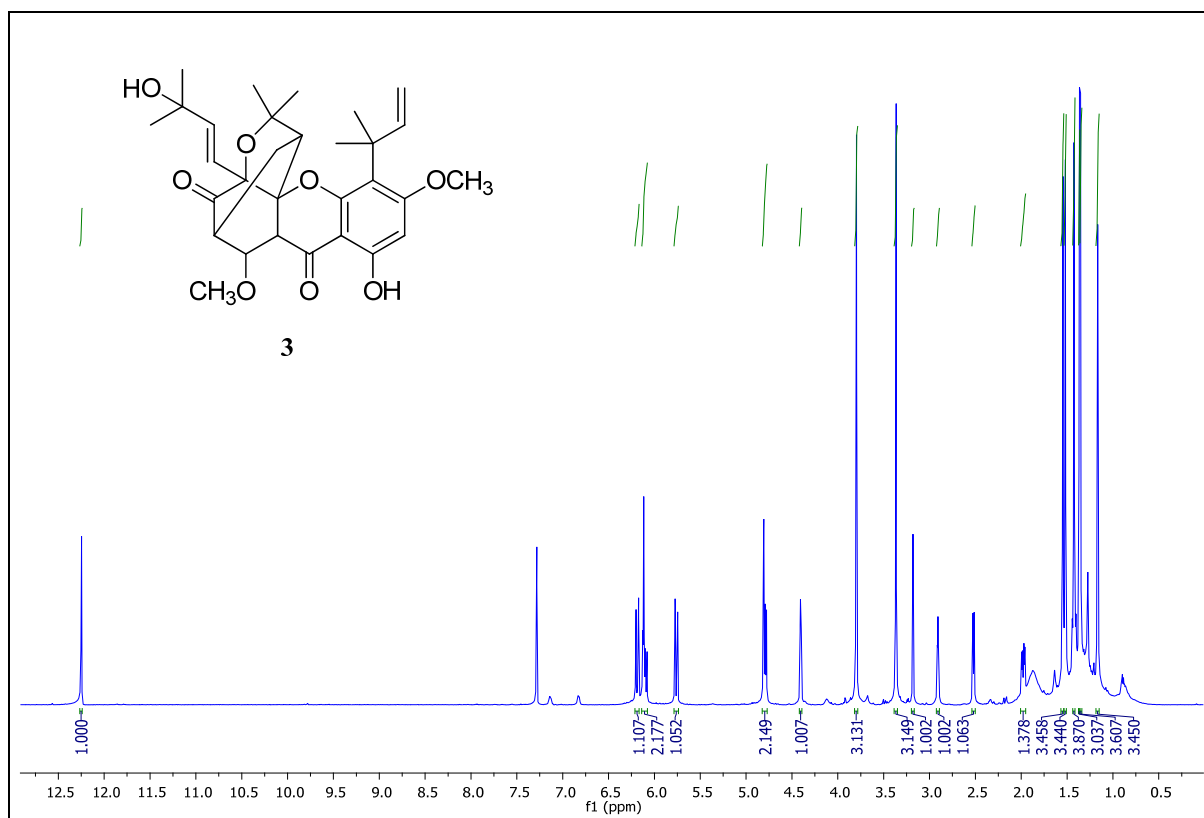


Figure S17. ¹H NMR spectrum of compound **3** in CDCl₃ (600 MHz).

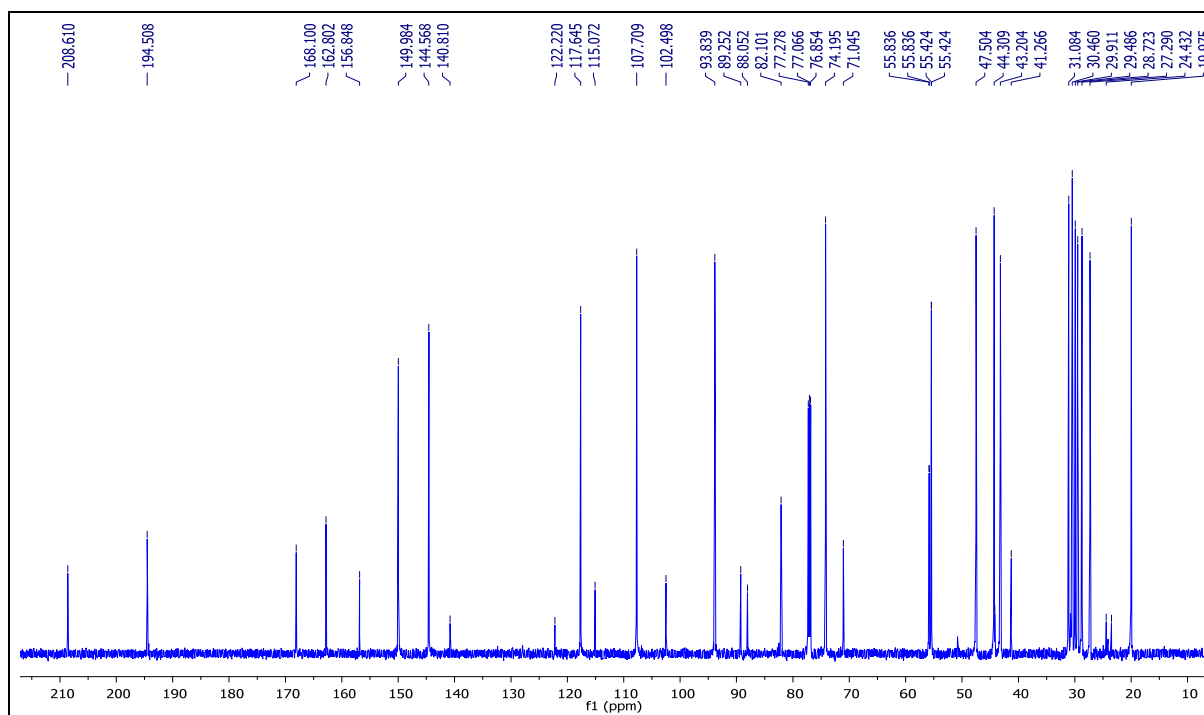


Figure S18. ¹³C NMR spectrum of compound **3** in CDCl₃ (150 MHz).

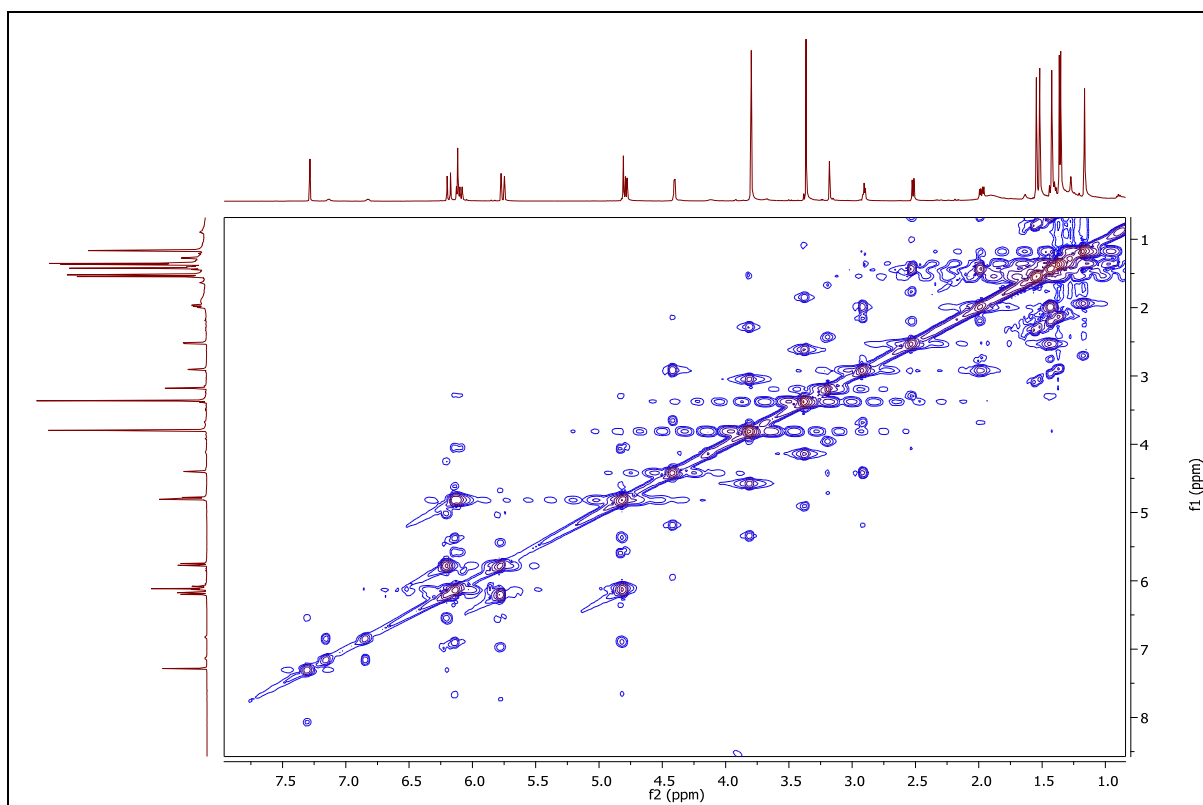


Figure S19. COSY spectrum of compound **3** in CDCl₃ (600 MHz).

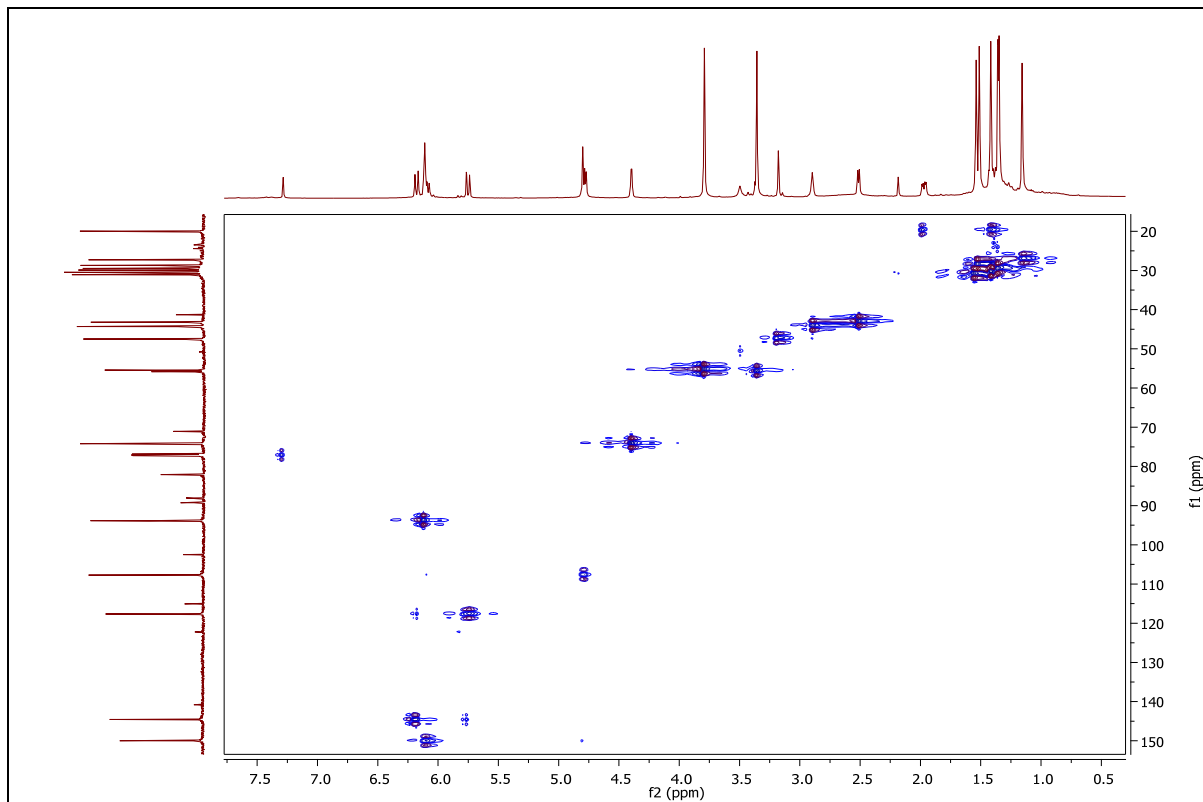


Figure S20. HSQC spectrum of compound **3** in CDCl₃ (600 MHz).

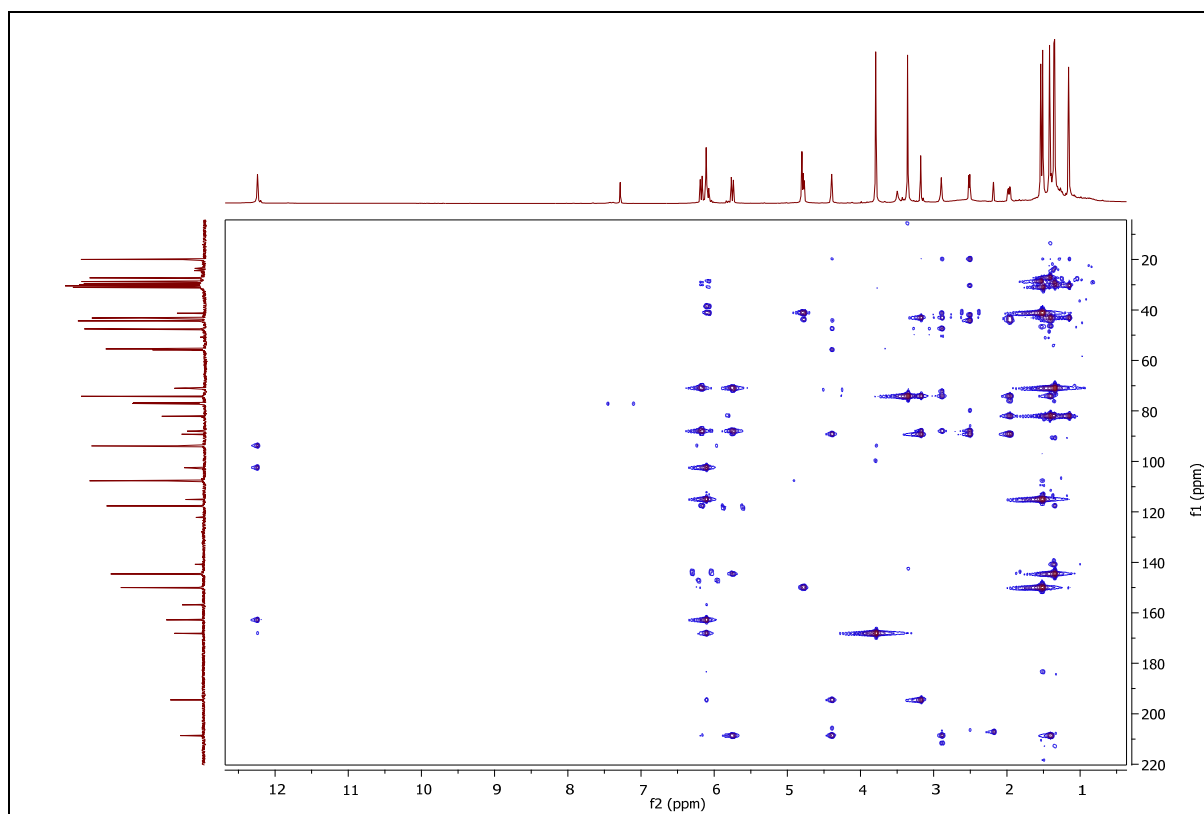


Figure S21. HMBC spectrum of compound **3** in CDCl_3 (600 MHz)

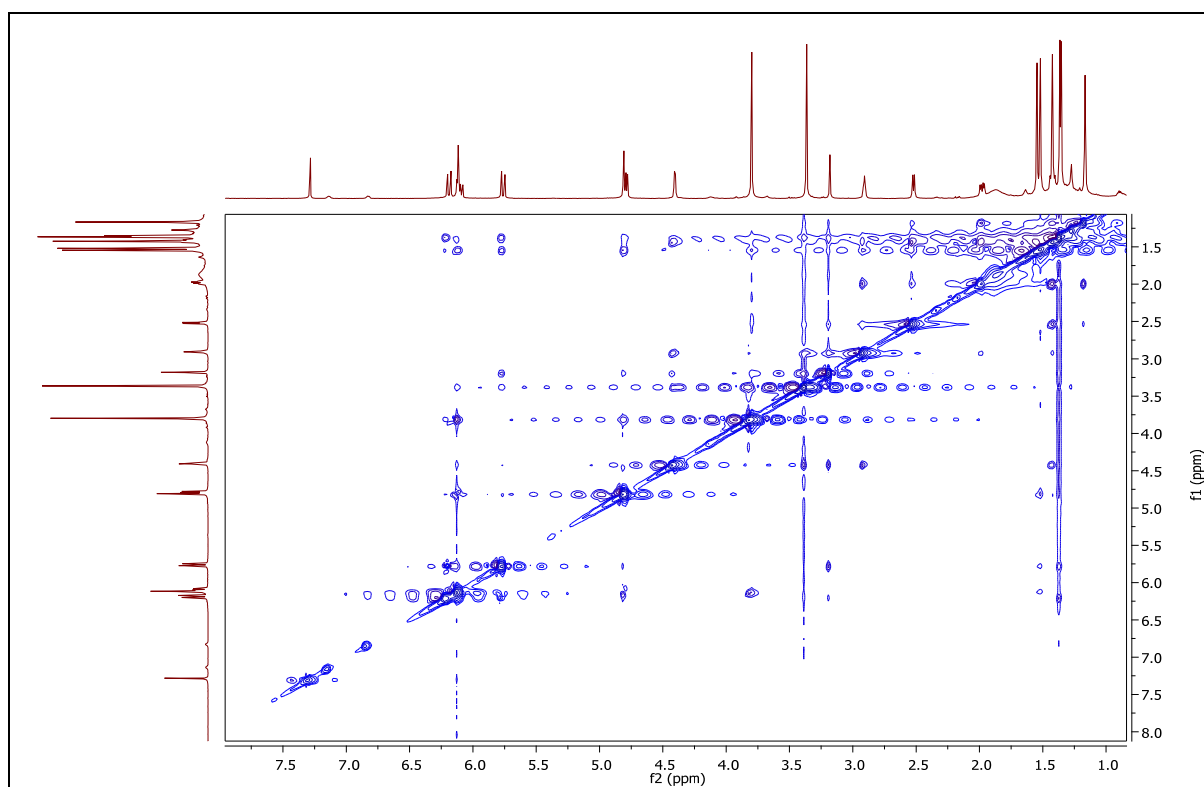


Figure S22. NOESY spectrum of compound (+)-**3** in CDCl_3 (600 MHz).

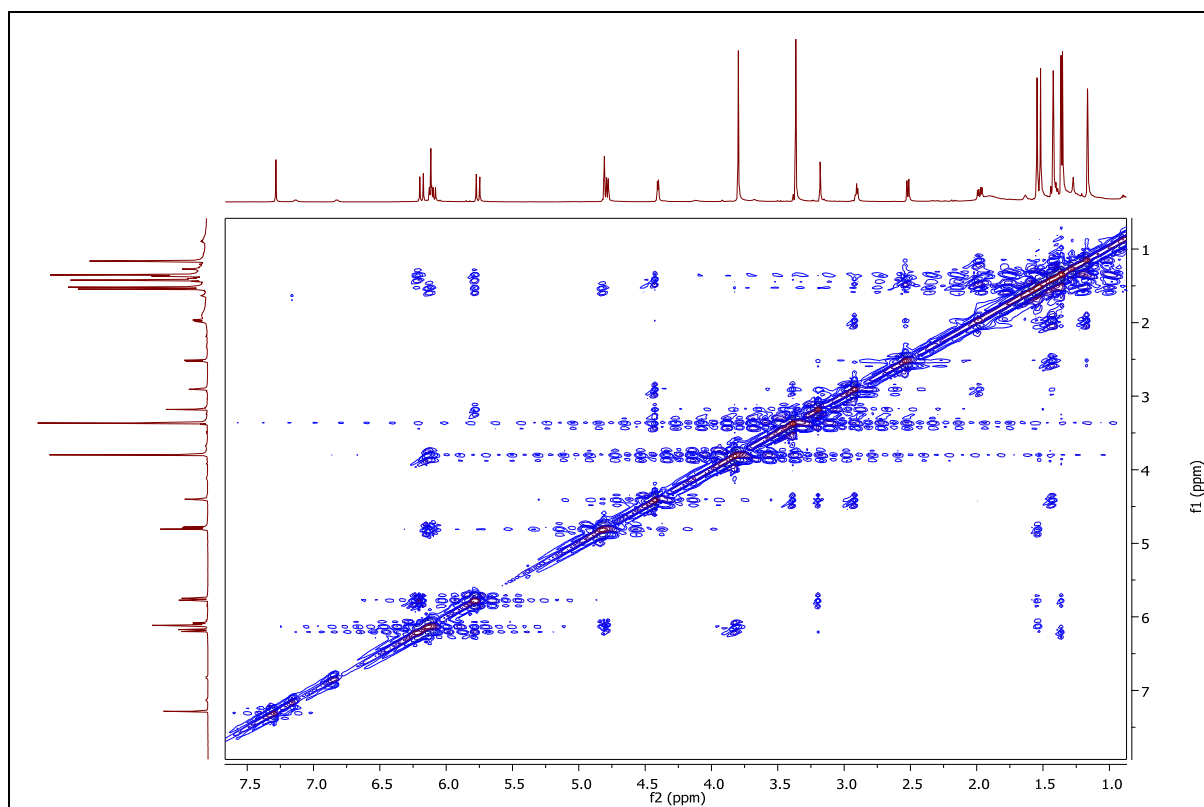


Figure S23. NOESY spectrum of compound **(-)-3** in CDCl_3 (600 MHz).

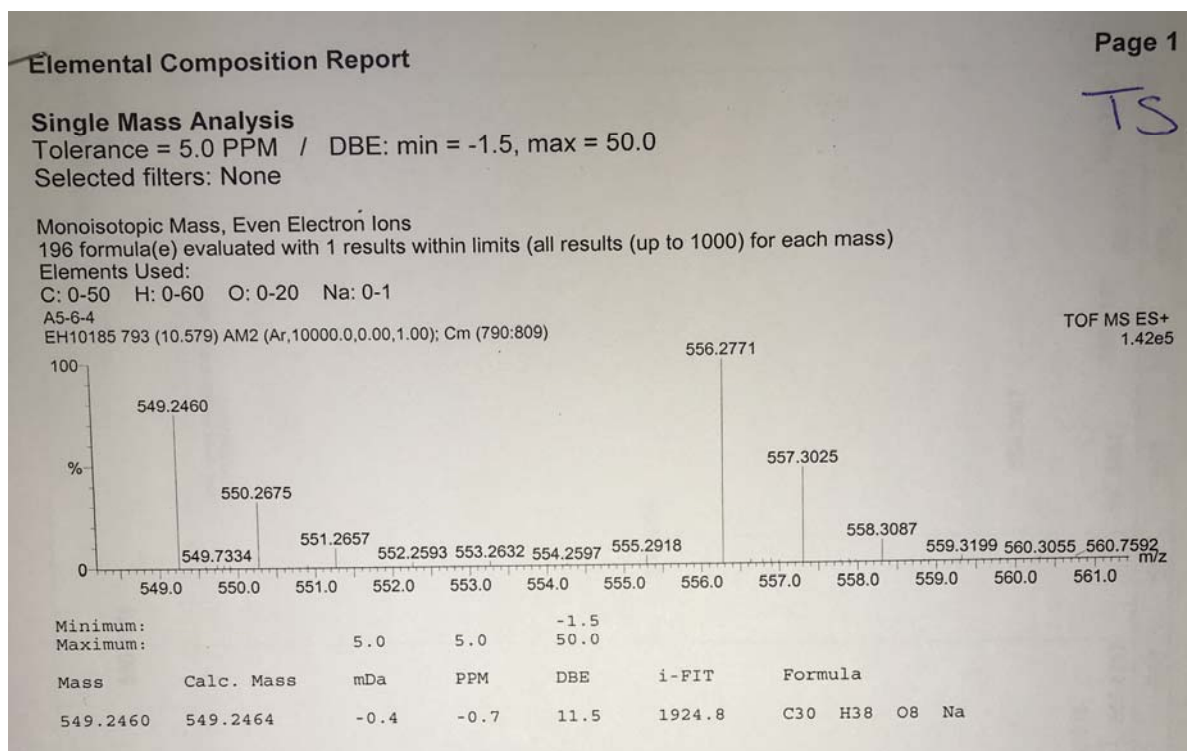


Figure S24. ESI-TOF-MS of compound **3**.

Table S3. ^1H , ^{13}C and HMBC Spectroscopic Data of **3** in CDCl_3 .

Position	3			HMBC
	δ_{C} , type		δ_{H} , (J in Hz)	
1	162.8	C	-	-
2	93.8	CH	6.11, s	1,3,9a
3	168.1	C	-	-
4	115.1	C	-	-
4a	156.9	C	-	-
5	88.1	C	-	-
6	208.6	C	-	-
7	44.3	CH	2.90, m	5,6,8,8a,22
8	74.2	CH	4.40, d (3.3)	6,7,8a,9,10a,OMe-8
8a	47.5	CH	3.18, m	5,8,9,10a,22
9	194.5	C	-	-
9a	102.5	C	-	-
10a	89.3	C	-	-
11	41.3	C	-	-
12	150.0	C	6.09, dd (17.6, 10.9)	4,11,14,15
13	107.7	CH ₂	4.80, d (17.6) 4.78, d (10.9)	11,12
14	31.1	CH ₃	1.54, s	4,11,12,15
15	28.7	CH ₃	1.51, s	4,11,12,14
16	117.7	CH ₂	5.75, d (16.0)	5,6,17,18
17	144.6	CH	6.18, d (16.0)	5,16,18
18	71.1	C	-	-
19	29.5	CH ₃	1.35, s	17,18,20
20	29.9	CH ₃	1.36, s	17,18,19
21	20.0	CH ₂	1.97, dd (14.6, 5.8) 1.43, m	7,8,10a,22, 23
22	43.2	CH	2.51, d (8.3)	5,7,10a,21,24
23	82.1	C	-	-
24	27.3	CH ₃	1.42, s	22,23,25
25	30.5	CH ₃	1.16, s	22,23,24
OH-1	-	-	12.24, s	1,2,9a
OMe-3	55.4	OCH ₃	3.79, s	3
OMe-8	55.8	OCH ₃	3.36, s	8

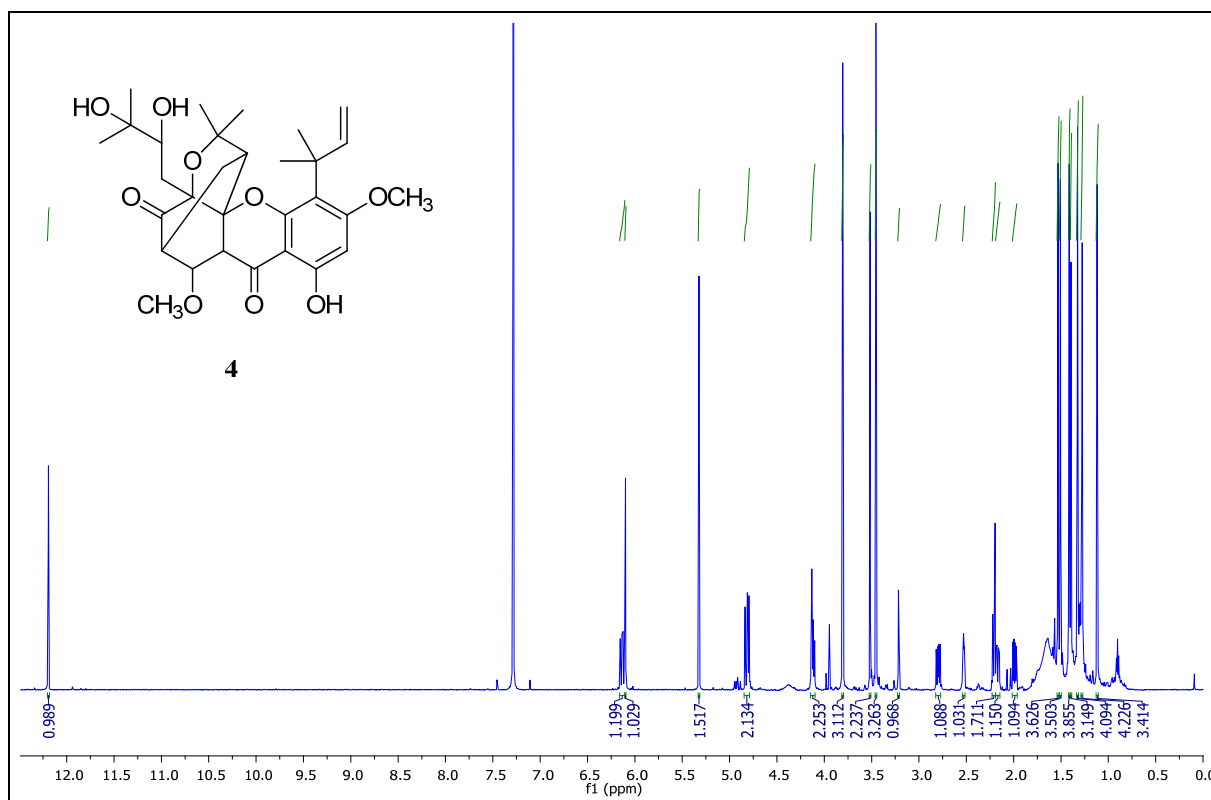


Figure S25. ¹H NMR spectrum of compound **4** in CDCl₃ (600 MHz).

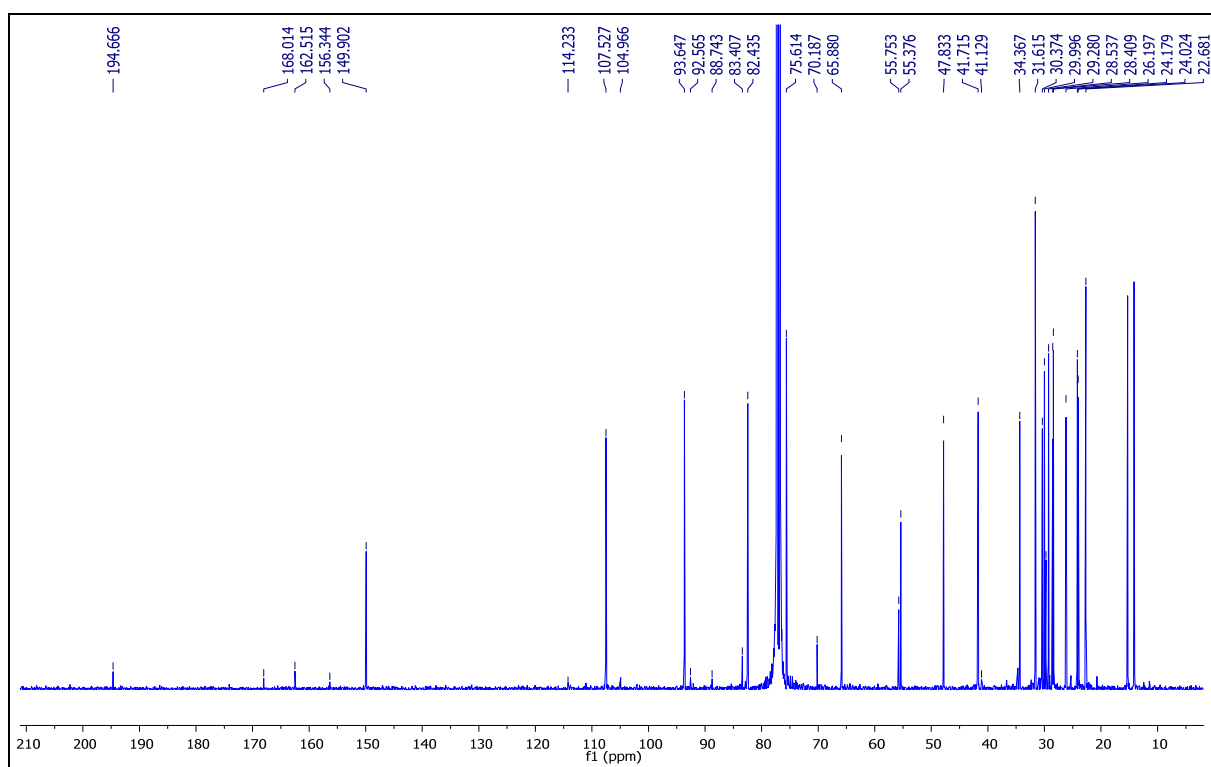


Figure S26. ¹³C NMR spectrum of compound **4** in CDCl₃ (150 MHz).

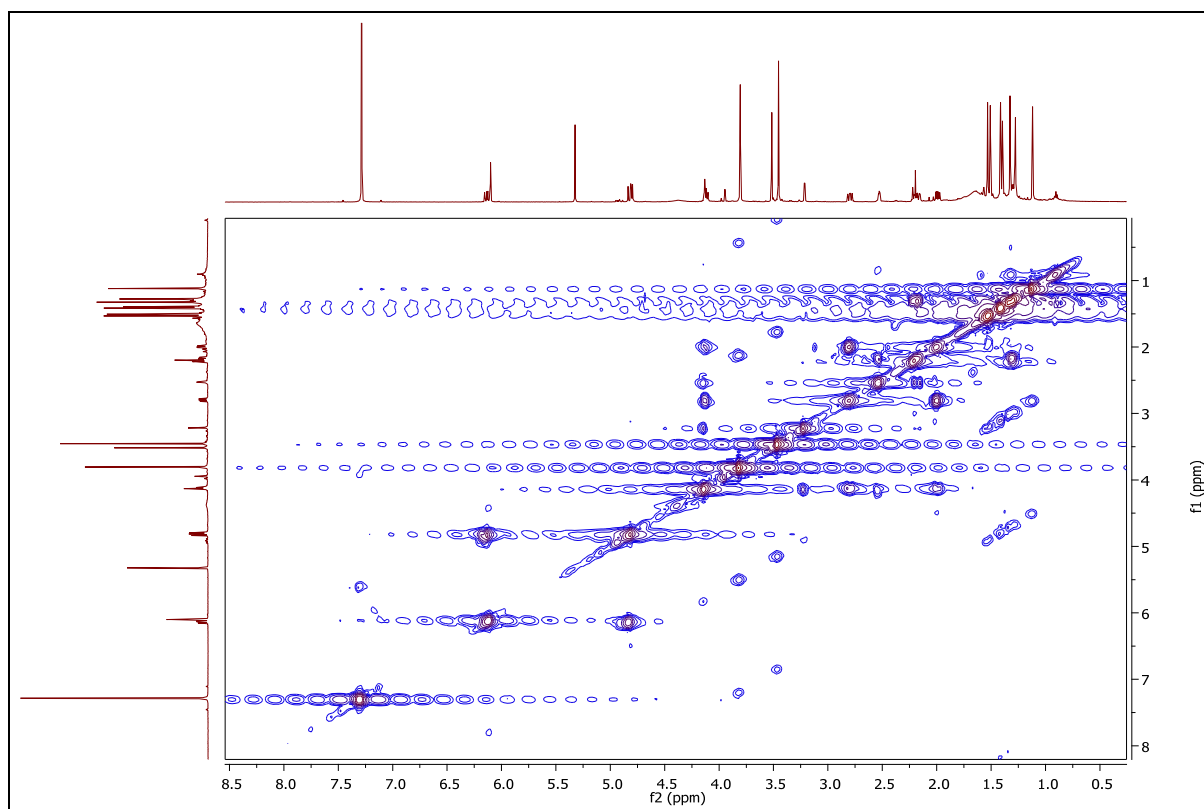


Figure S27. COSY spectrum of compound **4** in CDCl₃ (600 MHz).

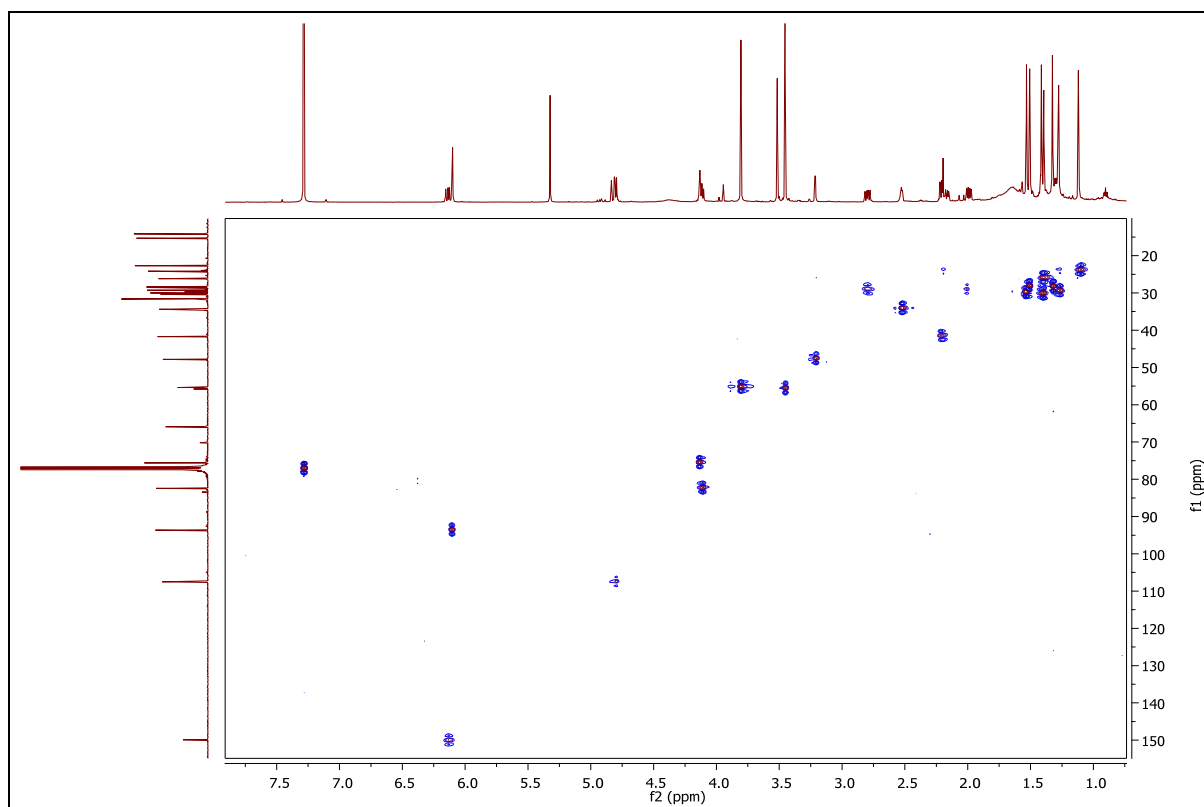


Figure S28. HSQC spectrum of compound **4** in CDCl₃ (600 MHz).

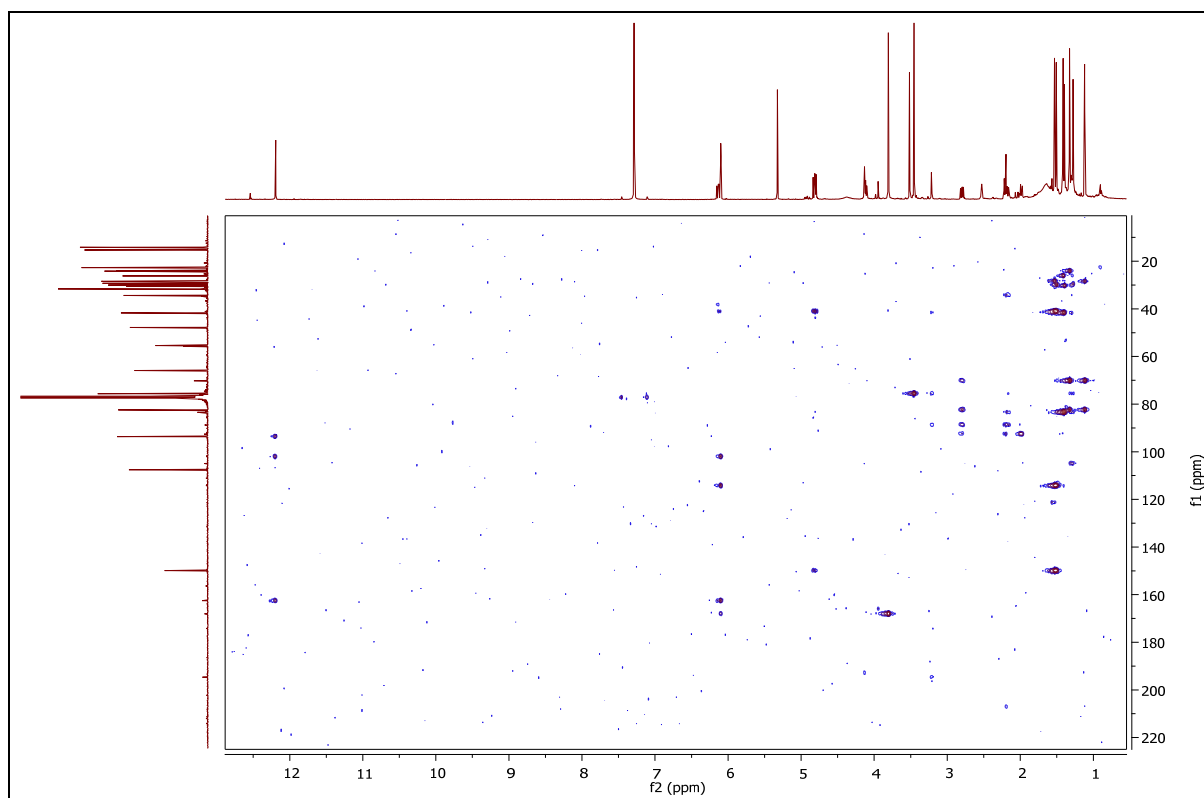


Figure S29. HMBC spectrum of compound **4** in CDCl₃ (600 MHz).

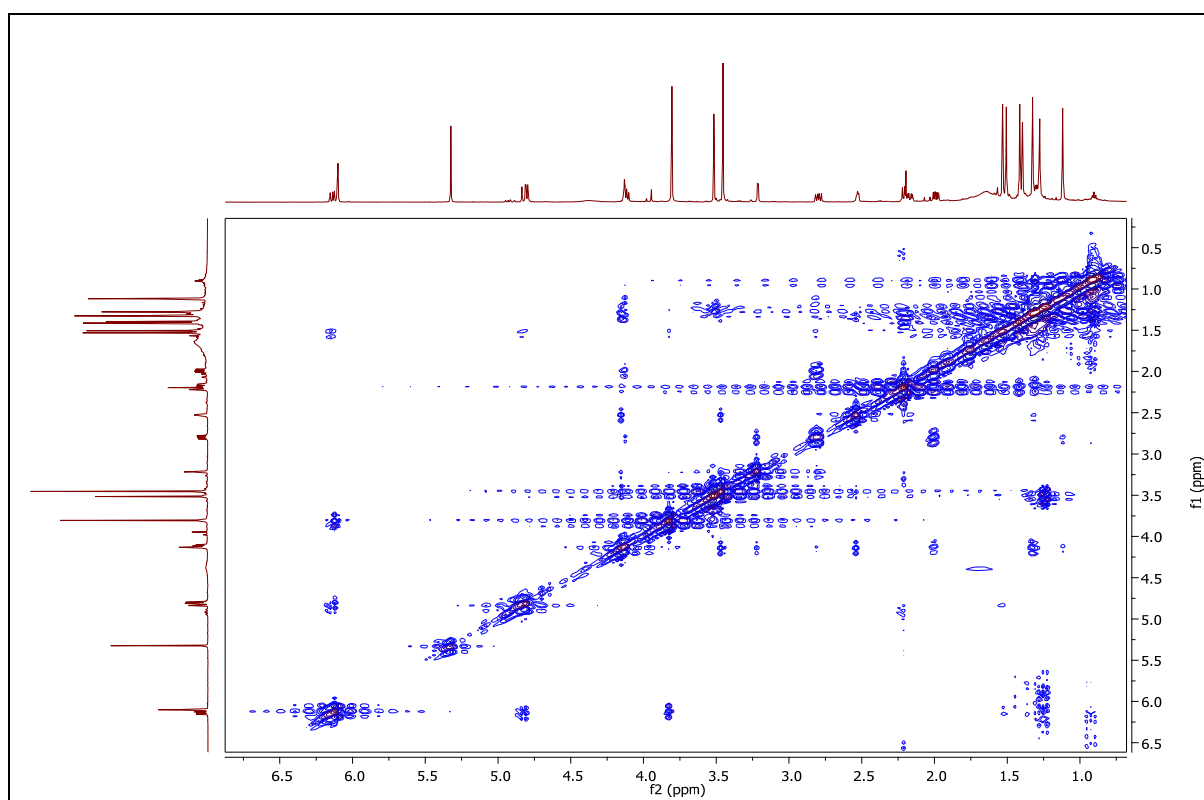


Figure S30. NOESY spectrum of compound (+)-**4** in CDCl₃ (600 MHz).

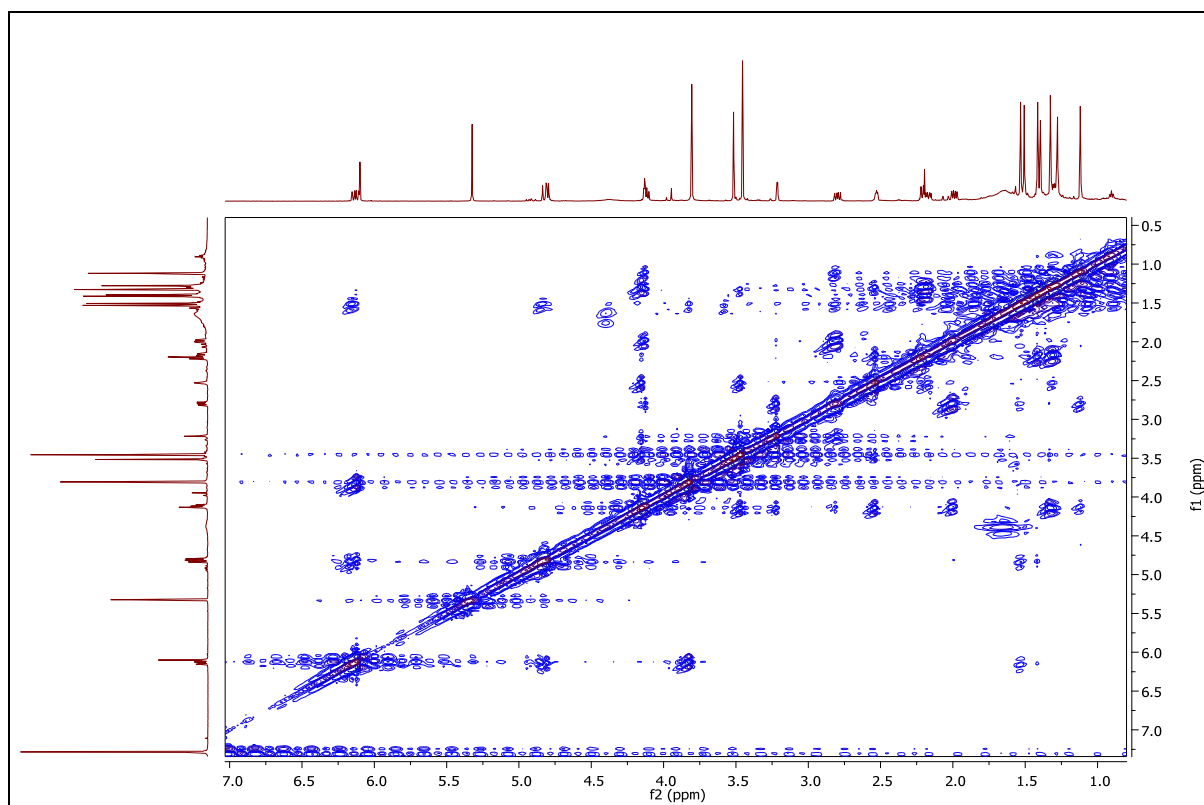


Figure S31. NOESY spectrum of compound (-)-4 in CDCl₃ (600 MHz).

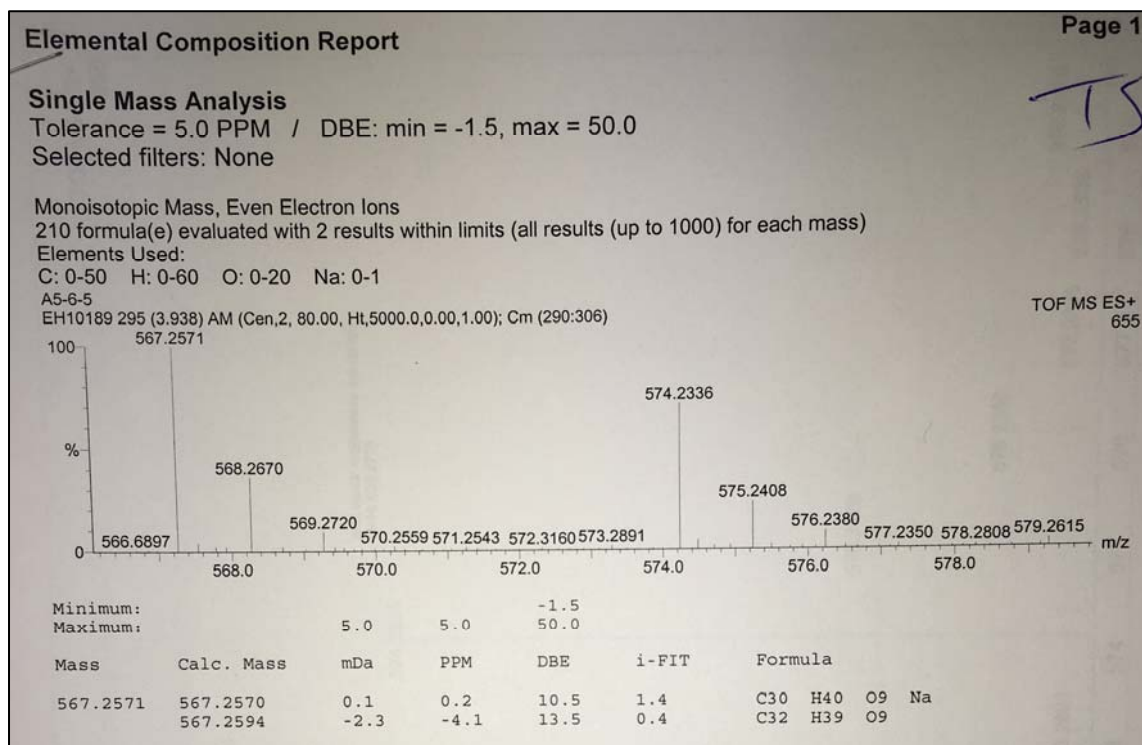


Figure S32. ESI-TOF-MS of compound 4.

Table S4. ^1H , ^{13}C and HMBC Spectroscopic Data of **4** in CDCl_3 .

Position	4		δ_{H} , (J in Hz)	HMBC
	δ_{C} , type			
1	162.5	C	-	
2	93.7	CH	6.10, s	1,3,4
3	168.0	C	-	
4	114.2	C	-	
4a	156.3	C	-	
5	92.6	C	-	
6	207.0	C	-	
7	41.7	CH	2.20, m	6,22
8	75.6	CH	4.13, m	9
8a	47.8	CH	3.21, d (3.5)	7,8,9,10a
9	194.7	C	-	-
9a	105.0	C	-	-
10a	88.6	C	-	-
11	41.1	C	-	-
12	149.9	CH	6.13, dd (17.5, 10.6)	4,11
13	107.5	CH ₂	4.82, d (17.5) 4.81, d (10.6)	11,12
14	30.0	CH ₃	1.53, s	4,11,12,15
15	28.4	CH ₃	1.51, s	4,11,12,14
16	28.9	CH ₂	2.80, dd (15.0, 9.1) 1.99, dd (15.0, 7.1)	5,10a,17,18
17	82.4	CH	4.11, dd (7.1, 9.1)	18
18	70.1	C	-	-
19	28.5	CH ₃	1.33, s	17,18,20
20	24.2	CH ₃	1.12, s	17,18,19
21	23.6	CH ₂	2.17, dd (15.3, 5.9) 1.40, m	8,10a,22, 23
22	34.0	CH	2.53, dd (4.6, 3.5)	7,8a
23	83.4	C	-	-
24	26.2	CH ₃	1.40, s	23,25
25	30.5	CH ₃	1.41, s	23,24
OH-1	-		12.19, s	1,2,9a
OMe-3	55.4	OCH ₃	3.81, s	3
OMe-8	55.8	OCH ₃	3.45, s	8

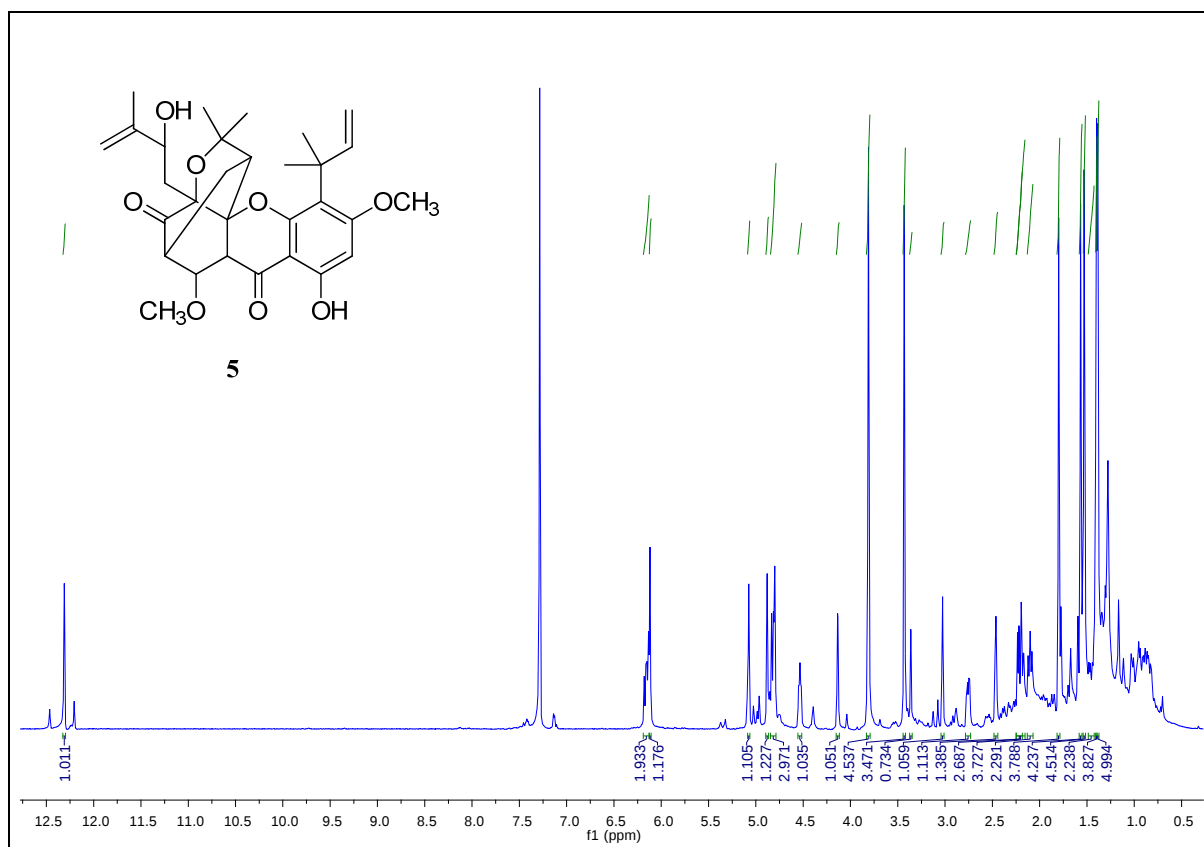


Figure S33. ¹H NMR spectrum of compound **5** in CDCl₃ (600 MHz).

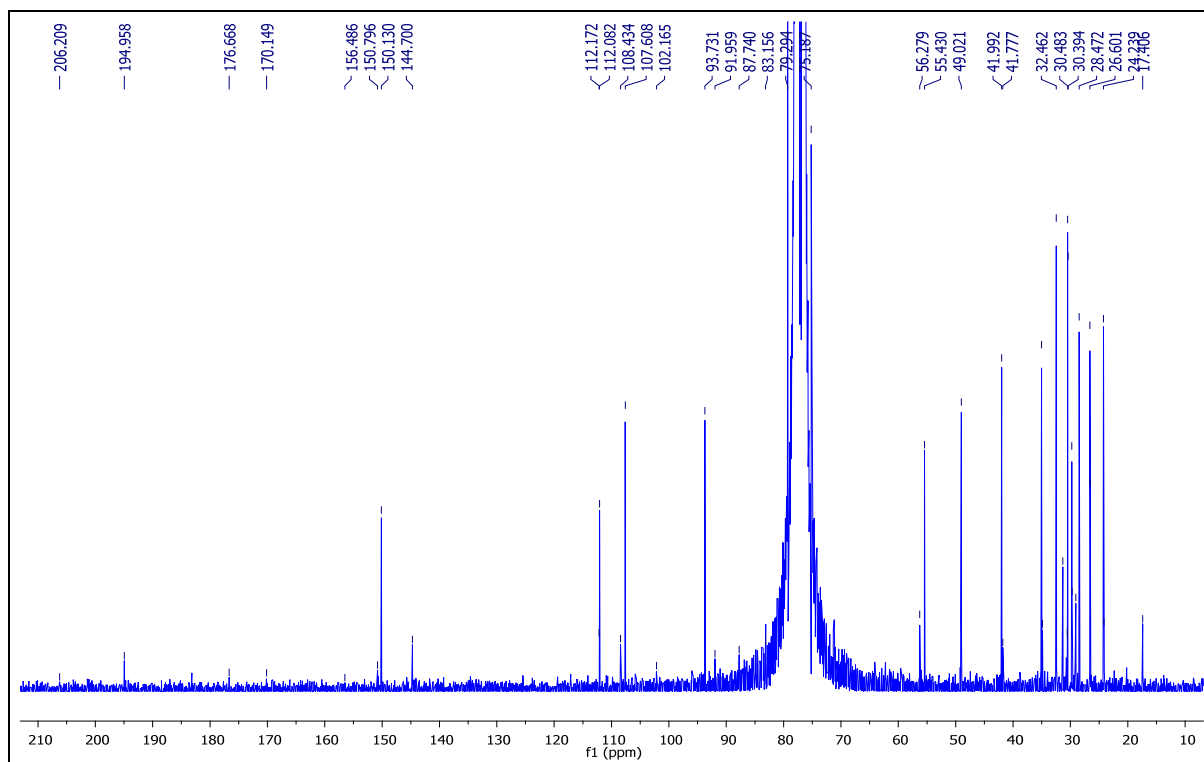


Figure S34. ¹³C NMR spectrum of compound **5** in CDCl₃ (150 MHz).

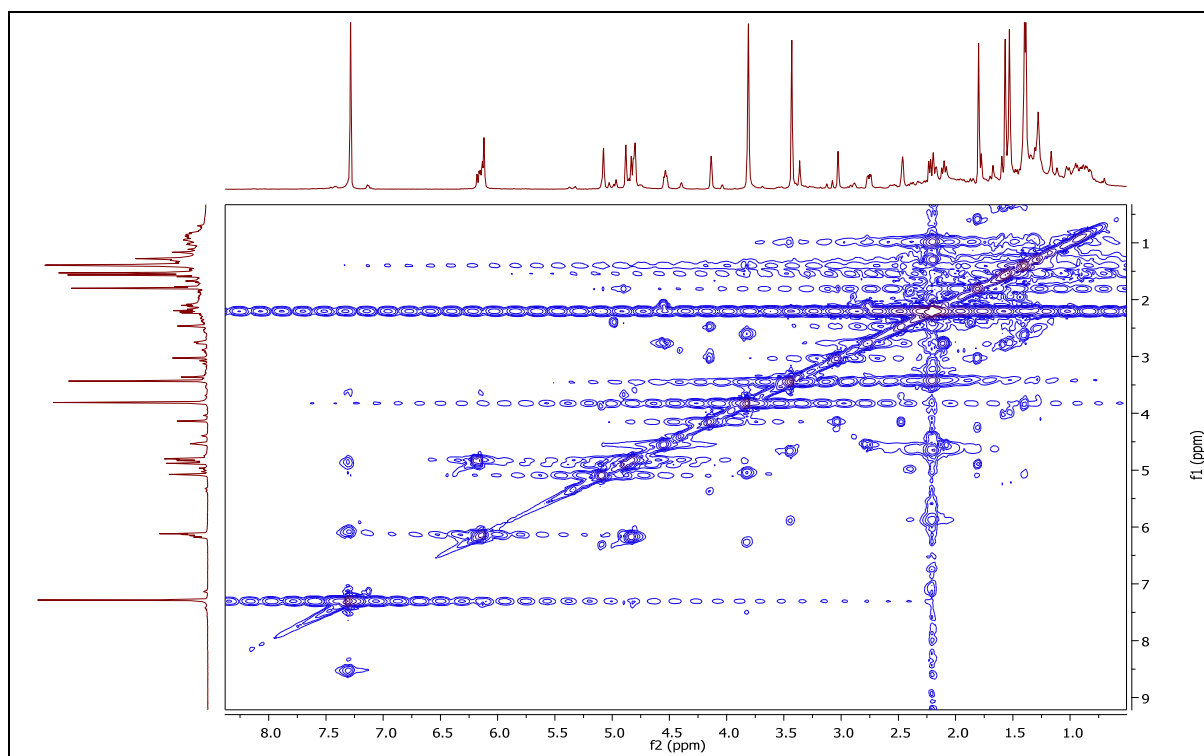


Figure S35. COSY spectrum of compound **5** in CDCl₃ (600 MHz).

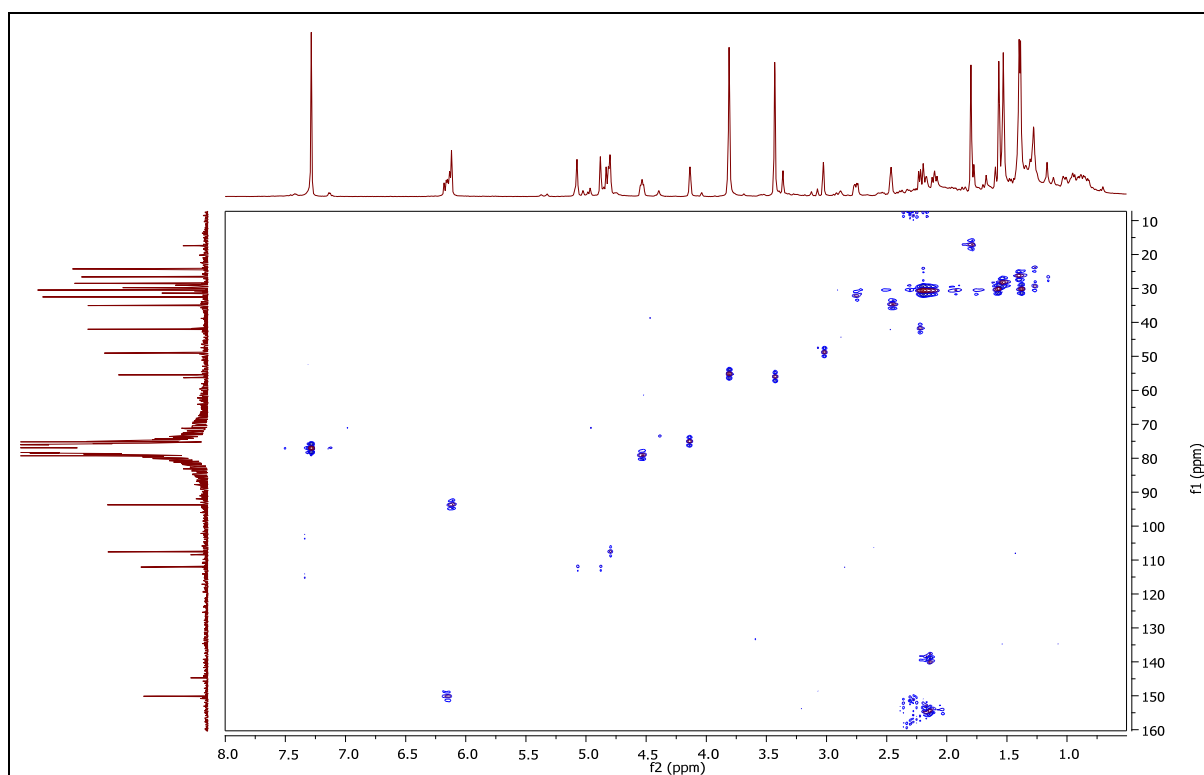


Figure S36. HSQC spectrum of compound **5** in CDCl₃ (600 MHz).

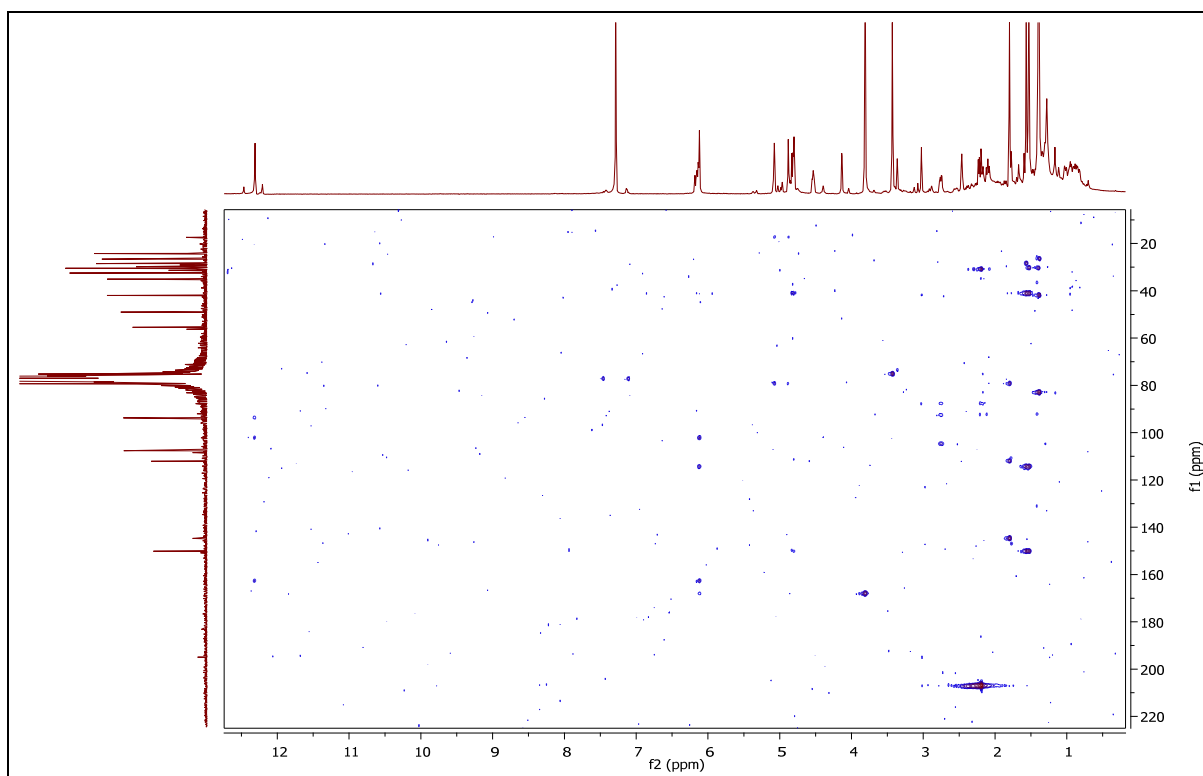


Figure 37. HMBC spectrum of compound **5** in CDCl₃ (600 MHz).

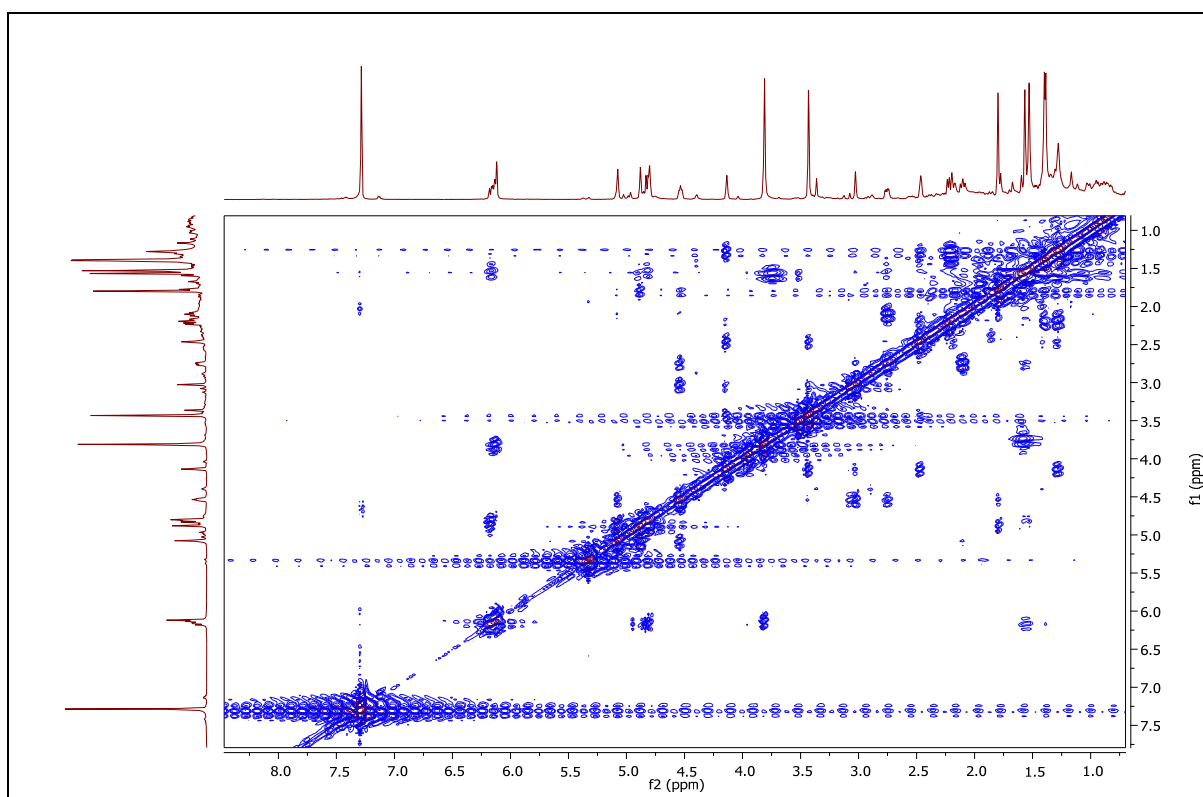


Figure S38. NOESY spectrum of compound (+)-**5** in CDCl₃ (600 MHz).

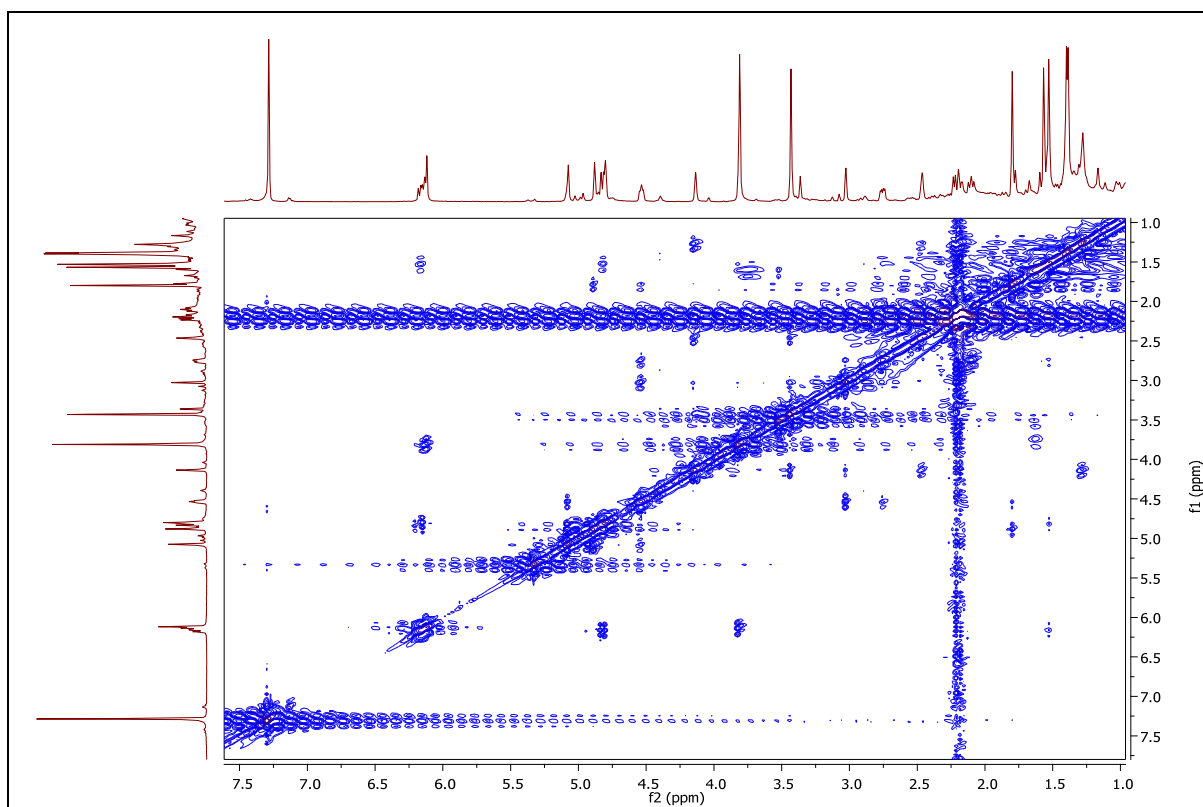


Figure S39. NOESY spectrum of compound **(-)-5** in CDCl_3 (600 MHz).

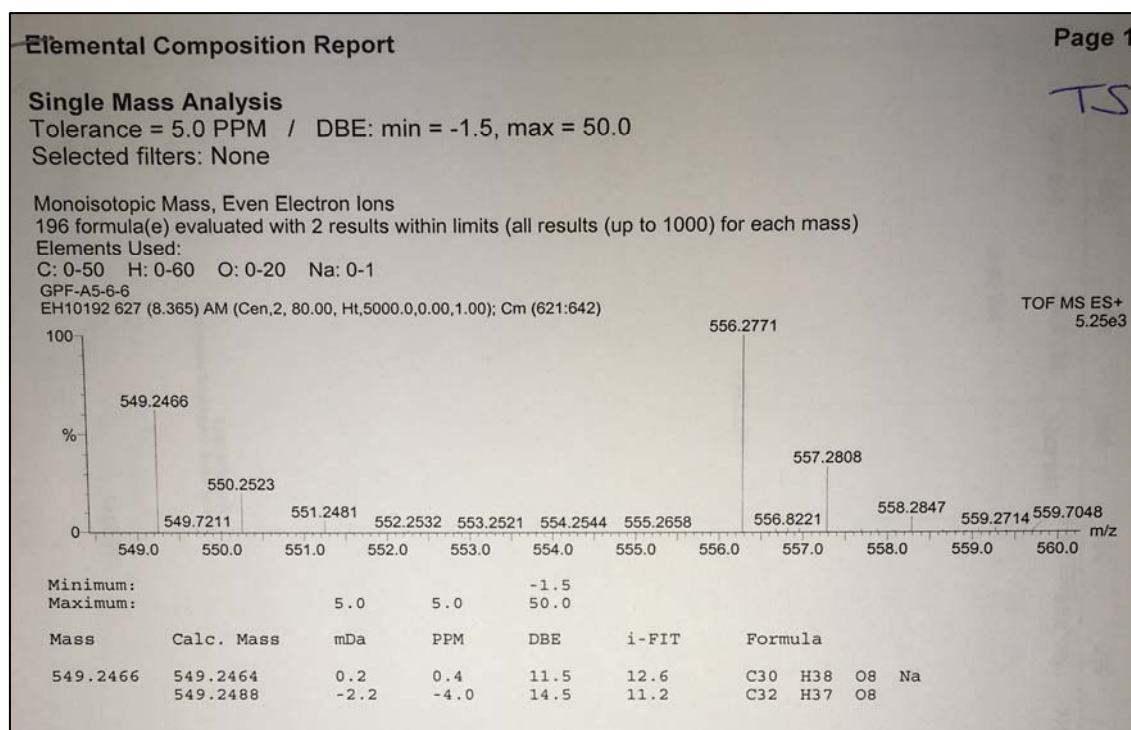


Figure S40. ESI-TOF-MS of compound **5**.

Table S5. ^1H , ^{13}C and HMBC Spectroscopic Data of **5** in CDCl_3 .

Position	5		δ_{H} , (J in Hz)	HMBC
	δ_{C} , type			
1	162.5 C	-		
2	93.7 CH	6.12, s		1,3,4,9a
3	168.0 C	-		
4	114.3 C	-		
4a	156.5 C	-		
5	92.0 C	-		
6	207.2 C	-		
7	34.7 CH	2.46, m		
8	75.2 CH	4.13, m		
8a	49.0 CH	3.03, m		9,10a,22
9	195.0 C	-		
9a	102.2 C	-		
10a	87.7 C	-		
11	41.0 C	-		
12	150.1 CH	6.16, dd (17.2, 10.8)		11,13
13	107.6 CH ₂	4.82, d (17.2) 4.81, d (10.8)		11,12
14	30.5 CH ₃	1.57, s		4,11,12,15
15	28.5 CH ₃	1.53, s		4,11,12,14
16	32.5 CH ₂	2.76, dd (13.9, 6.2) 2.10, m		5,6,18
17	79.3 CH	4.53, t (8.1)		18, 19
18	144.7 C	-		-
19	112.1 CH ₂	5.08, s 4.88, s		
20	17.4 CH ₃	1.80, s		17,18, 19
21	24.2 CH ₂	2.18, m 1.27, m		7,10a
22	41.8 CH	2.22, m		5, 7, 10a
23	83.2 C	-		
24	26.6 CH ₃	1.40, s		22,23,25
25	30.4 CH ₃	1.39, s		22,23,24
OH-1	-	12.31, s		1,2,9a
OMe-3	55.4 OCH ₃	3.81, s		3
OMe-8	56.0 OCH ₃	3.43, s		8

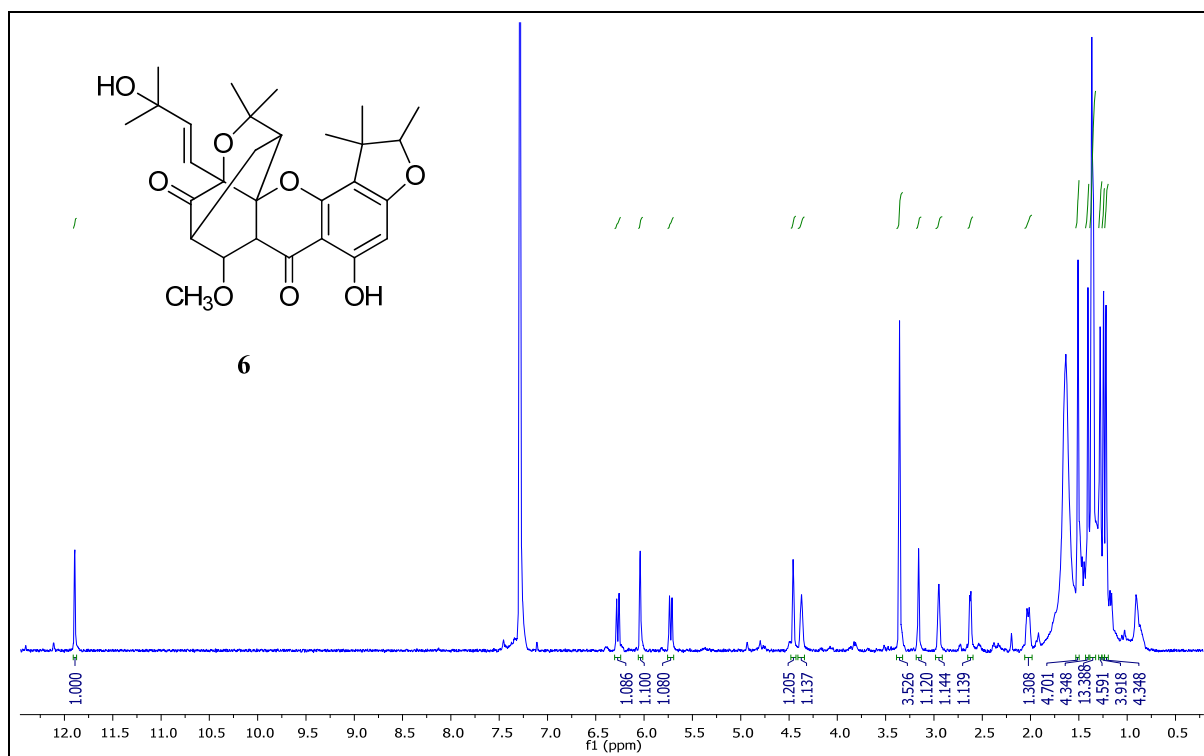


Figure S41. ^1H NMR spectrum of compound **6** in CDCl_3 (600 MHz).

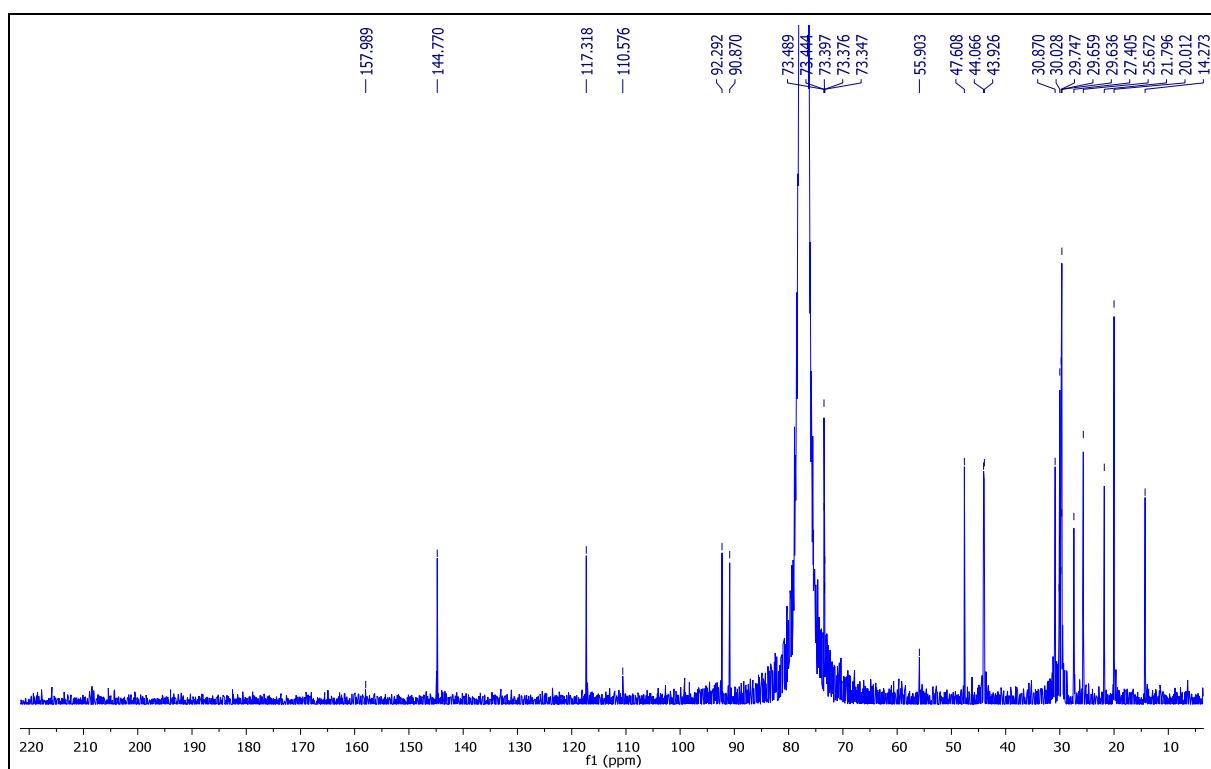


Figure S42. ^{13}C NMR spectrum of compound **6** in CDCl_3 (150 MHz).

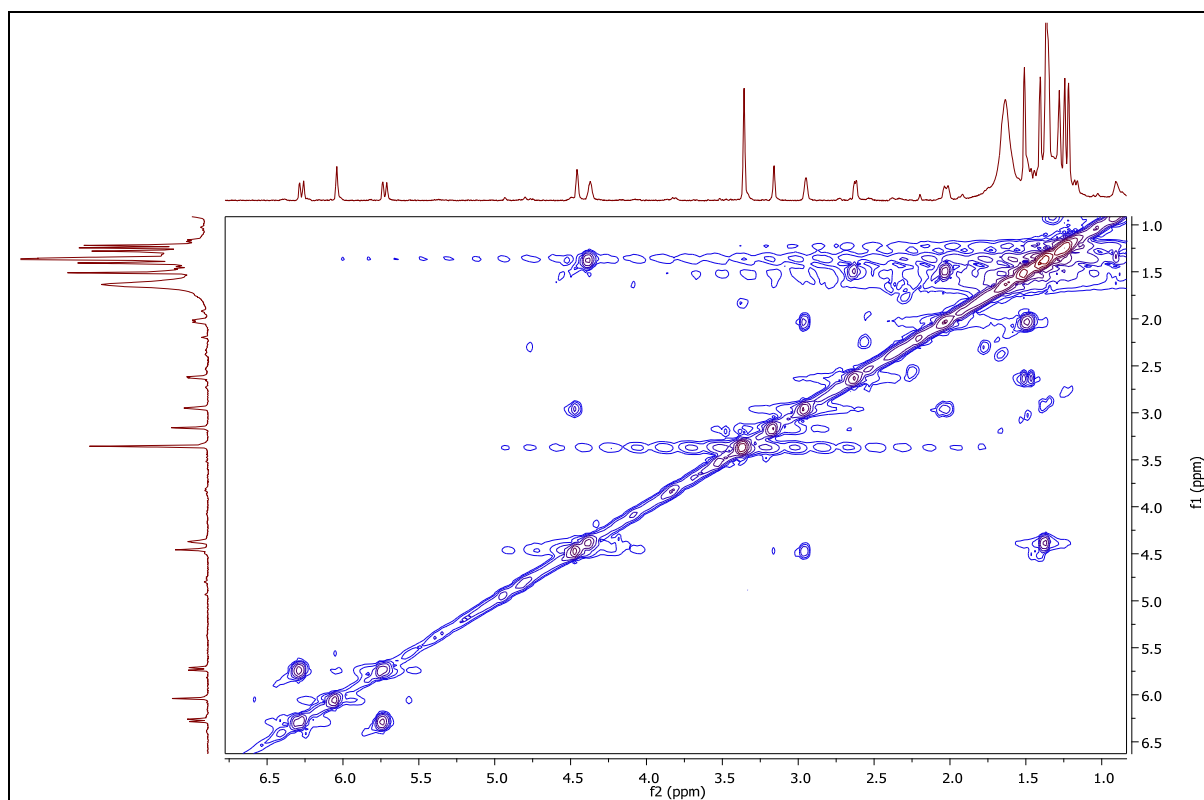


Figure S43. COSY spectrum of compound **6** in CDCl₃ (600 MHz).

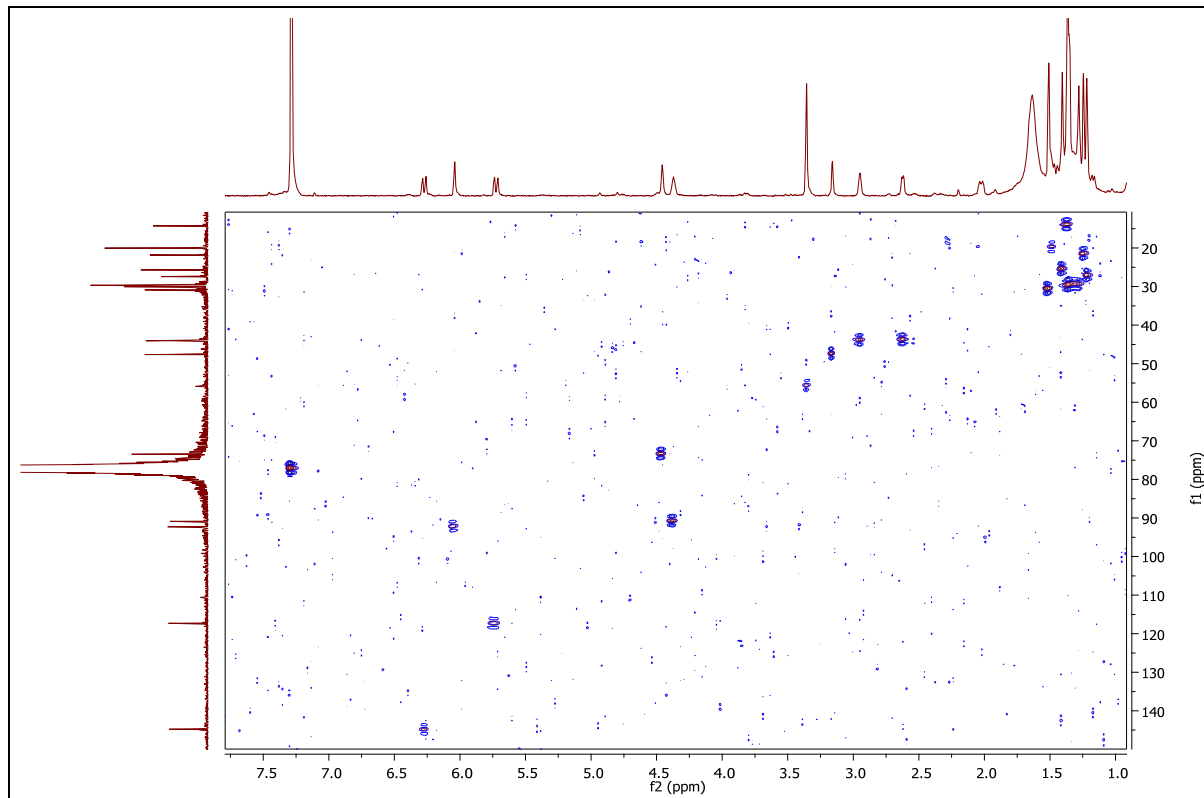


Figure S44. HSQC spectrum of compound **6** in CDCl₃ (600 MHz).

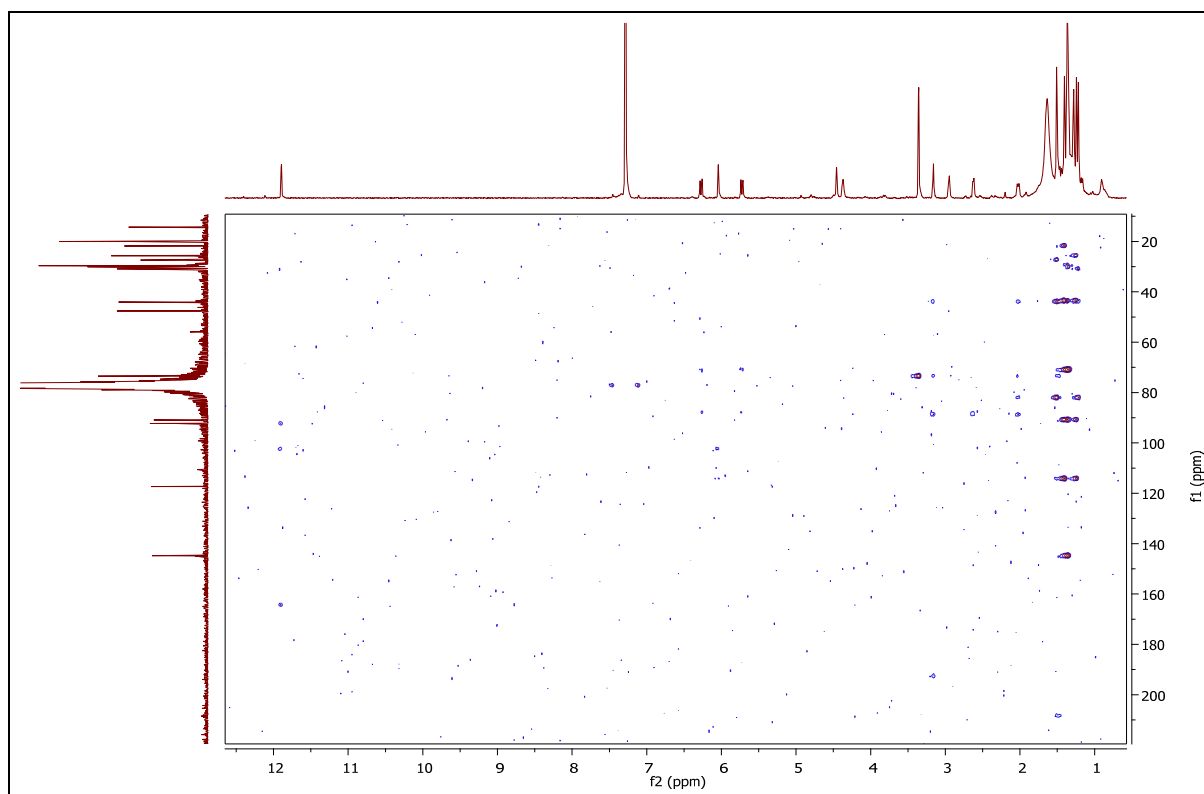


Figure S45. HMBC spectrum of compound **6** in CDCl₃ (600 MHz).

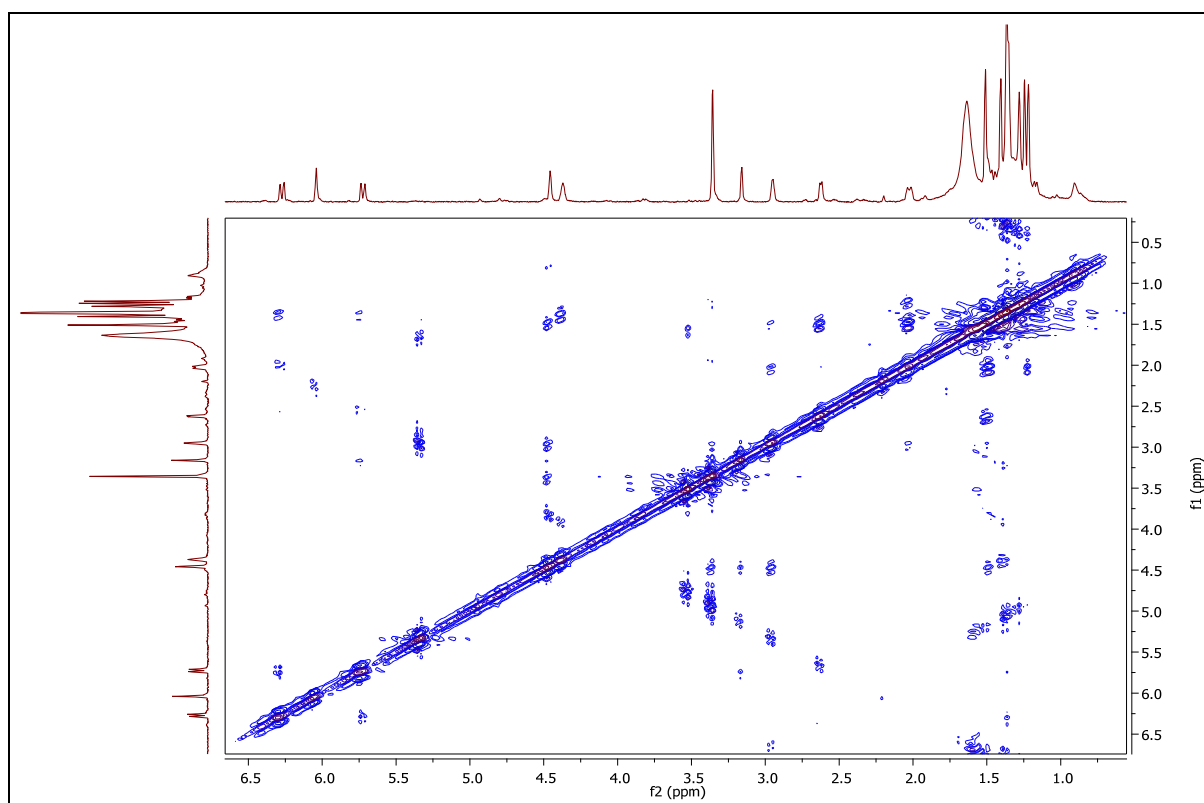


Figure S46. NOESY spectrum of compound (+)-**6** in CDCl₃ (600 MHz).

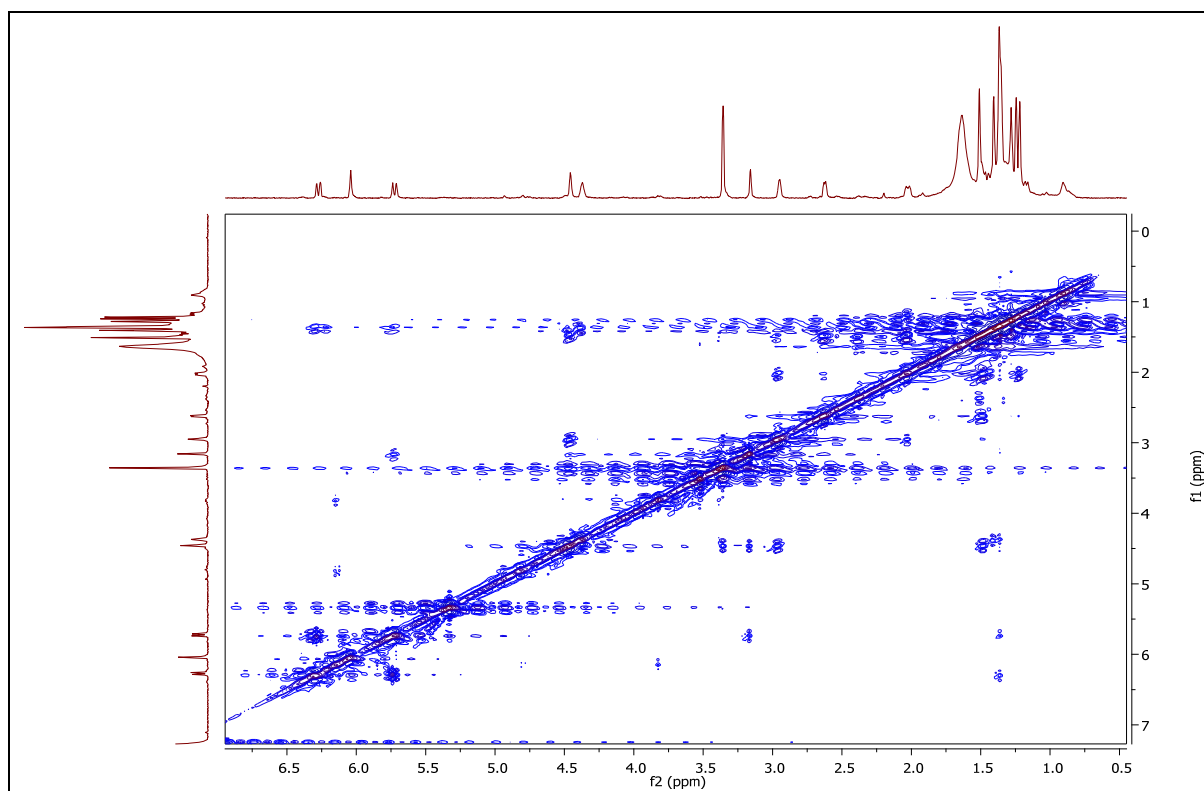


Figure S47. NOESY spectrum of compound (-)-6 in CDCl₃ (600 MHz).

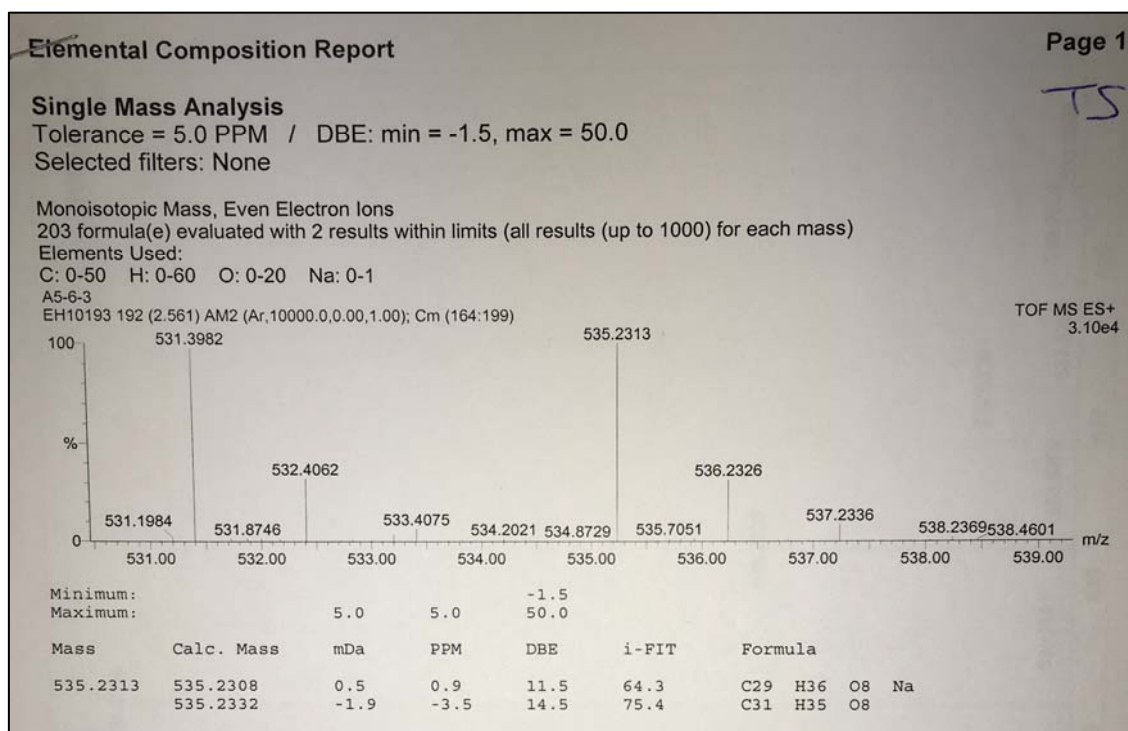


Figure S48. ESI-TOF-MS of compound 6.

Table S6. ^1H , and HMBC Spectroscopic Data of **6** in CDCl_3 .

Position	6		δ_{H} , (<i>J</i> in Hz)	HMBC
	δ_{C} , type			
1	164.3	C	-	
2	92.3	CH	6.07, s	1,3,4,9a
3	169.6	C	-	
4	114.2	C	-	
4a	158.0	C	-	
5	87.7	C	-	
6	208.4	C	-	
7	44.1	CH	2.95, m	8a
8	73.4	CH	4.46, m	
8a	47.6	CH	3.16, m	7,8,9,10a
9	192.6	C	-	
9a	102.3	C	-	
10a	88.6	C	-	
11	43.4	C	-	
12	90.9	CH	4.37, m	13
13	14.3	CH_3	1.37, d (7.2)	11,12
14	25.7	CH_3	1.41, s	4,11,12,15
15	21.8	CH_3	1.25, s	4,11,12,14
16	117.3	CH	5.72, d (15.8)	5,18
17	144.8	CH	6.27, d (15.8)	5,18
18	71.2	C	-	
19	29.7	CH_3	1.36, s	17,18
20	30.0	CH_3	1.35, s	17,18
21	20.0	CH_2	2.02, m 1.49, m	6,8,10a,22,23
22	43.9	CH	2.62, m	10a
23	82.0	C	-	
24	30.9	CH_3	1.22, s	22,23,25
25	27.4	CH_3	1.51, s	22,23,24
OH-1	-		12.00, s	1,2,9a
OMe-3				
OMe-8	55.9	OCH_3	3.36, s	8

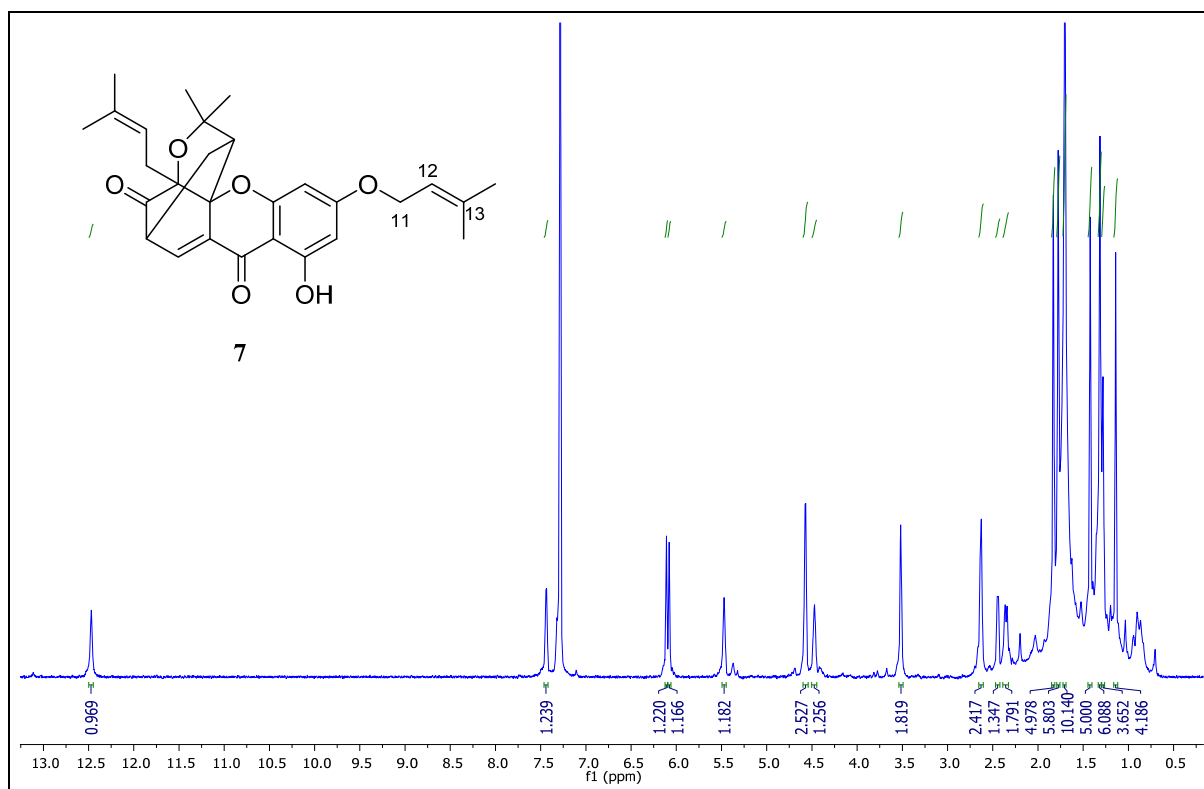


Figure S49. ^1H NMR spectrum of compound **7** in CDCl_3 (600 MHz).

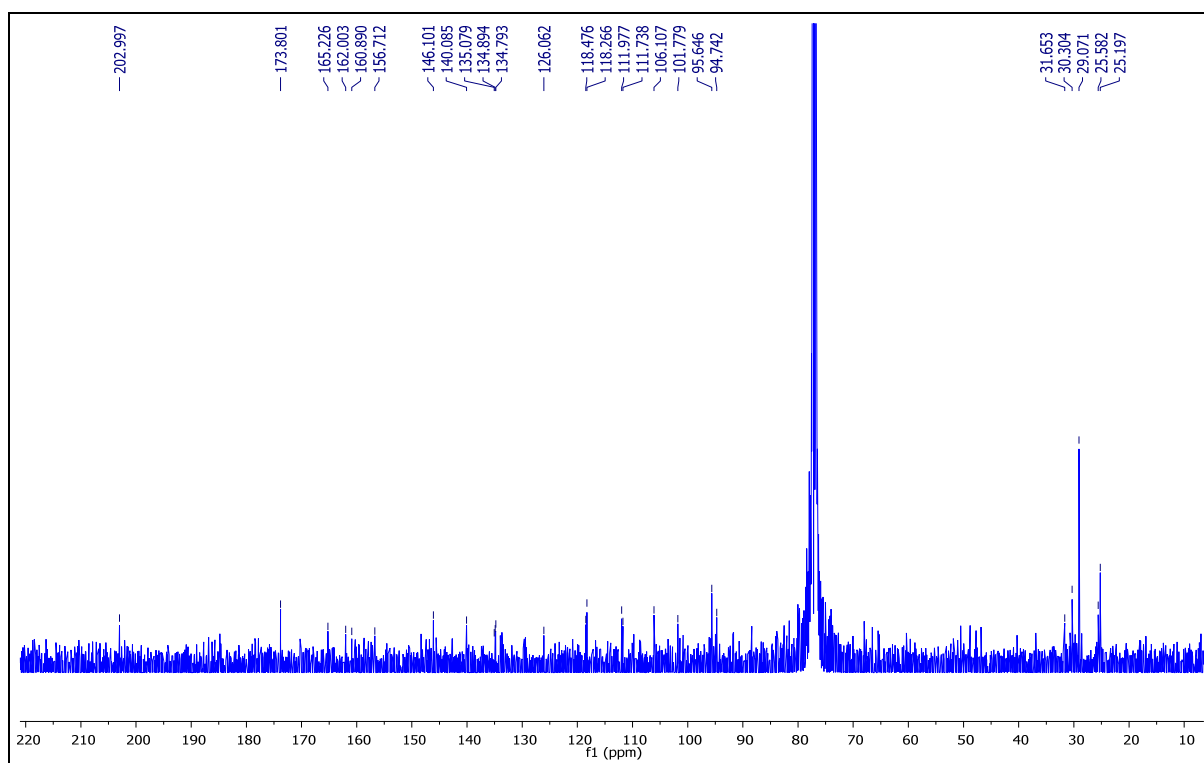


Figure S50. ^{13}C NMR spectrum of compound **7** in CDCl_3 (150 MHz).

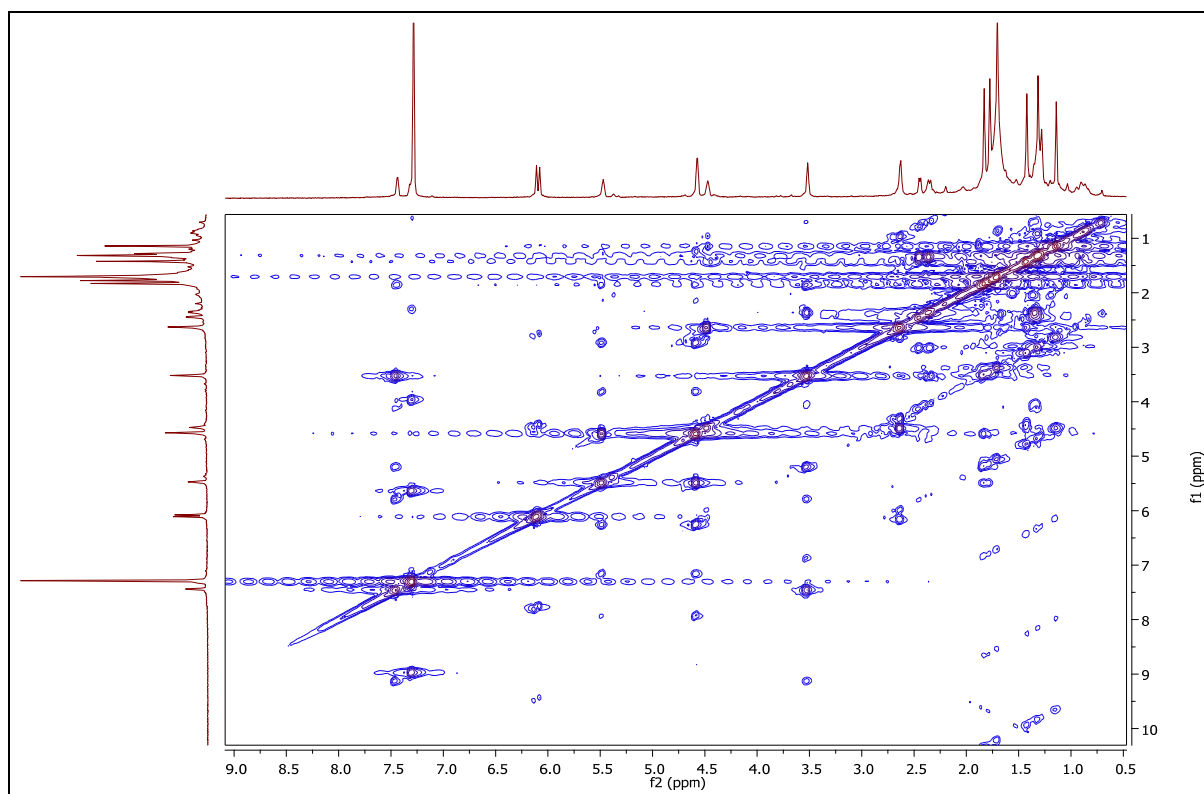


Figure S51. COSY spectrum of compound **7** in CDCl₃ (600 MHz).

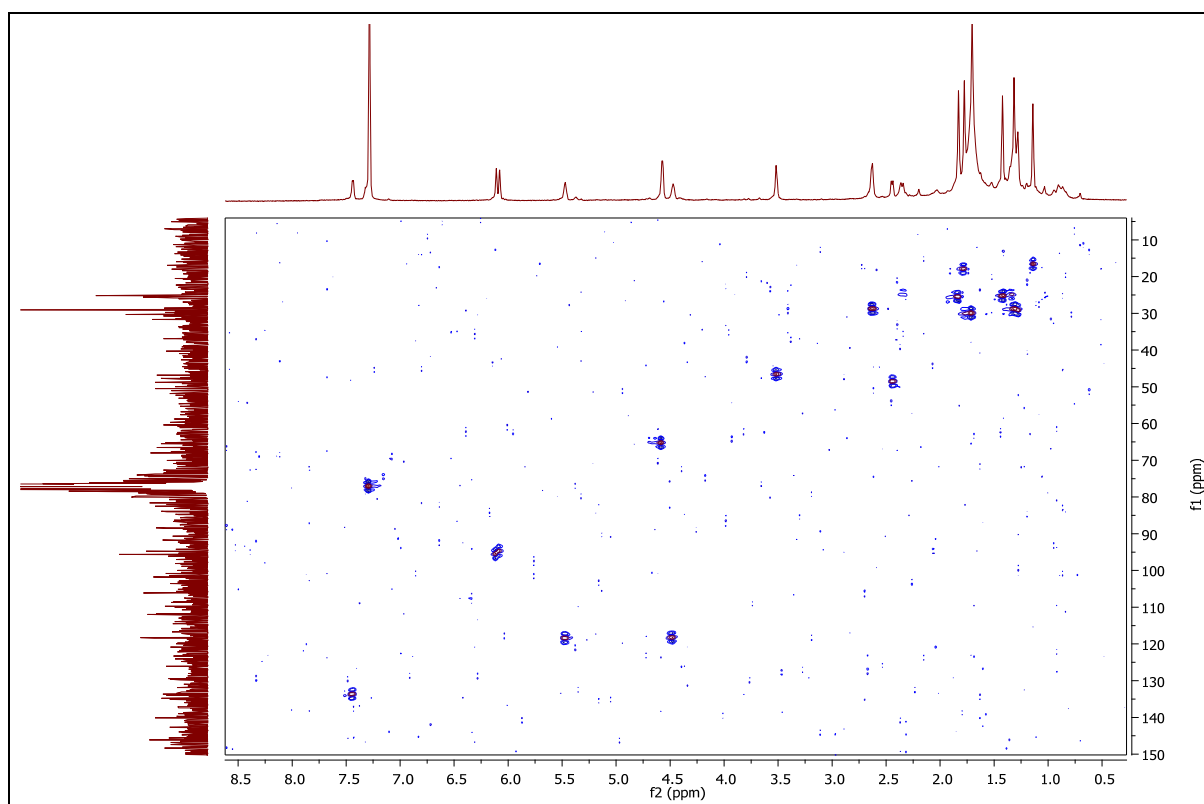


Figure S52. HSQC spectrum of compound **7** in CDCl₃ (600 MHz).

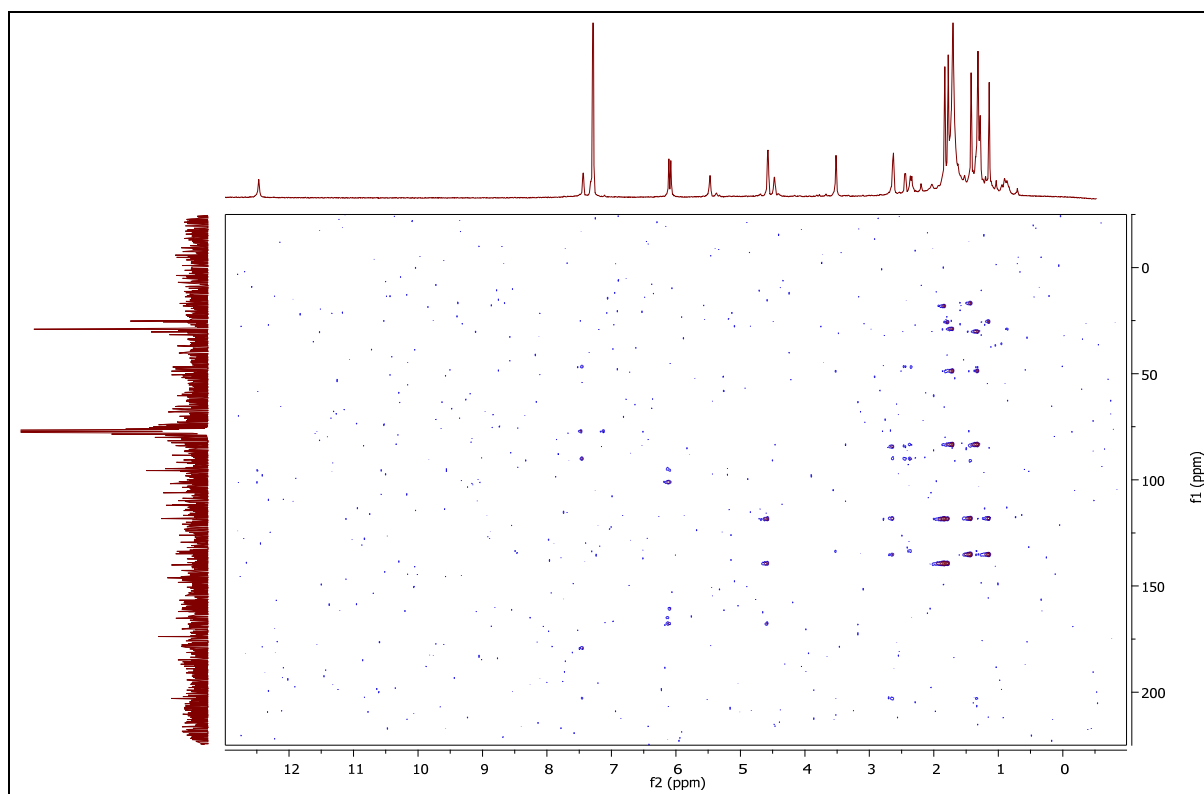


Figure S53. HMBC spectrum of compound **7** in CDCl_3 (600 MHz).

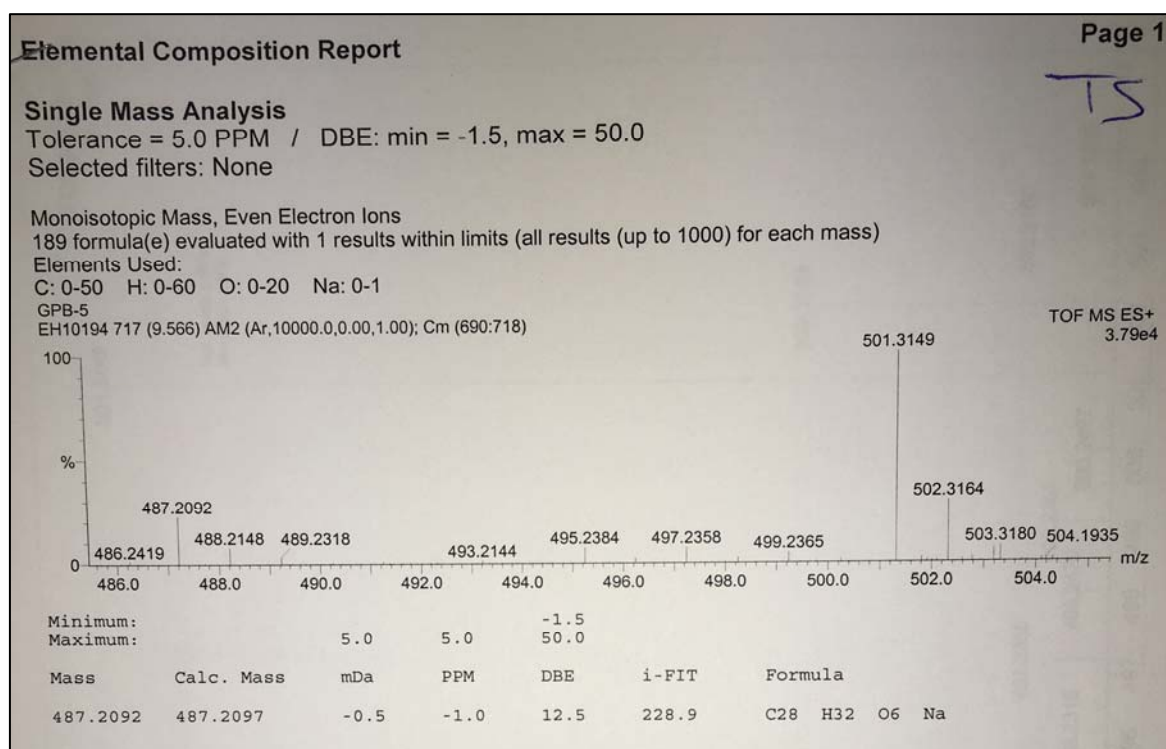


Figure S54. ESI-TOF-MS of compound **7**.

Table S7. ^1H , ^{13}C and HMBC Spectroscopic Data of **7** in CDCl_3 .

Position	7			HMBC
	δ_{C} , type		δ_{H} , (J in Hz)	
1	164.9	C	-	
2	95.7	CH	6.11, brs	1,3,4,9a
3	167.6*	C	-	
4	94.7	CH	6.08, brs	2,3,4a,9a
4a	160.7	C	-	
5	84.2*	C	-	
6	202.9	C	-	
7	46.5	CH	3.52, m	8,22
8	133.7	CH	7.44, d (4.9)	6,7,8a,9
8a	135.4	C	-	
9	179.3*	C	-	
9a	101.1	C	-	
10a	90.0*	C	-	
11	65.2	CH ₂	4.57, m	3,12,13
12	118.5	CH	5.47, m	
13	139.4	C		
14	25.4	CH ₃	1.83, s	12,13,15
15	17.9*	CH ₃	1.78, s	12,13,14
16	28.8	CH ₂	2.63, m	5,6,10a,17,18
17	118.3	CH	4.47, m	
18	135.2	C	-	
19	25.2	CH ₃	1.42, s	17,18,20
20	16.7*	CH ₃	1.14, s	17,18,19
21	24.9*	CH ₂	2.35, d (15.5)	7,8,10a,22
			1.33, m	
22	48.5	CH	2.44, d (8.8)	5,7,10a
23	83.3*	C	-	
24	28.8	CH ₃	1.32, s	22,23,25
25	29.9*	CH ₃	1.70, s	22,23,24
OH-1	-		12.47, s	1,2,9a
OH-3	-			

*Assigned from HMBC

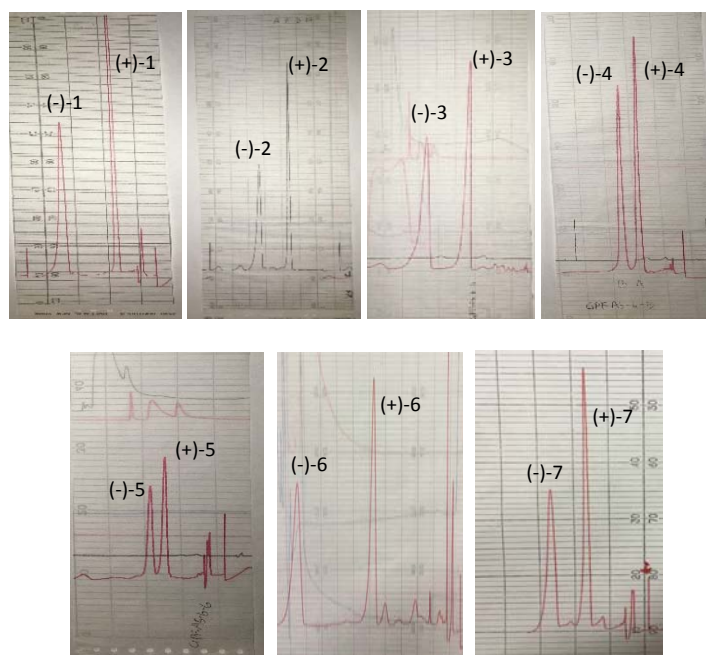


Figure S55. Chiral HPLC chromatogram of **1-7**.

1. Chiral HPLC analysis and separation of enantiomers of compounds **1-7** was performed by semi-preparative HPLC on a chiral column (CHIRALCEL OD-H column, flow rate 2 mL/min, 49:1 *n*-hexane-*i*PrOH).

2. All chromatograms are running from right (short retention time) to left (longer retention time) and the retention times of compounds **1-7** are listed below:

(+)-**1** (t_R = 8 min), (-)-**1** (t_R = 15 min), (+)-**2** (t_R = 14 min), (-)-**2** (t_R = 20 min), (+)-**3** (t_R = 17 min), (-)-**3** (t_R = 30 min), (+)-**4** (t_R = 9 min), (-)-**4** (t_R = 11 min), (+)-**5** (t_R = 6 min), (-)-**5** (t_R = 8 min), (+)-**6** (t_R = 30 min), (-)-**6** (t_R = 34 min), (+)-**7** (t_R = 9 min) and (-)-**7** (t_R = 12 min).