Supplementary Information

Withanolides from Leaves of *Nicandra physalodes*

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Table S1. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data for the known compounds **5-10** (δ in ppm, J in Hz)

Position	**5**[a]		**6**[b]		**7**[a]		**8**[a]		**9**[a]		**10**[a]	
	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H
1	204.0	–	205.9	–	203.2	–	204.2	–	204.1	–	203.9	–
2	129.2	6.07, dd (2.0, 10.0)	129.3	5.79, dd (2.4, 10.0)	129.3	6.00, d (9.9)	129.6	6.02, dd (10.0, 2.0)	129.6	5.96, m	129.3	6.17, dd (10.1, 1.8)
3	141.5	6.62, m	142.7	6.65, m	141.4	6.59, m	140.9	6.57, m	140.8	6.55, m	141.3	6.60, ddd (10.2, 5.3, 2.1)
4	38.3	2.67, dd (4.7, 18.1) 2.74, m	38.3	2.86, m 2.52, dd (19.0, 5.0)	38.1	2.56, dd (5.0, 14.9)	38.2	2.53, dd (1.8, 10.0)	38.0	2.48, dd (19.0, 4.8) 2.63, m	38.3	2.81, m 2.62, dd (18.7, 4.7)
5	73.8	–	74.5	–	74.3	–	74.4	–	74.3	–	73.9	–
6	57.4	3.33, d (2.1)	57.8	3.22, d (3.9)	56.6	3.16, d (3.3)	56.8	3.12, d (3.7)	56.7	3.88, d (3.2)	55.0	3.30, d (3.8)
7	54.6	4.08, s	56.0	4.00, m	56.0	3.30, s	56.3	3.30, s	57.3	3.11, m	57.4	3.10, m
8	40.2	3.08, m	40.2	3.08, d (11.0)	36.4	2.20, m	37.6	2.86, m	36.9	2.16, m	39.8	3.05, m
9	32.3	2.45, td (3.7, 11.0, 11.0)	33.2	1.98, m	38.7	3.96, dd (2.4, 13.0)	36.2	2.19, m	36.4	2.16, m	32.7	2.06, m
10	52.7	–	54.9	–	52.6	–	52.1	–	52.1	–	52.6	–
11	24.7	1.59, q 3.08, m	25.7	2.86, m 1.82, m	39.4	2.75, d (13.1) 2.68, d (8.7)	33.5	1.74, m	21.9	3.11, m	25.1	3.05, m
12	30.0	2.74, m 2.79, m	30.6	1.53, m 2.86, m	213.3	–	35.1	2.32, m	35.5	1.62, m	30.2	2.81, m
13	145.0	–	143.1	–	58.2	–	49.6	–	47.7	–	137.4	–

Table S1. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data for the known compounds **5-10** (*δ* in ppm, *J* in Hz) (cont.)

Position	**5**[a]		**6**[b]		**7**[a]		**8**[a]		**9**[a]		**10**[a]	
	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H
14	138.5	–	138.1	–	43.9	2.05, q (10.9)	47.3	1.74, m	62.0	1.75	136.8	–
15	126.2	7.74, m	126.7	7.35, d (7.9)	24.0	1.60, m	22.6	3.17, m	77.0	4.99, m	125.0	7.64, d (8.0)
16	126.0	7.96, d (4.5)	125.6	7.00, d (8.0)	27.4	1.45, m	24.0	1.74, m	130.6	5.97, m	125.2	7.39, d (7.9)
17	136.2	–	137.2	–	53.9	1.50, m	85.4	–	156.8	–	143.3	–
18	129.2	7.76, s	129.6	6.97, s	15.1	1.28, s	16.4	1.09, s	15.4	1.23, s	129.5	7.19, s
19	14.4	1.24, s	18.8	1.23, s	11.8	0.98, d (7.0)	15.2	1.19, s	19.1	1.02, s	14.4	1.23, d (7.1)
20	198.0	–	44.7	2.74, m	40.6	1.70, m	42.1	2.07, m	35.2	2.32, m	45.2	
21	26.9	2.57, s	18.1	1.21, s	13.9	1.14, s	14.5	0.98, d (7.0)	17.2	1.08, d (6.8)	16.5	1.56, d (7.0)
22	–	–	69.7	4.00, m	66.6	4.30, m	67.8	4.68, m	67.5	4.36, m	76.0	4.08, m
23	–	–	35.6	2.86, m	31.0	1.83, d (7.0)	34.6	1.87, m	34.5	1.94, m	42.7	1.8, m
				1.53, m								
24	–	–	64.3	–	63.1	–	63.5	–	62.8	–	74.3	–
25	–	–	64.0	–	63.9	–	63.0	–	62.9	–	77.5	–
26	–	–	92.9	4.98, s	93.1	5.50, s	92.8	5.46, m	92.9	5.45, s	98.8	5.35, d (4.1)
27	–	–	17.1	1.33, s	19.2	1.38, s	17.6	1.49, s	19.4	1.34, s	19.1	1.96, s
28	–	–	14.8	1.31, s	17.6	1.48, s	19.2	1.32, s	17.6	1.47, s	24.0	1.87, s

[a]Measured in pyridine-$d_{5;}$ [b]measured in MeOH.

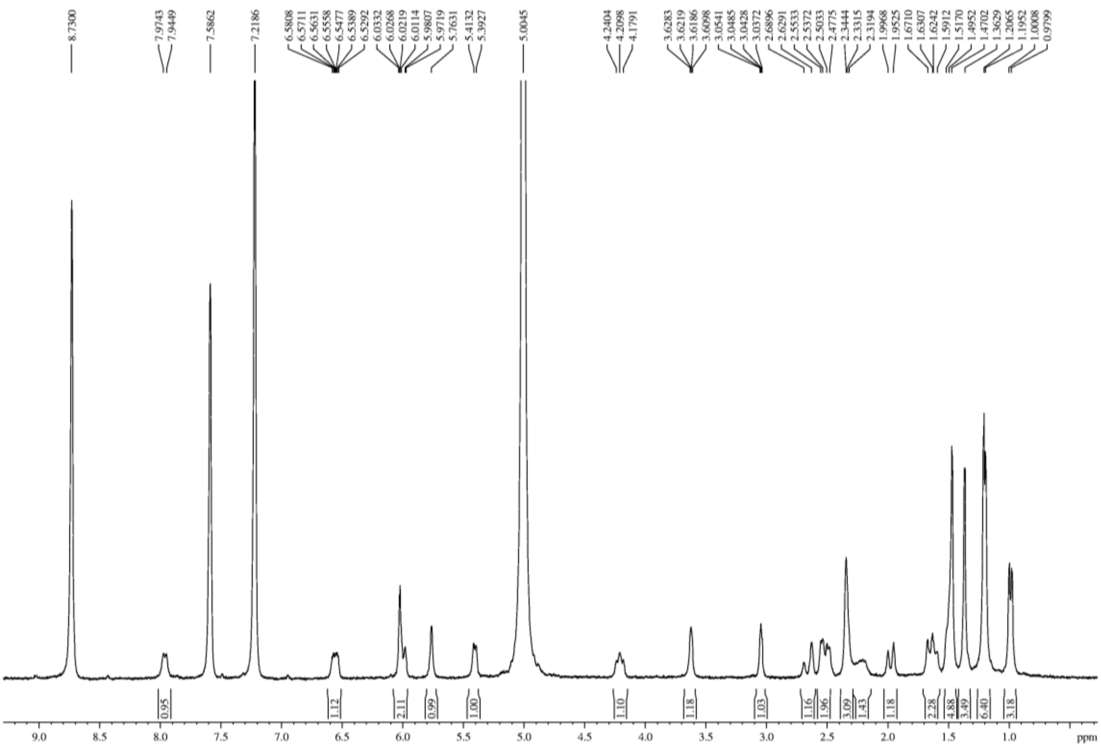

Figure S1. ^{1}H NMR (500 MHz, C_5D_5N) spectrum of compound **1**.

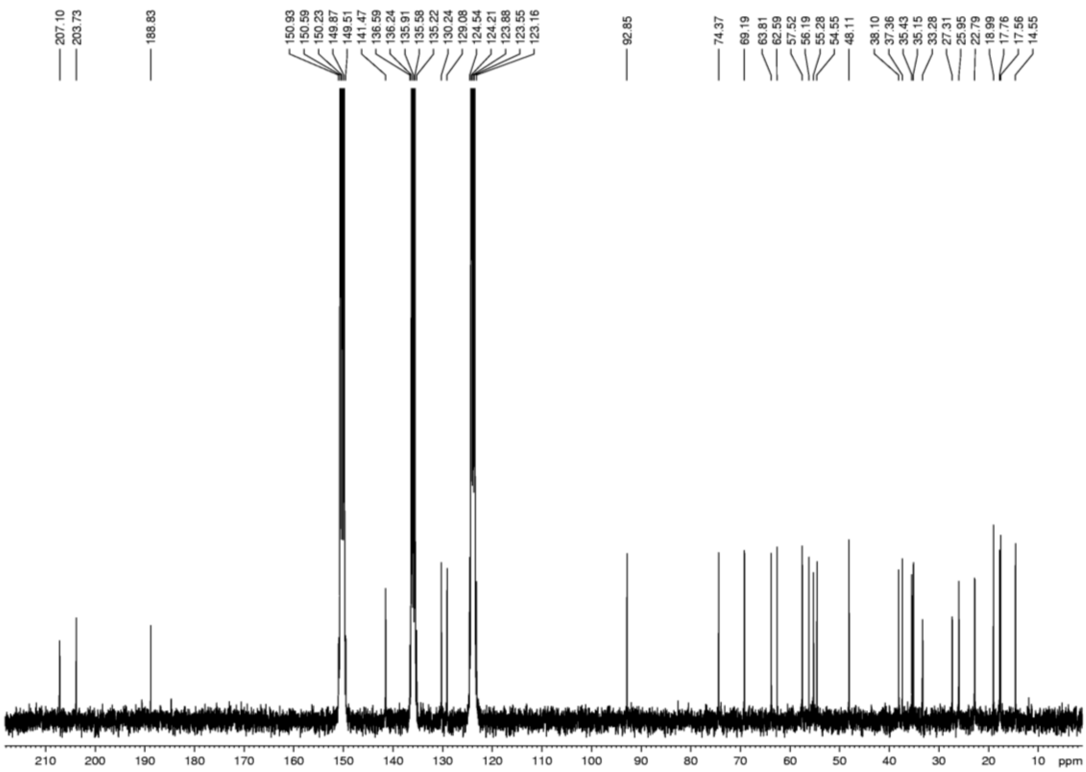

Figure S2. ^{13}C NMR (75 MHz, C_5D_5N) spectrum of compound **1**.

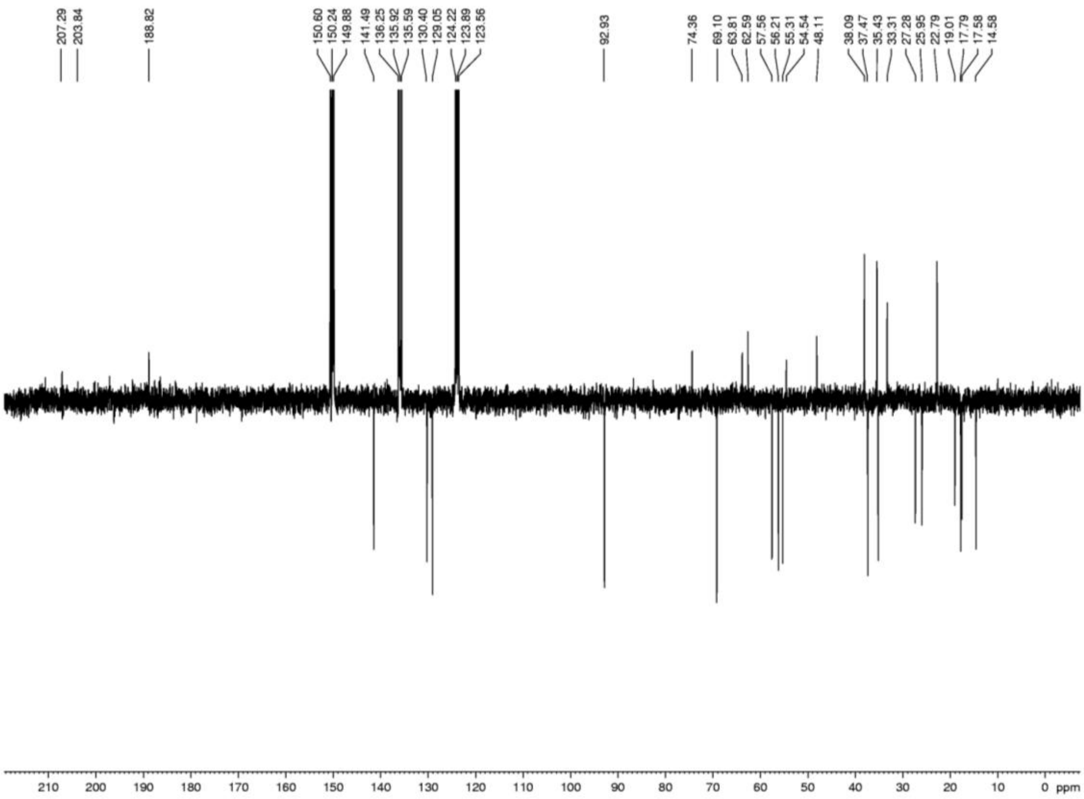

Figure S3. ^{13}C NMR DEPT 135° (75 MHz, C_5D_5N) spectrum of compound **1**.

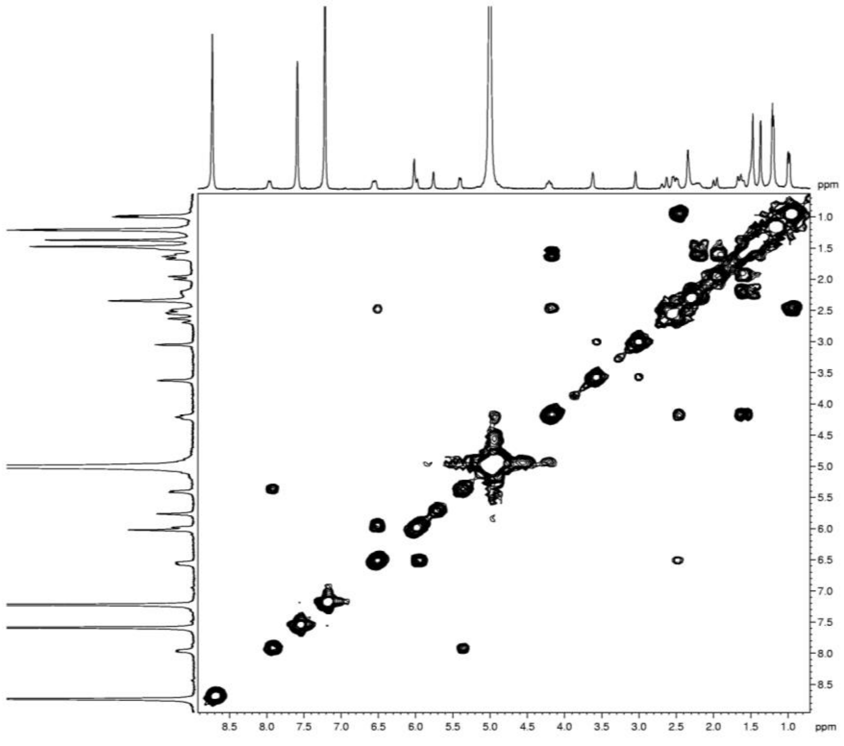

Figure S4. ^{1}H,^{1}H-COSY spectrum of compound **1**.

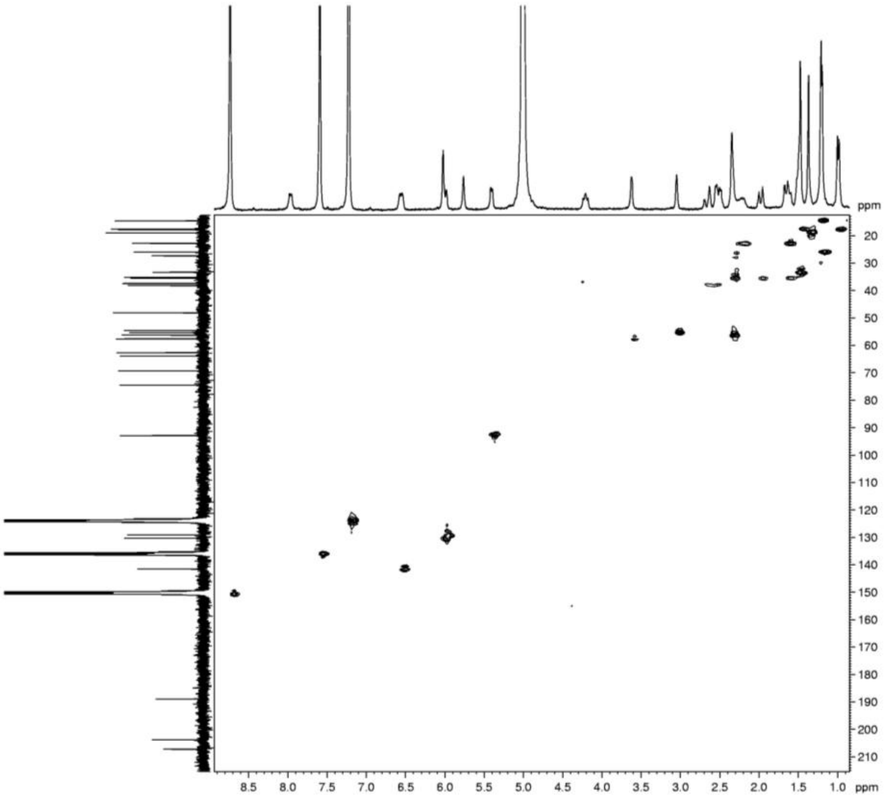

Figure S5. $^{1}H,^{13}C$-HSQC spectrum of compound **1**.

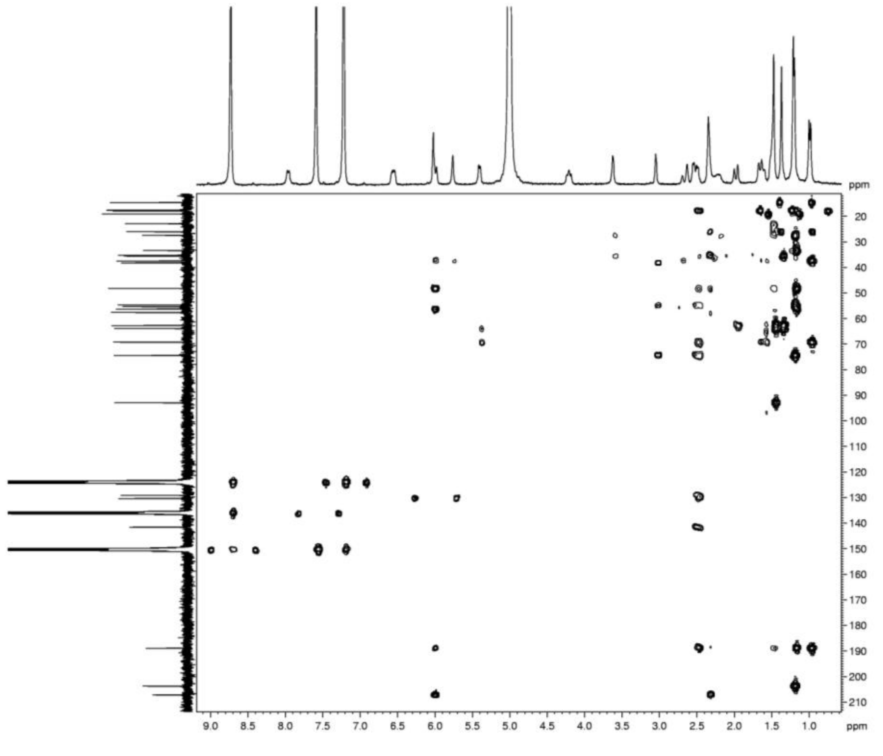

Figure S6. $^{1}H,^{13}C$-HMBC spectrum of compound **1**.

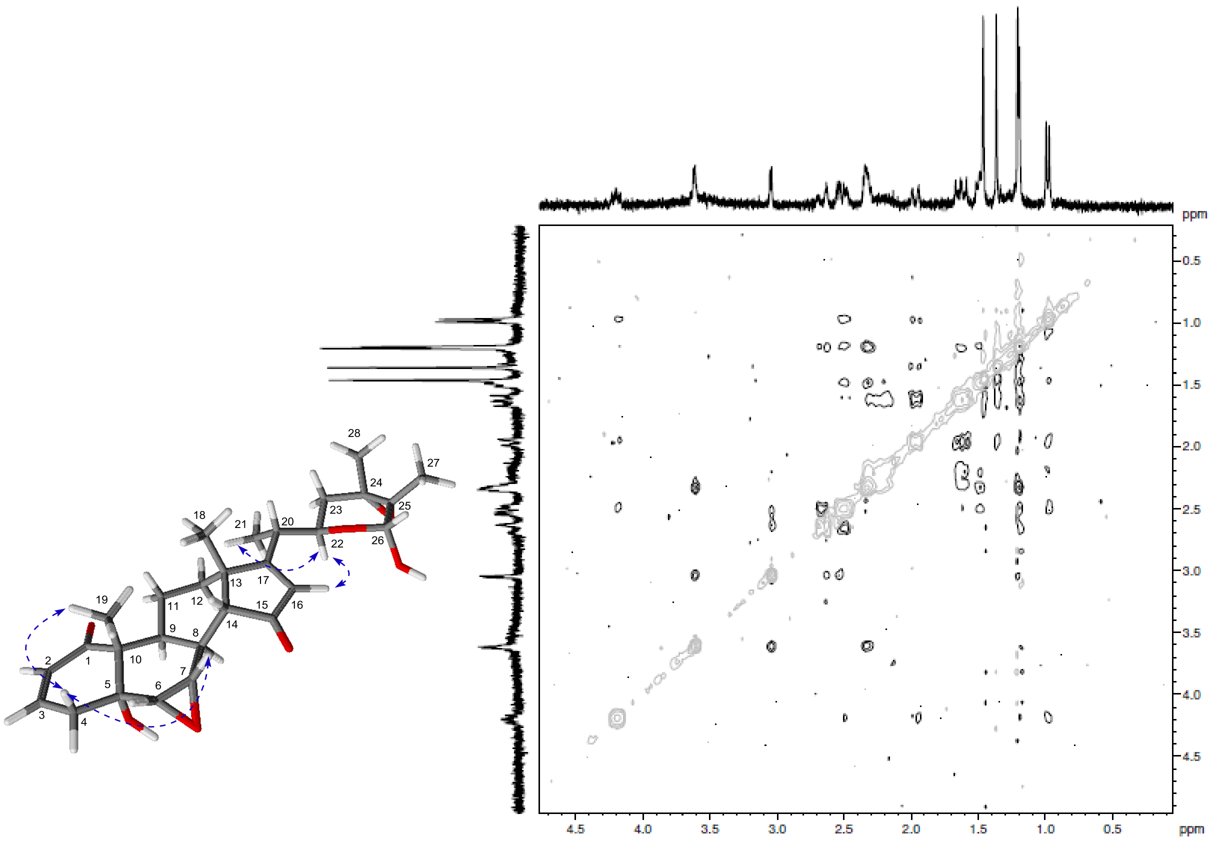

Figure S7. ^{1}H,^{1}H-NOESY spectrum of compound **1**.

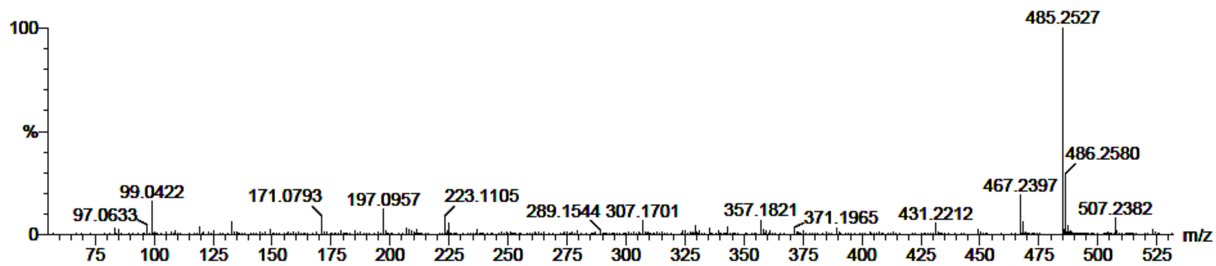

Figure S8. HRESIMS (positive mode) spectrum of compound **1**.

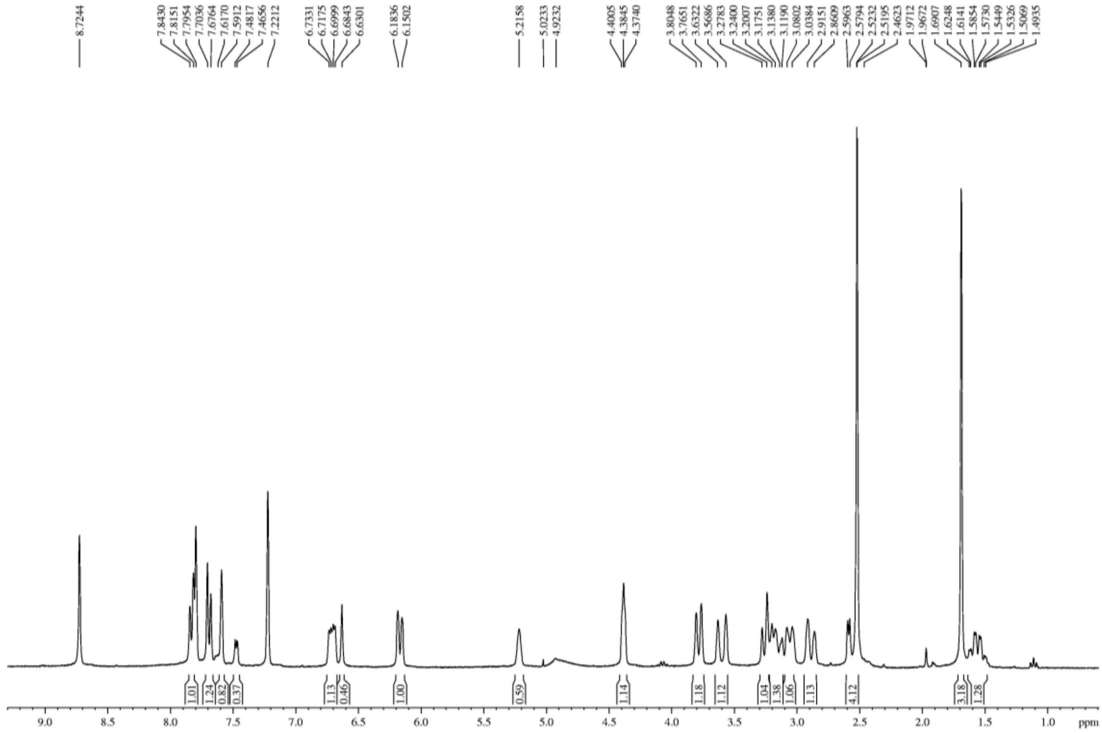

Figure S9. ^{1}H NMR (500 MHz, C_5D_5N) spectrum of compound **2**.

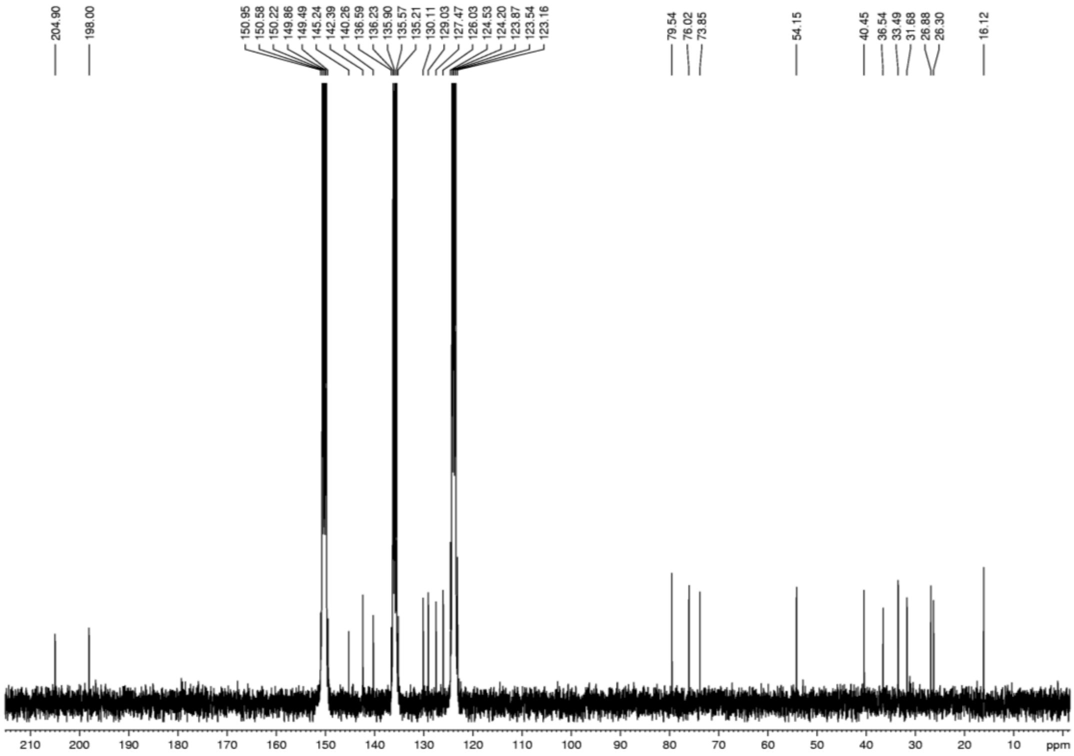

Figure S10. ^{13}C NMR (75 MHz, C_5D_5N) spectrum of compound **2**.

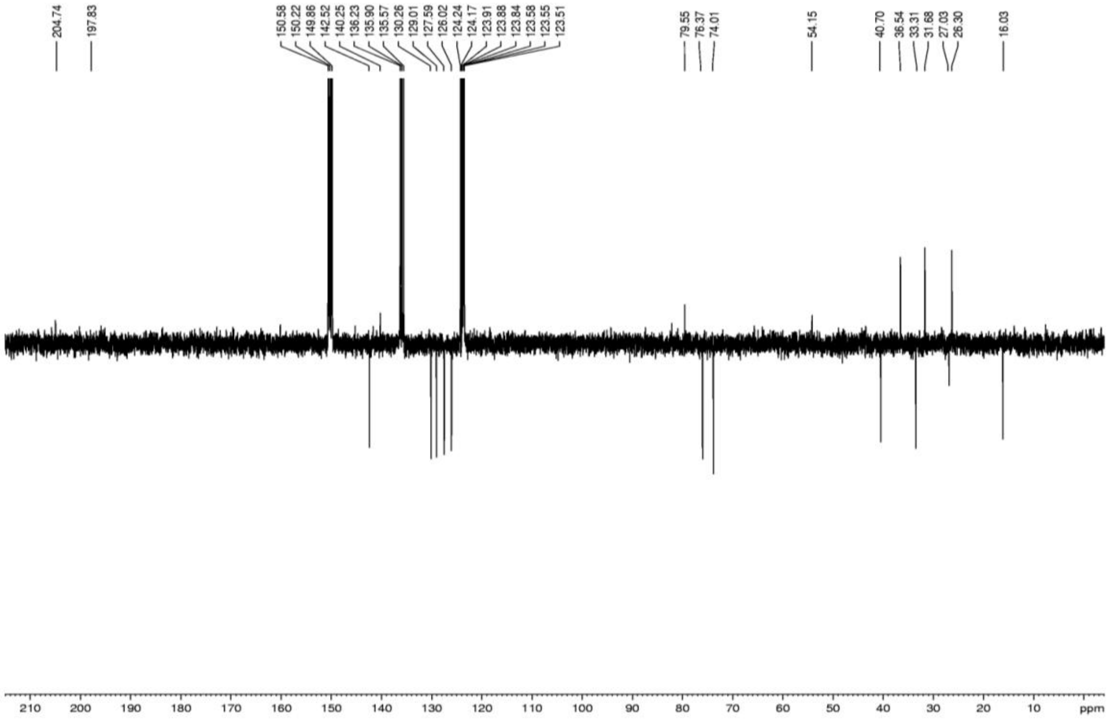

Figure S11. ^{13}C NMR DEPT 135° (75 MHz, C_5D_5N) spectrum of compound **2**.

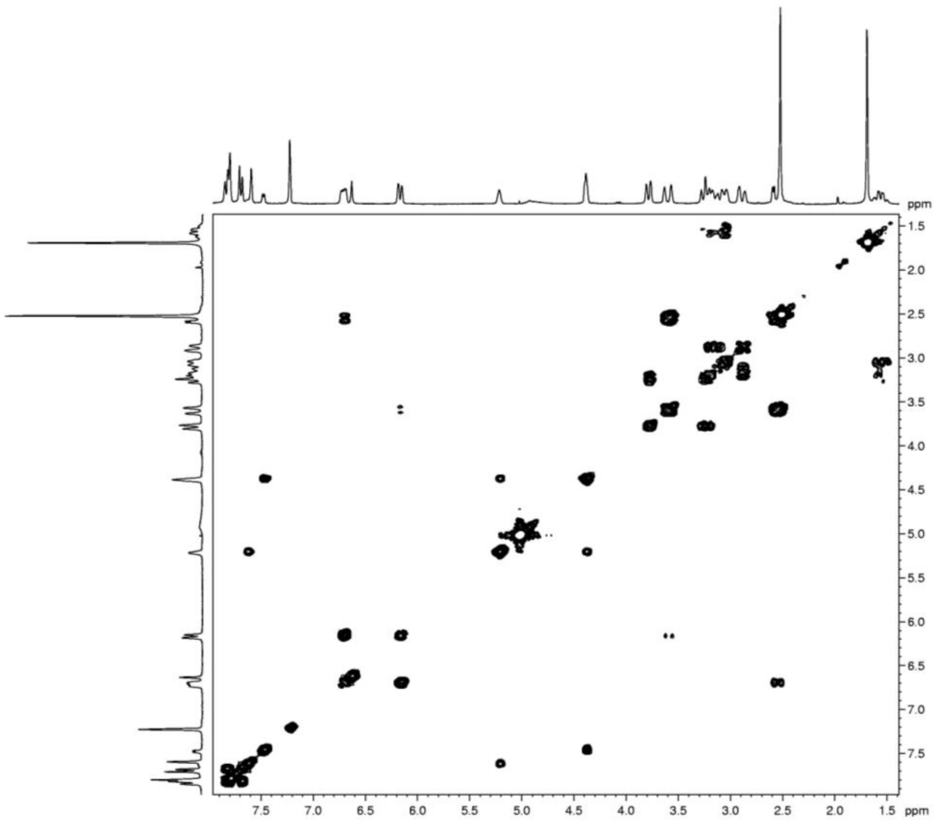

Figure S12. ^{1}H,^{1}H-COSY spectrum of compound **2**.

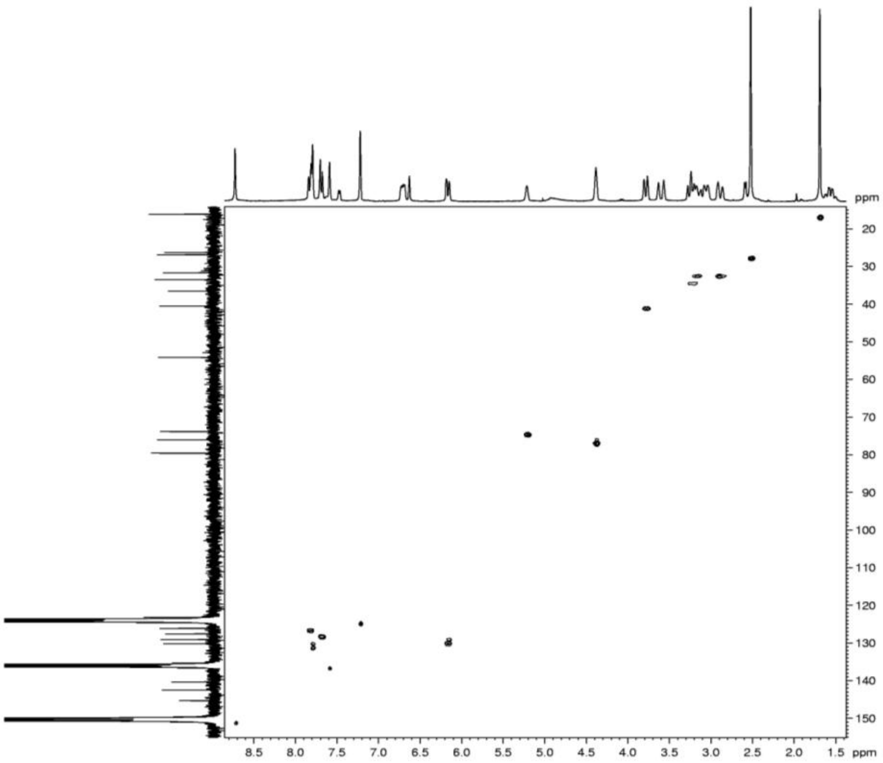

Figure S13. ^{1}H,^{13}C-HSQC spectrum of compound **2**.

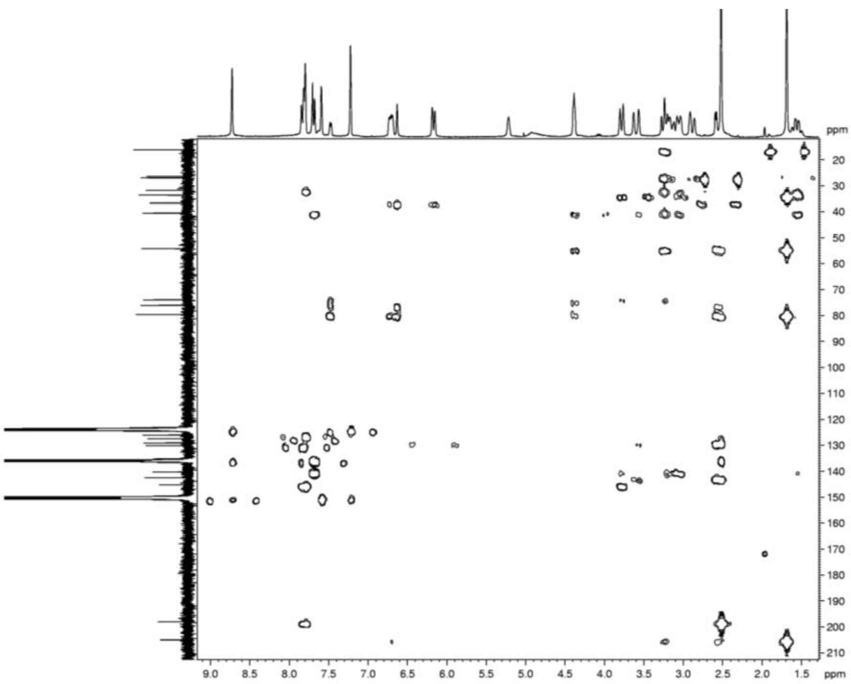

Figure S14. ^{1}H,^{13}C-HMBC spectrum of compound **2**.

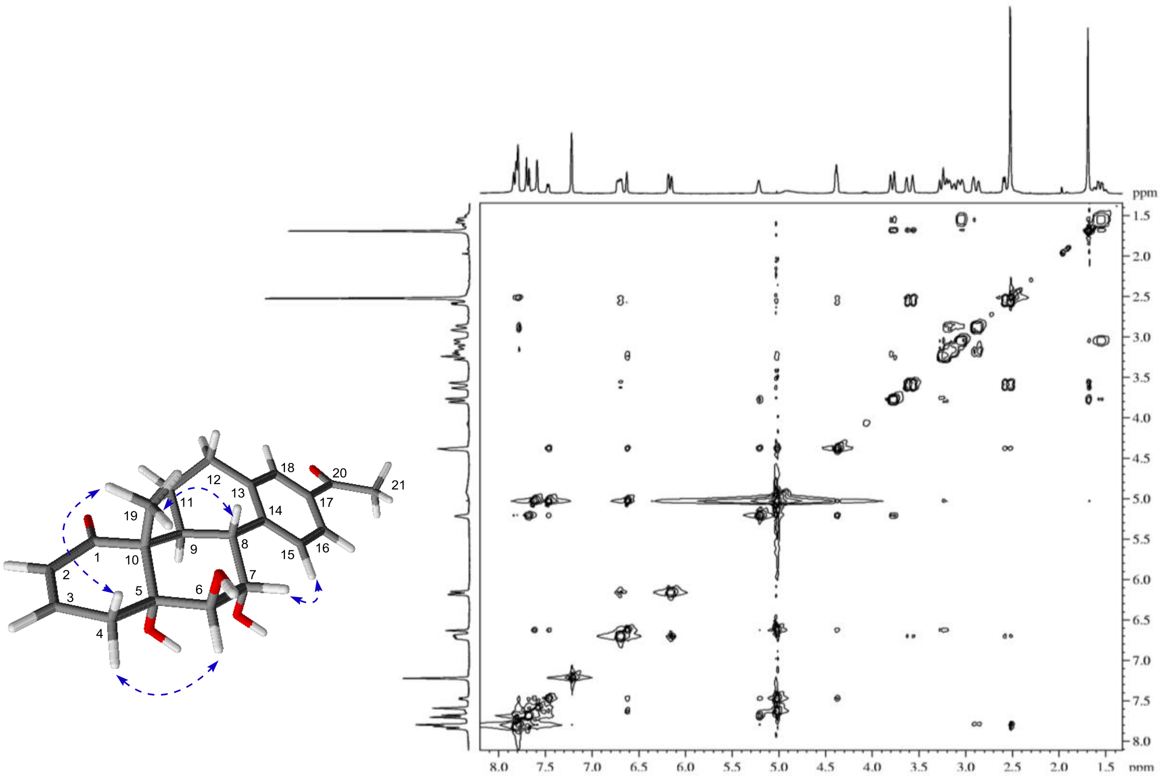

Figure S15. $^{1}H,^{1}H$-NOESY spectrum of compound **2**.

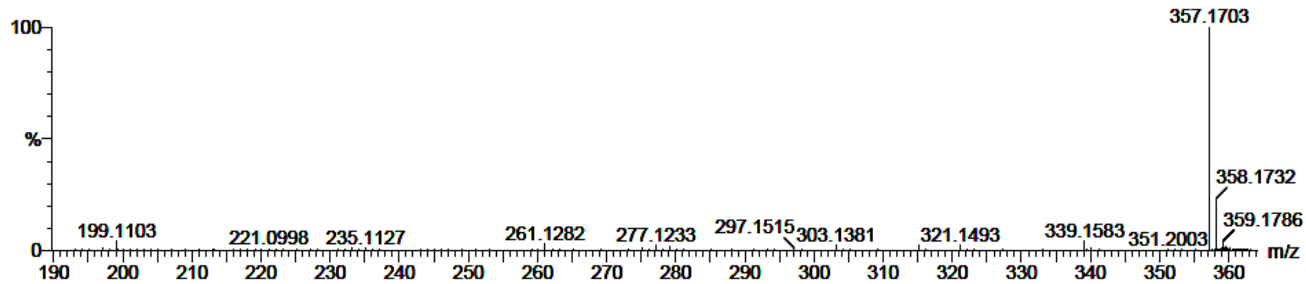

Figure S16. HRESIMS (positive mode) spectrum of compound **2**.

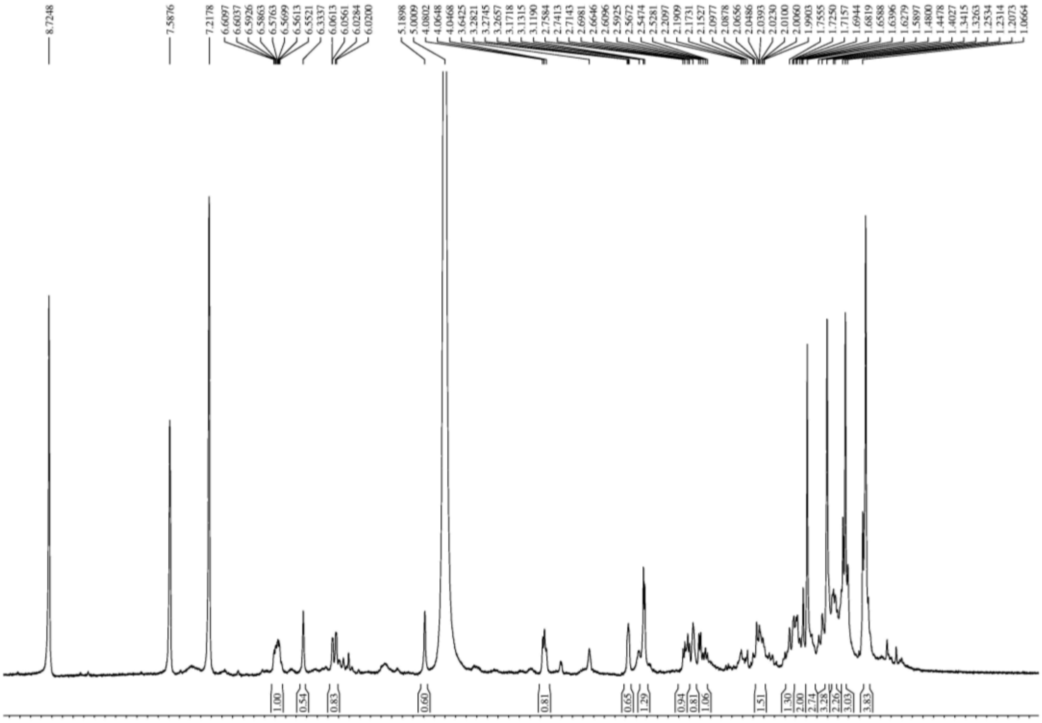

Figure S17. ^{1}H NMR (500 MHz, C_5D_5N) spectrum of compound **3**.

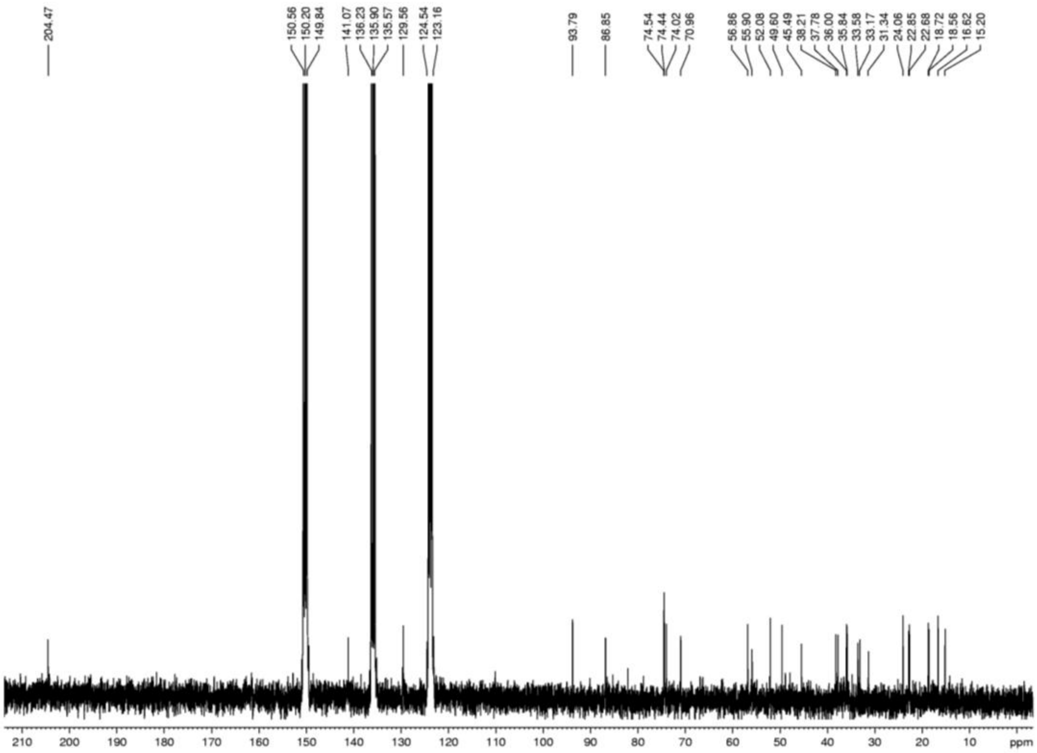

Figure S18. ^{13}C NMR (500 MHz, C_5D_5N) spectrum of compound **3**.

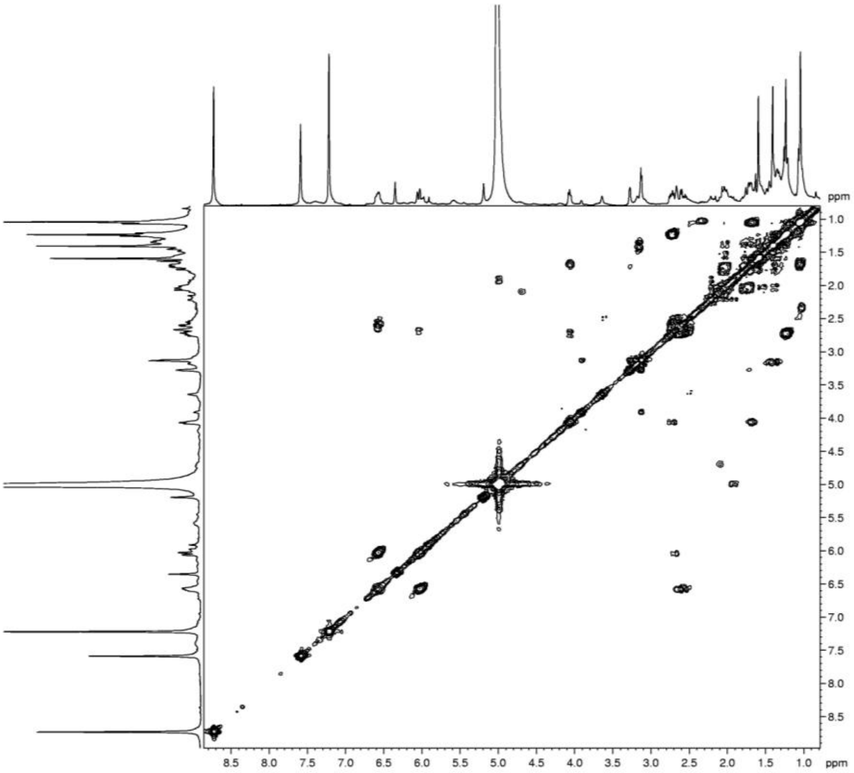

Figure S19. ^{1}H,^{1}H-COSY spectrum of compound **3**.

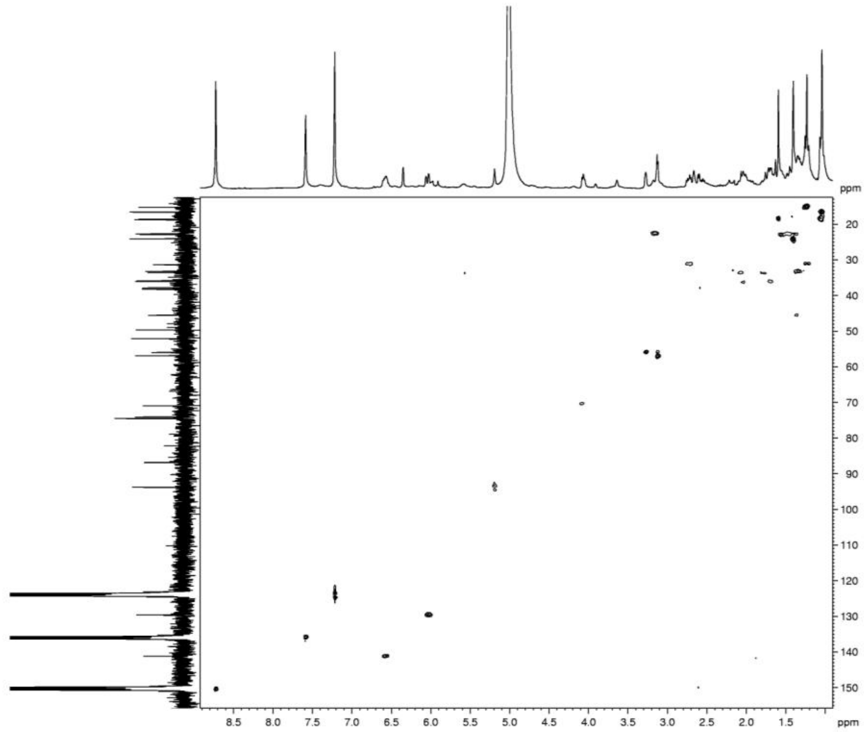

Figure S20. ^{1}H,^{13}C-HSQC spectrum of compound **3**.

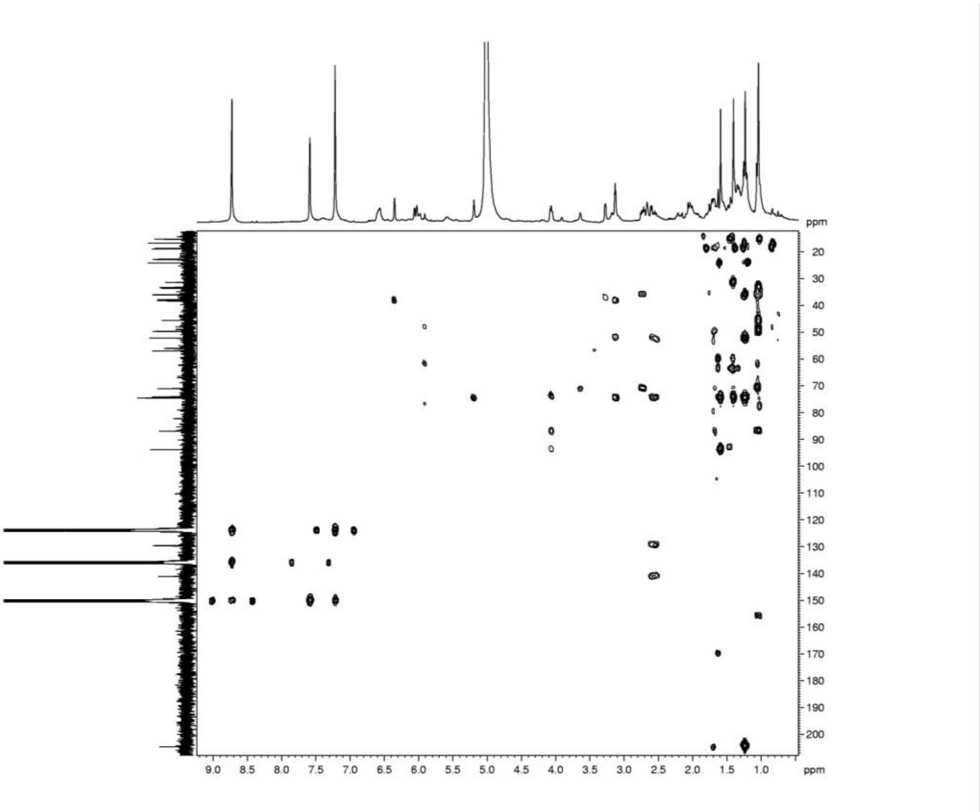

Figure S21. $^{1}H,^{13}C$-HMBC spectrum of compound **3**.

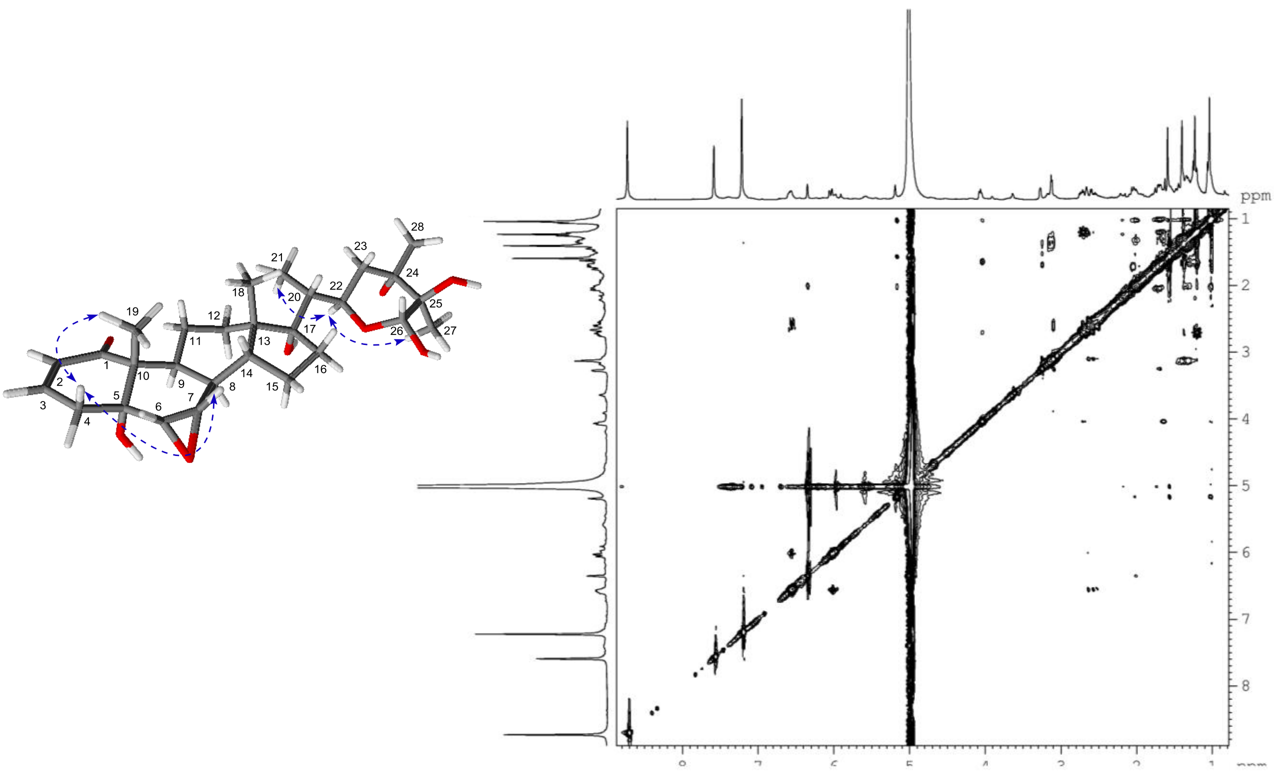

Figure S22. $^{1}H,^{1}H$-NOESY spectrum of compound **3**.

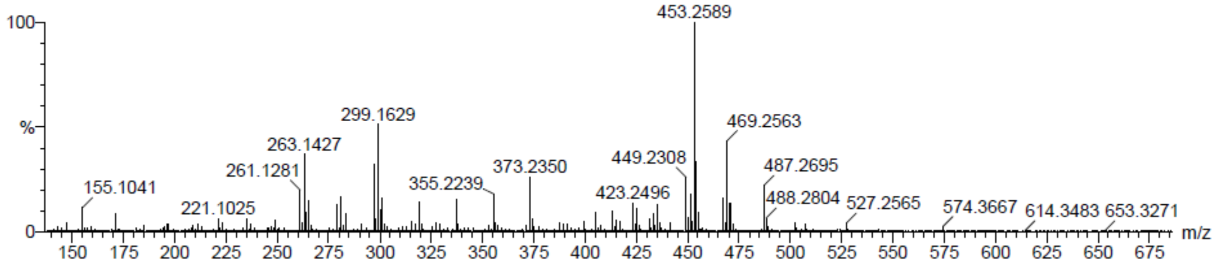

Figure S23. HRESIMS (positive mode) spectrum of compound **3**.

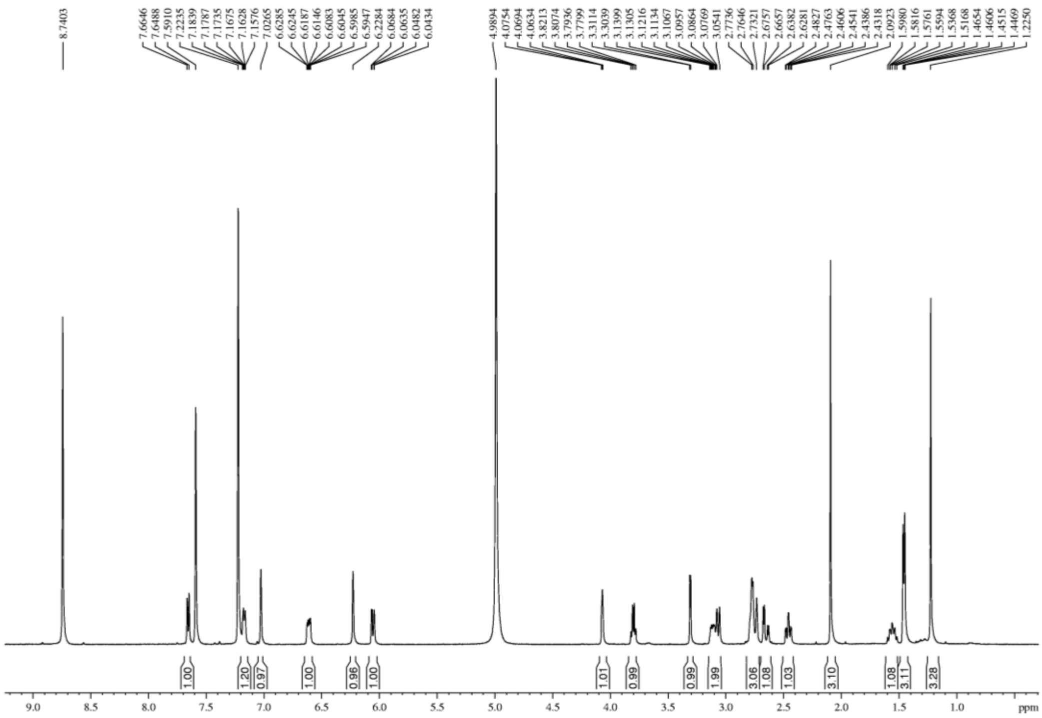

Figure S24. [1]H NMR (500 MHz, C_5D_5N) spectrum of compound **4**.

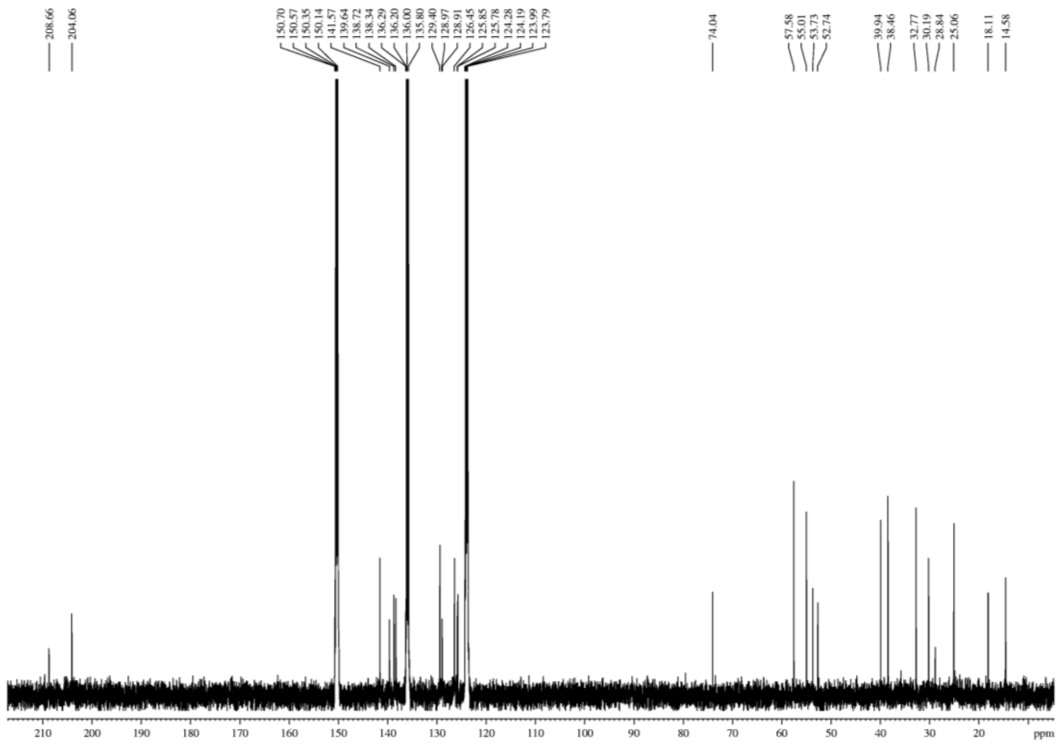

Figure S25. ^{13}C NMR (75 MHz, C_5D_5N) spectrum of compound **4**.

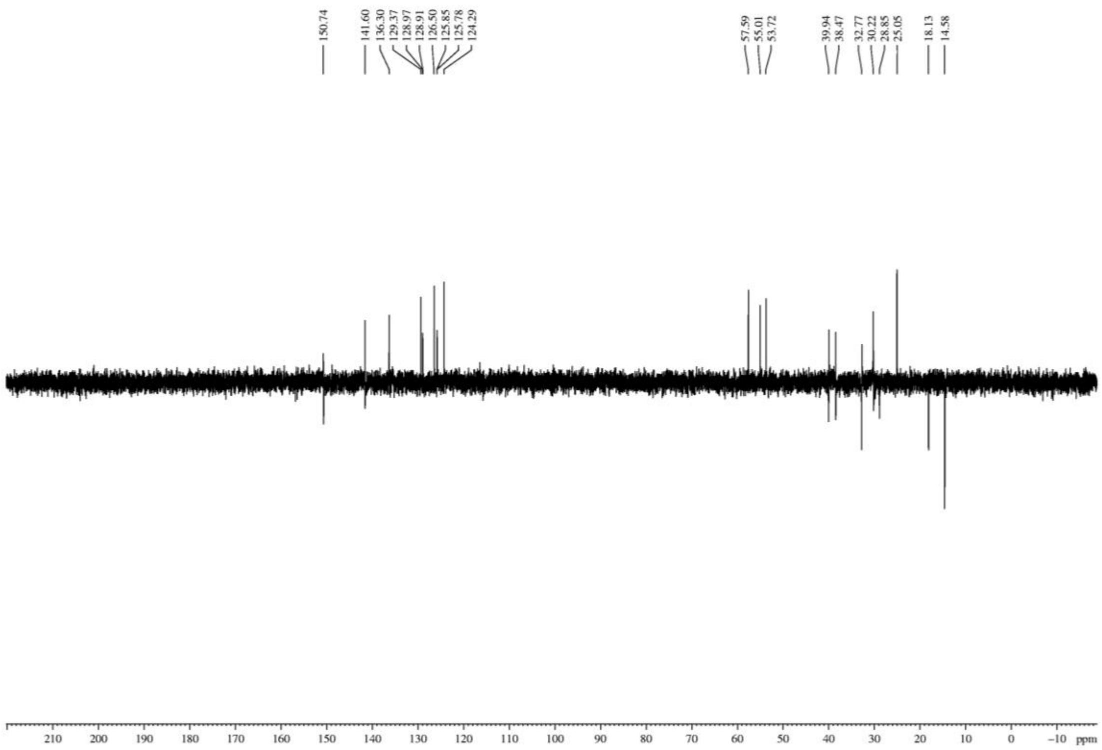

Figure S26. ^{13}C NMR DEPT 135° (75 MHz, C_5D_5N) spectrum of compound **4**.

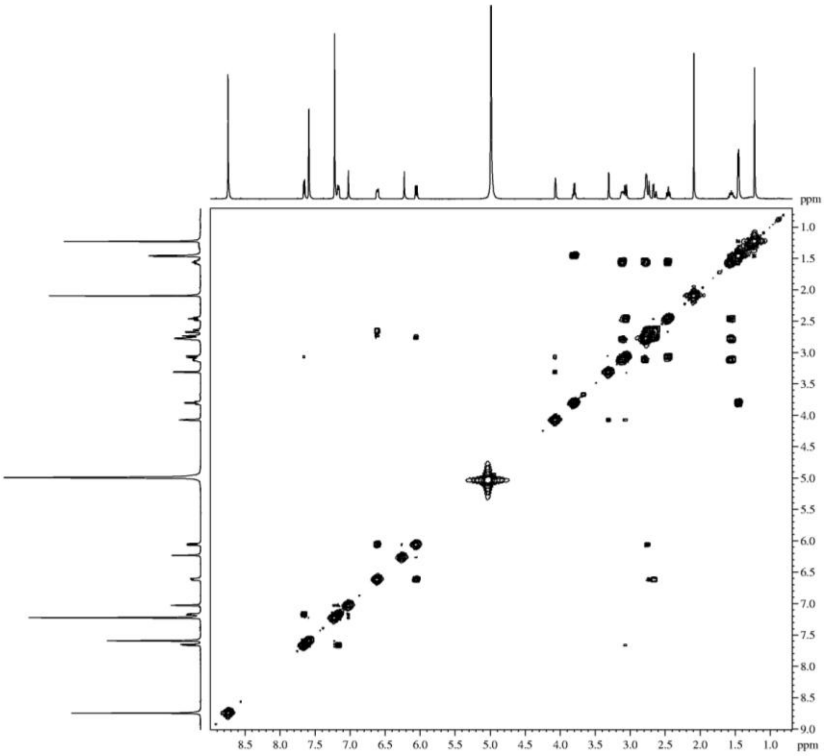

Figure S27. $^{1}H,^{1}H$-COSY spectrum of compound **3**.

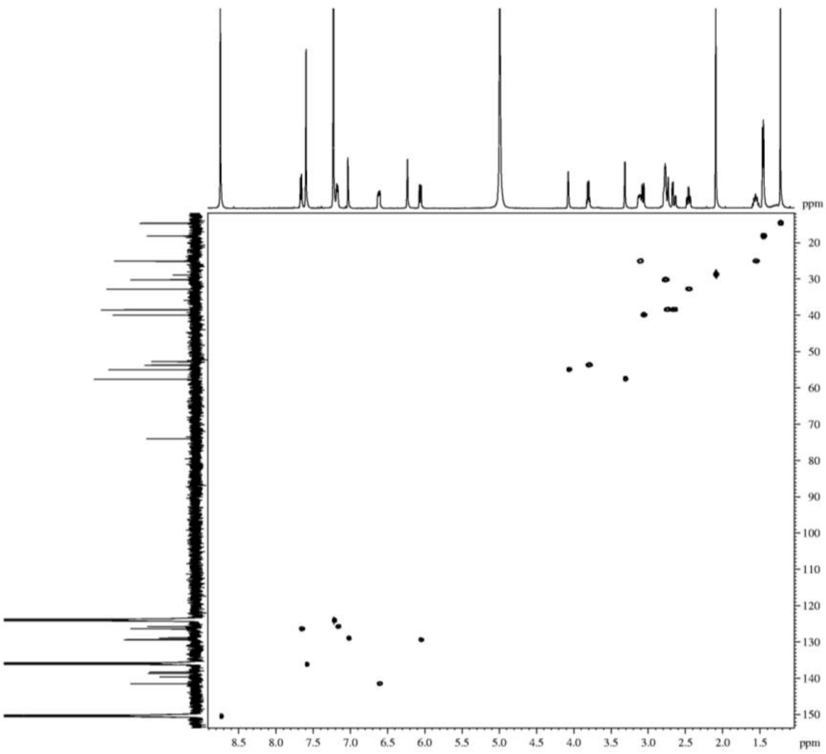

Figure S28. $^{1}H,^{13}C$-HSQC spectrum of compound **4**.

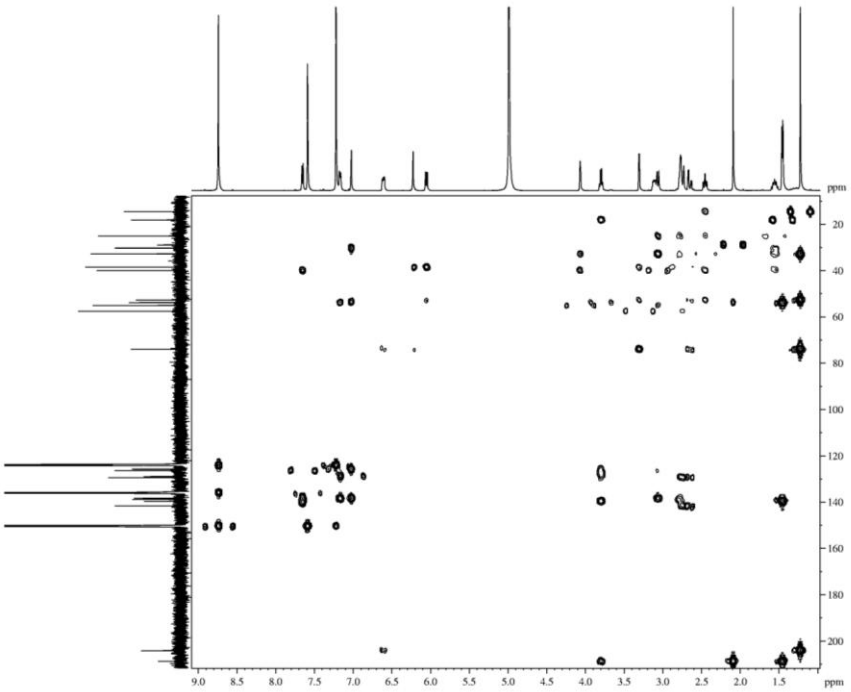

Figure S29. ^{1}H,^{13}C-HMBC spectrum of compound **4**.

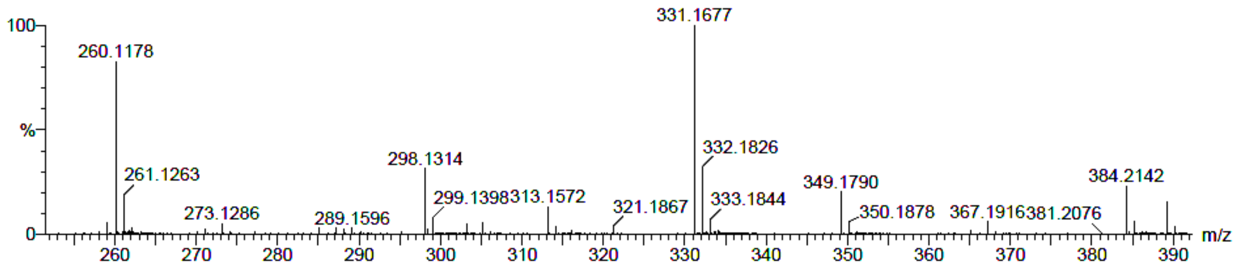

Figure S30. HRESIMS (positive mode) spectrum of compound **4**.