Supporting Information

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Chemical Constituents of *Siegesbeckia orientalis* and Their Anti-proliferative Activity

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Table of Contents **Page**

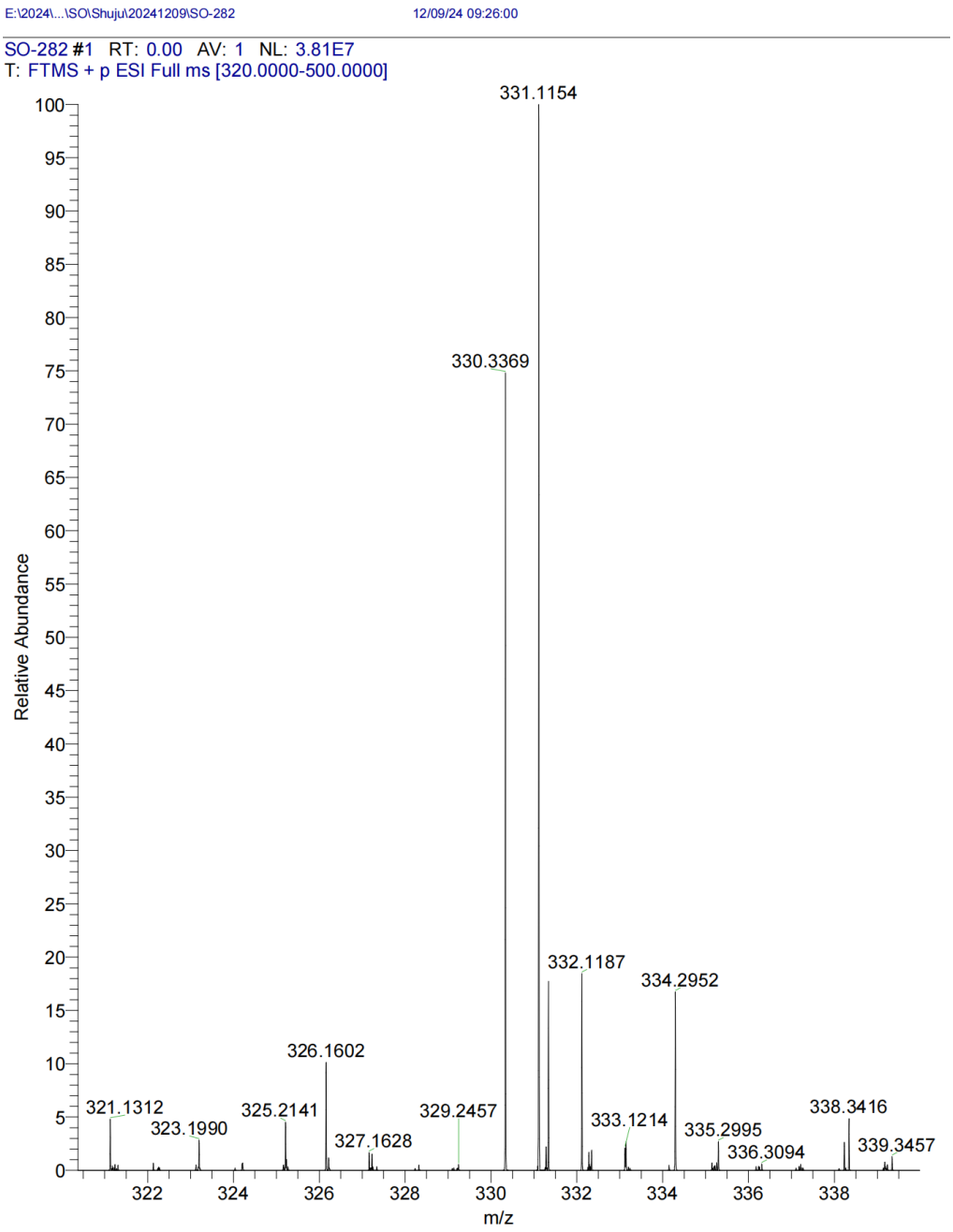


Figure S1: HR-ESI-MS Spectrum of **1**.

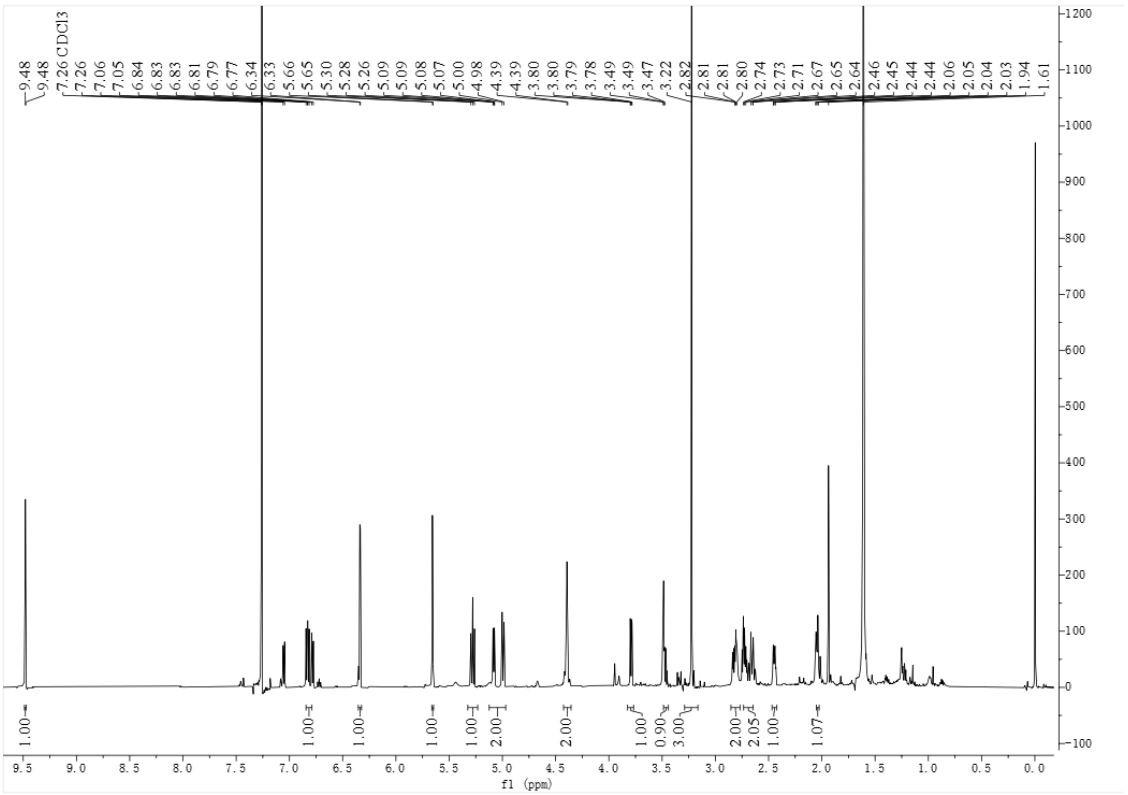


Figure S2: ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of **1**.

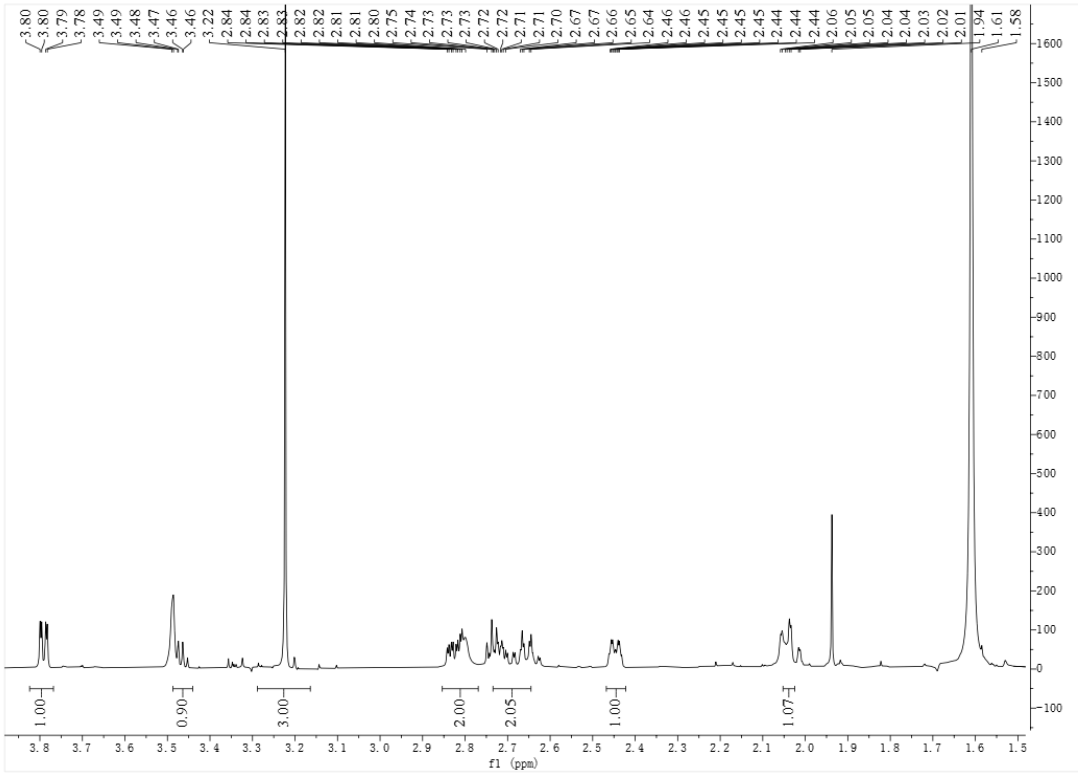


Figure S3: ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of **1** (From δ_H 1.6 ppm to δ_H 3.8 ppm).

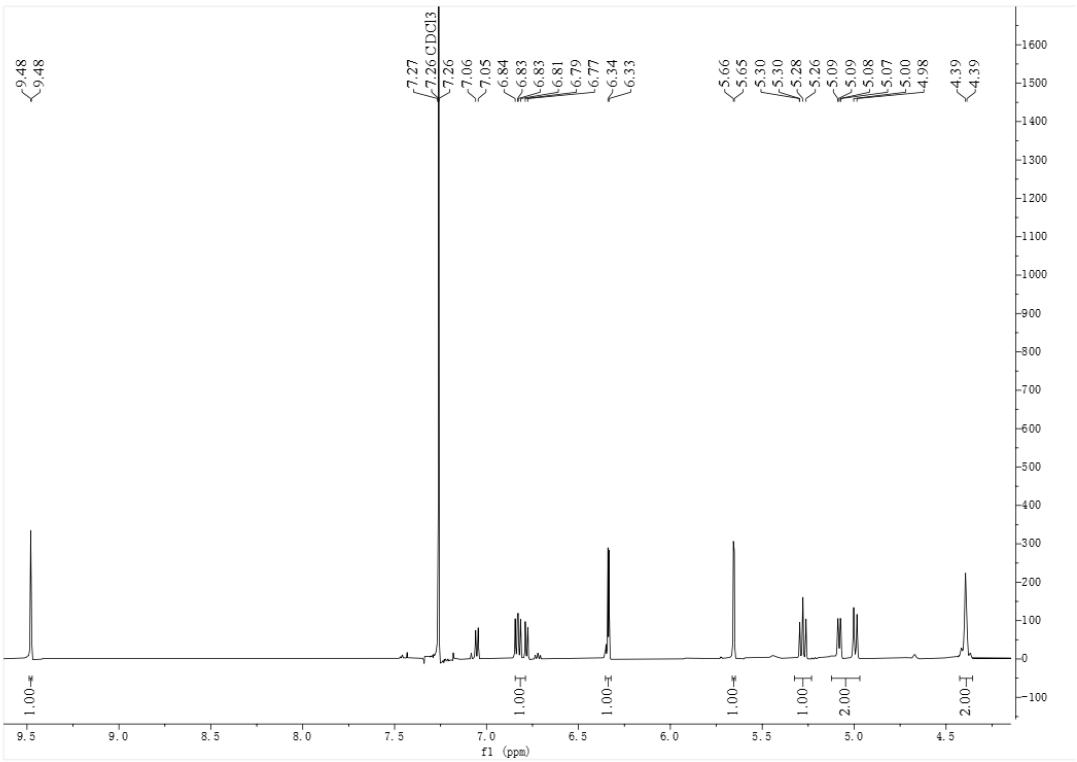


Figure S4: ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of **1** (From δ_H 4.4 ppm to δ_H 9.5 ppm).

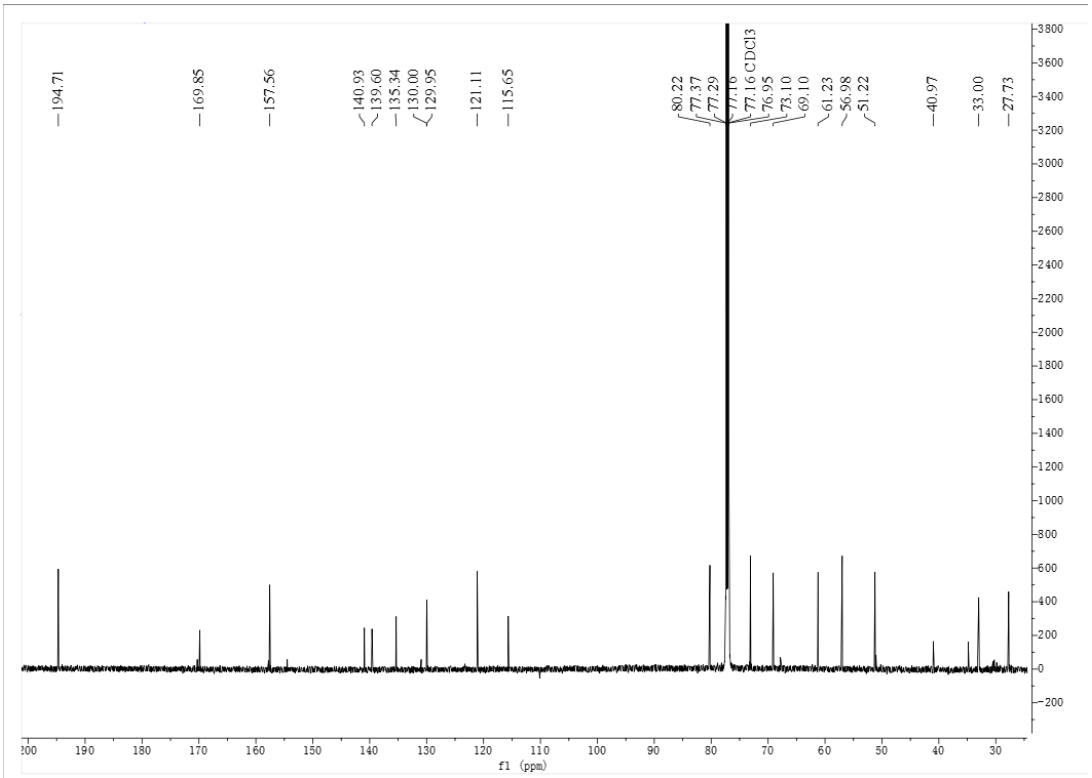


Figure S5: ^{13}C-NMR (600 MHz, $CDCl_3$) Spectrum of **1**.

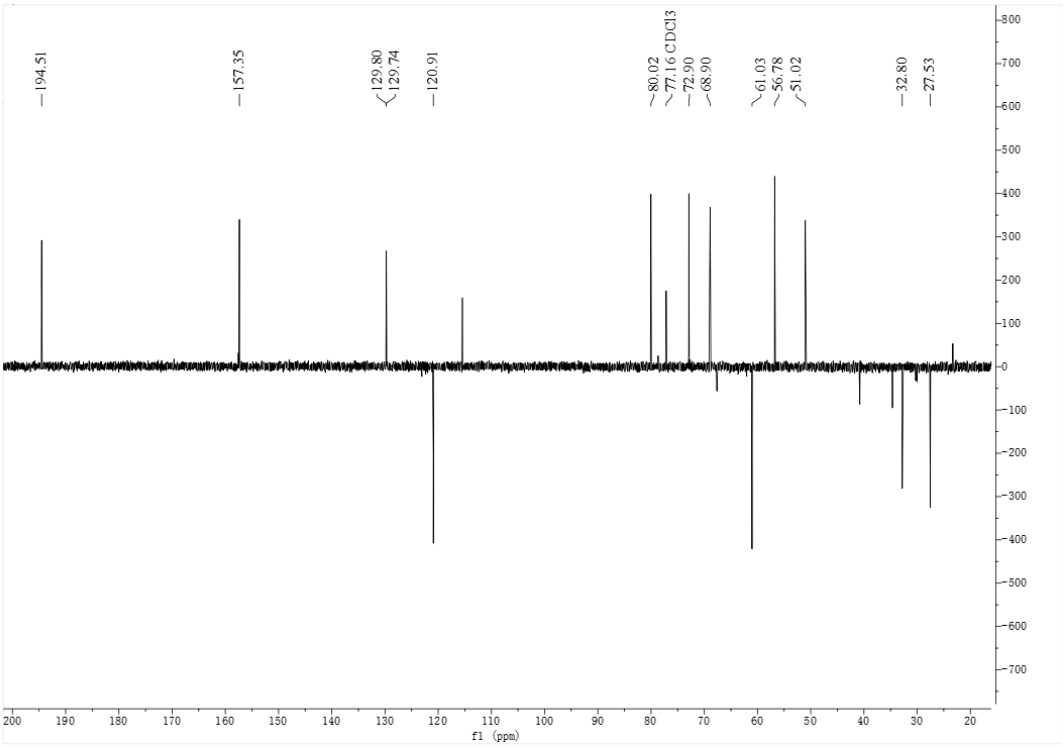


Figure S6: DEPT135 (600 MHz, $CDCl_3$) Spectrum of **1**.

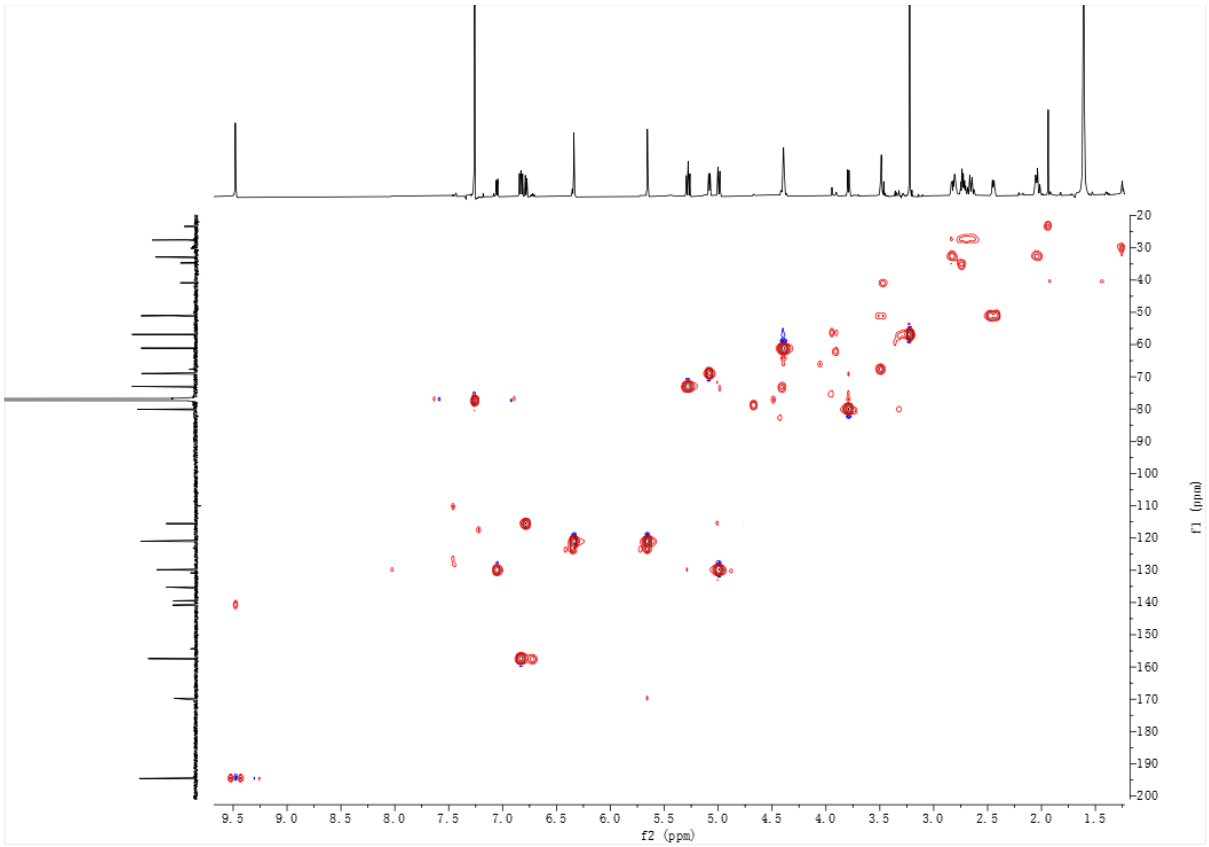


Figure S7: HSQC Spectrum of **1**.

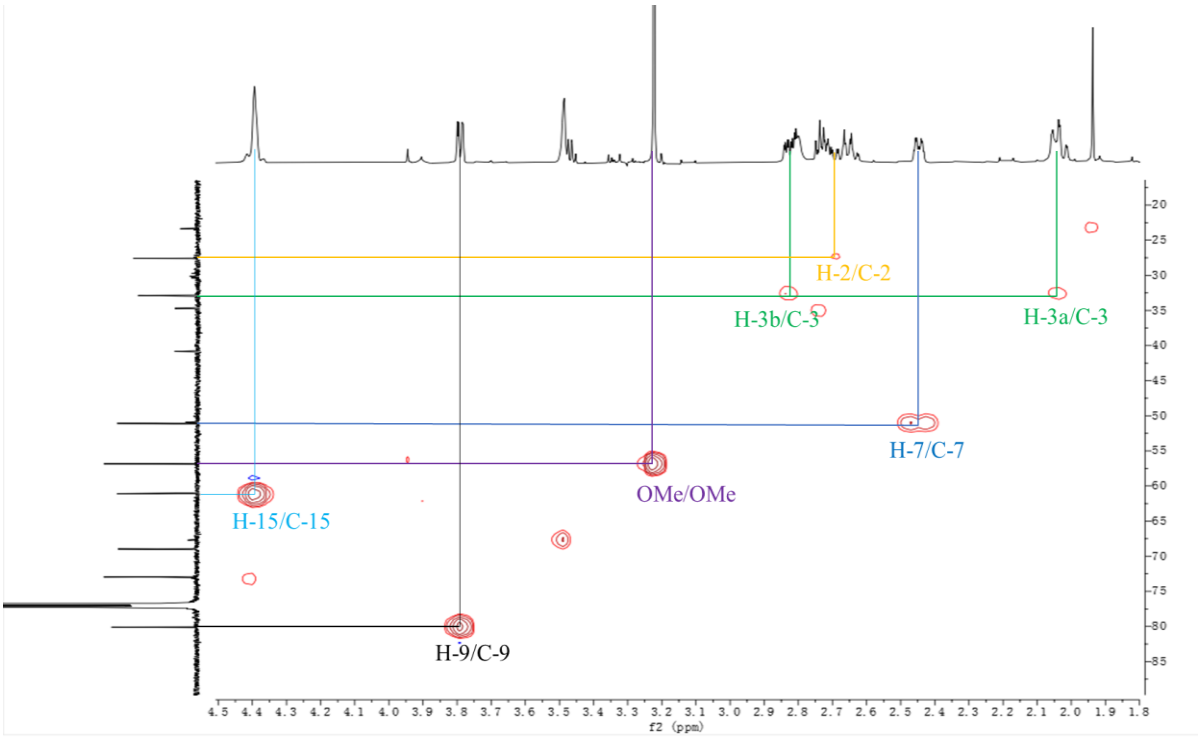


Figure S8: HSQC Spectrum of **1** (From δ_H 1.9 ppm to δ_H 4.4 ppm).

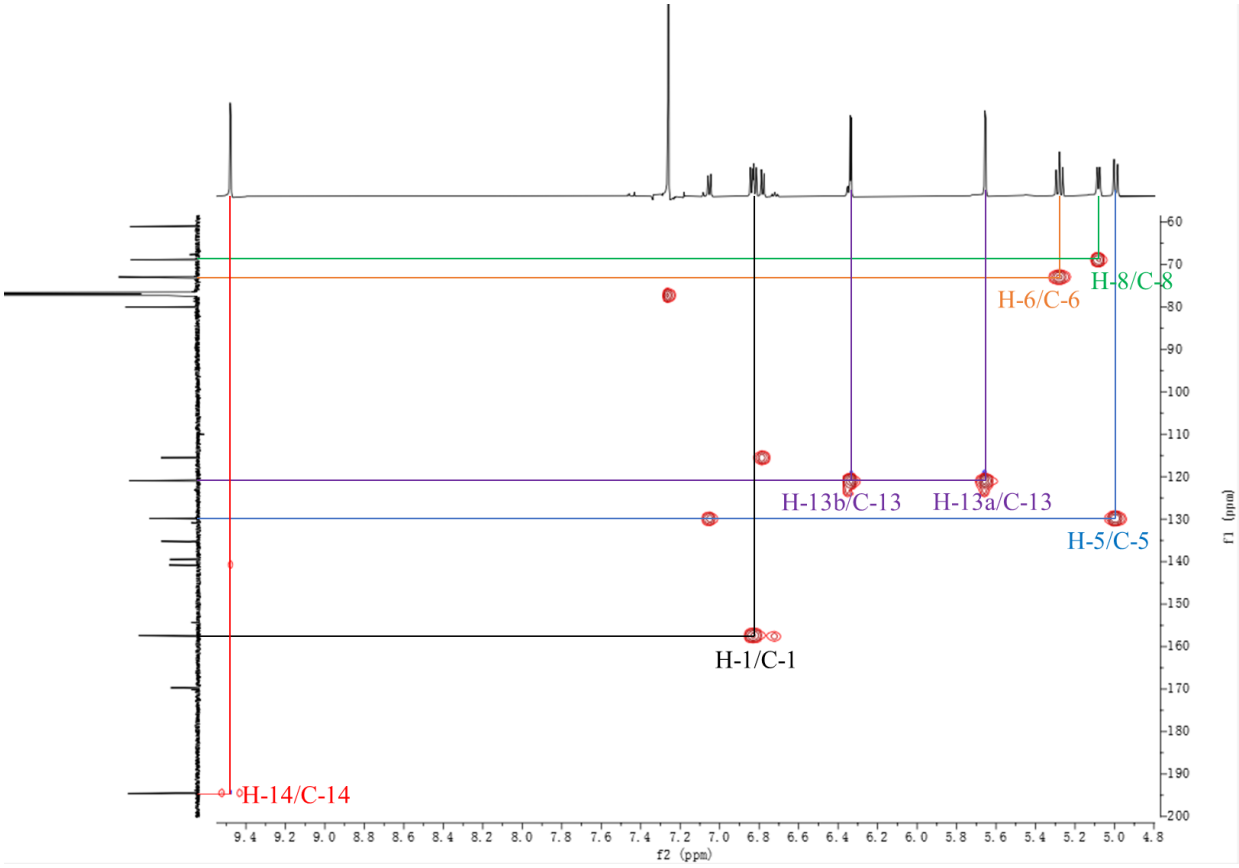


Figure S9: HSQC Spectrum of **1** (From δ_H5.0 ppm to δ_H 9.5 ppm).

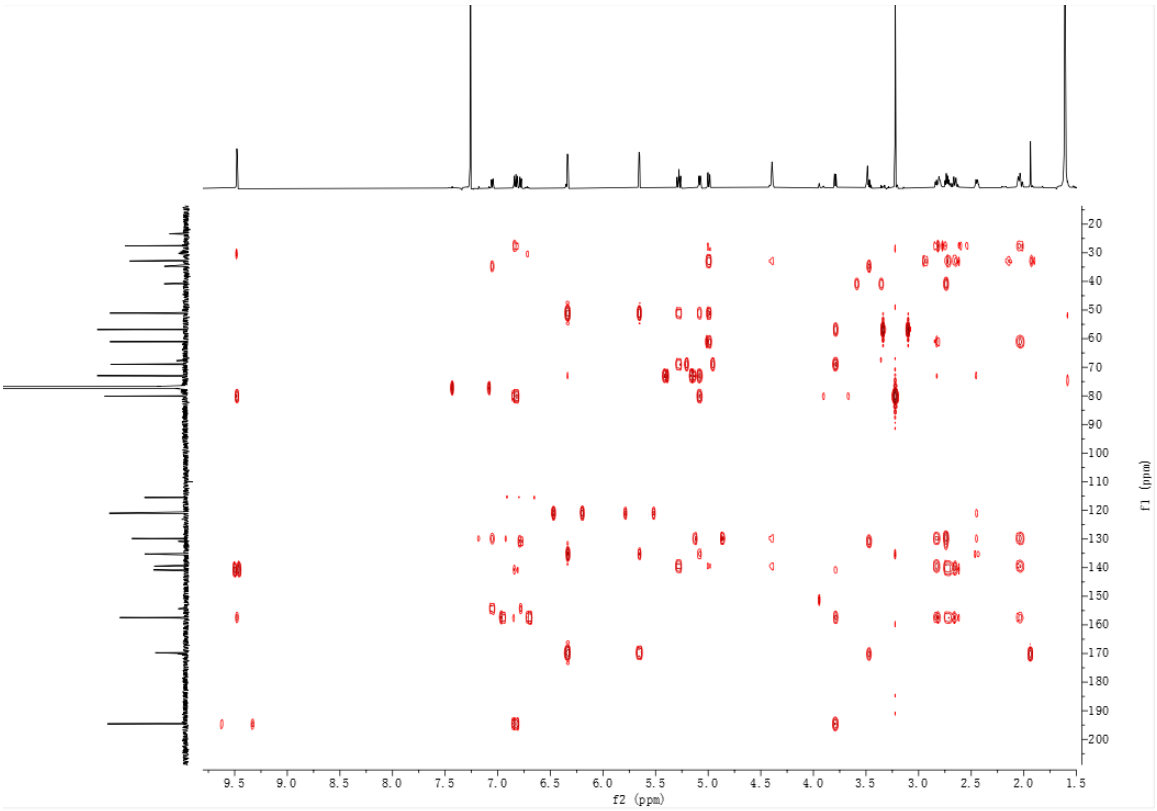


Figure S10: HMBC Spectrum of **1**.

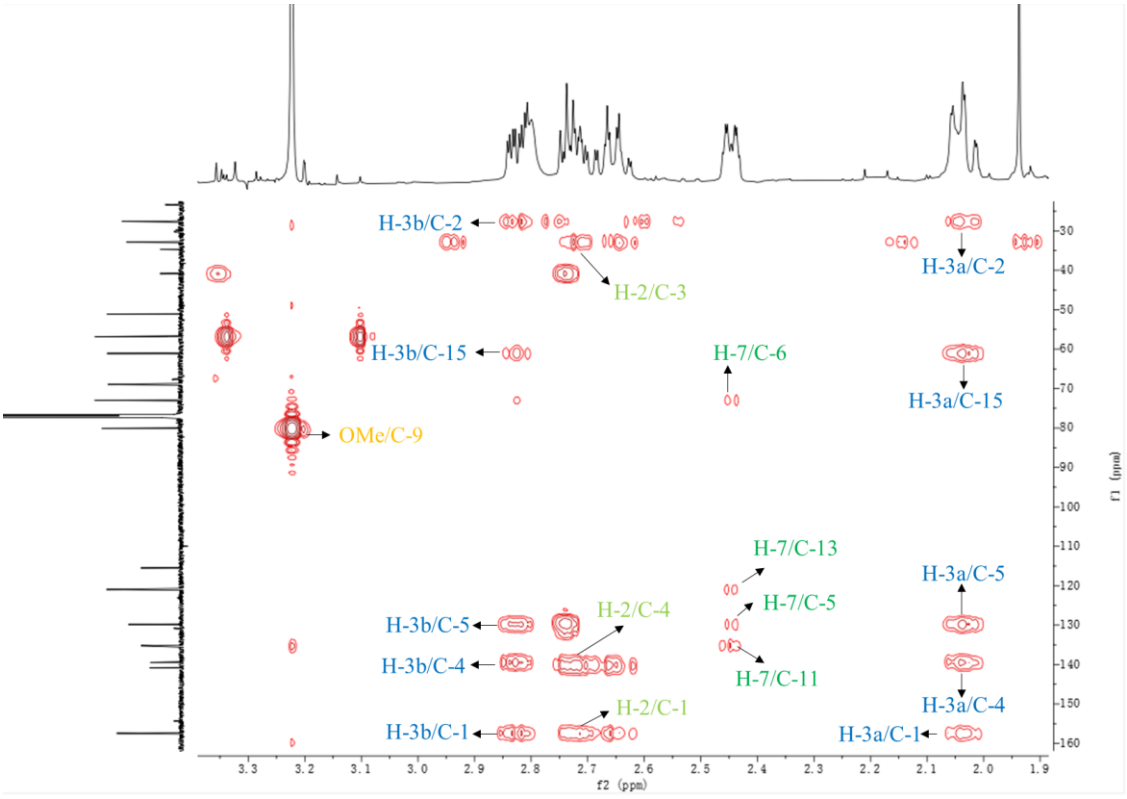


Figure S11: HMBC Spectrum of **1** (From δ_H 1.9 ppm to δ_H 3.2 ppm).

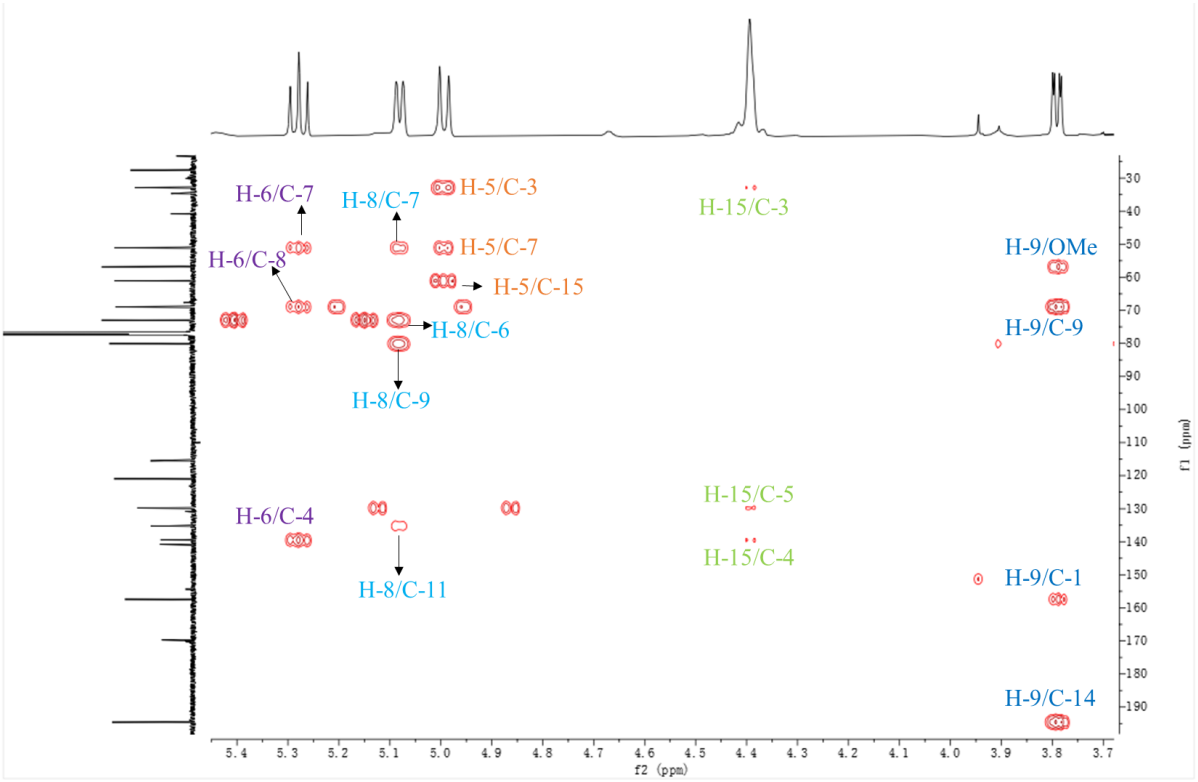


Figure S12: HMBC Spectrum of **1**(From δ_H 3.8 ppm to δ_H 5.3 ppm).

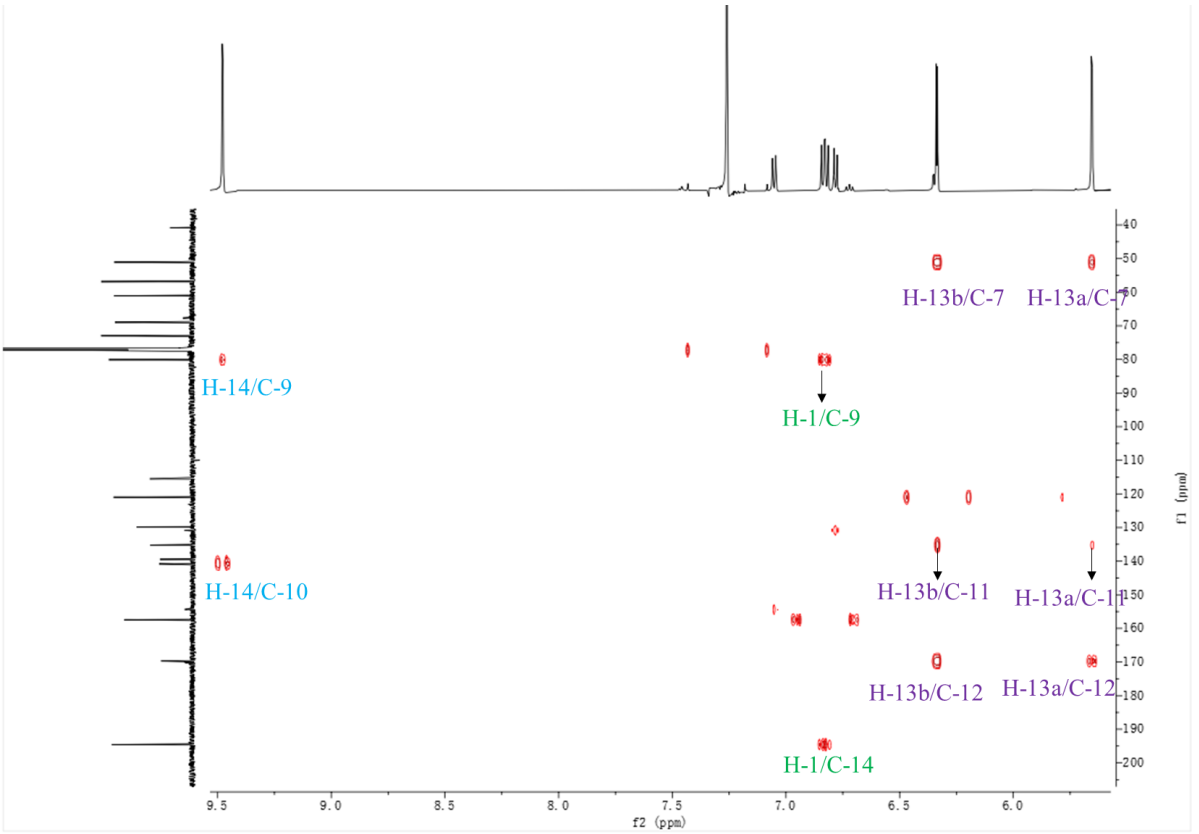


Figure S13: HMBC Spectrum of **1** (From δ_H 5.6 ppm to δ_H 9.5 ppm).

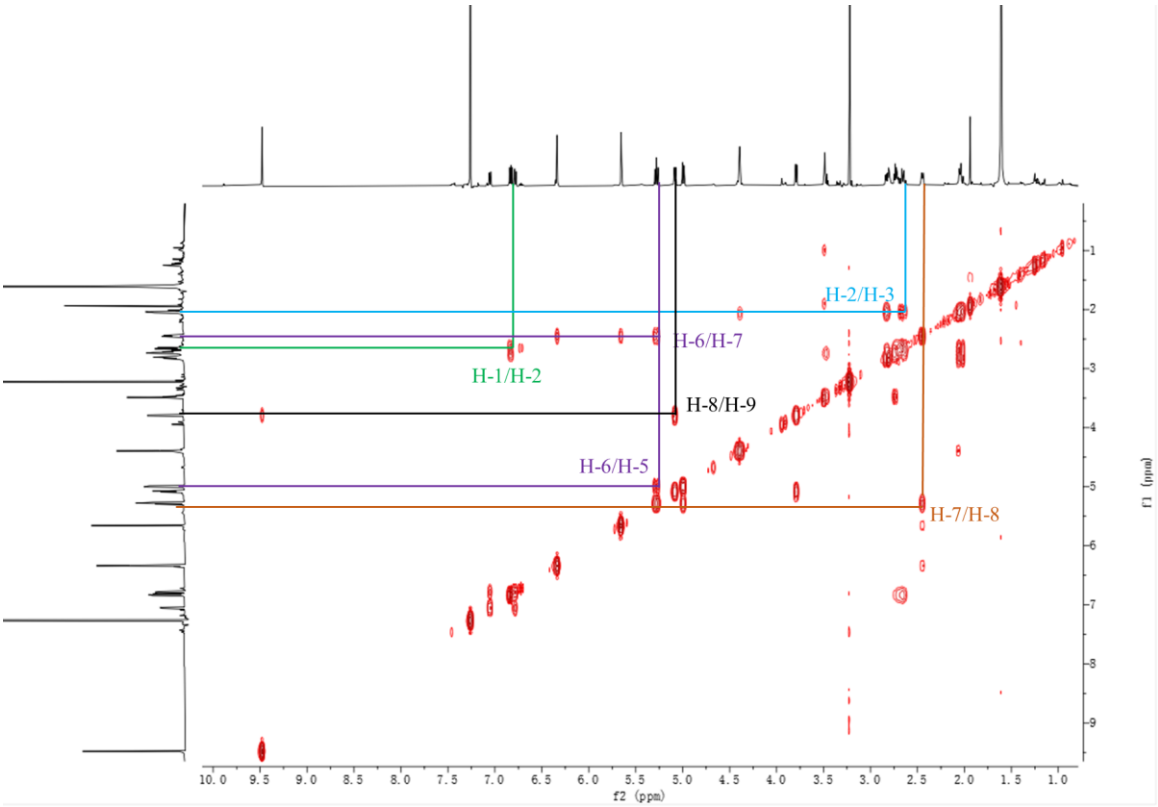


Figure S14: ^{1}H-^{1}H COSY Spectrum of **1**.

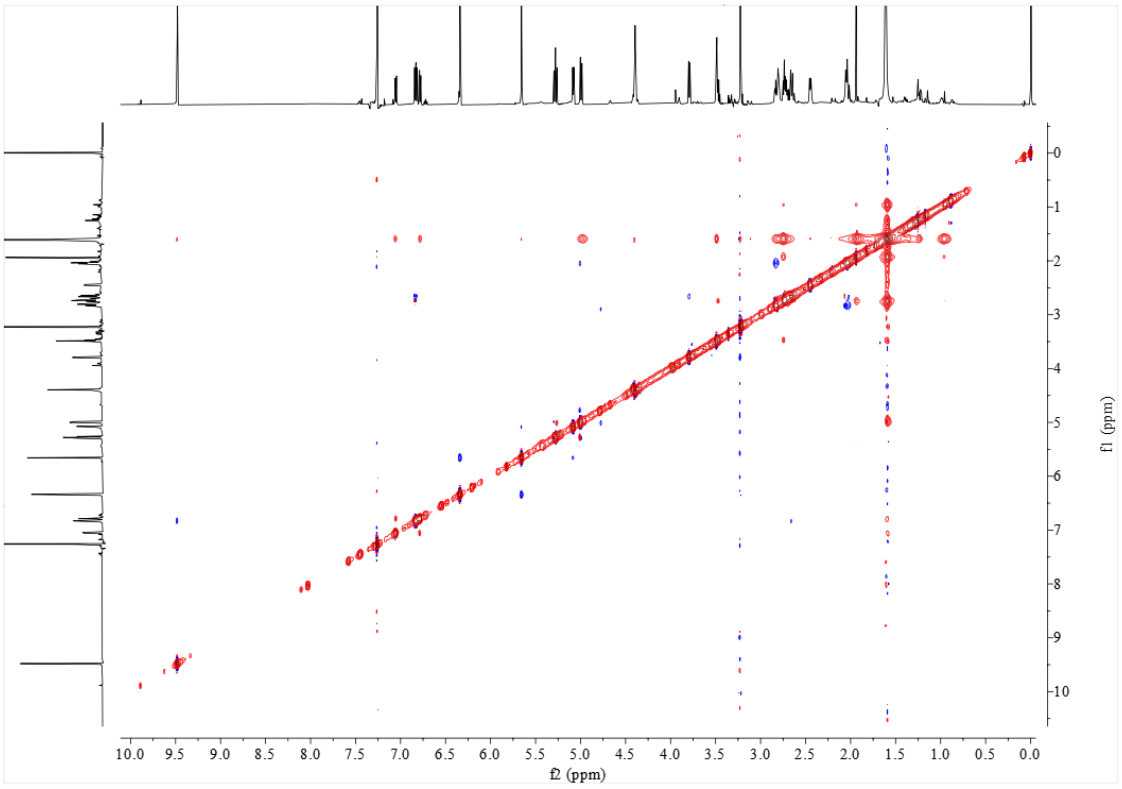


Figure S15: ^{1}H-^{1}H NOESY Spectrum of **1**.

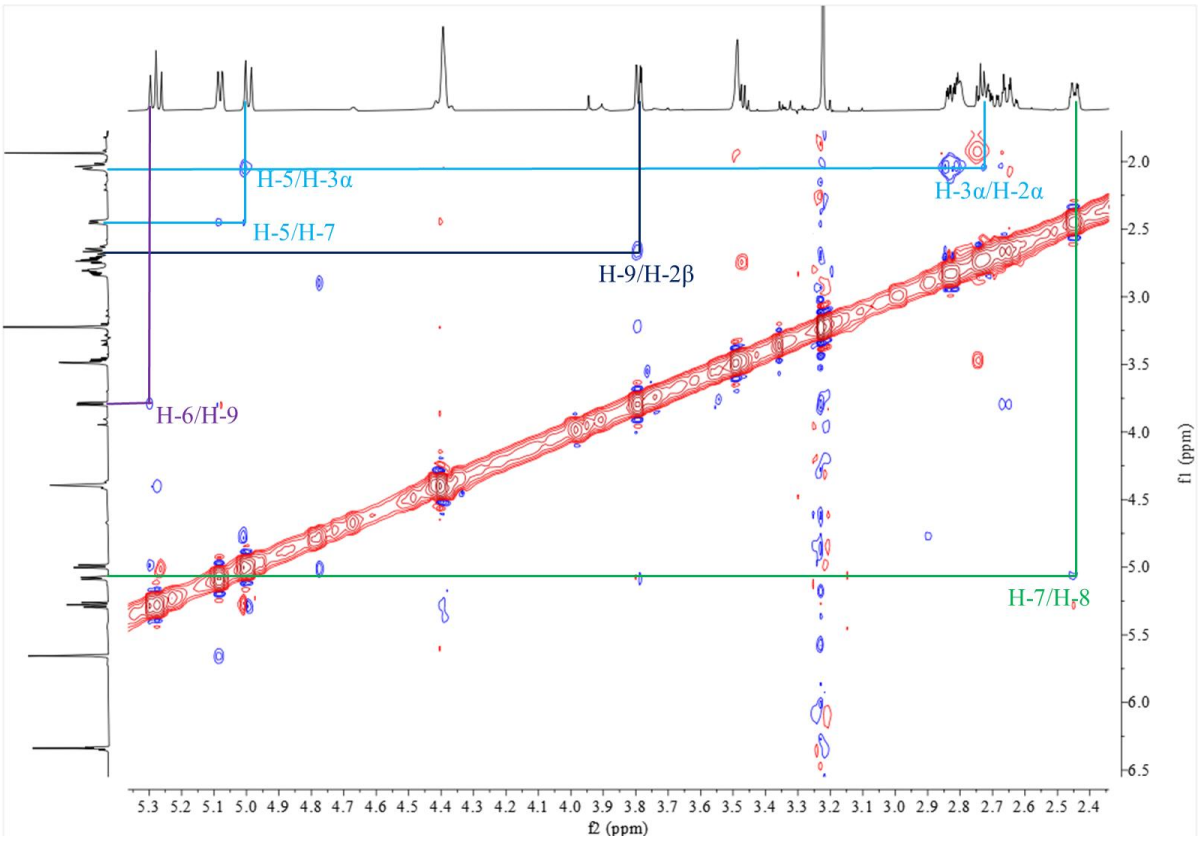


Figure S16: ^{1}H-^{1}H NOESY Spectrum of **1** (From δ_H 2.4 ppm to δ_H 5.3 ppm).

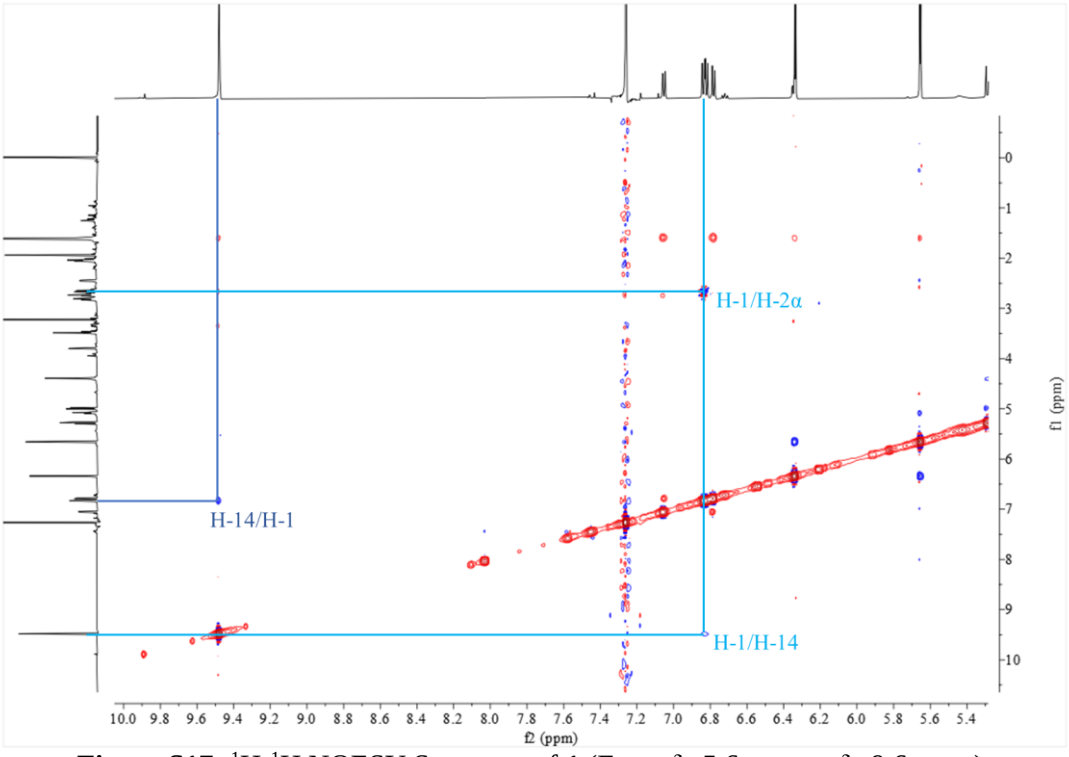


Figure S17: ^{1}H-^{1}H NOESY Spectrum of **1** (From δ_H 5.6 ppm to δ_H 9.6 ppm).

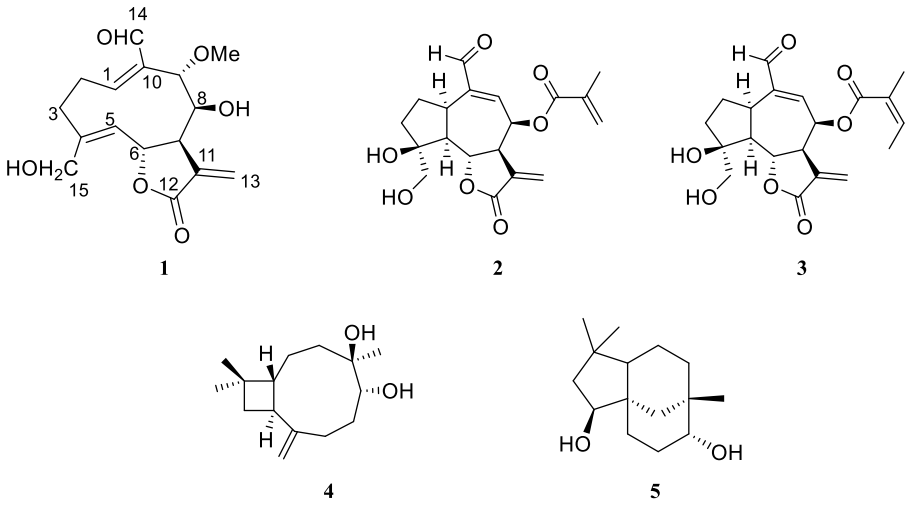


Figure S18: The structures of compounds **1-5**.

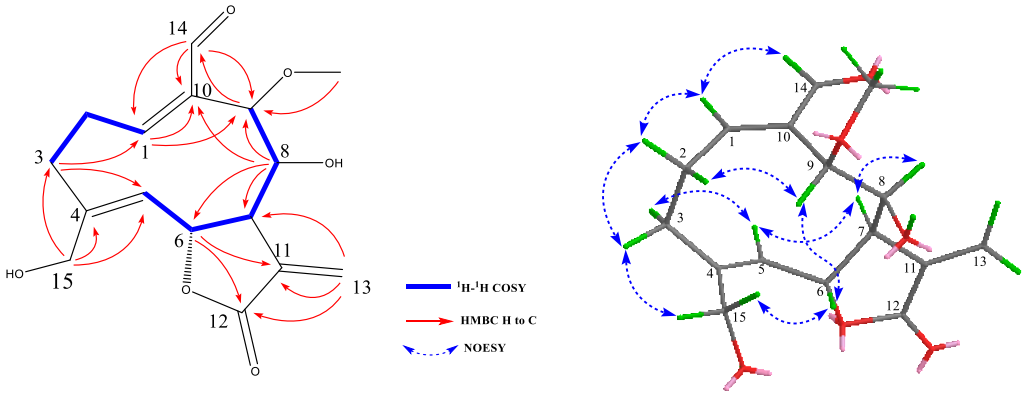


Figure S19: COSY, HMBC and NOESY correlations of compound **1**.

Table S1: NMR spectral data for compound **1** in $CDCl_3$ (600/150 MHz).

No.	**1**				
	δ_H (*J*, Hz)	δ_C	^{1}H-^{13}C HMBC	^{1}H-^{1}H COSY	^{1}H-^{1}H NOESY
1	6.81 dd (10.0, 7.6)	157.6	C-3, C-9, C-10, C-14	H-2	H-2α, H-14
2α	2.66 m	27.7	C-1,C-3,C-4	H-1	H-1, H-3α
2β	2.73 m				H-9
3α	2.04 m	33.0	C-1, C-2, C-5, C-15		H-2α, H-5, H-15α
3β	2.82 m				
4		139.6			
5	4.99 d (10.6)	130.0	C-3, C-4, C-7, C-15	H-6	H-3α, H-7
6	5.28 t (10.2)	73.1	C-4, C-7, C-8	H-5, H-7	H-15β, H-9
7	2.45 m	51.2	C-5, C-6, C-8, C-13	H-6, H-8	H-5, H-8
8	5.08 d (8.0)	69.1	C-6, C-7, C-10, C-9	H-7, H-9	H-7
9	3.79 dd (8.0, 2.2)	80.2	C-1, C-8, C-10, C-14		H-2β, H-6
10		140.9			
11		135.3			
12		169.9			
13a	5.65 d (3.1)	121.1	C-7, C-11, C-12		
13b	6.34 d (3.5)				
14	9.48 d	194.7	C-1, C-9, C-10		H-1
15	4.39 s (2H)	61.2	C-3, C-4, C-5		H-3α
					H-6
-OMe	3.22 s	57.0	C-9		

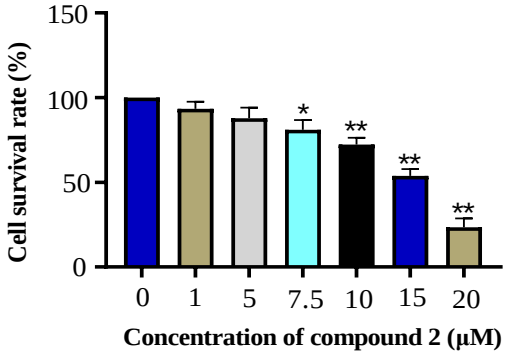


Figure S20: Compound **2** had cytotoxic effect on MDA-MB-231 cells.

Table S2: Anti-breast cancer activity of isolated compounds (IC_{50} in μM).

	1	2	3	4	5	Adriamycin
MDA-MB-231	＞20	13.73 ± 1.24	＞20	＞20	＞20	4.35 ± 1.08

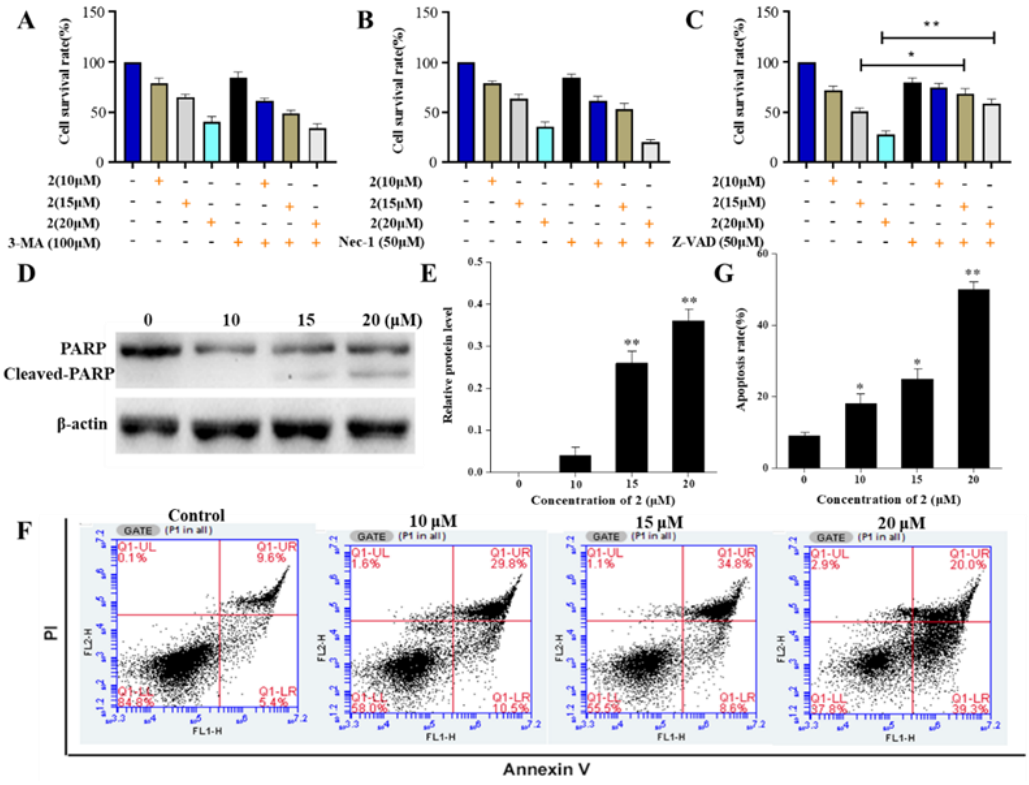


Figure S21. Apoptosis induced by Compound **2** in MDA-MB-231 cells.

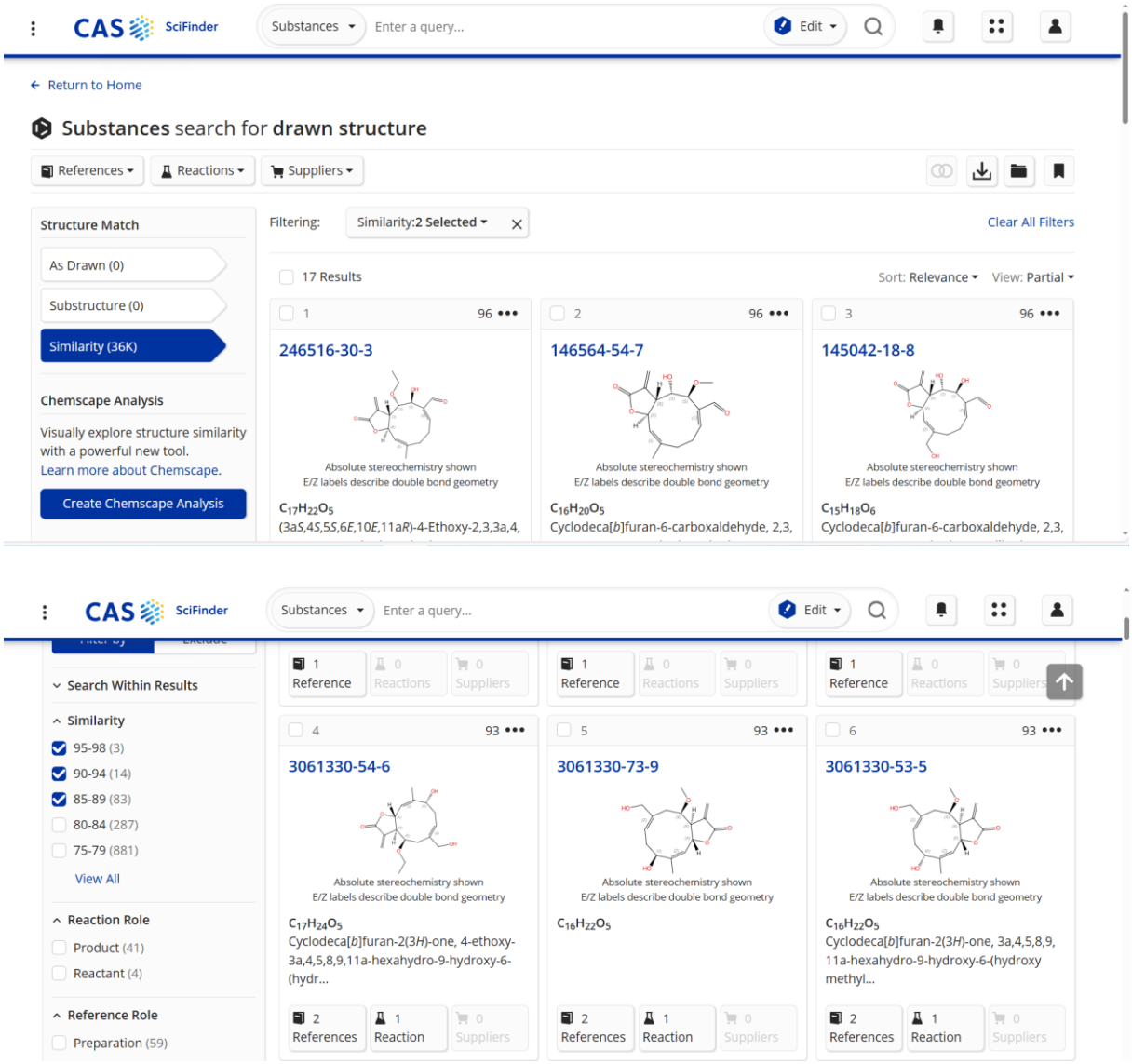
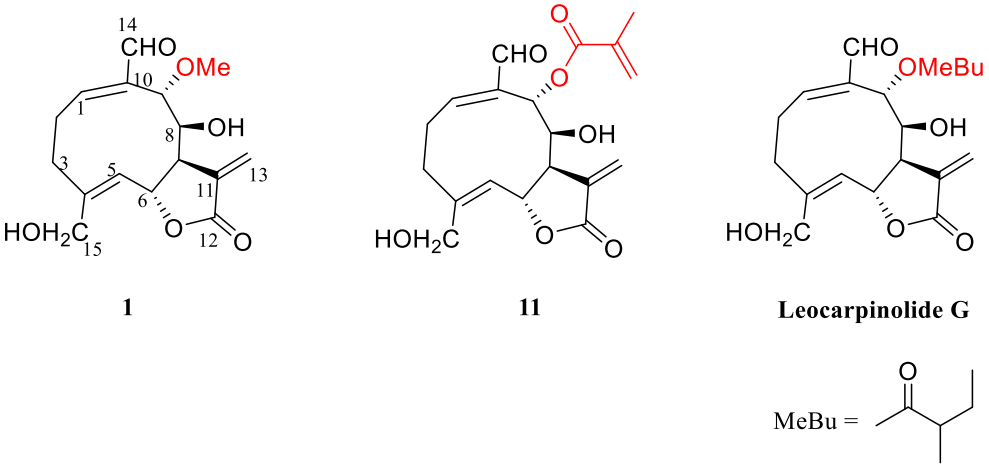


Figure S22: The Scifinder similarity report for new compound **1**.



1 **11** **Leocarpinolide G**

Figure S23: The structure is most similar to compound **1**.

Table S3: The ^{1}H NMR data for compound **1** and the similar compounds.

Position	1 (600MHz, $CDCl_3$)	11 [1] (600MHz, $CDCl_3$)	LeocarpinolideG [2] (400MHz, $CDCl_3$)
1	6.81 dd (10.0, 7.6)	6.77 dd (10.0, 7.6)	6.61 dd
2	2.66 m	2.69 m	2.50 dddd
	2.73 m	3.01 m	2.79 dddd
3	2.04 m	2.03 t (12.1)	2.04 ddd
	2.82 m	2.82 m	2.72 ddd
5	4.99 d (10.6)	5.03 d (10.6)	5.17 d
6	5.28 t (10.2)	5.43 t (10.2)	5.31 dd
7	2.45 m	2.48 d (9.5)	2.49 dddd
8	5.08 d (7.9)	5.31 d (8.2)	5.46 dd
9	3.79 dd (8.0, 2.2)	5.37 dd (8.3, 1.6)	5.56 br d
13	5.65 d (3.1)	5.67 d (3.1)	5.68 d
	6.34 d (3.5)	6.36 d (3.1)	6.42 d
14	9.48 d	9.46 s	9.40 d
15	4.39 s	4.49 m	4.06 br s
2′			2.41 tq
3′		6.13 s	1.60 ddq
		5.62 s	1.42 ddq
4′		1.92 s	0.85 t
5′			1.07 d

Table S4: The ^{13}C NMR data for compound **1** and the similar compounds.

Position	1 (600MHz,$CDCl_3$)	11 [1] (600MHz, $CDCl_3$)	LeocarpinolideG [2] (400MHz, $CDCl_3$)
1	157.6	158.9	155.04
2	27.6	28.0	27.39
3	33.0	33.0	32.49
4	139.6	140.6	140.30
5	130.0	129.5	128.99
6	73.1	73.0	73.75
7	51.2	52.0	51.51
8	69.1	68.5	70.38
9	80.2	73.2	71.24
10	140.9	141.4	139.51
11	135.3	135.9	133.99
12	169.9	169.6	168.95
13	121.1	120.8	123.10
14	194.7	194.4	195.37
15	61.2	61.3	60.72
1′		167.2	176.03
2′		135.6	41.24
3′		127.2	26.79
4′		18.4	11.48
5′			16.78
-OMe	56.8		

[1] N. Liu, C. Wu, J. H. Yu, K. K. Zhu, M. N. Song, F. Y. Yang, R. L. Feng, Y. Y. Zhang, W. Q. Chang and H. Zhang (2019). Germacrane-type sesquiterpenoids with cytotoxic activity from Sigesbeckia orientalis, *Bioorg Chem*. **92**, 103196.

[2] F. A. Macías and N. H. Fischer (1992). Melampolides from Lecocarpus pinnatifidus, Phytochemistry. **31**(**8**), 2747-2754.

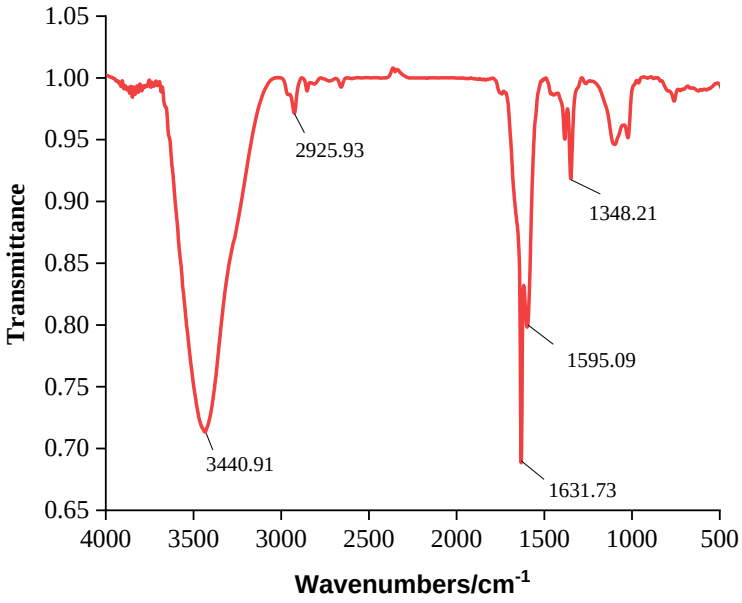


Figure S24: IR spectrum of compound **1**.

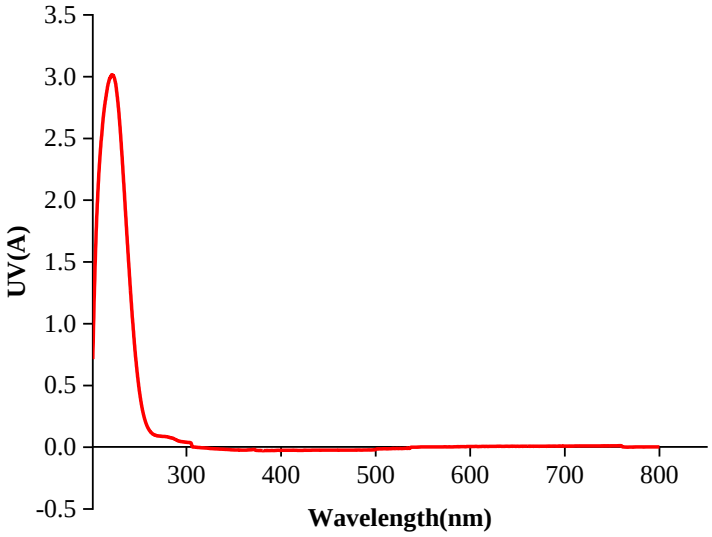


Figure S25: UV spectrum of compound **1**.

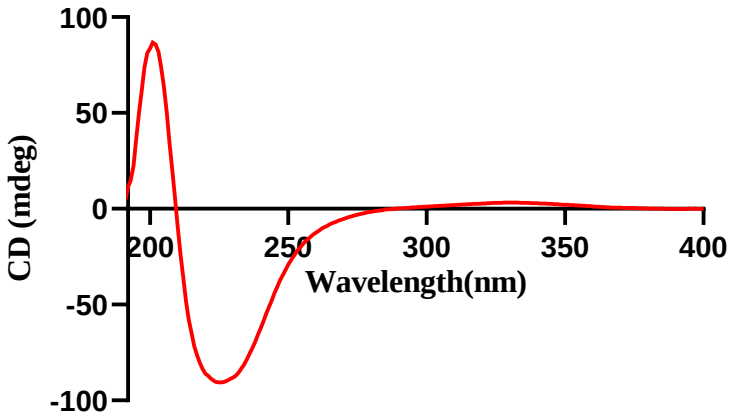


Figure S26: CD spectrum of compound **1**.

Compound1.zip

Figure S27: FID (NMR) files of compound **1**.