Supporting Information

***Rec. Nat. Prod.* X:X (2023) XX-XX**

A Novel Phenanthrene and An Undescribed Alkaloid from the Roots of *Stephania tetrandra*

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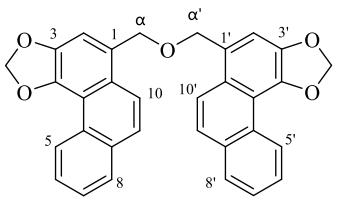
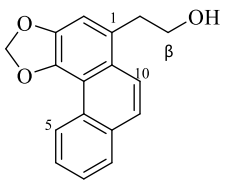


1

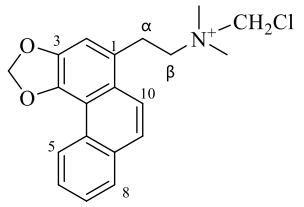


artapilosine B

Table 1. The most similar compound data to compound **1**

Position	**1**		artapilosine B	
	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C
1 (1')		131.1		128.7
2 (2')	7.32 s	109.8	7.18 s	111.0
3 (3')		145.0		144.9
4 (4')		143.5		142.5
4a (4a')		117.3		117.1
4b (4b')		128.7		129.0
5 (5')	9.09 dd (7.8, 1.8)	127.0	9.10 dd (8.0, 2.0)	127.3
6 (6')	7.62 overlapped	126.5	7.58 overlapped	126.3
7 (7')	7.62 overlapped	127.4	7.62 overlapped	126.8
8 (8')	7.85 dd (7.8, 1.8)	127.9	7.84 dd (8.0, 2.0)	127.6
8a (8a')		132.1		131.9
9 (9')	7.62 overlapped	125.8	7.60 d (10.0)	125.2
10 (10')	7.93 d (9.0)	122.6	7.86 d (10.0)	122.6
10a (10a')		126.2		126.2
α (α')	5.11 s	63.9	3.33 t (6.8)	36.7
β (β')			3.37 t (6.8)	63.2
OCH_2O (OCH_2O')	6.26 s	101.4	6.24 s	101.1

Recorded in $CDCl_3$



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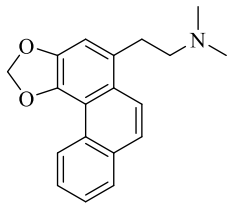
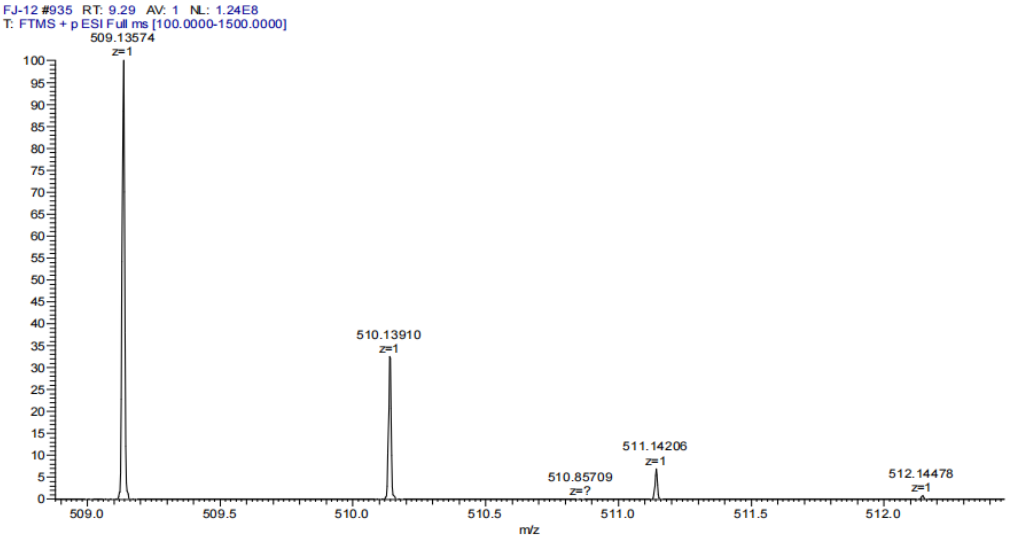


stephenanthrine

Table 2. The most similar compound data to compound **2**

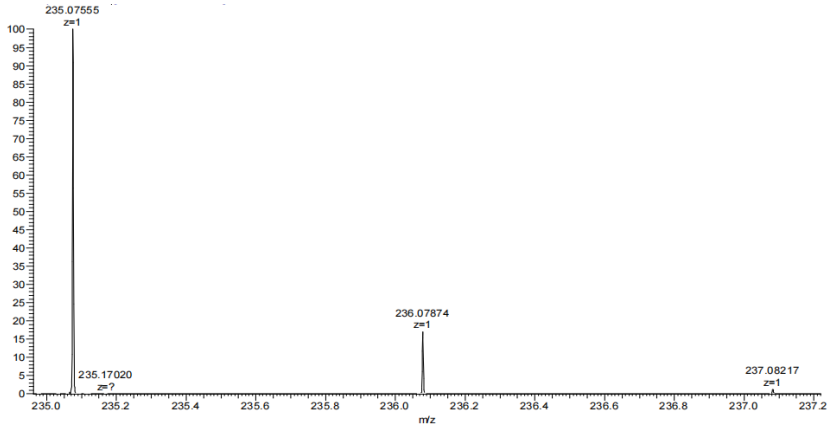
Position	**2**[a]		stephenanthrine[b]	
	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C
1		126.5		131.9
2	7.37 s	112.3	7.16 s	110.1
3		146.8		145.0
4		144.7		142.3
4a		118.4		117.1
4b		129.8		128.6
5	9.12 dd (7.8, 1.8)	128.3	9.08 br d (9.6)	127.3
6	7.63 overlapped	128.3	7.83 br d (9.6)	127.3
7	7.63 overlapped	127.7	7.58-7.61 m	126.8
8	7.90 overlapped	128.9	7.58-7.61 m	126.3
8a		133.4		131.3
9	7.73 d (9.6)	127.3	7.62 br d (9.6)	125.5
10	7.90 overlapped	122.7	7.87 d (9.6)	122.4
10a		127.4		125.9
α	3.63 m	27.2	3.38 ddd (16.8, 11.2, 5.6)	30.9
β	3.76 m	64.3	2.85 ddd (16.8, 11.2, 5.6)	60.2
OCH_2O	6.30 s	102.9	6.21 s	101.1
N-CH_3	3.41 s	50.3	2.56 s	44.5
N-CH_2Cl	5.48 s	69.6		

[a]Recorded in CD_3OD, [b]Recorded in $CDCl_3$.



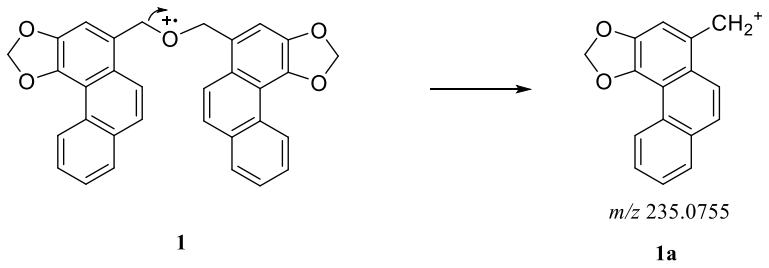
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
509.13574	509.13594	-0.4	21.5	C32 H22 O5 Na	M+Na

Figure S1: The HR-ESIMS spectrum of compound **1**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
235.07555	235.07536	0.82	11.5	C16 H11 O2

Figure S2: The HR-ESIMS data between *m/z* 50 to 350 in compound **1**



1 **1a**

Figure S3: Fragment ion of compound **1**

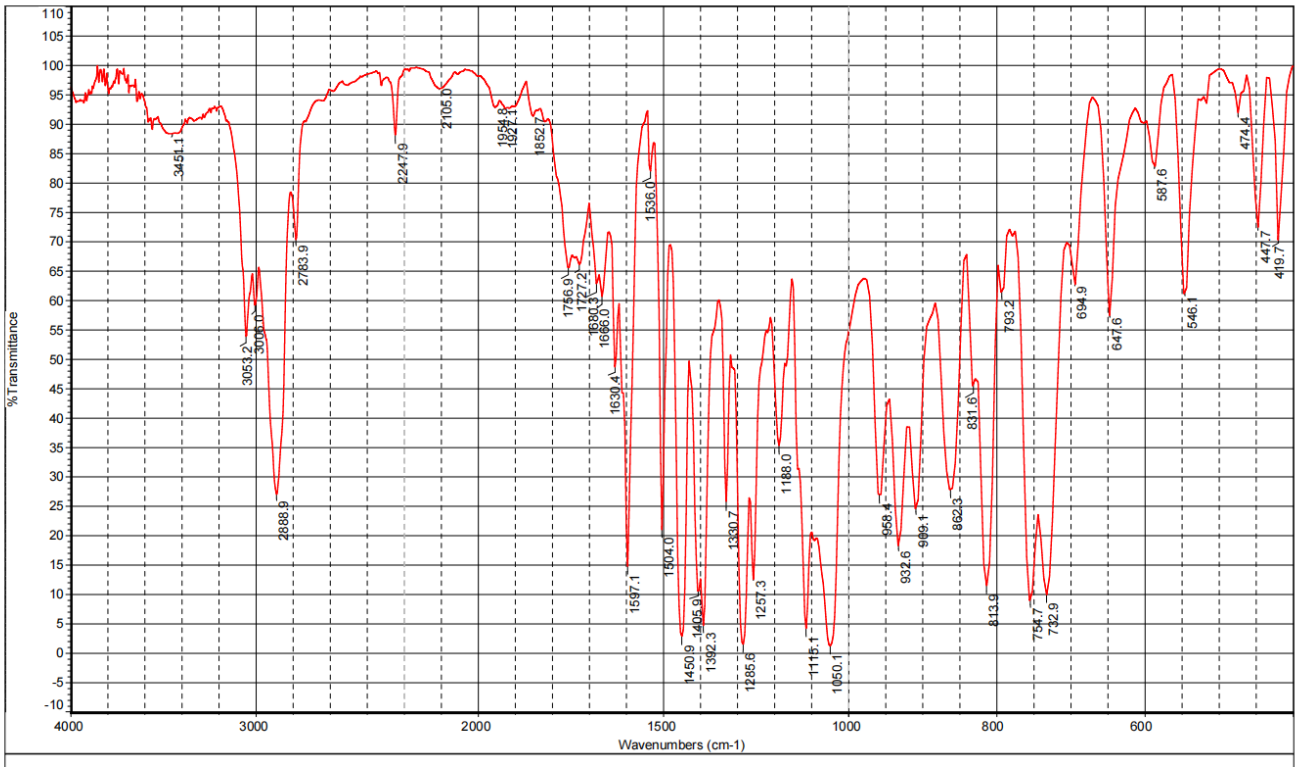


Figure S4: The IR spectrum of compound **1**

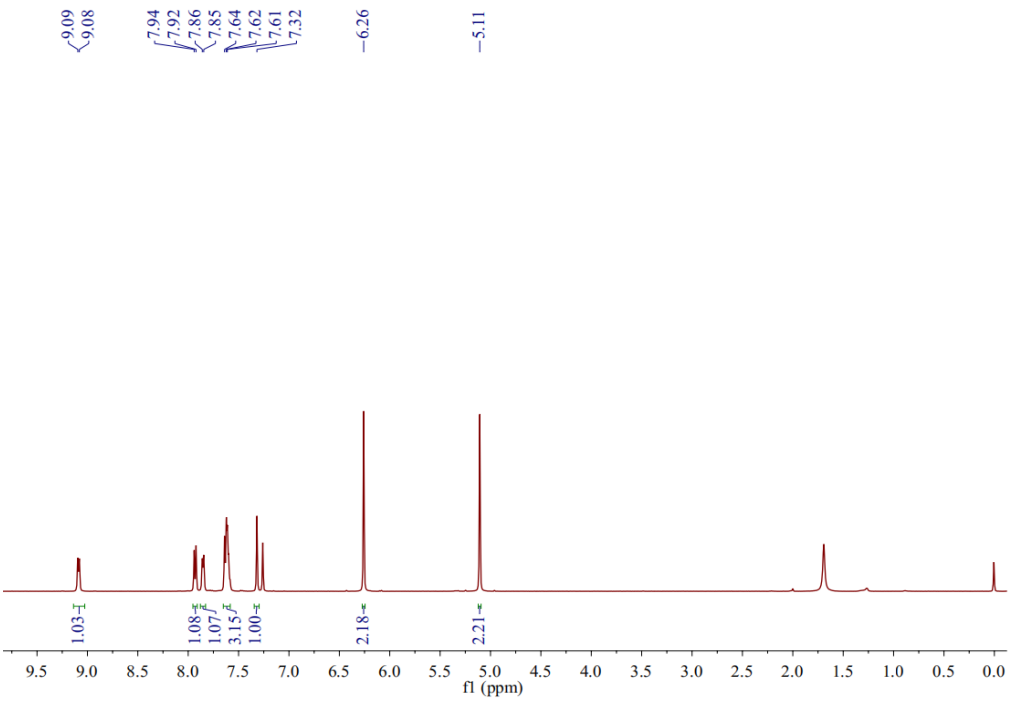


Figure S5: The ^{1}H-NMR spectrum of compound **1** in $CDCl_3$ (600 MHz)

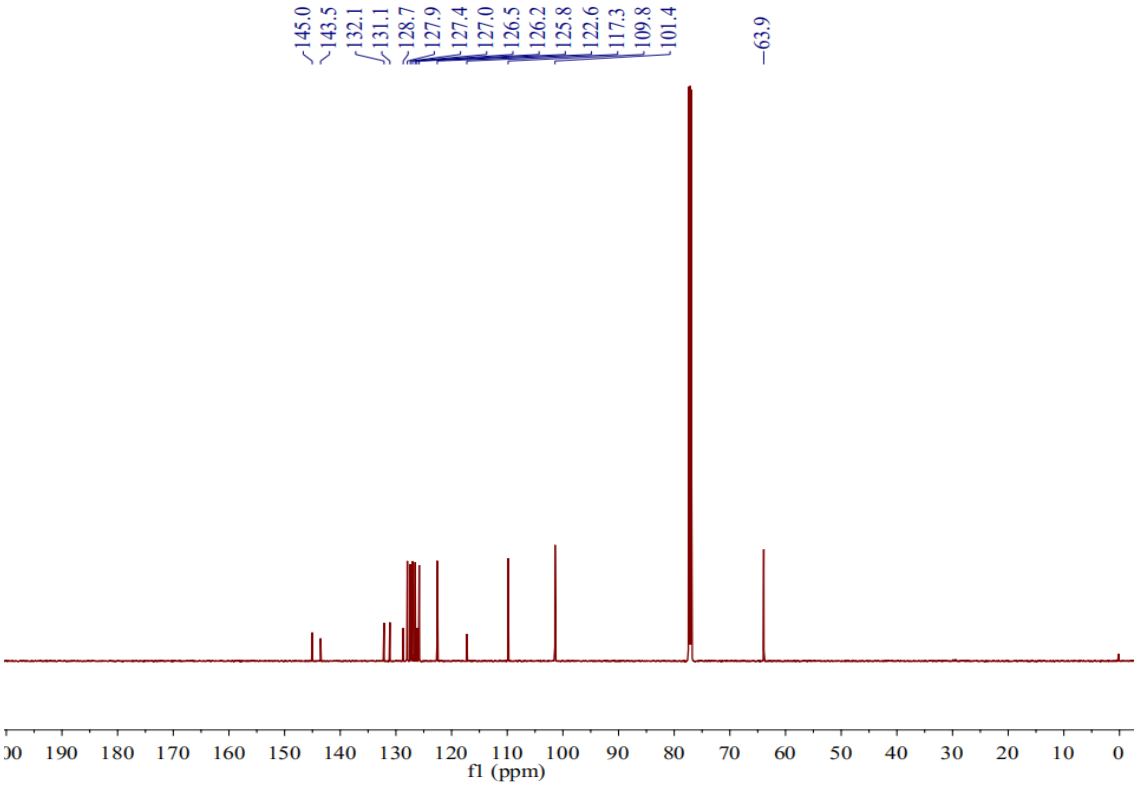


Figure S6: The ^{13}C-NMR spectrum of compound **1** in $CDCl_3$ (150 MHz)

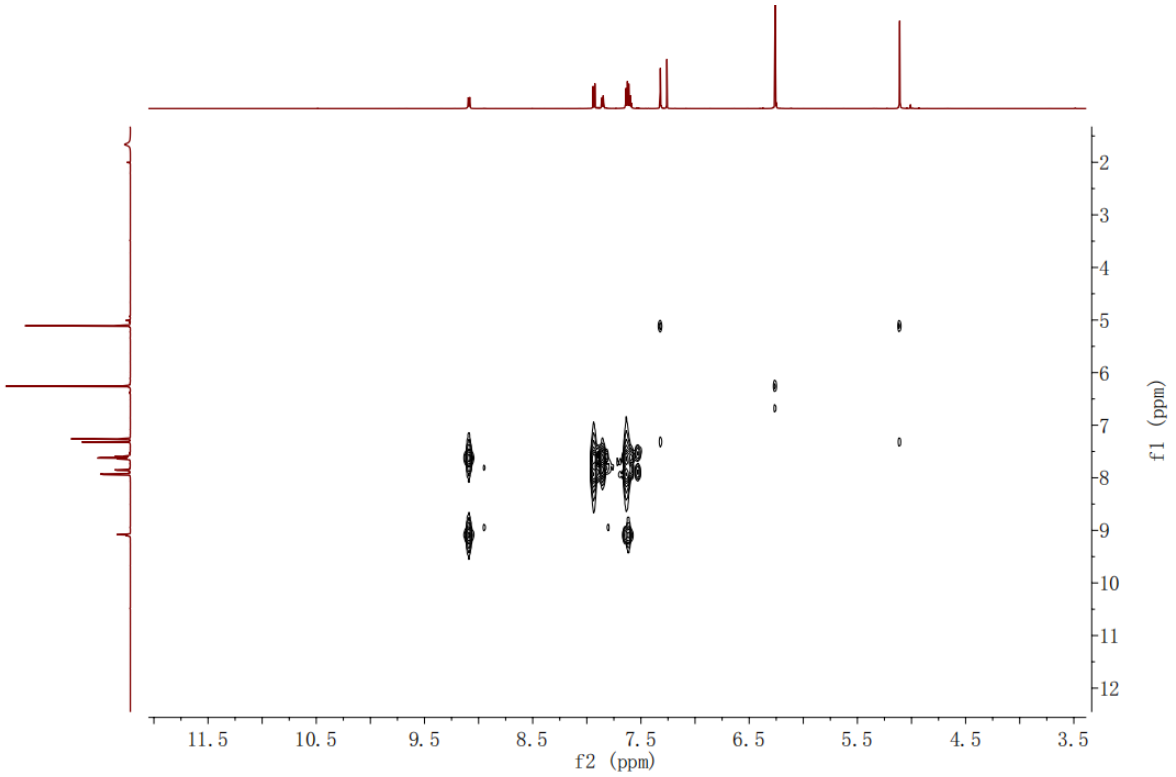


Figure S7: The ^{1}H-^{1}H COSY spectrum of compound **1** in $CDCl_3$

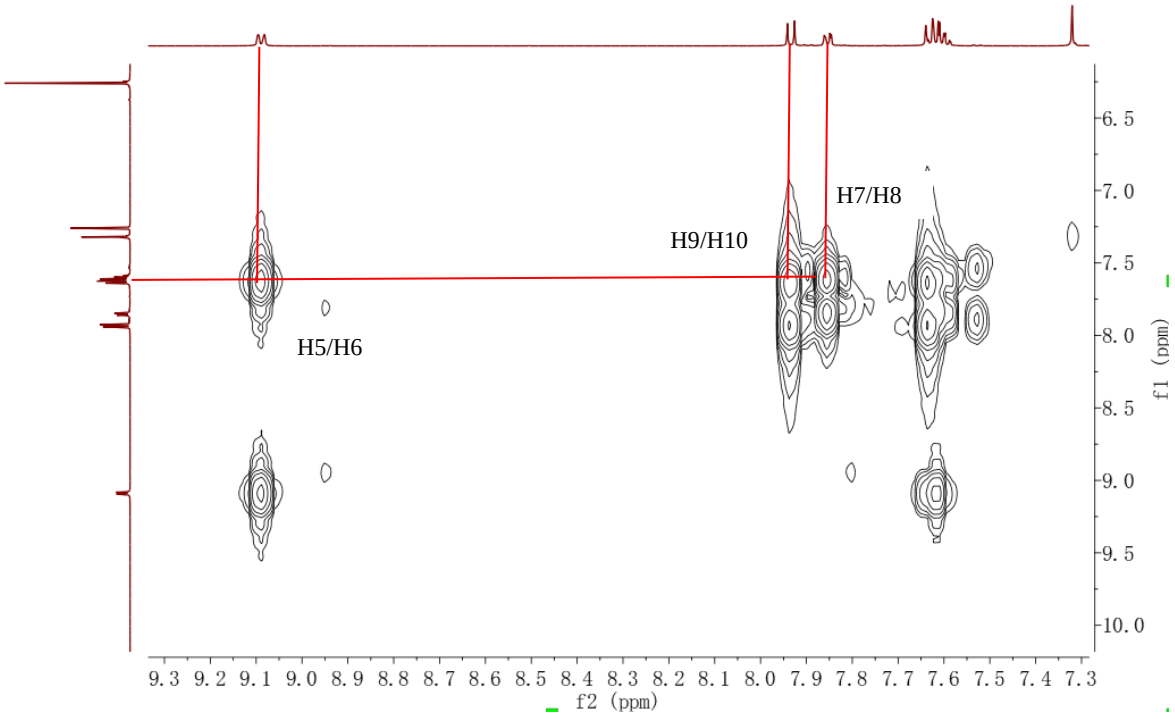


Figure S8: The ^{1}H-^{1}H COSY spectrum of compound **1** in $CDCl_3$ (From δ_H 7.3 to 9.3)

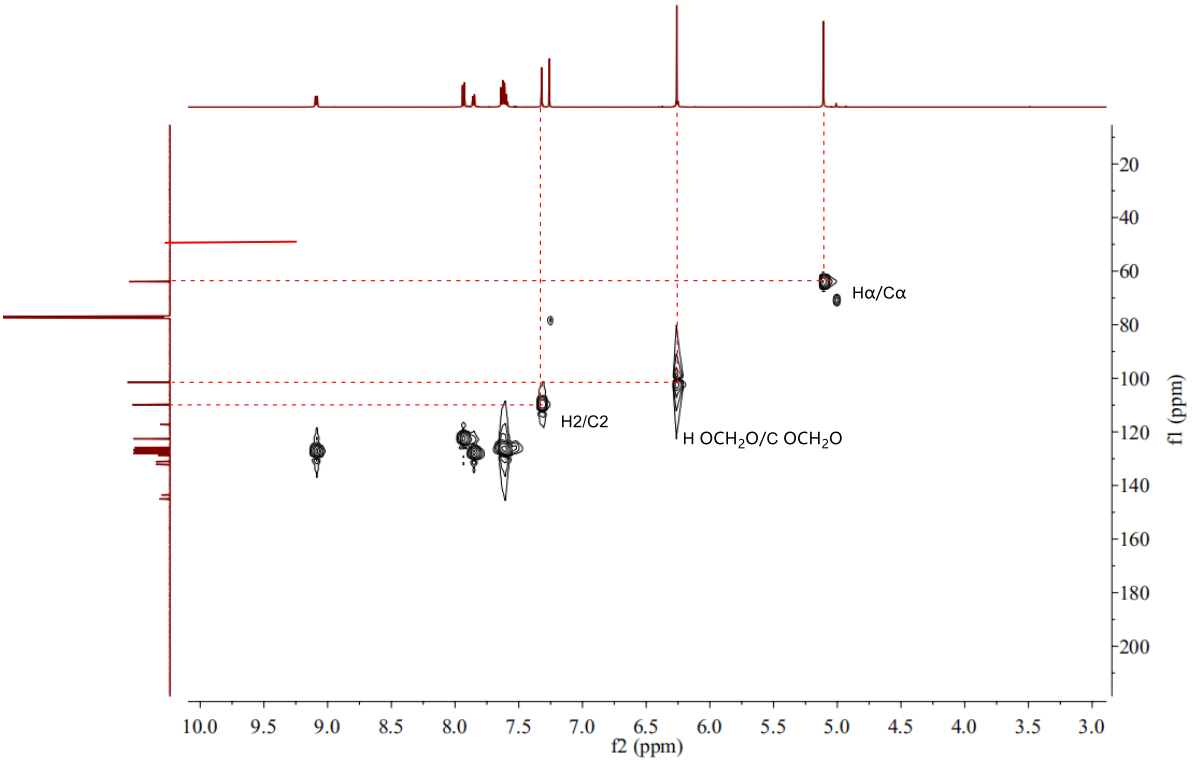


Figure S9: The HSQC spectrum of compound **1** in $CDCl_3$

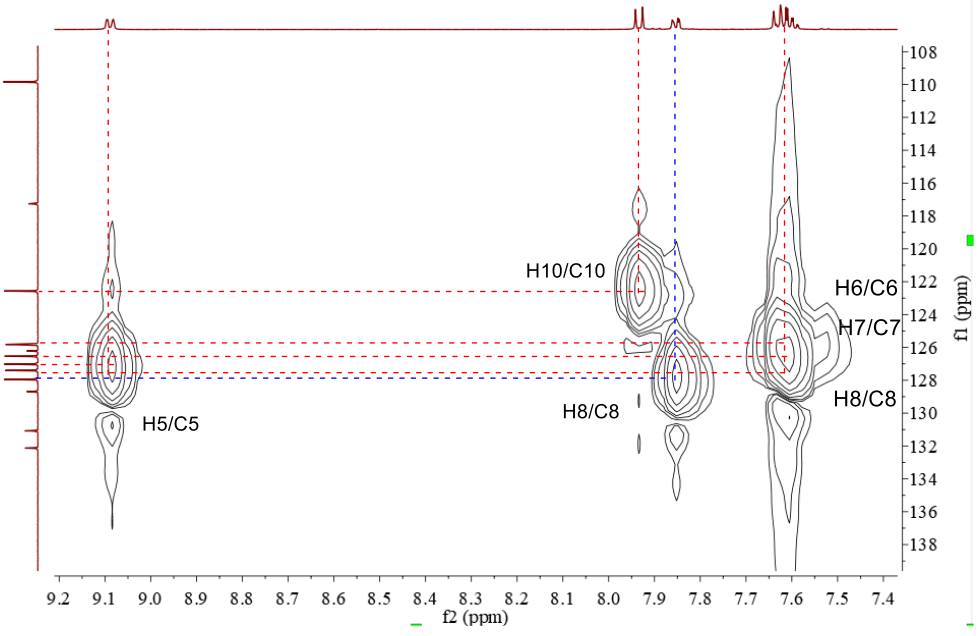


Figure S10: The HSQC spectrum of compound **1** in $CDCl_3$ (From δ_C 108 to 138)

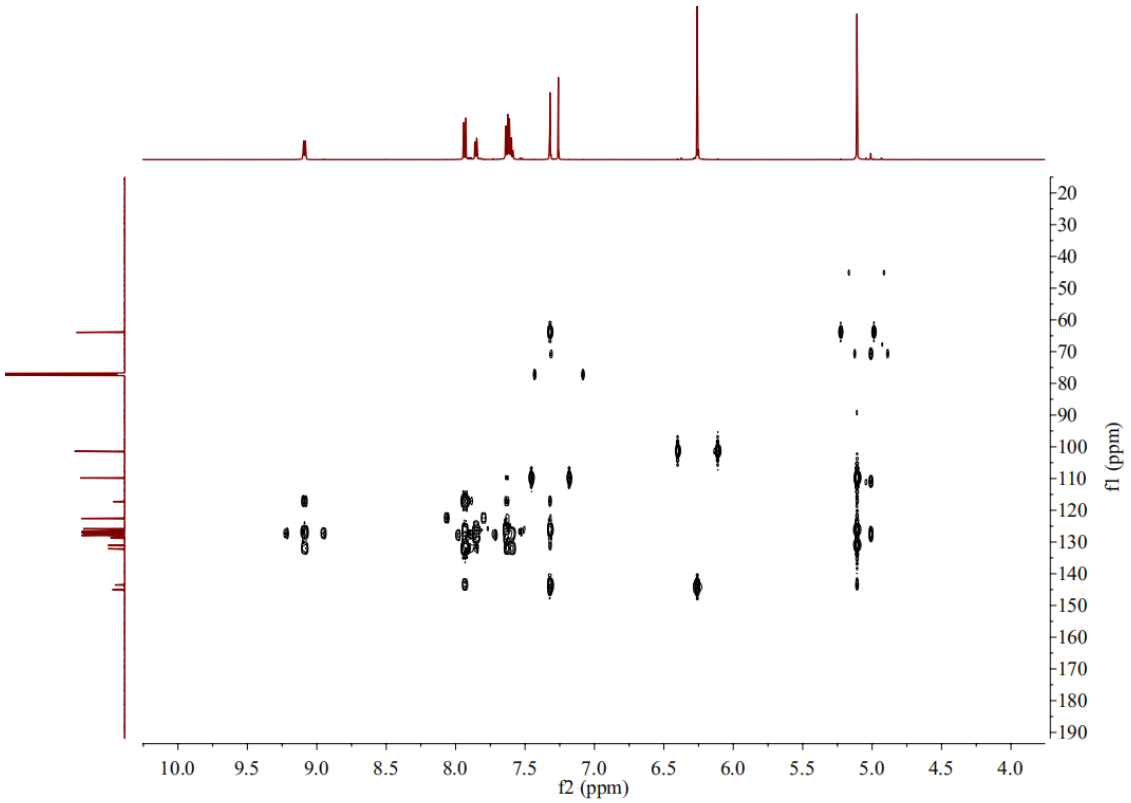


Figure S11: The HMBC spectrum of compound **1** in $CDCl_3$

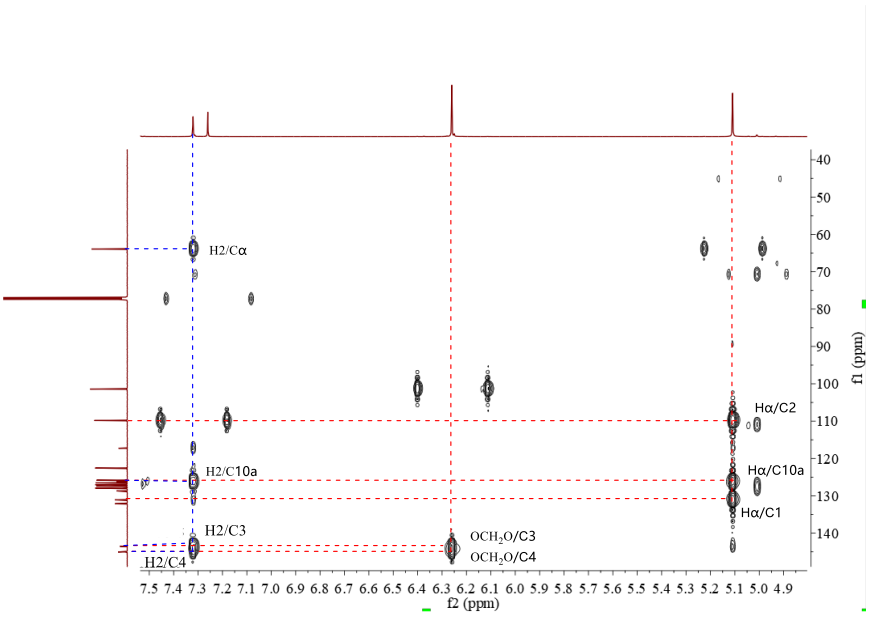


Figure S12: The HMBC spectrum of compound **1** in $CDCl_3$ (From δ_H 4.9 to 7.5)

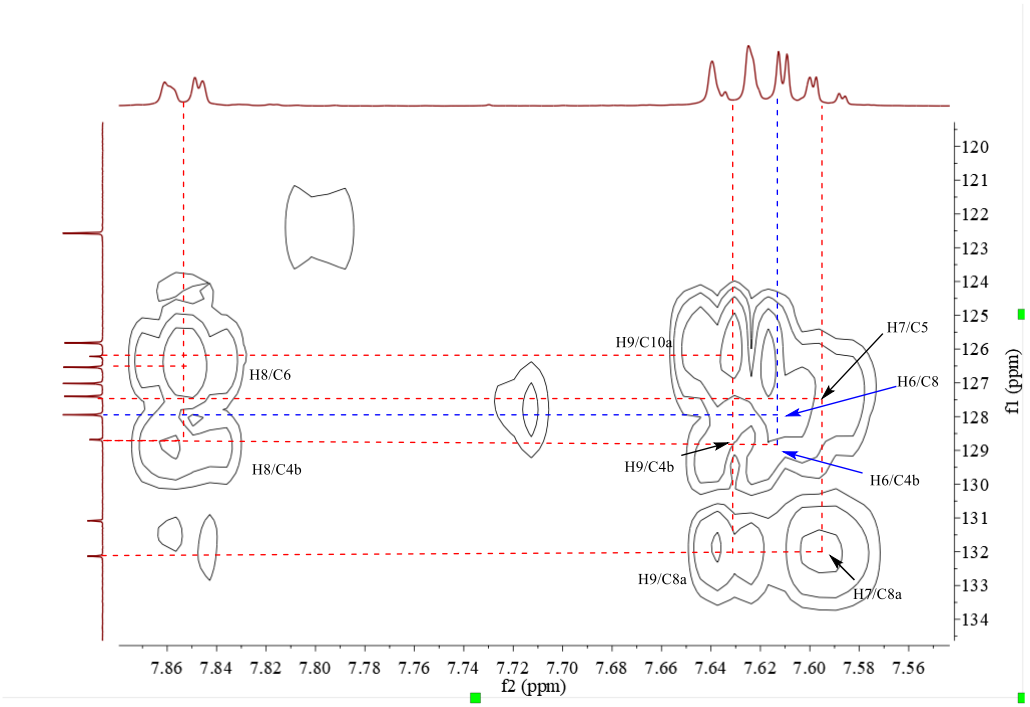


Figure S13: The HMBC spectrum of compound **1** in $CDCl_3$ (From δ_H 7.5 to 7.9)

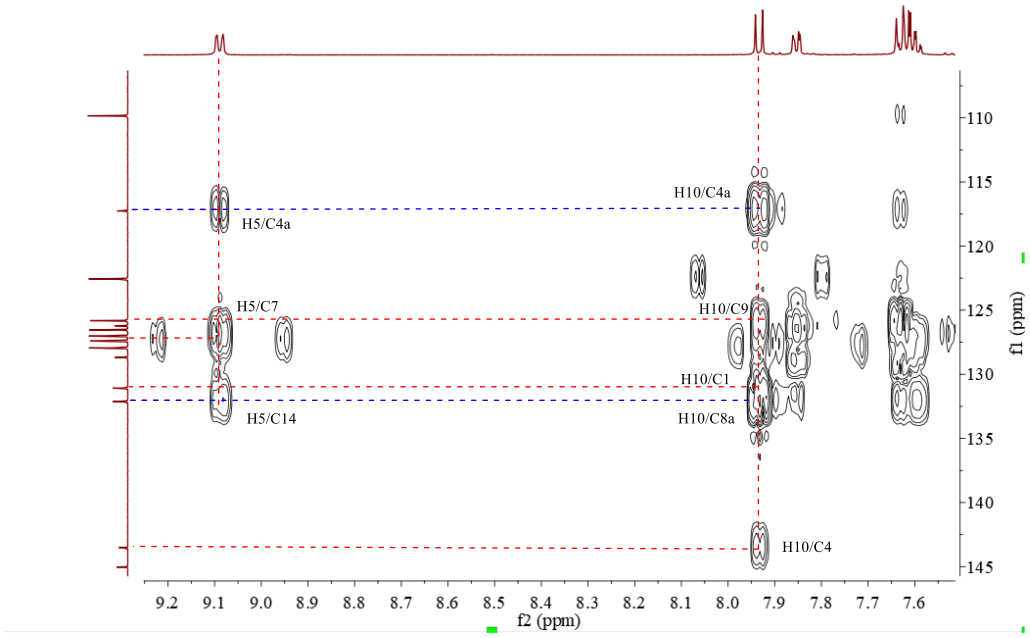
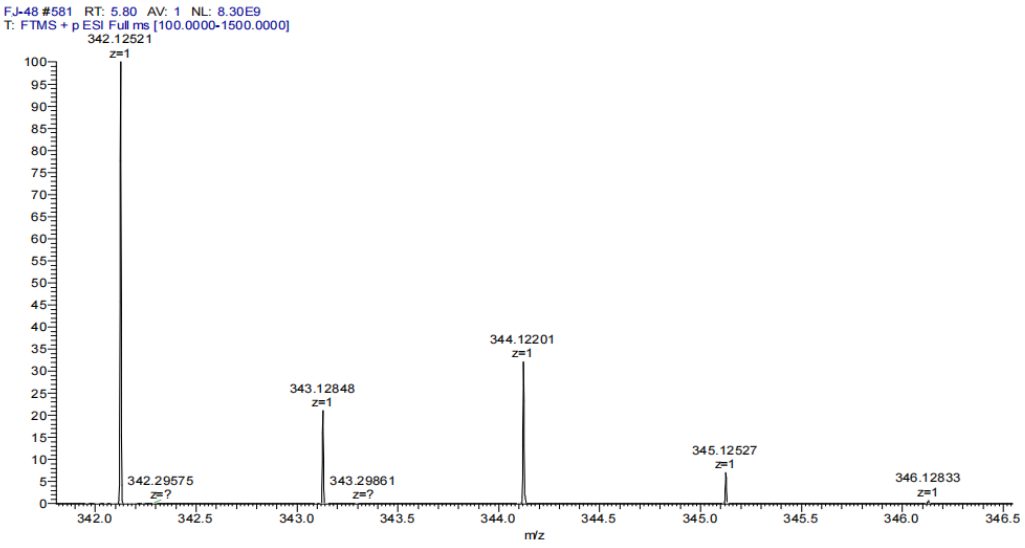


Figure S14: The HMBC spectrum of compound **1** in $CDCl_3$ (From δ_H 7.9 to 9.2)



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
342.12521	342.12553	-0.94	10.5	C20 H21 O2 N Cl	M+H

Figure S15: The HR-ESIMS spectrum of compound **2**

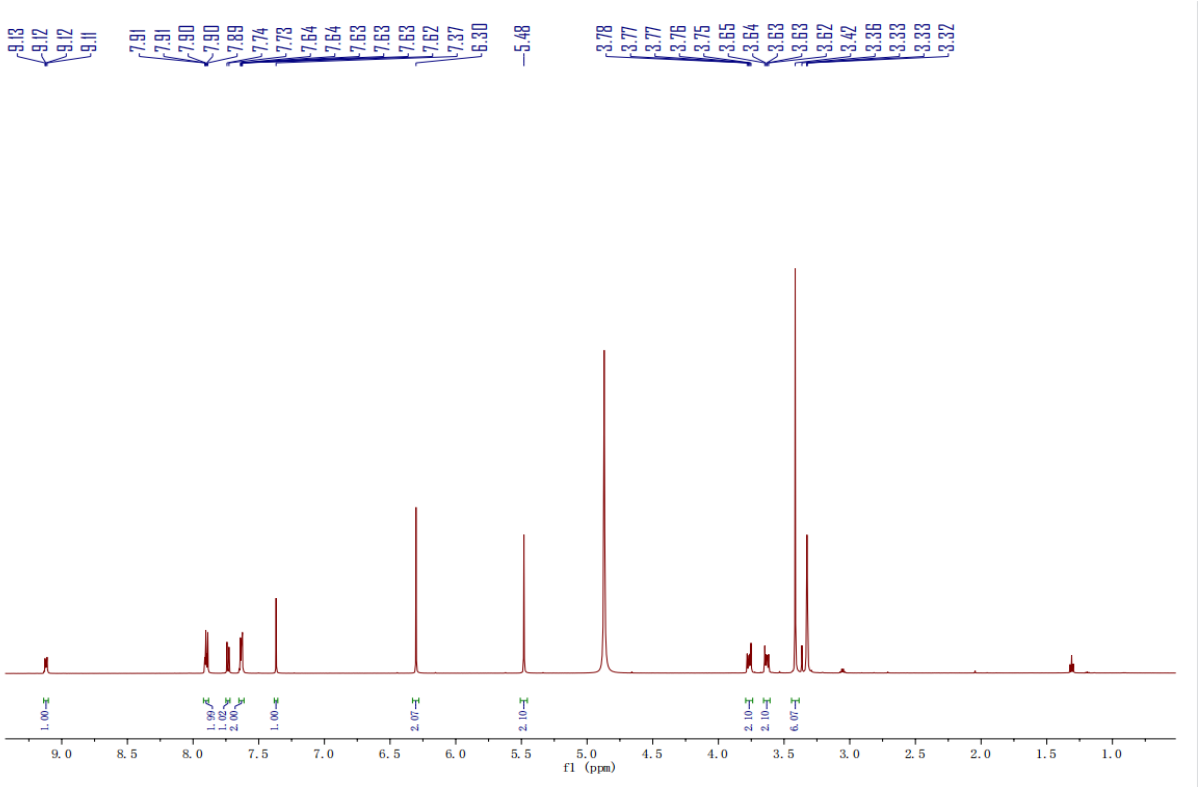


Figure S16: The ^{1}H-NMR spectrum of compound **2** in CD_3OD (600 MHz)

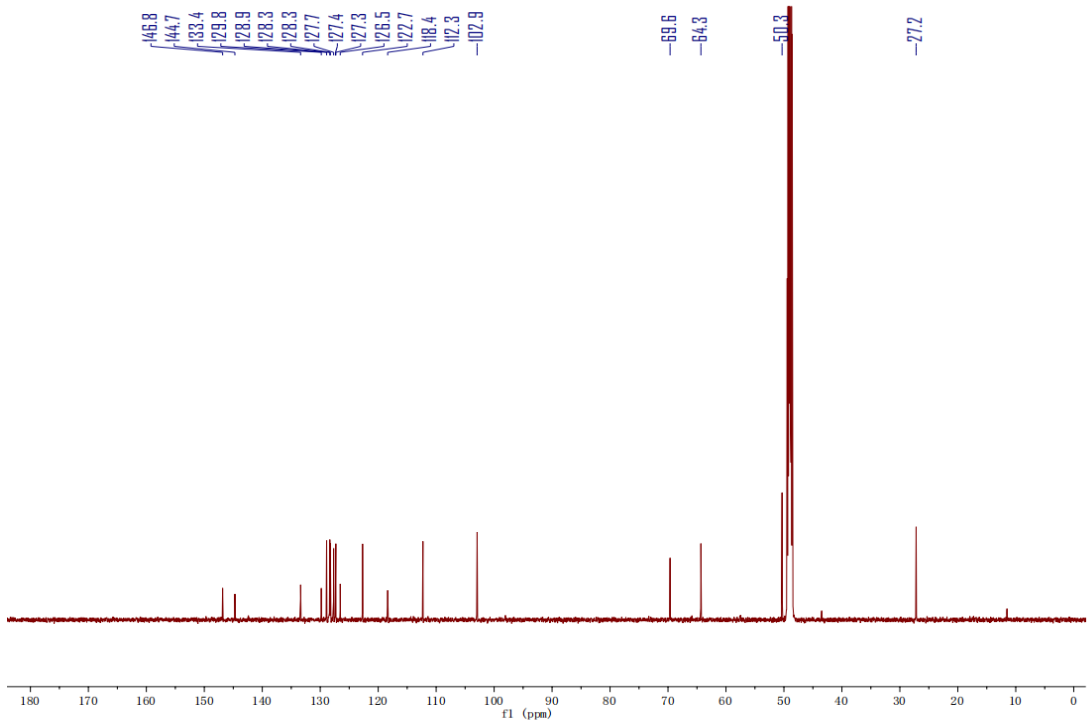


Figure S17: The ^{13}C-NMR spectrum of compound **2** in CD_3OD (150 MHz)

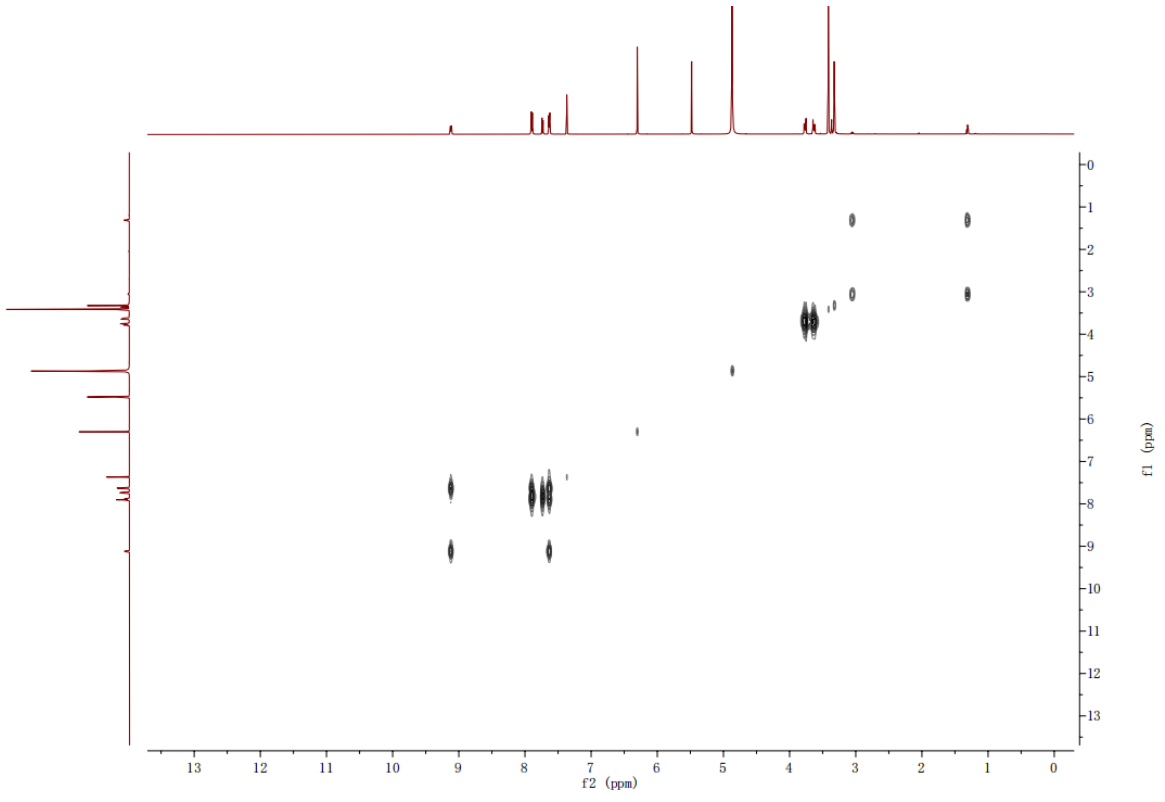


Figure S18: The ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD

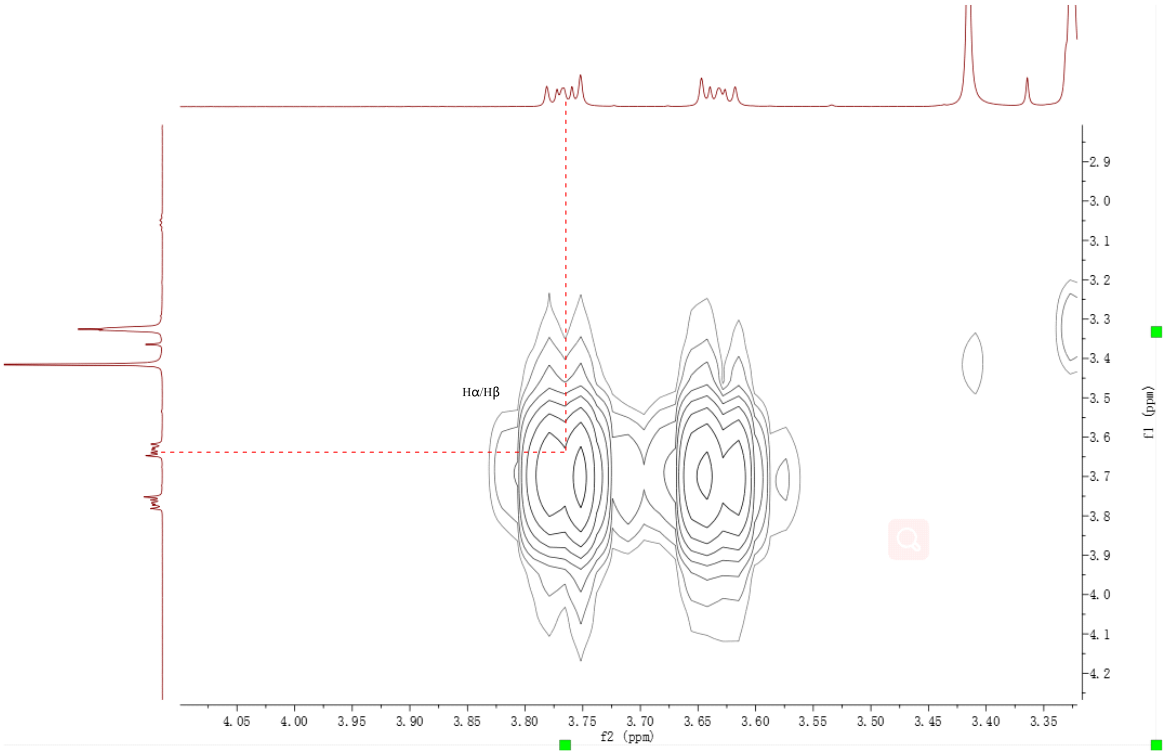


Figure S19: The ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD (From δ_H 2.9 to 4.2)

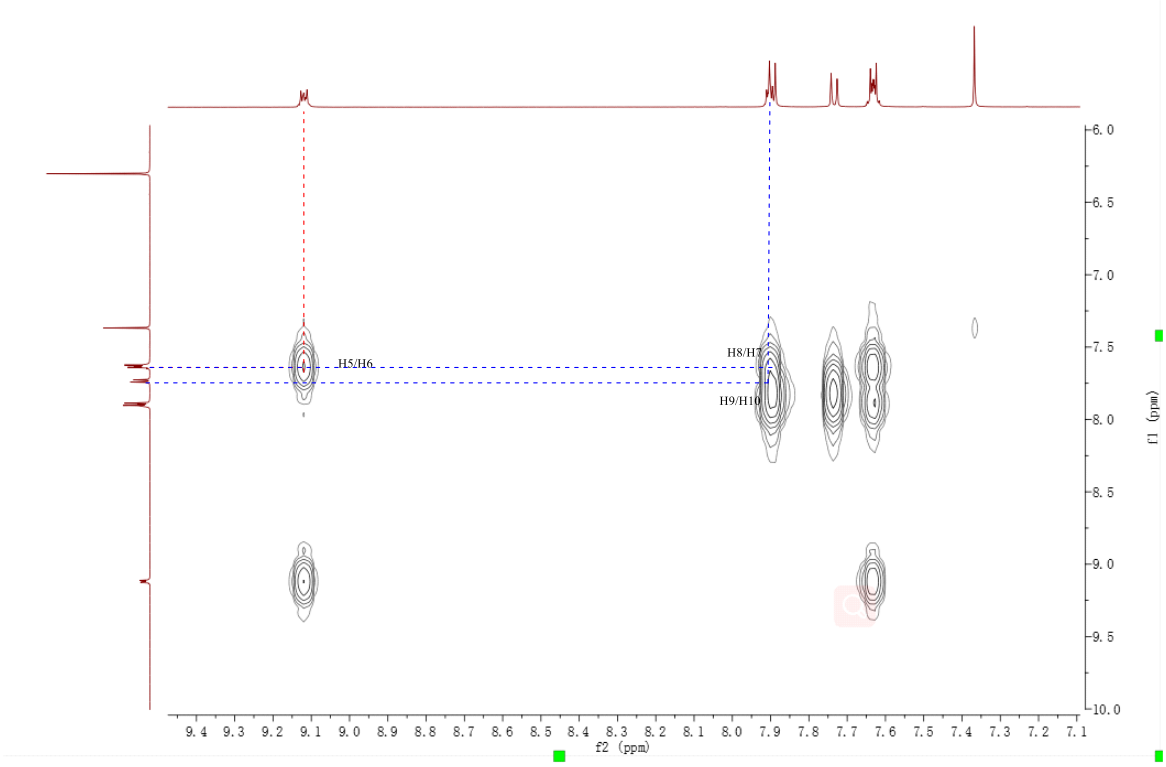


Figure S20: The ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD (From δ_H 6.0 to 10)

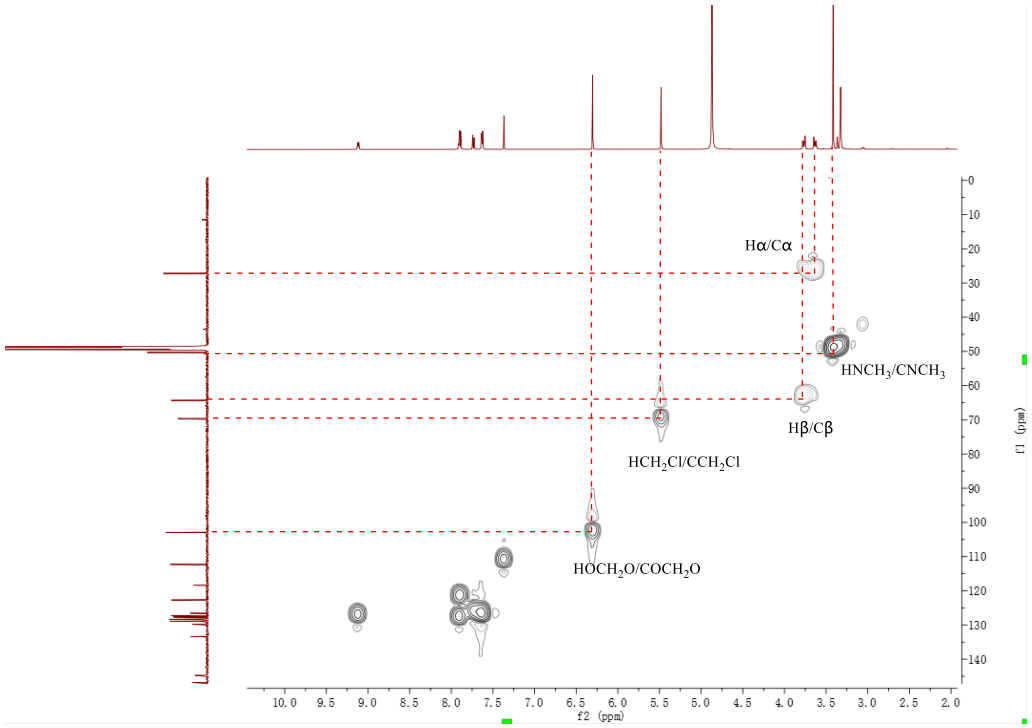


Figure S21: The HSQC spectrum of compound **2** in CD_3OD

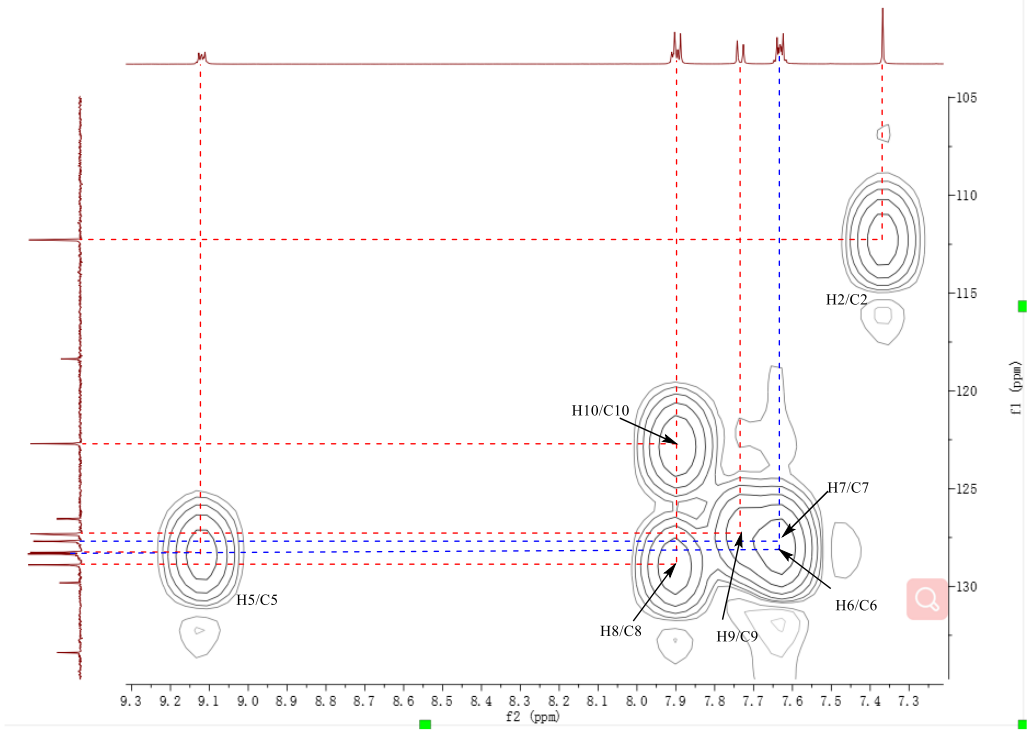


Figure S22: The HSQC spectrum of compound **2** in CD_3OD (From δ_C 110 to 140)

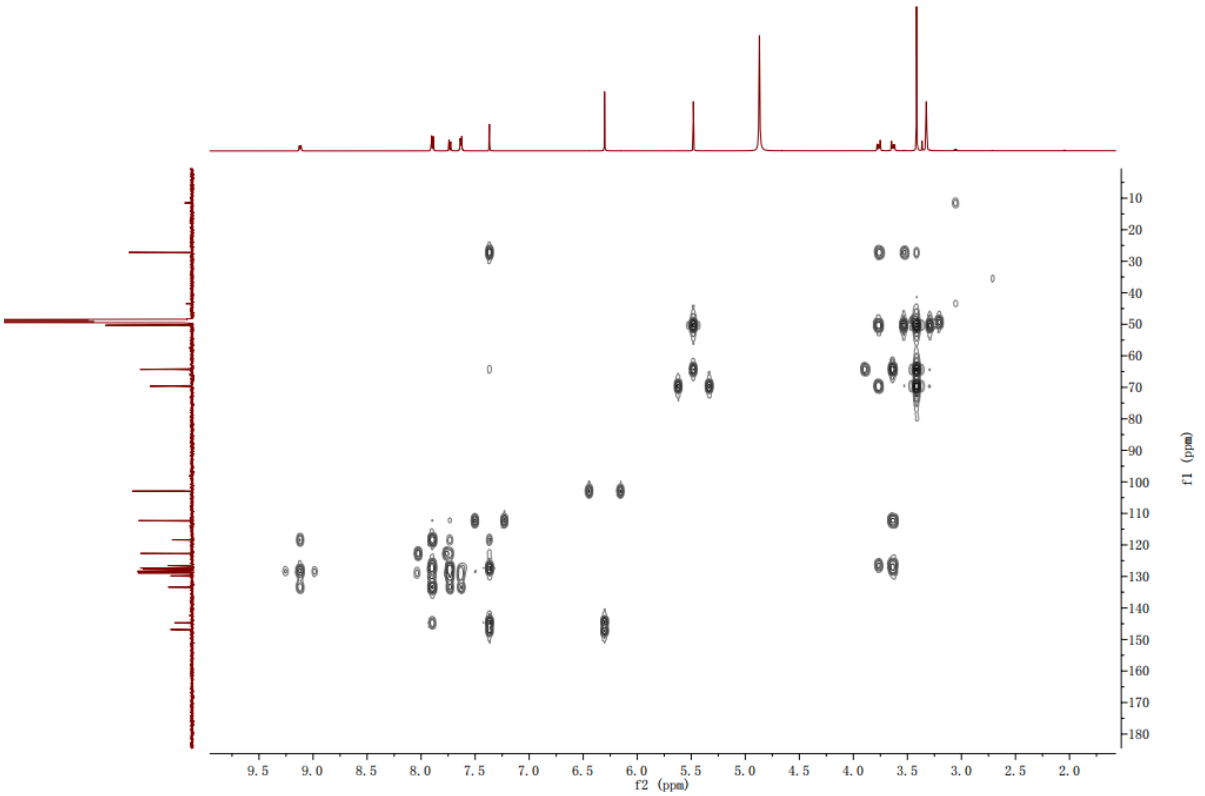


Figure S23: The HMBC spectrum of compound **2** in CD_3OD

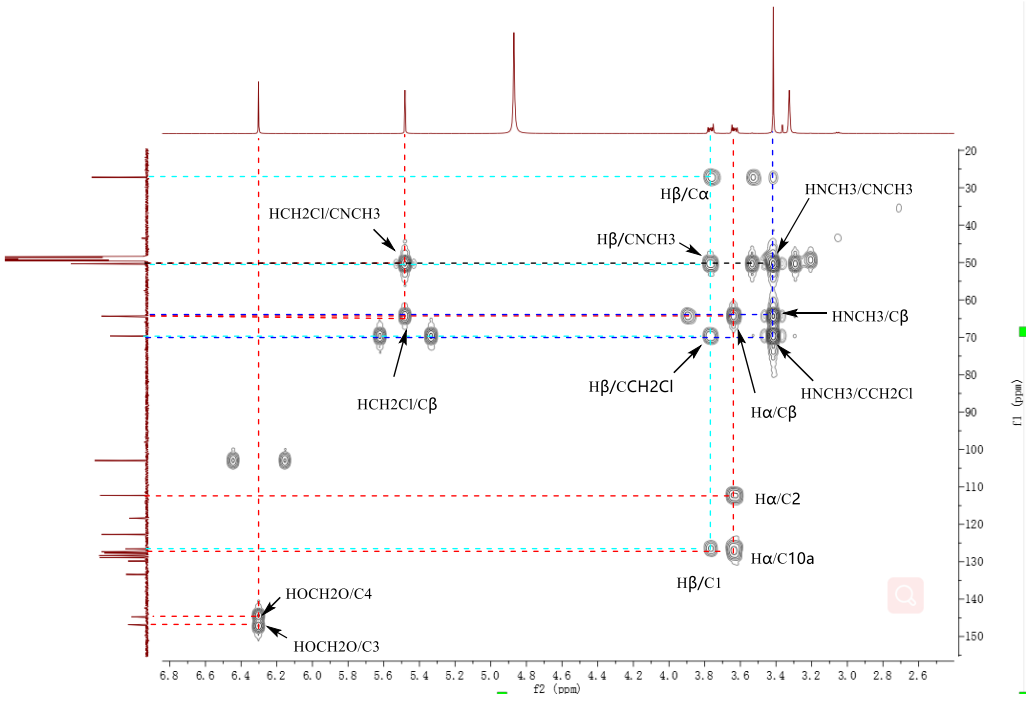


Figure S24: The HMBC spectrum of compound **2** in CD_3OD (From δ_H 2.6 to 6.8)

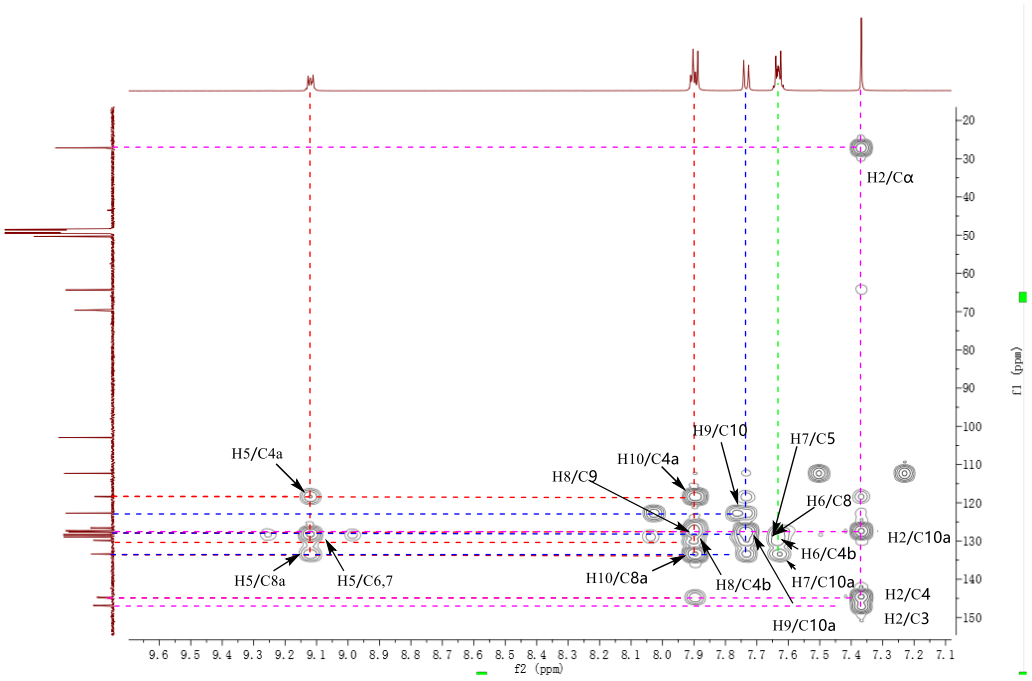


Figure S25: The HMBC spectrum of compound **2** in CD_3OD (From δ_H 7.1 to 9.6)

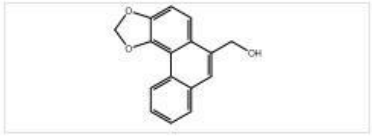
CAS SciFinder^{n}

Substances (2)

View in SciFinder^{n}

1 — Similarity Score: 99

500554-75-6



$C_{16}H_{12}O_3$

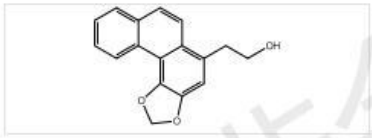
Phenanthro[3,4-*d*]-1,3-dioxole-6-methanol

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	252.27	-
Boiling Point (Predicted)	489.2±14.0 °C	Press: 760 Torr
Density (Predicted)	1.381±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.03±0.10	Most Acidic Temp: 25 °C

2 — Similarity Score: 96

2881056-41-1



$C_{17}H_{14}O_3$

Phenanthro[4,3-*d*]-1,3-dioxole-5-ethanol

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	266.29	-
Boiling Point (Predicted)	488.4±14.0 °C	Press: 760 Torr
Density (Predicted)	1.337±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	14.66±0.10	Most Acidic Temp: 25 °C

Figure S26: SciFinder search report for the non dimer version of compound **1** with 90-99 % similarity.

CAS SciFinder^{n}

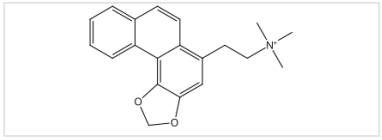
Substances (1)

View in SciFinder^{n}

1

Similarity Score: **91**

785744-42-5



$C_{20}H_{22}NO_2$

N,N,N-Trimethylphenanthro[3,4-*d*]-1,3-dioxole-5-ethanaminium

3 References | 11 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	308.39	-

Figure S27: SciFinder search report of compound **2** with 90-99 % similarity.

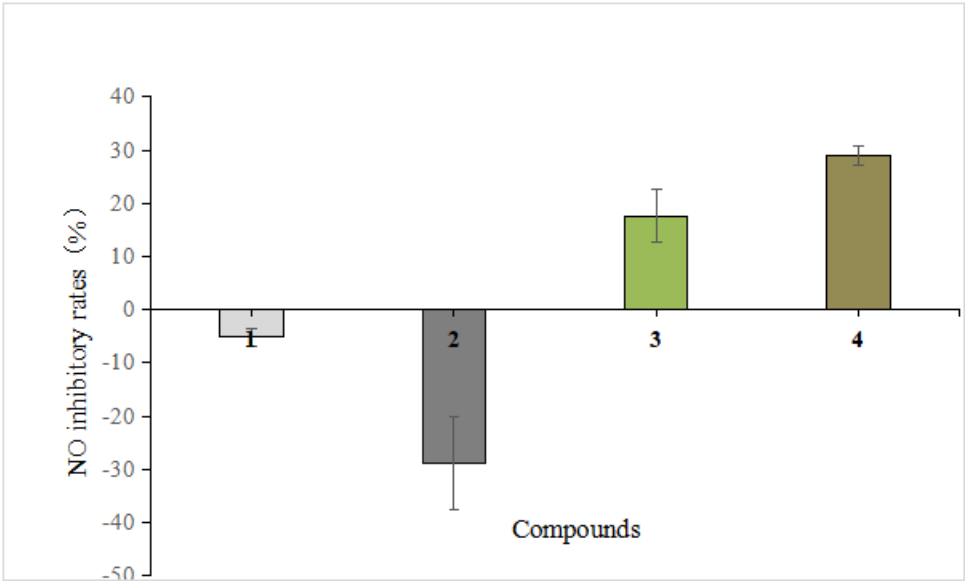


Figure S28: The NO inhibitory rates of compounds **1-4** at the concentration of 10 μM

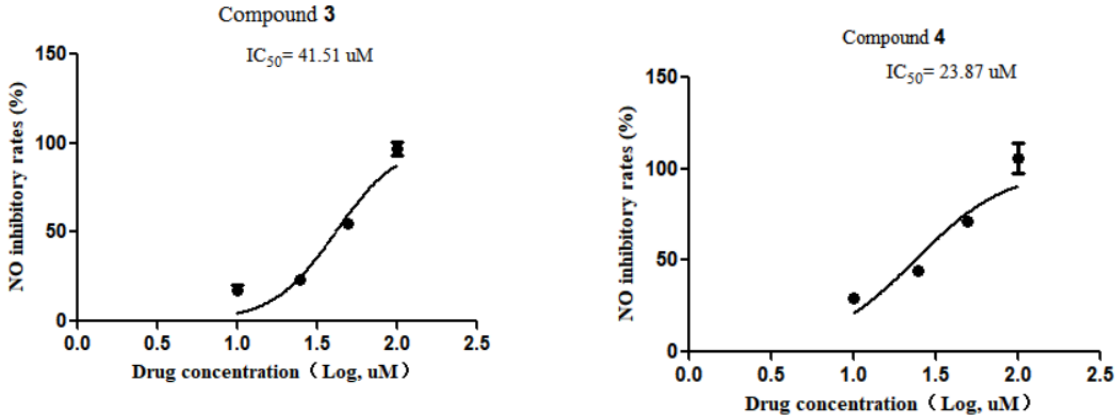


Figure S29: NO inhibition curve of compounds **3** and **4**