Supporting Information

***Rec. Nat. Prod*. 19:3 (2025) 296-301**

Structures and Biological Evaluation of 8,4′-oxyneolignans from the roots of *Platycodon grandifloras*

Lang Ding [1], Yang Yu [1,2,3], Ling Zhang [1], Shuang-Ying Gui [*1], Ju-Tao Wang [*1,2,3], and Bai-Xiang Cai [*1,2]

[1] *School of Pharmacy, Anhui University of Chinese Medicine, Hefei, 230012, PR China*

[2] *Anhui Province Key Laboratory of Bioactive Natural Products, Hefei, 230012, PR China*

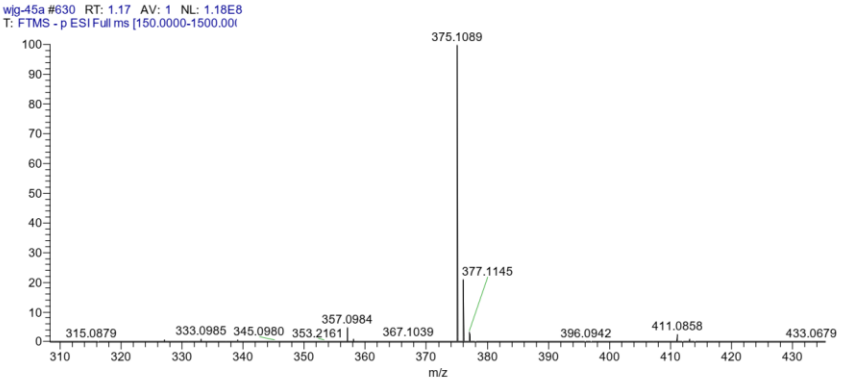
[3] *Institute of Medicinal Chemistry, Anhui Academy of Chinese Medicine, Hefei 230012, PR China*

Table of Contents — **Pages**

Figure S1-1: HR-ESI-MS spectrum of **1**. 3
Figure S1-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **1**. 3
Figure S1-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **1**. 4
Figure S1-4: HSQC spectrum of **1**. 5
Figure S1-5: HSQC spectrum of **1** (From δ_H 3.0 ppm to δ_H 8.0 ppm). 5
Figure S1-6: HMBC spectrum of **1**. 6
Figure S1-7: HMBC spectrum of **1** (From δ_H 3.4 ppm to δ_H 7.6 ppm). 6
Figure S1-8: ^{1}H-^{1}H COSY spectrum of **1**. 7
Figure S1-9: ROESY spectrum of **1**. 8
Figure S1-10: ECD spectra for compound **1**. 8
Figure S1-11: Scifinder search report of **1**. 9
Figure S2-1: HR-ESI-MS spectrum of **2**. 10
Figure S2-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **2**. 10
Figure S2-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **2**. 11
Figure S2-4: HSQC spectrum of **2**. 11
Figure S2-5: HSQC spectrum of **2** (From δ_H 3.5 ppm to δ_H 8.0 ppm). 12
Figure S2-6: HMBC spectrum of **2**. 12
Figure S2-7: HMBC spectrum of **2** (From δ_H 3.6 ppm to δ_H 8.2 ppm). 13
Figure S2-8: ^{1}H-^{1}H COSY spectrum of **2** 13
Figure S2-9: ROESY spectrum of **2**. 14
Figure S2-10: ECD spectra for compound **2**. 14
Figure S2-11: Scifinder search report of **2**. 15
Table S2-12: The NMR spectroscopic data for **1** and **2** with similar compound **1′** (δ in ppm and J in Hz) 16
Figure S3-1: HR-ESI-MS spectrum of **3**. 17
Figure S3-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **3**. 18
Figure S3-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **3**. 18
Figure S3-4: HSQC spectrum of **3**. 19

[*]Corresponding authors: E- Mail: guishy0520@ahtcm.edu.cn (Shuang-Ying Gui); wjt591@ahtcm.edu.cn (Ju-Tao Wang); caibx@ahtcm.edu.cn (Bai-Xiang Cai).

Figure S3-5: HSQC spectrum of **3** (From δ_H 3.5 ppm to δ_H 8.0 ppm). 19
Figure S3-6: HMBC spectrum of **3**. 20
Figure S3-7: HMBC spectrum of **3** (From δ_H 3.0 ppm to δ_H 7.5 ppm). 20
Figure S3-8: ^{1}H-^{1}H COSY spectrum of **3**. 21
Figure S3-9: ROESY spectrum of **3**. 21
Figure S3-10: ECD spectra for compound **3**. 22
Figure S3-11: Scifinder search report of **3**. 23
Figure S4-1: HR-ESI-MS spectrum of **4**. 24
Figure S4-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **4**. 25
Figure S4-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **4**. 25
Figure S4-4: HSQC spectrum of **4**. 26
Figure S4-5: HSQC spectrum of **4** (From δ_H 1.5 ppm to δ_H 7.5 ppm). 26
Figure S4-6: HMBC spectrum of **4**. 27
Figure S4-7: HMBC spectrum of **4** (From δ_H 1.0 ppm to δ_H 7.6 ppm). 27
Figure S4-8: ^{1}H-^{1}H COSY spectrum of **4**. 28
Figure S4-9: ROESY spectrum of **4**. 28
Figure S4-10: ECD spectra for compound **4**. 29
Figure S4-11: Scifinder search report of **4**. 30
Table S4-12: The NMR spectroscopic data for **3** and **4** with similar compound **2′** (δ in ppm and J in Hz) 31
S5-1: General Experimental Procedures. 31



Meas. m/z	Pred. m/z	Df. ppm	Formula	Ion
375.1089	375.1085	1.0664	$C_{19}H_{20}O_8$	$[M-H]^-$

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

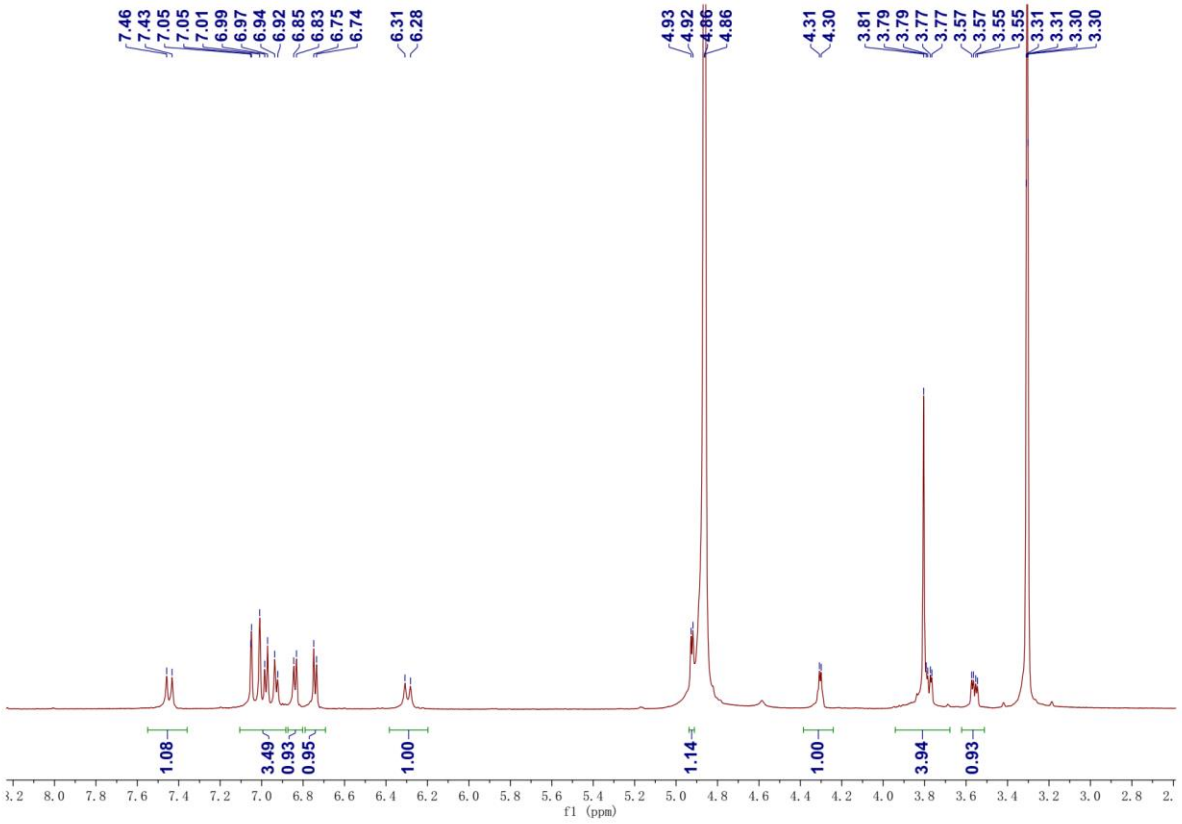


Figure S1-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **1.**

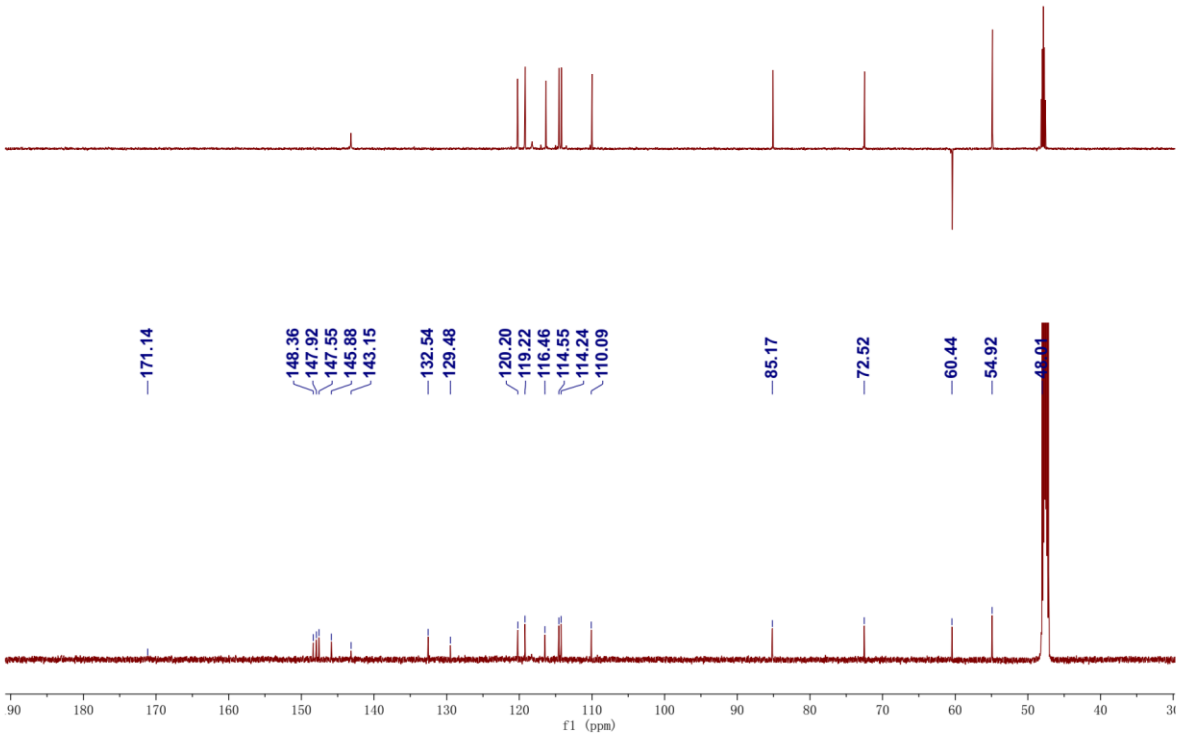


Figure S1-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **1.**

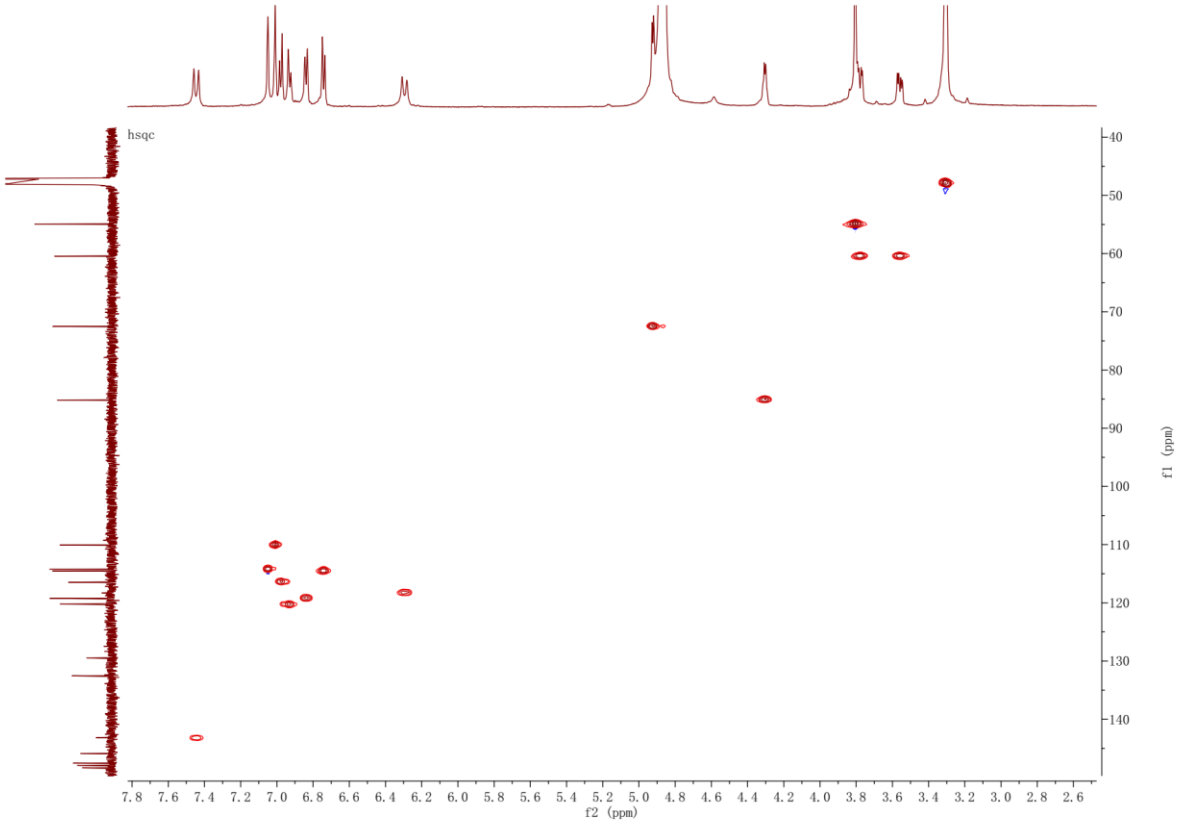


Figure S1-4: HSQC spectrum of **1.**

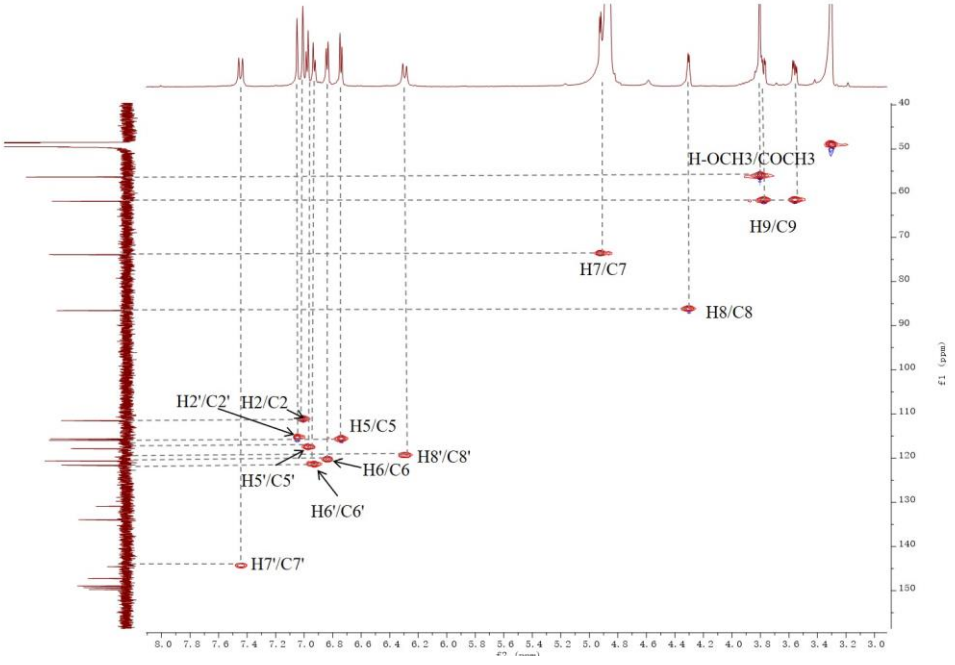


Figure S1-5: HSQC spectrum of **1** (From δ_H 3.0 ppm to 8.0 ppm)**.**

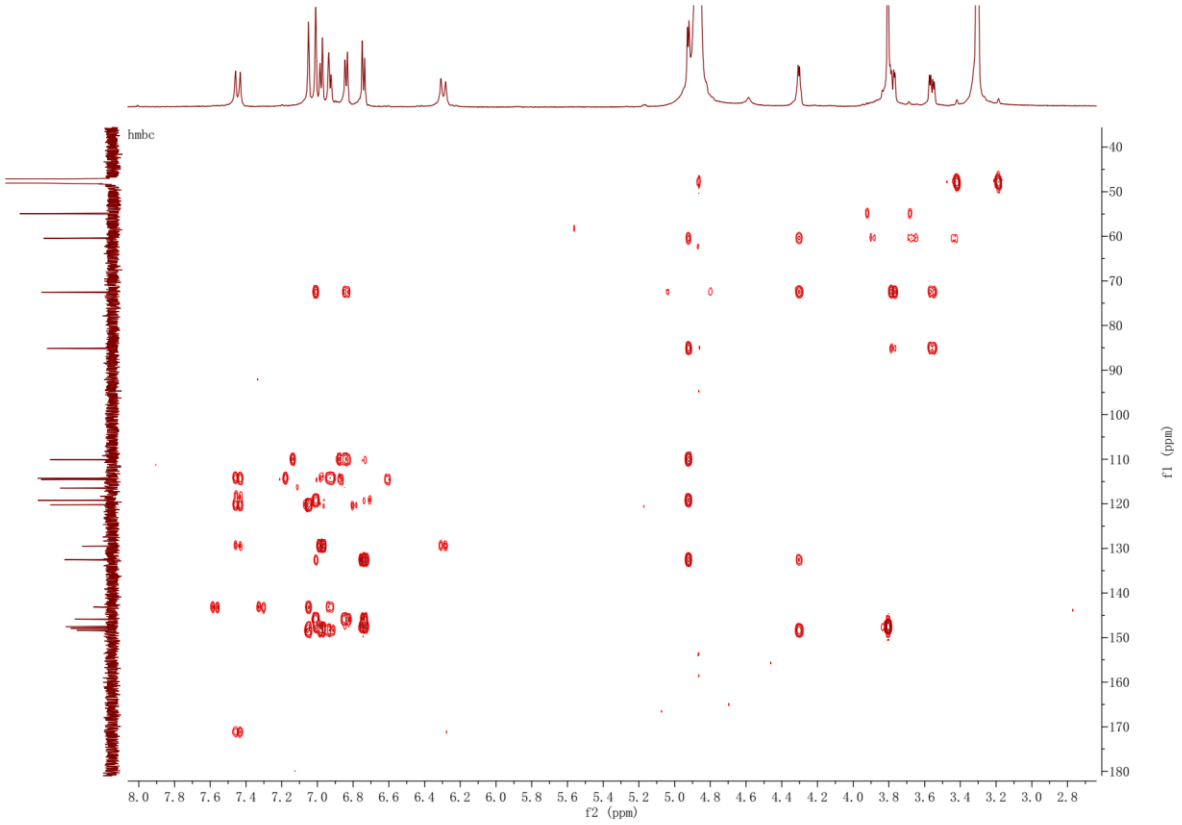


Figure S1-6: HMBC spectrum of **1**.

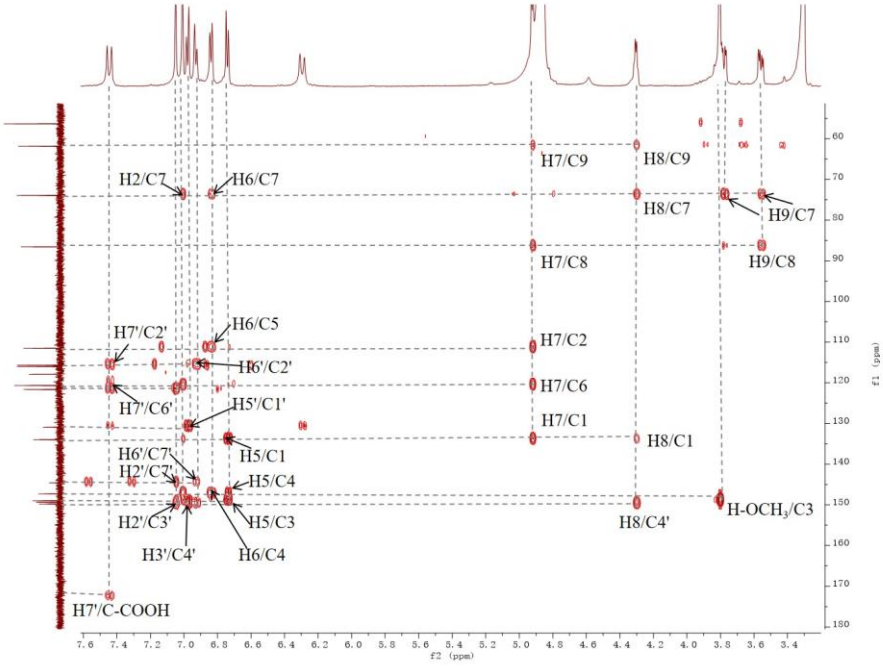


Figure S1-7: HMBC spectrum of **1** (From δ_H 3.4 ppm to 7.6 ppm).

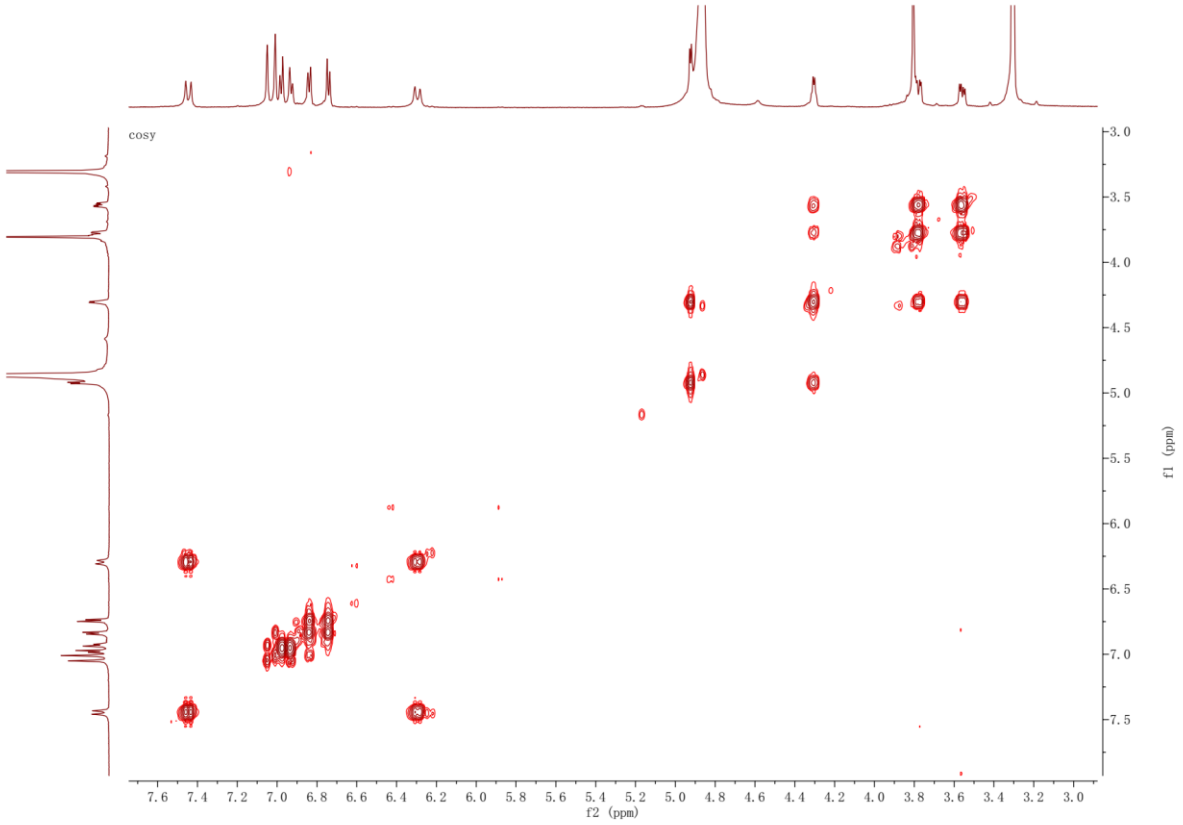


Figure S1-8: ^{1}H-^{1}H COSY spectrum of **1**.

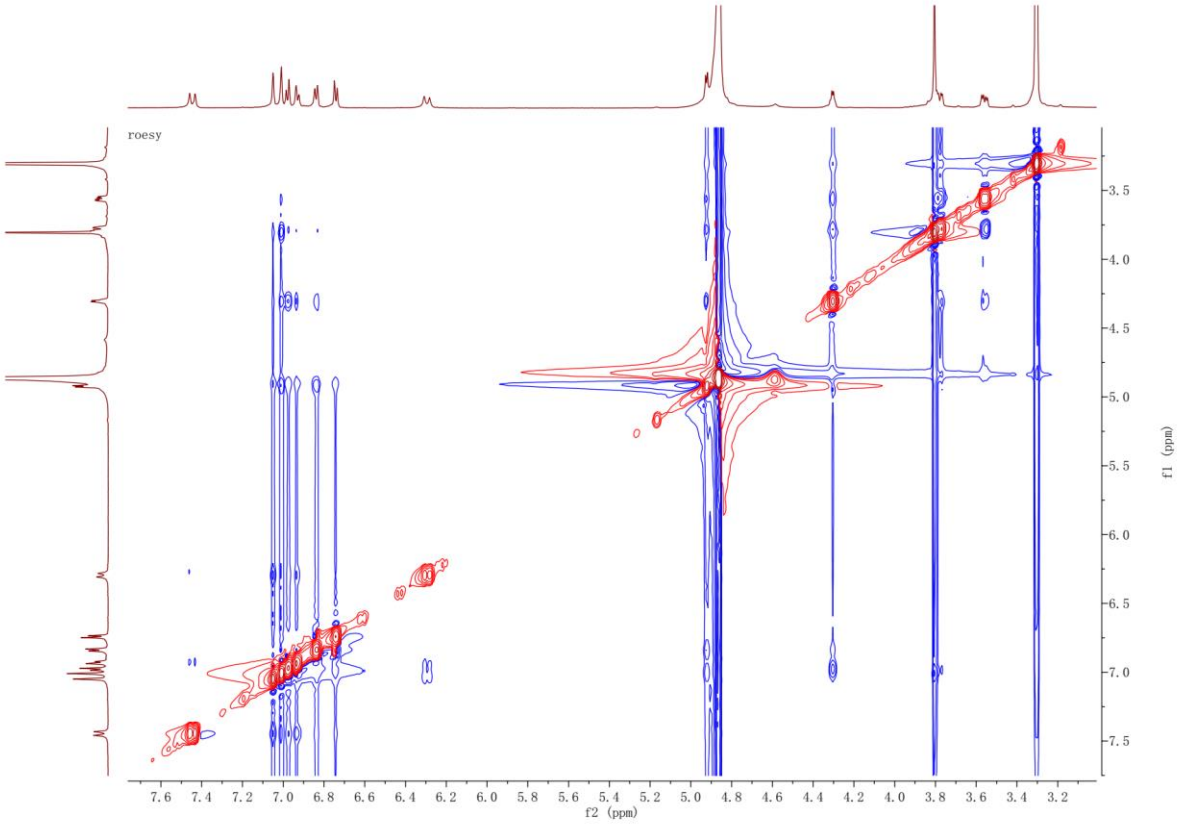


Figure S1-9: ROESY spectrum of **1**.

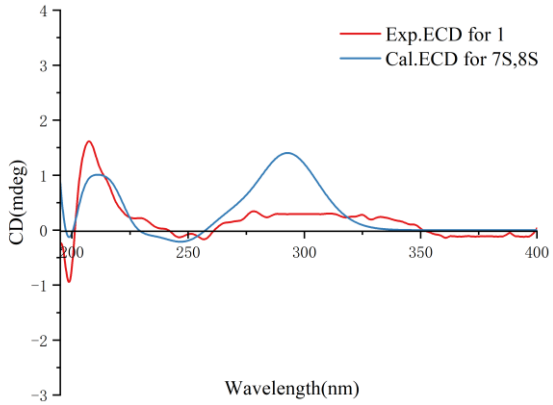


Figure S1-10: ECD spectra for compound **1**.

CAS SciFinder

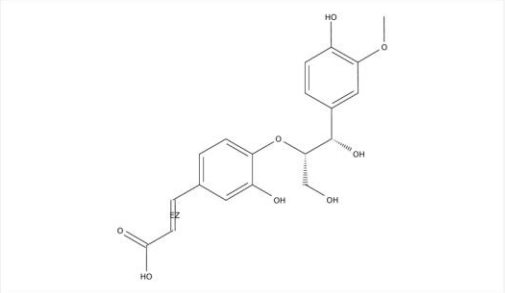
Task History

Initiating Search

March 14, 2025, 1:28 PM

Substances:

Filtered By:



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	View Results

CAS SciFinder

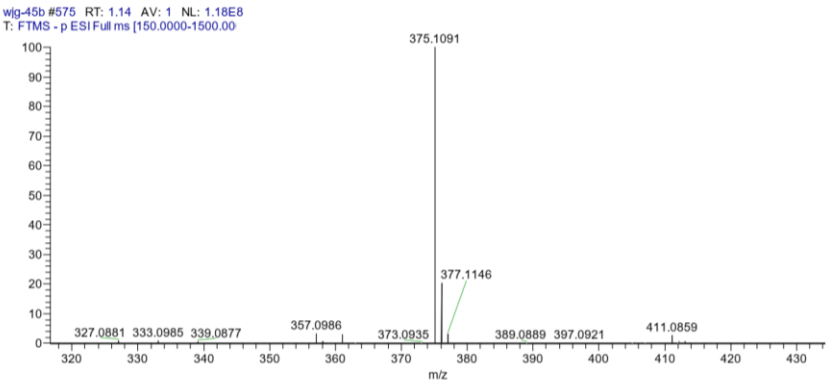
Substances (0)

View in CAS SciFinder

We couldn't find any results. Please update your search query and try again.

Substances with (0) results

Figure S1-11: Scifinder search report of **1**.



Meas. m/z	Pred. m/z	Df. ppm	Formula	Ion
375.1091	375.1085	1.5995	$C_{19}H_{20}O_8$	$[M-H]^-$

Figure S2-1: HR-ESI-MS spectrum of **2**.

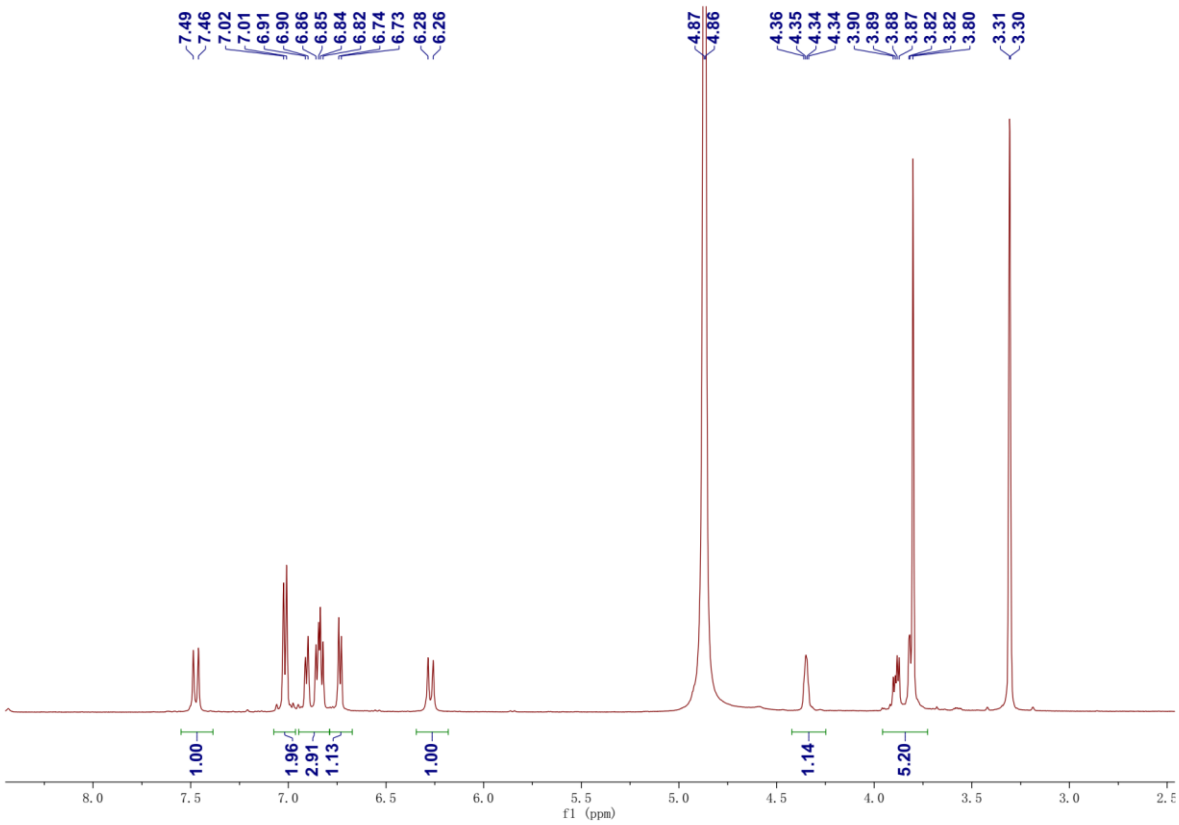


Figure S2-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **2**.

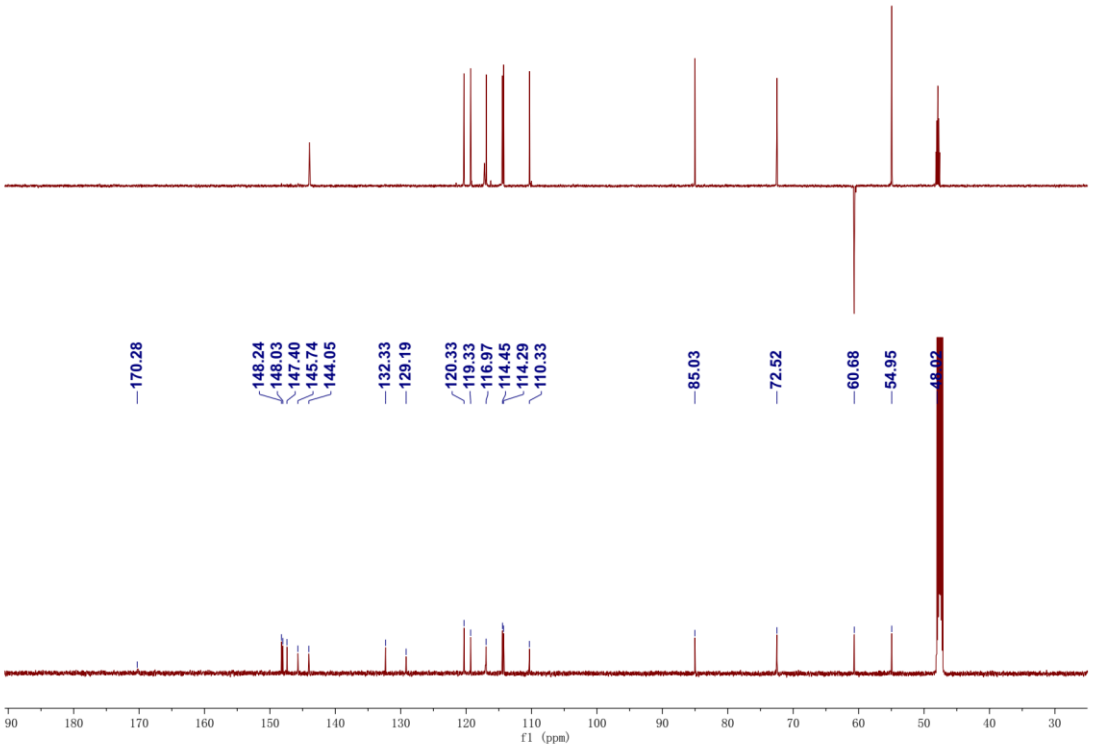


Figure S2-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **2**.

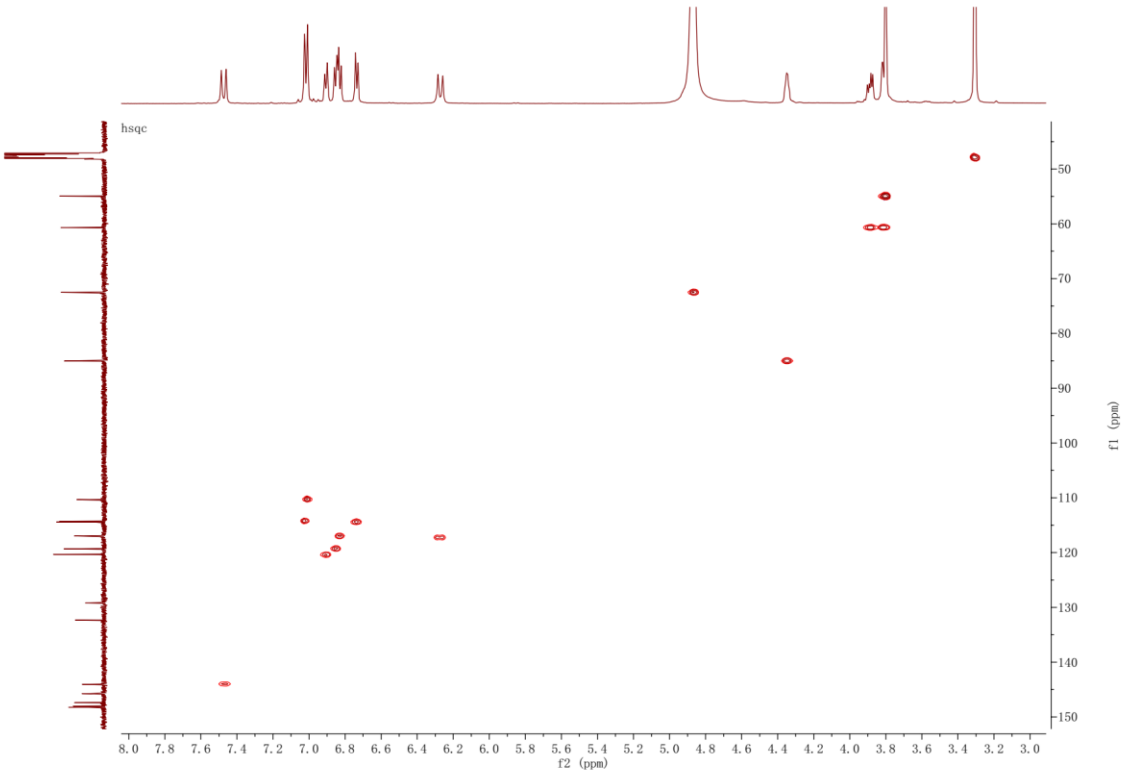


Figure S2-4: HSQC spectrum of **2**.

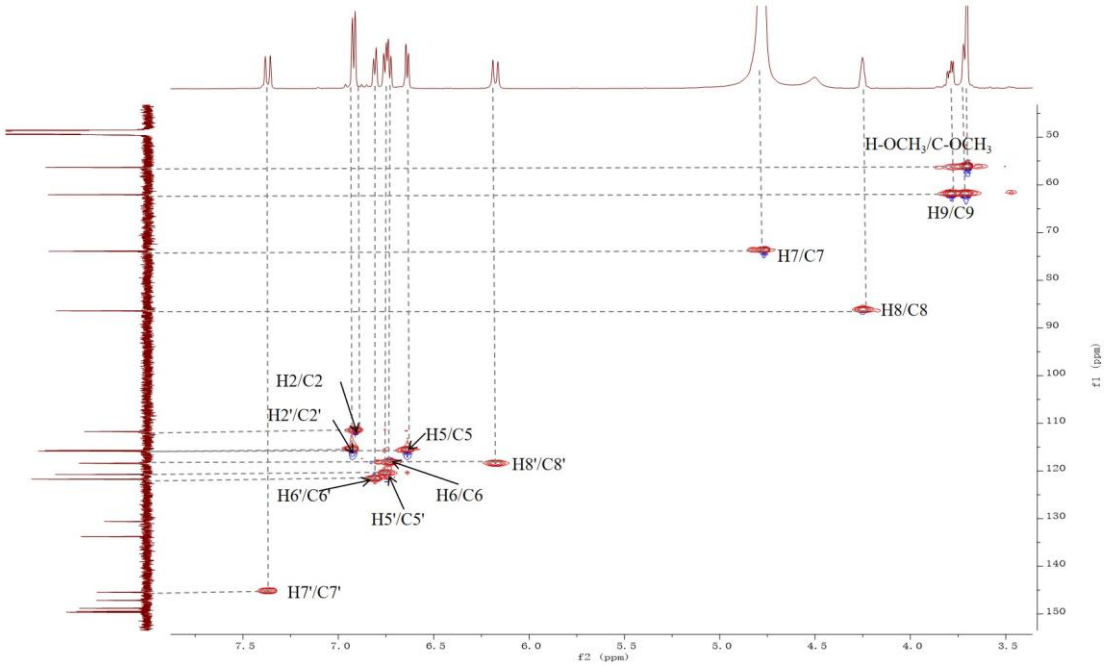


Figure S2-5: HSQC spectrum of **2** (From δ_H 3.5 ppm to 8.0 ppm).

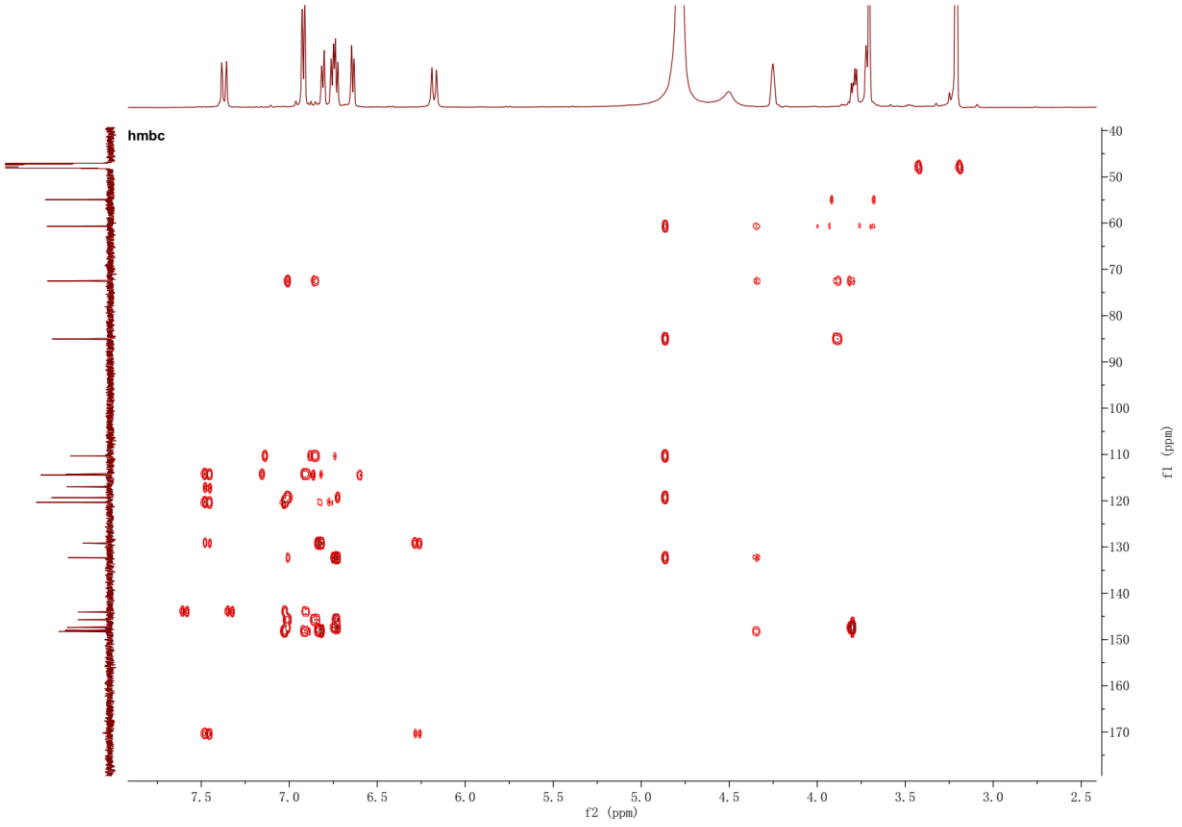


Figure S2-6: HMBC spectrum of **2**.

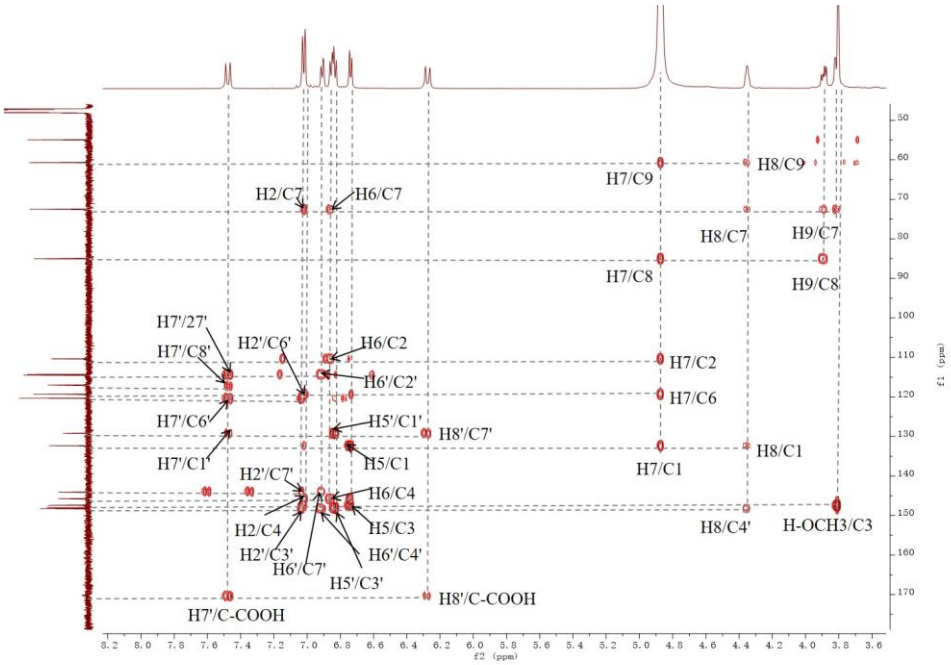


Figure S2-7: HMBC spectrum of **2** (From δ_H 3.6 ppm to 8.2 ppm).

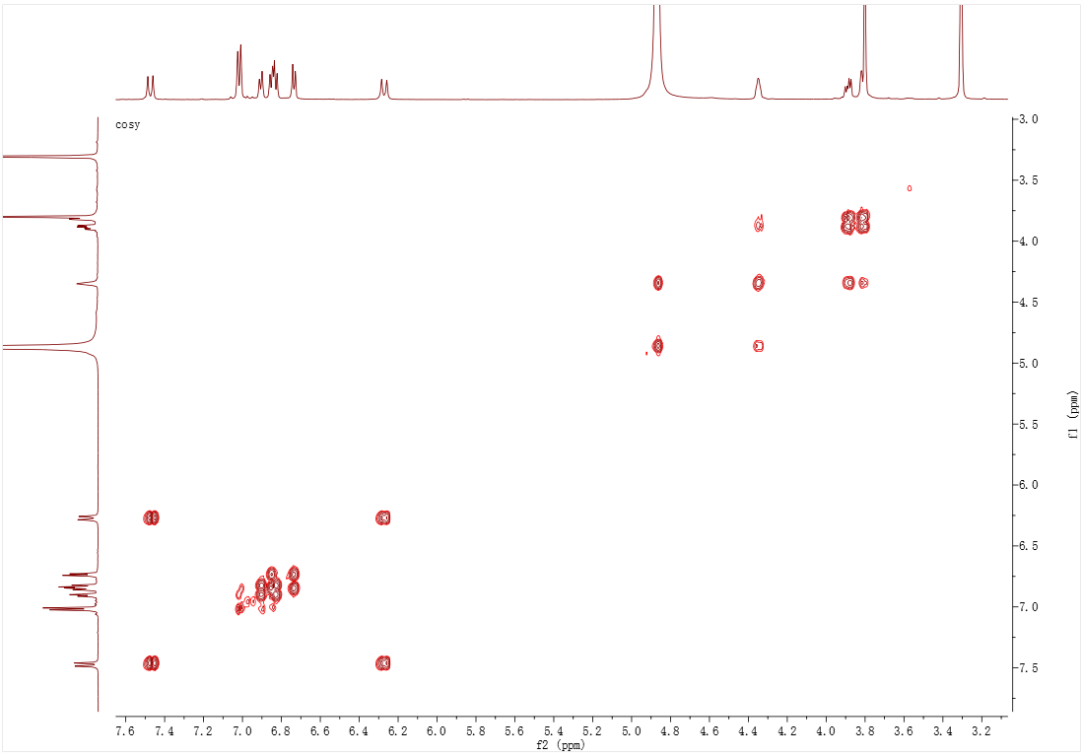


Figure S2-8: ^{1}H-^{1}H COSY spectrum of **2**.

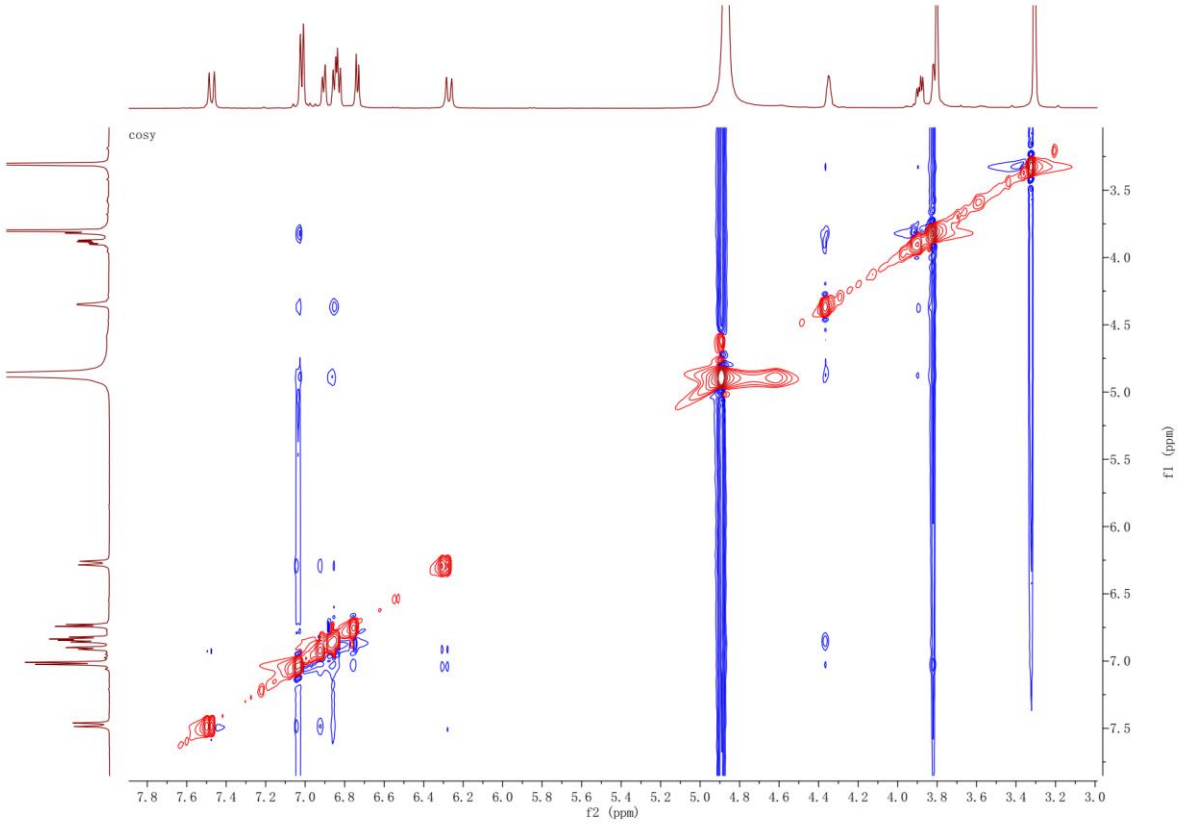


Figure S2-9: ROESY spectrum of **2**.

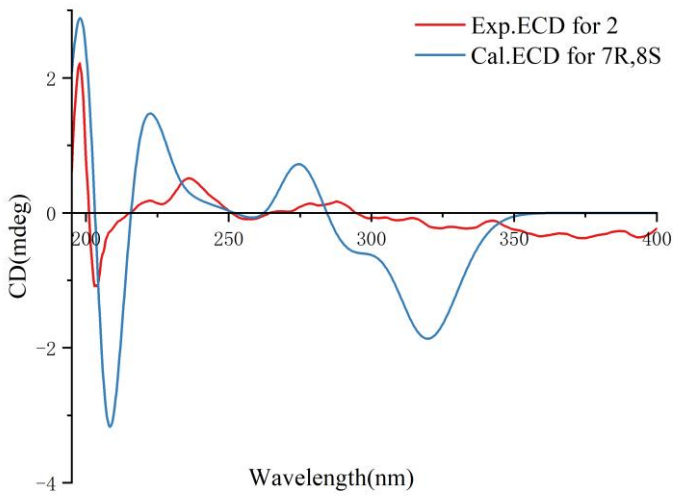


Figure S2-10: ECD spectra for compound **2**.

CAS SciFinder

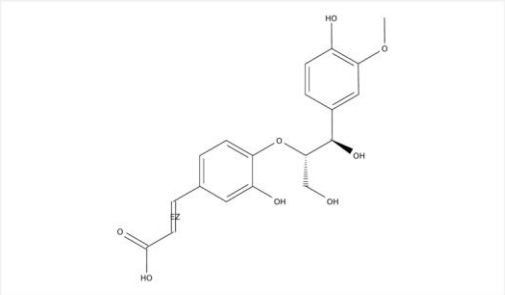
Task History

Initiating Search

March 14, 2025, 1:30 PM

Substances:

Filtered By:



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	View Results

CAS SciFinder

Substances (0)

View in CAS SciFinder

We couldn't find any results. Please update your search query and try again.

Substances with (0) results

Figure S2-11: Scifinder search report of **2**.

Table S2-12: The NMR spectroscopic data for **1** and **2** with similar compound **1′** (δ in ppm and J in Hz)

Position	**1**		**2**		**1′**	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	-	132.6	-	132.3	-	134.0
2	7.01 (s)	110.6	7.01 (s)	110.3	7.01 (d, 1.8)	111.5
3	-	147.5	-	147.4	-	149.0
4	-	145.9	-	145.7	-	147.4
5	6.74 (d, 8.1)	114.5	6.74 (d, 8.1)	114.4	6.74 (d, 8.3)	116.0
6	6.84 (d, 8.1)	119.2	6.83 (d, 8.1)	119.3	6.84 (dd, 8.3, 1.8)	120.7
7	4.92 (d, 5.2)	72.5	4.87 (over lapped)	72.5	4.92 (d, 5.5)	74.0
8	4.30 (m)	85.2	4.34 (m)	85.0	4.28 (m)	86.7
9	3.56 (dd, 11.5, 4.9) 3.78 (dd, 11.9, 3.9)	60.8	3.82 (m) 3.89 (m)	60.6	3.54 (dd, 11.7, 5.3) 3.77 (dd, 11.7, 4.4)	61.9
1'	-	129.5	-	129.2	-	131.4
2'	7.05 (s)	114.2	7.02 (s)	114.3	7.04 (d, 2.3)	115.6
3'	-	147.9	-	148.0	-	149.4
4'	-	148.3	-	148.2	-	149.5
5'	6.97 (d, 8.1)	116.4	6.82 (d, 8.1)	116.9	6.97 (d, 8.3)	118.0
6'	6.92 (d, 8.1)	120.2	6.90 (d, 8.1)	120.3	6.92 (dd, 8.3, 1.8)	121.4
7'	7.45 (d, 15.8)	143.1	7.48 (d, 15.8)	144.1	7.38 (d, 16.0)	143.3
8'	6.30 (d, 15.8)	118.2	6.27 (d, 15.8)	117.2	6.31 (d, 16.0)	121.4
9'	-	171.1	-	170.2	-	172.6
3-OCH_3	3.81 (s)	54.9	3.80 (s)	54.9	3.81 (s)	56.3

The ^1H and ^{13}C NMR data of compound **1** and **2** were recorded at 600 MHz with CD_3OD as the solvent. Similarly, the ^1H and ^{13}C NMR data of compound **1'** reported in reference [1] were obtained using CD_3OD as the solvent.

Reference:

[1] M. Ichikawa, K. Ryu, J. Yoshida, N. Ide, Y. Kodera, T. Sasaoka, R. T. Rosen (2003). Identification of six phenylpropanoids from garlic skin as major antioxidants. *J. Agr. Food Chem.* **51**, 7313-7317.

Formula Predictor Report - WGJ-1.lcd

Data File: E:\DATA\2024\1011\WGJ-1.lcd

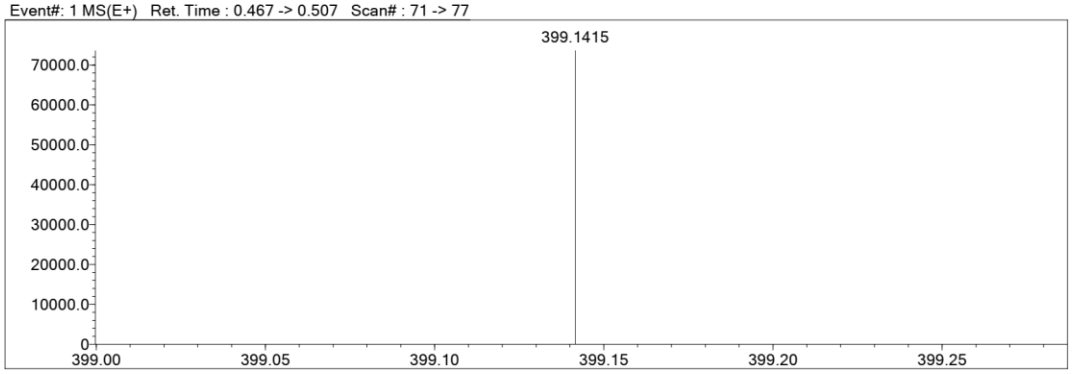
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	Sn	2	0	0	Na
B	3	0	0	Mg	2	0	0	Cu	2	0	0	I	3	0	0	
C	4	5	100	Si	4	0	0	Se	2	0	0	Ir	3	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0	Pt	2	0	0	
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 10
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

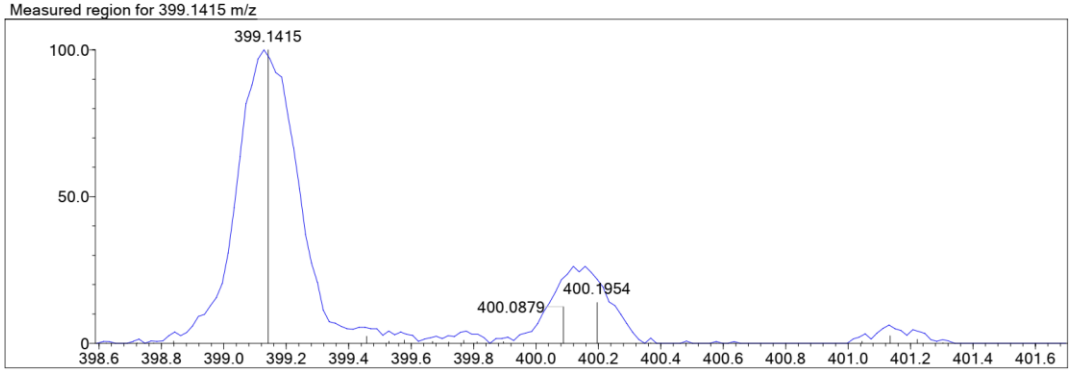
DBE Range: not fixed
Apply N Rule: no
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 30

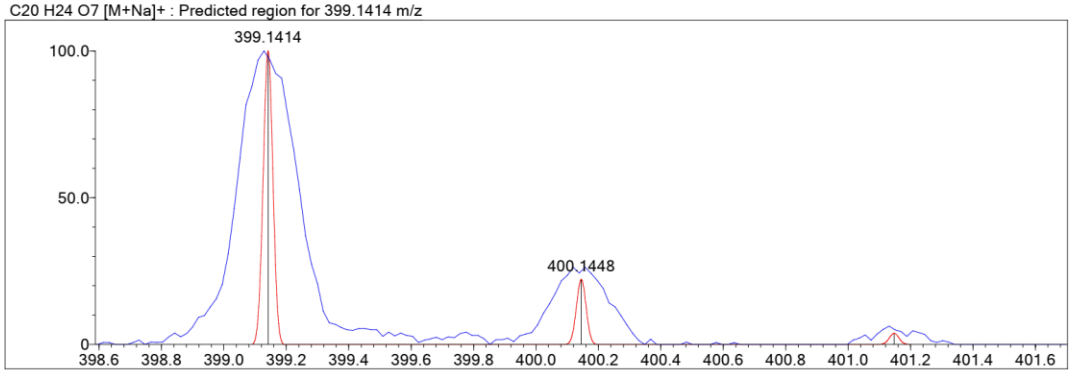
Event#: 1 MS(E+) Ret. Time : 0.467 -> 0.507 Scan# : 71 -> 77



Measured region for 399.1415 m/z



C20 H24 O7 [M+Na]+ : Predicted region for 399.1414 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C20 H24 O7	[M+Na]+	399.1415	399.1414	0.1	0.25	9.0

Figure S3-1: HR-ESI-MS spectrum of **3**.

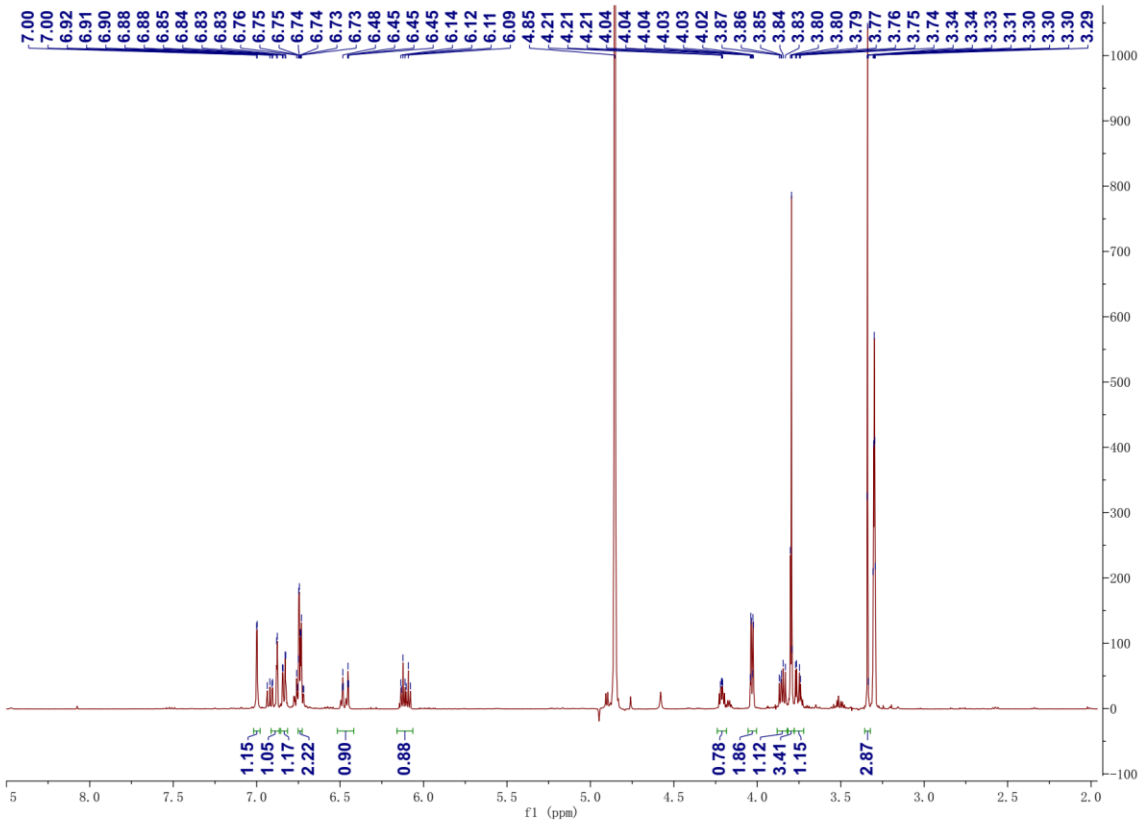


Figure S3-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **3**.

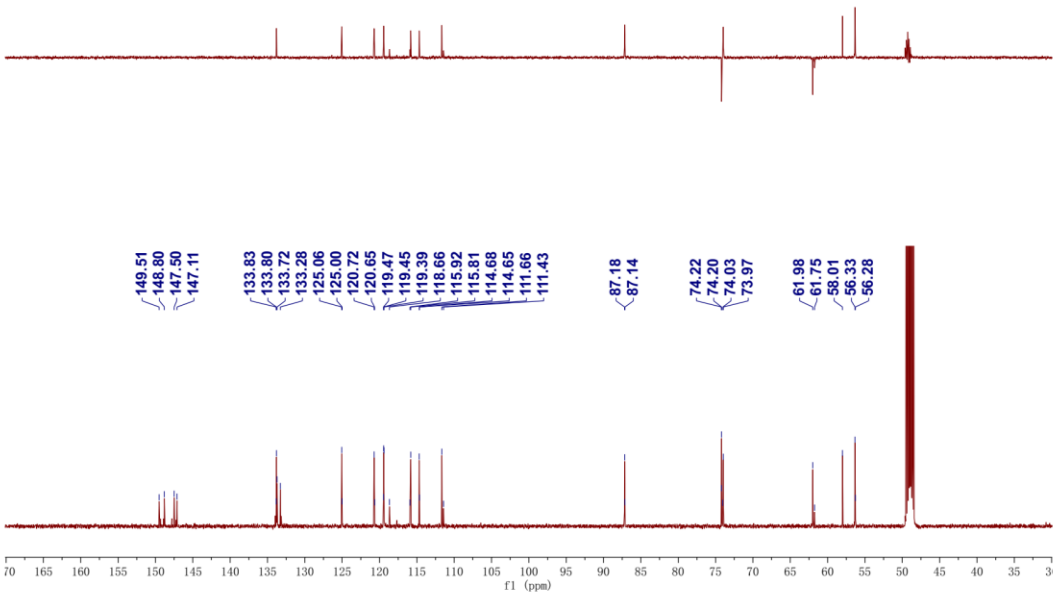


Figure S3-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **3**.

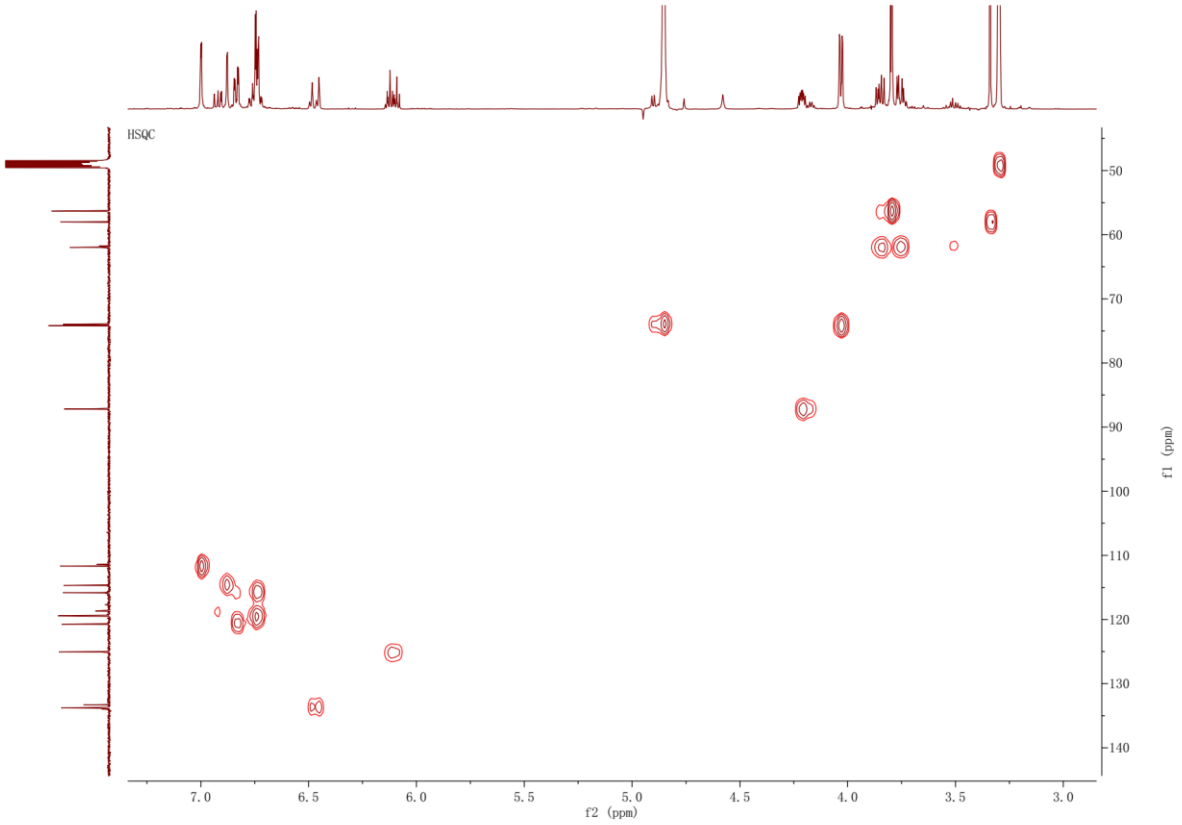


Figure S3-4: HSQC spectrum of **3**.

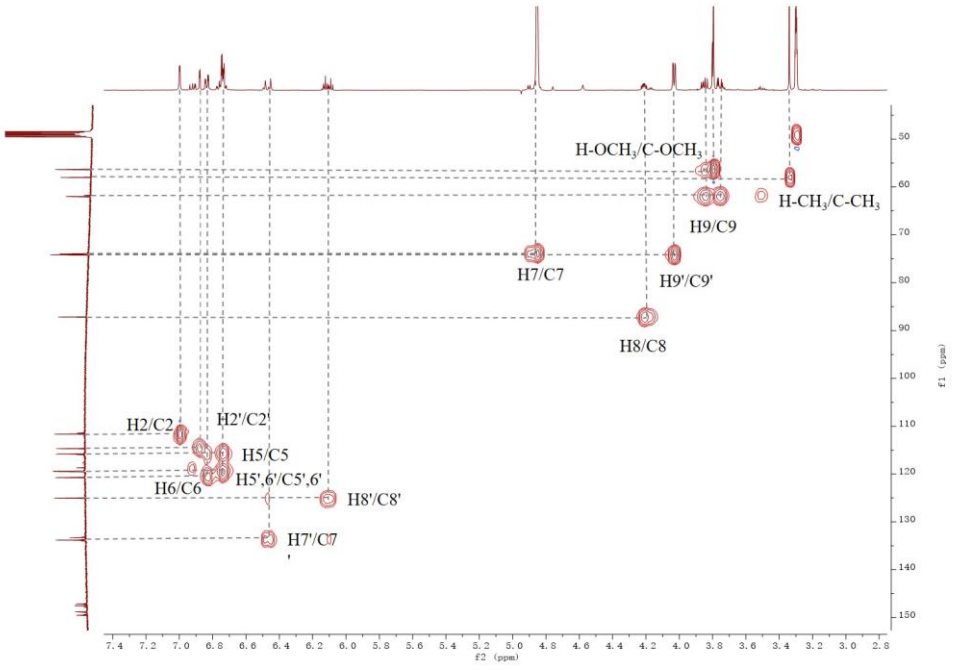


Figure S3-5: HSQC spectrum of **3** (From δ_H 2.8 ppm to 7.4 ppm).

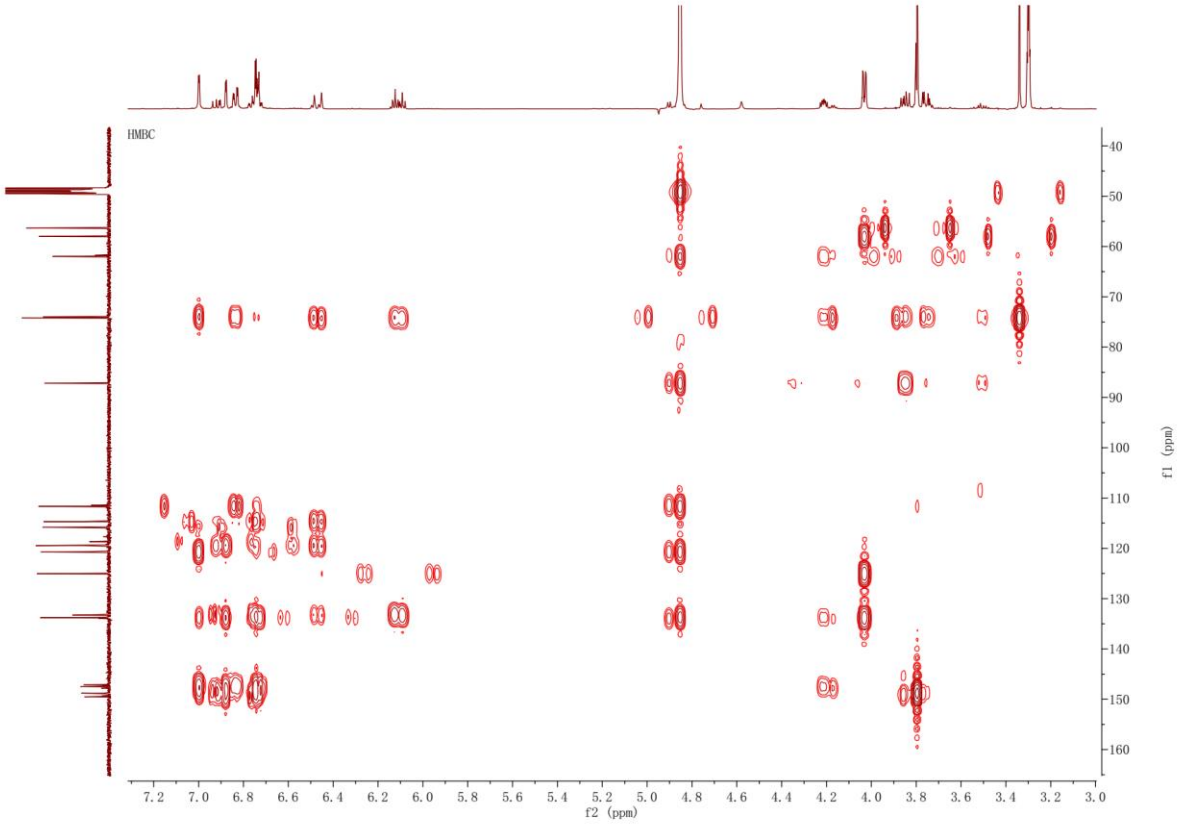


Figure S3-6: HMBC spectrum of **3**.

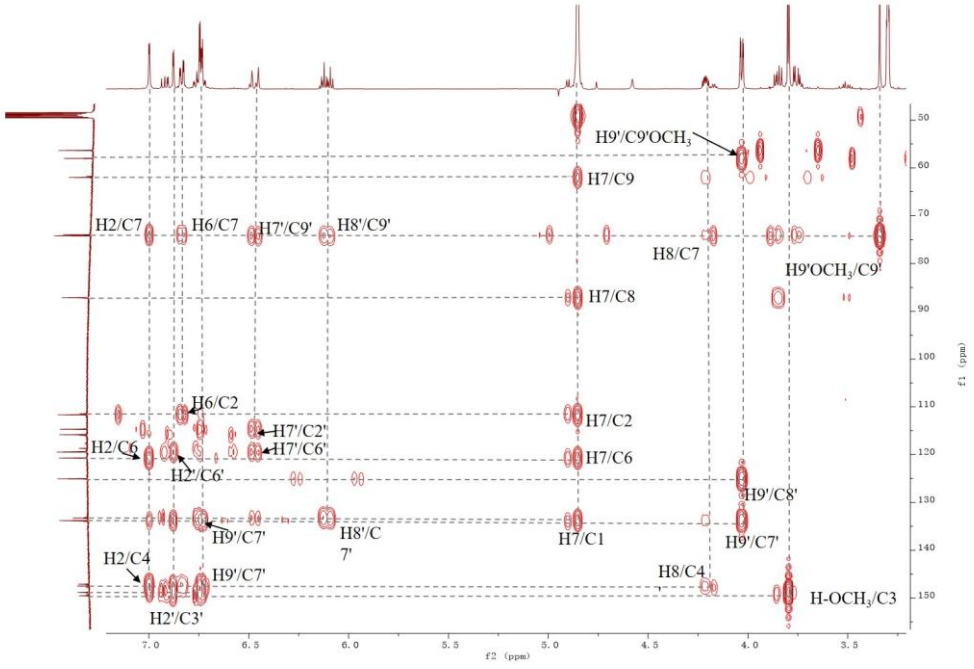


Figure S3-7: HMBC spectrum of **3** (From δ_H 3.0 ppm to 7.5 ppm).

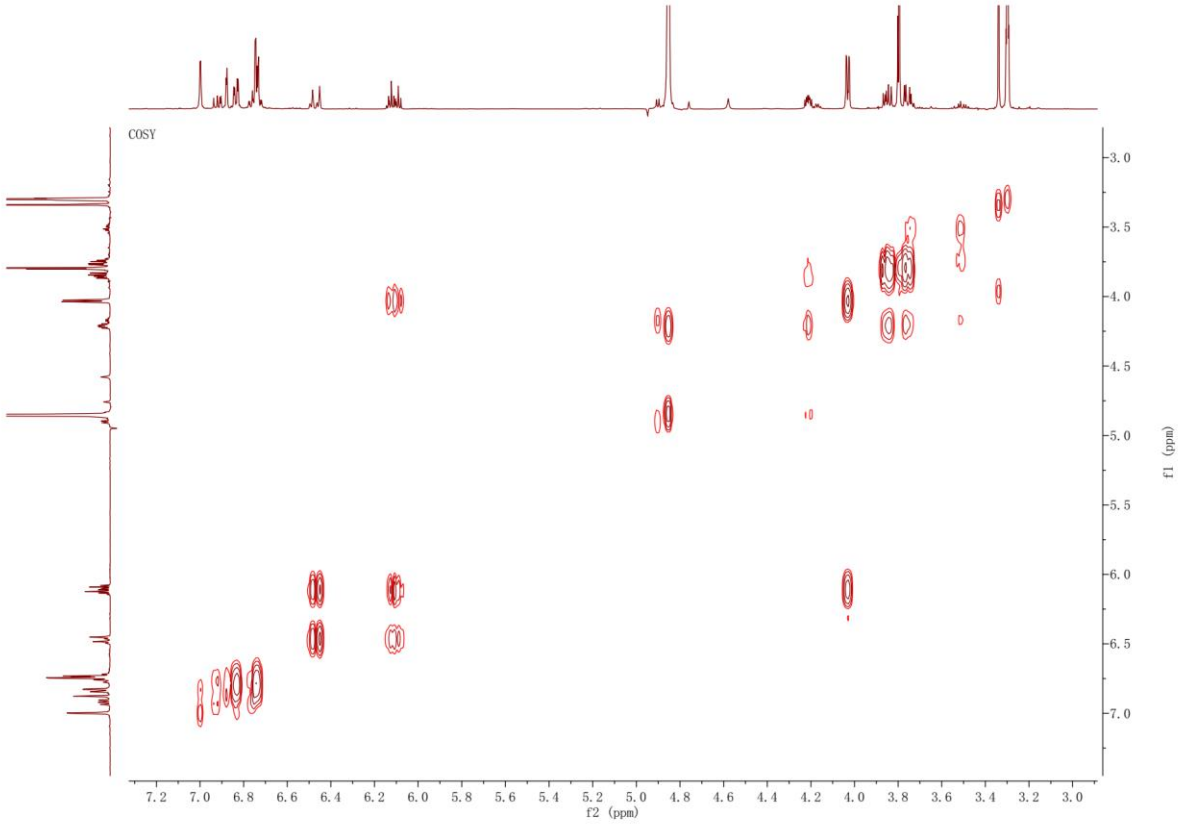


Figure S3-8: ^{1}H-^{1}H COSY spectrum of **3**.

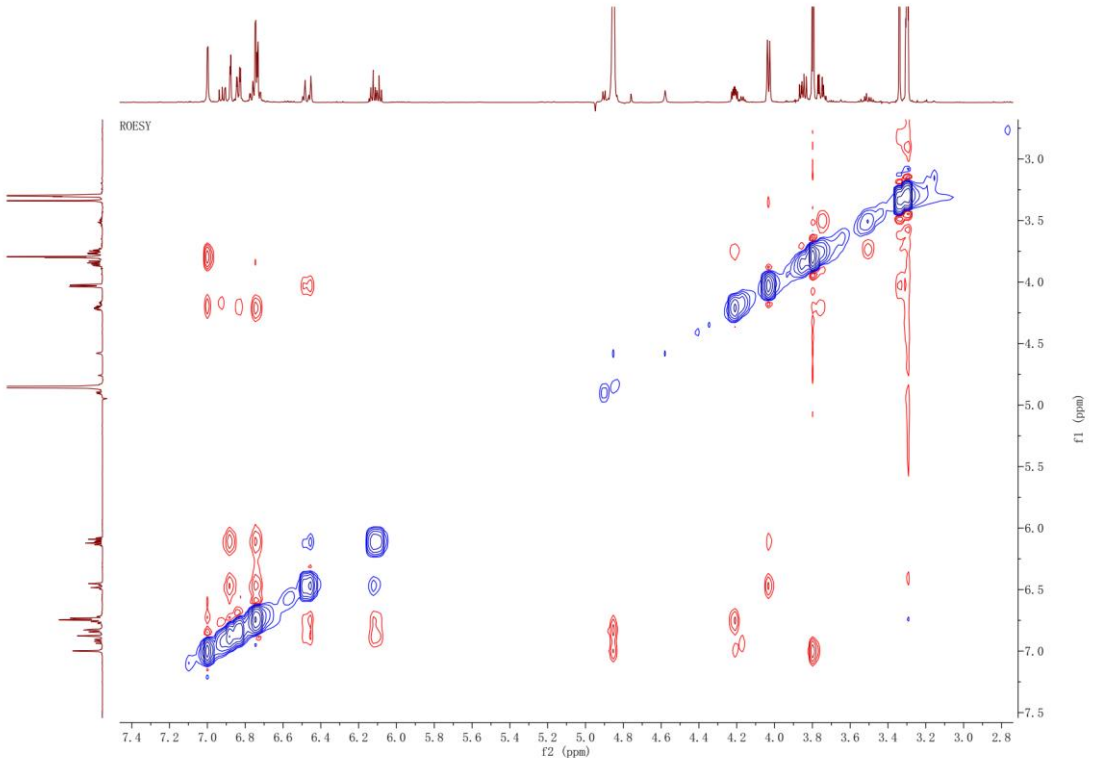


Figure S3-9: ROESY spectrum of **3**.

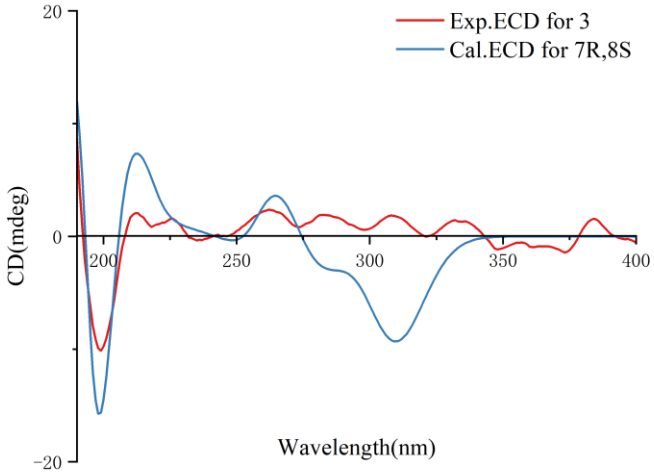


Figure S3-10: ECD spectra for compound **3**.

CAS SciFinder

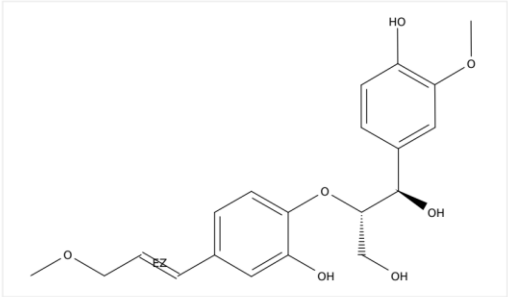
Task History

Initiating Search

March 14, 2025, 12:57 PM

Substances:

Filtered By:



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	View Results

CAS SciFinder

Substances (0)

View in CAS SciFinder

We couldn't find any results. Please update your search query and try again.

Substances with (0) results

Figure S3-11: Scifinder search report of **3**.

Formula Predictor Report - WGJ-2.lcd

Page 1 of 1

Data File: E:\DATA\2024\1011\WGJ-2.lcd

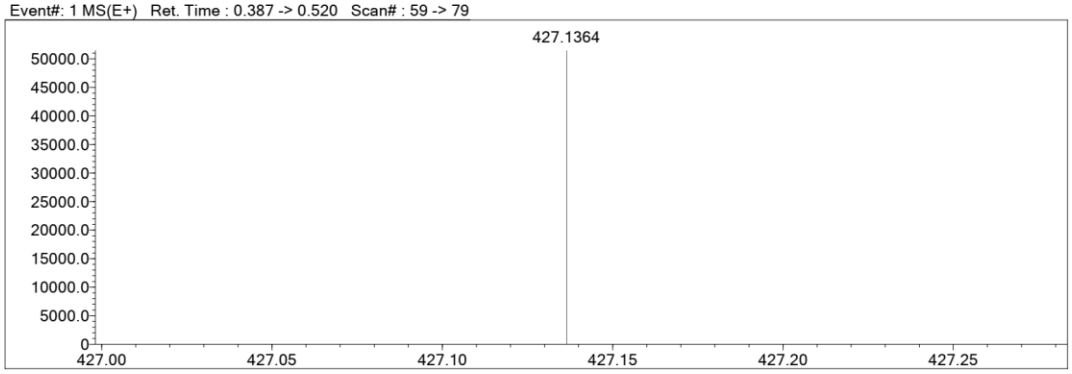
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	F	1	0	0	Cl	1	0	0	Ag	1	0	0	H
2H	1	0	0	Na	1	0	0	Co	2	0	0	Sn	2	0	0	Na
B	3	0	0	Mg	2	0	0	Cu	2	0	0	I	3	0	0	
C	4	5	100	Si	4	0	0	Se	2	0	0	Ir	3	0	0	
N	3	0	10	P	3	0	0	Br	1	0	0	Pt	2	0	0	
O	2	0	30	S	2	0	0	Pd	2	0	0					

Error Margin (ppm): 10
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

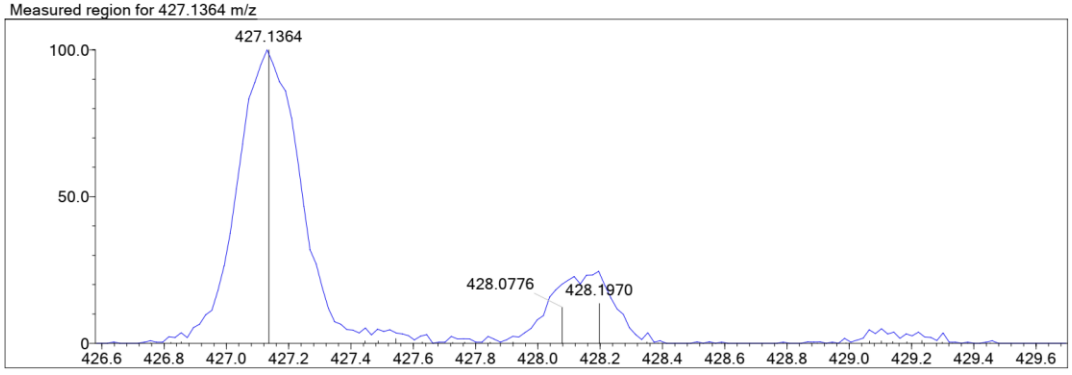
DBE Range: not fixed
Apply N Rule: no
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 30

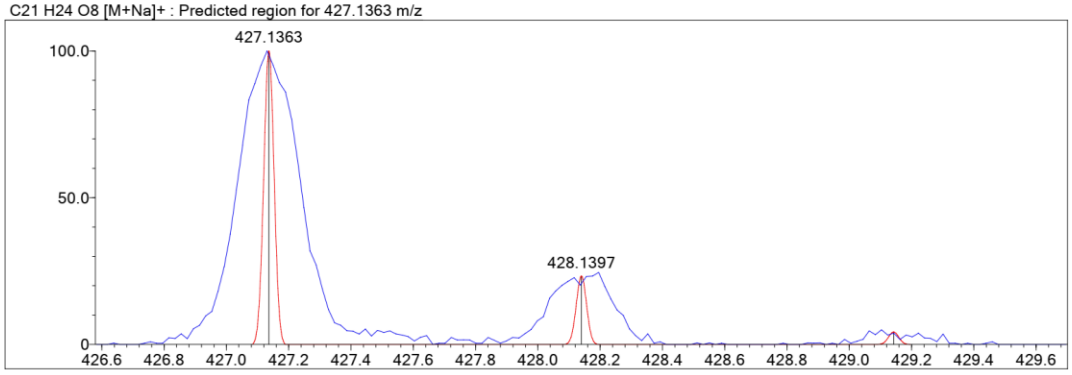
Event#: 1 MS(E+) Ret. Time : 0.387 -> 0.520 Scan# : 59 -> 79



Measured region for 427.1364 m/z



C21 H24 O8 [M+Na]+ : Predicted region for 427.1363 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C21 H24 O8	[M+Na]+	427.1364	427.1363	0.1	0.23	10.0

Figure S4-1: HR-ESI-MS spectrum of **4**.

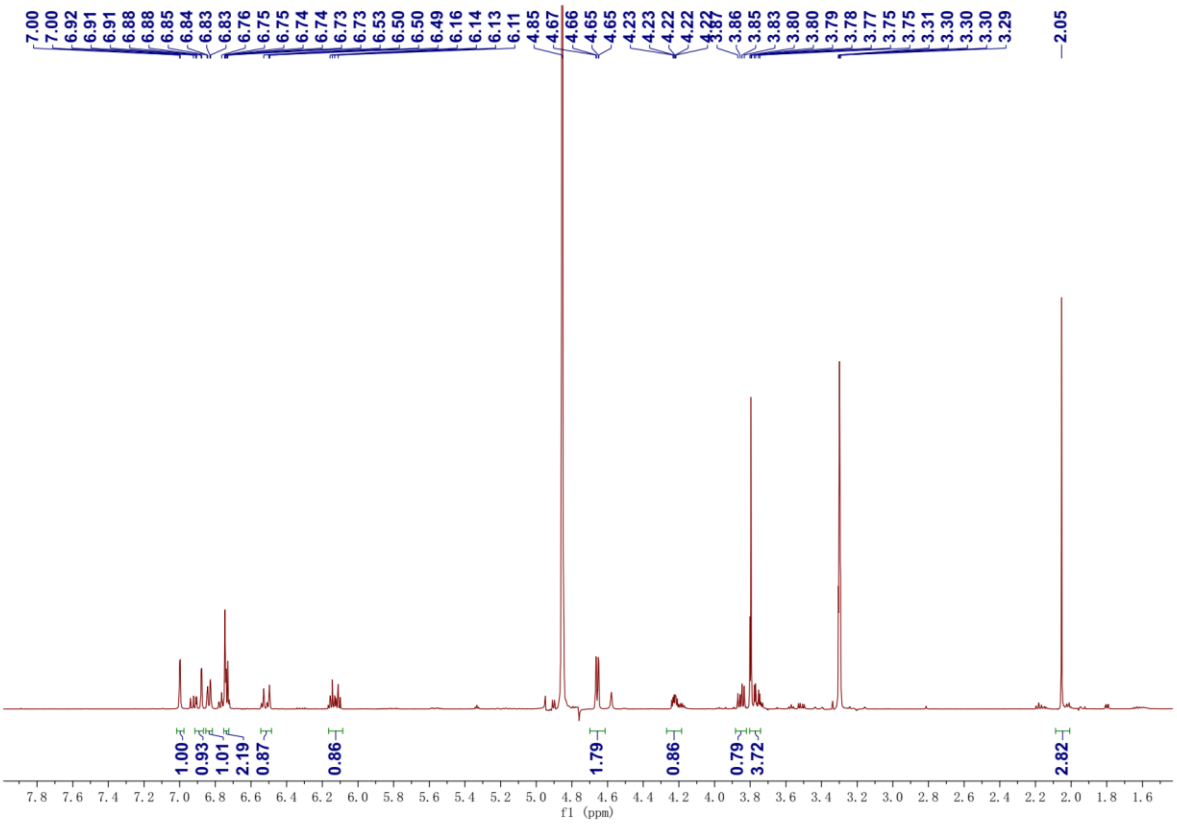


Figure S4-2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of **4**.

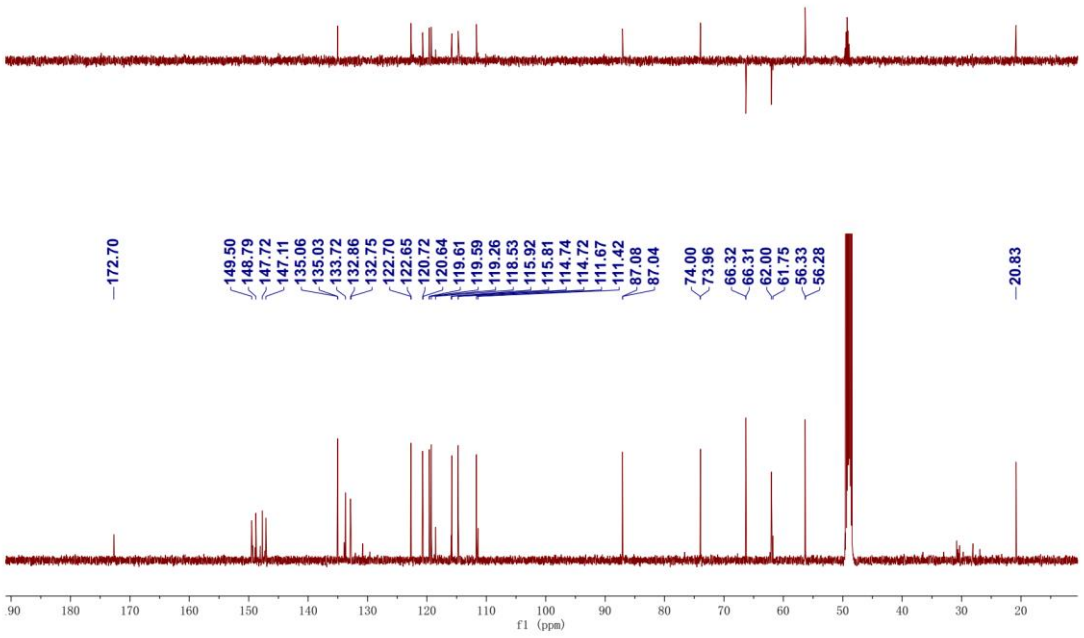


Figure S4-3: ^{13}C-NMR and DEPT (150 MHz, CD_3OD) spectrum of **4**.

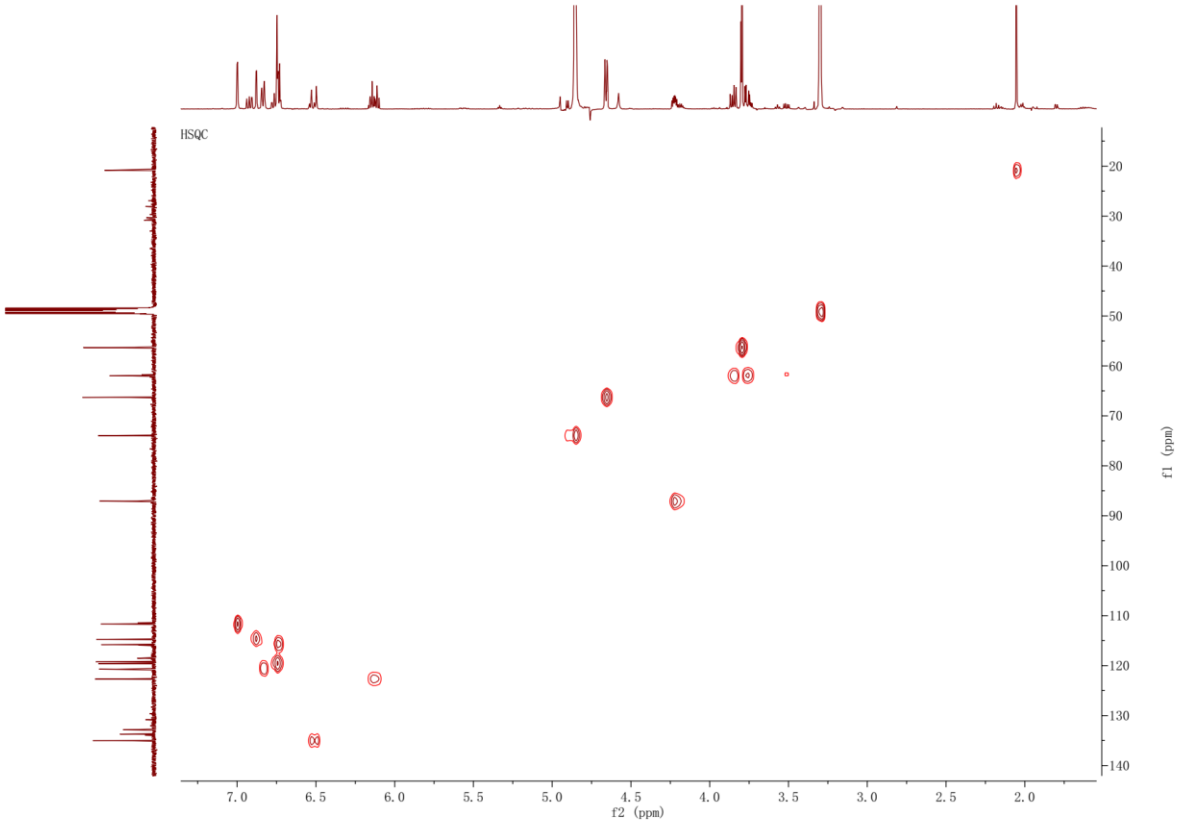


Figure S4-4: HSQC spectrum of **4**.

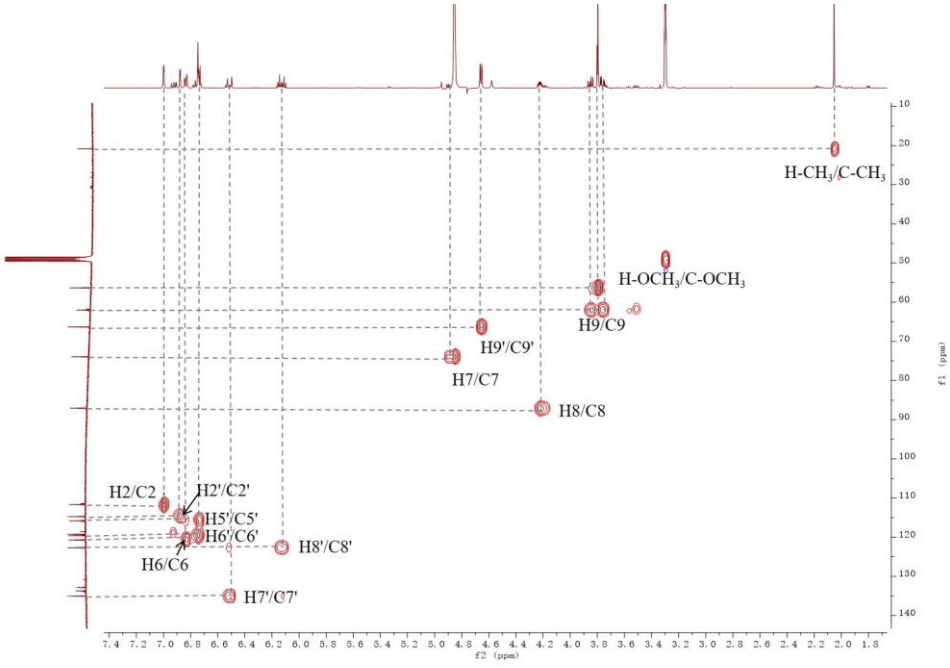


Figure S4-5: HSQC spectrum of **4** (From δ_H 1.5 ppm to 7.5 ppm).

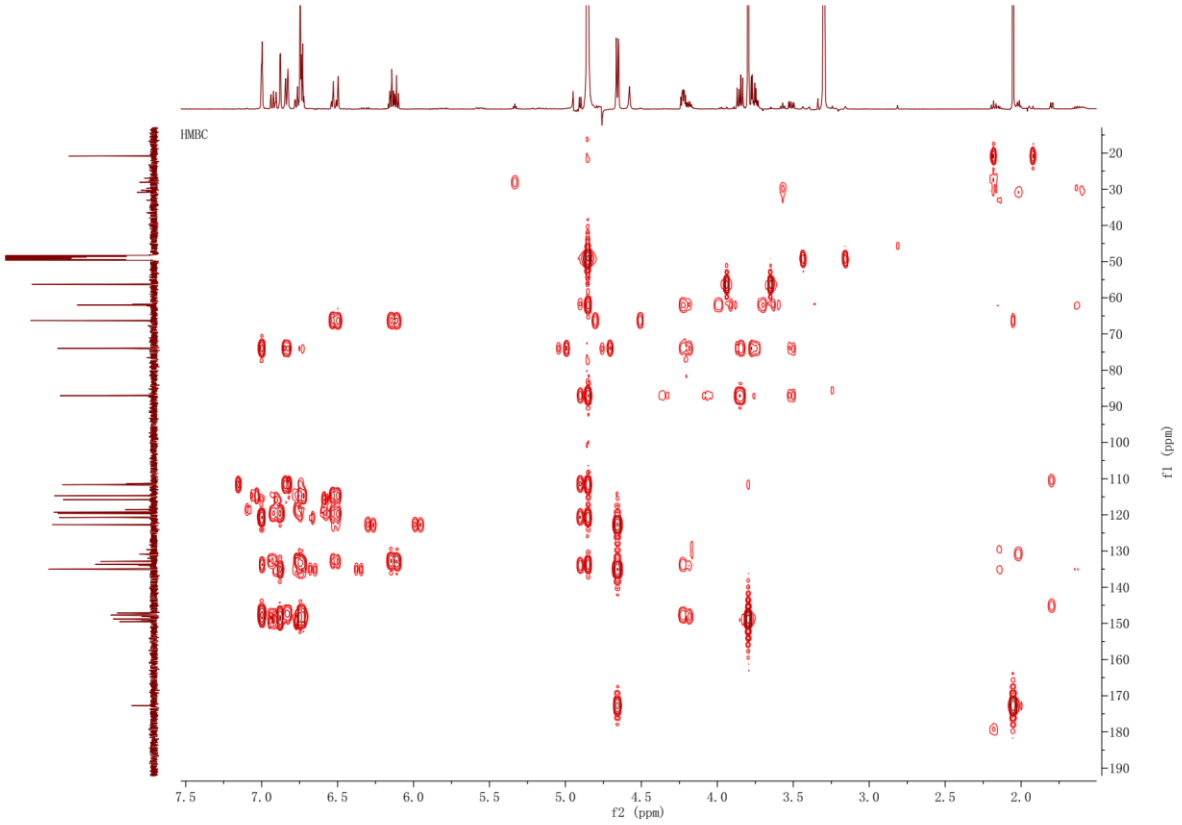


Figure S4-6: HMBC spectrum of **4**.

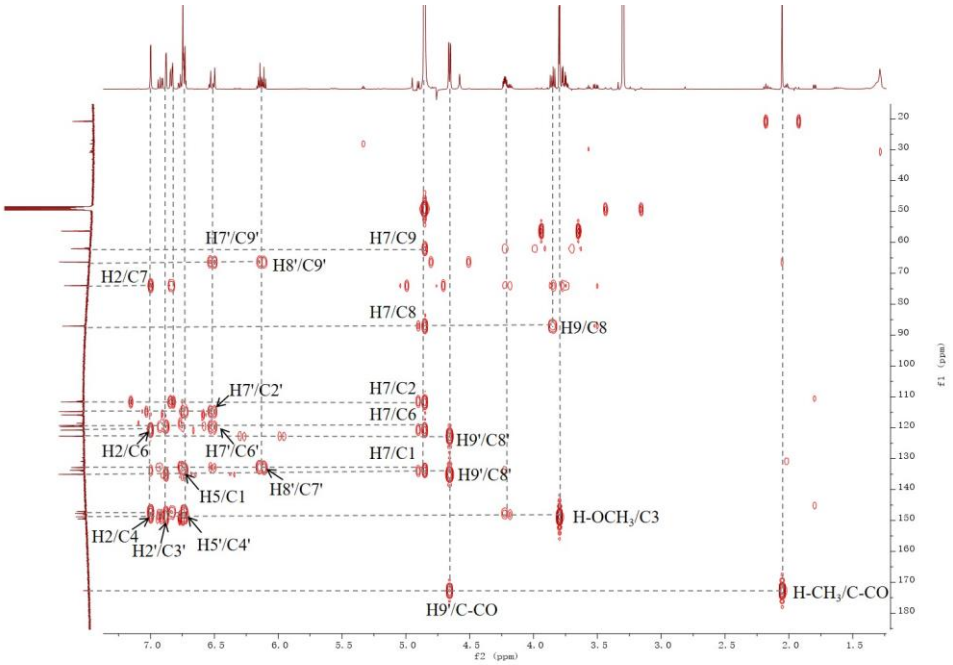


Figure S4-7: HMBC spectrum of **4** (From δ_H 1.0 ppm to 7.6 ppm).

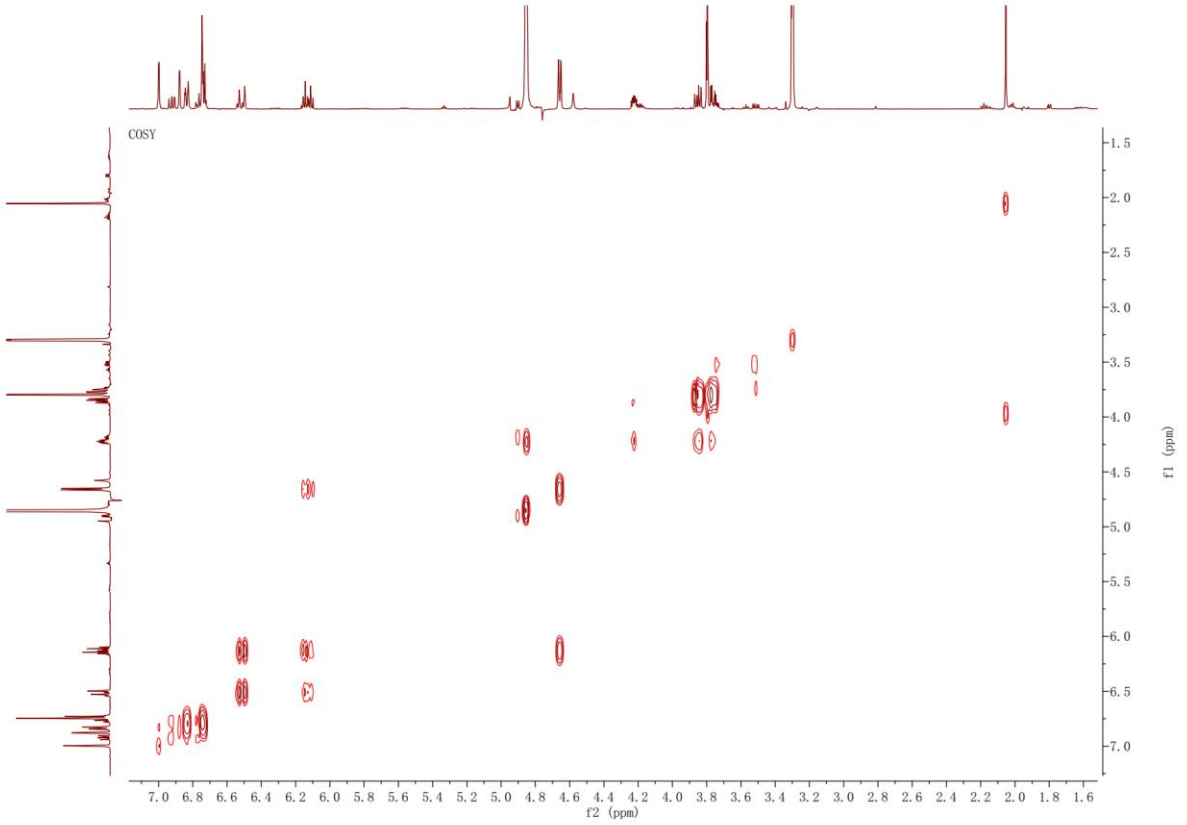


Figure S4-8: ^{1}H-^{1}H COSY spectrum of **4**.

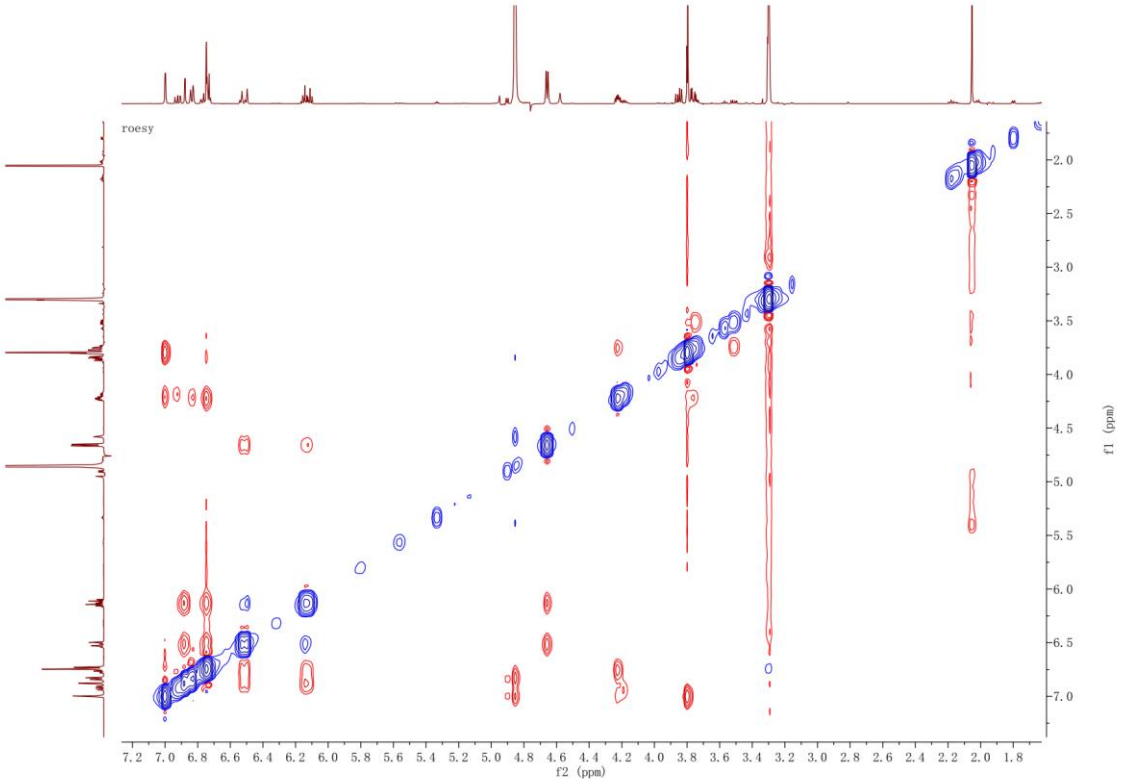


Figure S4-9: ROESY spectrum of **4**.

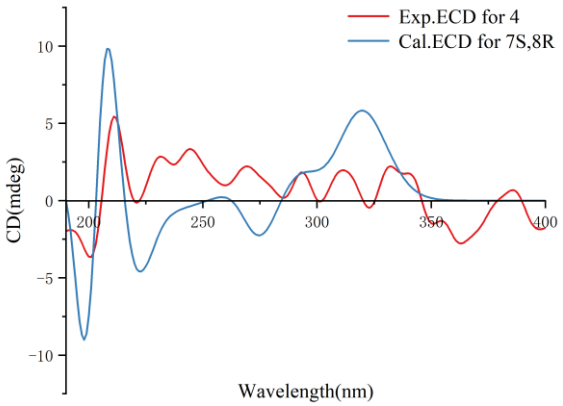


Figure S4-10: ECD spectra for compound **4**.

CAS SciFinder

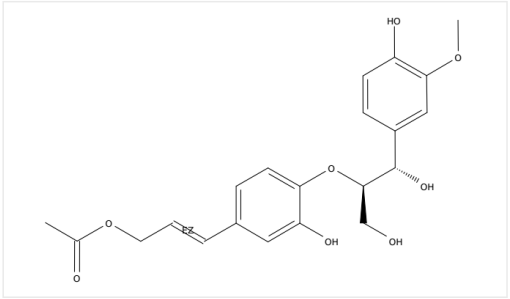
Task History

Initiating Search

March 14, 2025, 1:12 PM

Substances:

Filtered By:



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (0)	Substances	View Results

CAS SciFinder

Substances (0)

View in CAS SciFinder

We couldn't find any results. Please update your search query and try again.

Substances with (0) results

Figure S4-11: Scifinder search report of **4**.

Table S4-12: The NMR spectroscopic data for **3** and **4** with similar compound **2′** (δ in ppm and J in Hz)

Position	**3**		**4**		**2′**	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	-	133.7	-	133.7	-	133.4
2	6.99 (d, 1.8)	111.6	6.99 (d, 1.8)	111.7	7.04 (d, 2.0)	111.7
3	-	148.8	-	148.8	-	147.3
4	-	147.1	-	147.1	-	148.9
5	6.74 (over lapped)	115.8	6.73 (over lapped)	115.8	6.78 (d, 8.0)	114.7
6	6.83 (dd, 8.0, 1.8)	120.7	6.83 (dd, 8.1, 1.8)	120.7	6.77 (dd, 8.0, 2.0)	120.8
7	4.84 (over lapped)	73.9	4.85 (over lapped)	74.0	4.89 (d, 7.5)	74.0
8	4.21 (m)	87.2	4.22 (m)	87.1	4.24 (m)	87.3
9	3.75 (m) 3.85 (m)	62.0	3.76 (dd, 11.8, 3.5) 3.86 (dd, 11.8, 6.4)	62.0	4.19 (over lapped) 4.20 (dd, 5.8, 1.4)	63.8
1'	-	133.3	-	132.9	-	131.5
2'	6.87 (d, 1.8)	114.7	6.87 (d, 1.8)	114.7	6.91 (d, 2.0)	114.6
3'	-	149.5	-	149.5	-	147.1
4'	-	147.5	-	147.7	-	133.7
5'	6.73(over lapped)	119.4	6.74 (over lapped)	119.2	6.79(d, 8.0)	114.7
6'	6.73(over lapped)	119.4	6.74 (over lapped)	119.5	6.87(dd, 8.0, 2.0)	119.3
7'	6.47 (dd, 15.9, 6.1)	133.8	6.52 (dd, 15.9, 6.3)	135.0	6.48 (d, 15.8)	131.6
8'	6.11 (m)	125.0	6.13 (m)	122.7	6.21 (m)	128.4
9'	4.03 (dt, 6.1, 1.7)	74.2	4.66 (m)	66.3	3.79 (m) 3.89 (m)	62.0
3-OCH_3	3.80 (s)	56.3	3.79 (s)	56.4	3.83 (s)	56.4
1"	3.34 (s)	58.2	-	172.7	-	-
1"-CH_3	-	-	2.05 (s)	20.8	-	-

The ^1H and ^{13}C NMR data of compound **3** and **4** were recorded at 600 MHz with CD_3OD as the solvent. Similarly, the ^1H and ^{13}C NMR data of compound **2'** reported in reference [2] were obtained using CD_3OD as the solvent.

Reference:

[2] Y. J. Feng, X. X. Wang, P. Y. Zhuang, D. Y. Zhang, L. Gao, J. M. Chen, G. Han (2017). Chemical Component Research on *Codonopsis Pilosula*. *China J. Chin. Mater. Med.* **42**, 135-139.

S5-1: General Experimental Procedures.

The isolated compounds were evalutated using a 600 MHz NMR spectrometer (Bruker, Germany), with residual solvent signals serving as the internal standard. High resolution mass spectrometry (HRMS) data were acquired via LC-IT-TOFMS (Shimadzu, Japan) and LC-Orbitrap Exploris 120 (Thermo, USA) mass spectrometers. Optical rotations were measured with a P-2000 instrument (JASCO, Japan). Circular dichroism data were obtained using a P-1500 instrument (JASCO, Japan). A Waters 1525 HPLC system (Waters, USA) equipped with Waters Xbrige series C18 chromatographic columns (4.6 mm × 250 mm and 19 mm × 250 mm, 5 μm) were used for liquid phase separation. Both the column chromatography silica gel (200-300 mesh) and thin layer chromatography silica gel plates were produced by Shanxi Nuotai Silica Gel Reagent Factory. The reverse filling material (20-45 mm, Fuji Silysia Chemical, Japan) was RP-18 silicone. MPLC was

conducted via an RUIHE (China) pump system equipped with RP-18 silica gel-packed glass columns (26 mm× 460 mm and 15 mm × 230 mm, respectively). Pharmacia Sephadex LH-20 gel material was manufactured by the Sweden Amersham Biosciences Company. The colorants used were sulfuric acid-ethanol and sulfuric acid-vanillin.