

Supporting Information

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A New Lignan from the Herbaceous Stems of *Ephedra intermedia* Schrenket C. A. Meyer.

Xiling Fan ^{1,2}, Yangang Cao ^{1,2}, Mengnan Zeng ^{1,2}, Ru Wang ^{1,2}, Yanling Liu ^{1,2}, Chen Xu ^{1,2}, Xinyi Ma ^{1,2}, Yingjie Ren ^{1,2}, He Chen ^{1,2}, Xiangda Li ^{1,2}, Xiaoke Zheng ^{1,2*} and Weisheng Feng ^{1,2*}

¹School of Pharmacy, Henan University of Chinese Medicine, Zhengzhou 450046, China

²The Engineering and Technology Center for Chinese Medicine Development of Henan Province China, Zhengzhou 450046, China

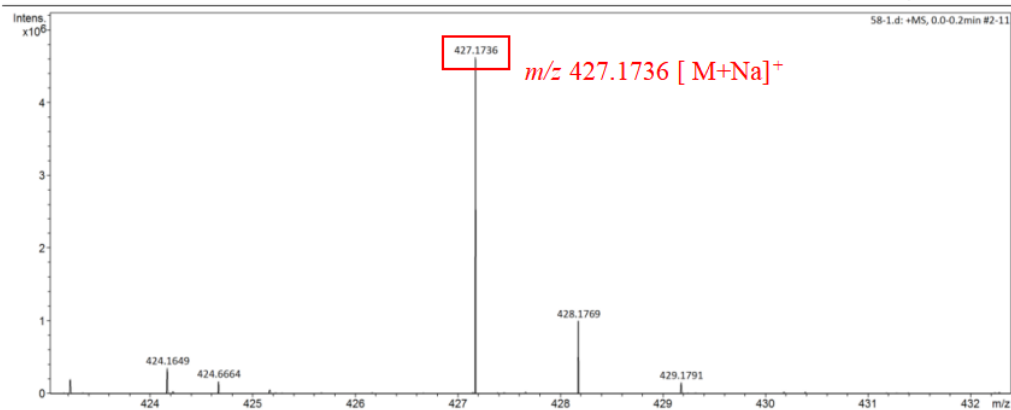
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Display Report

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Comment				

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Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 μ C



58-1.d
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by: ZMH
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Figure S1: HR-ESI-MS spectrum of compound 1

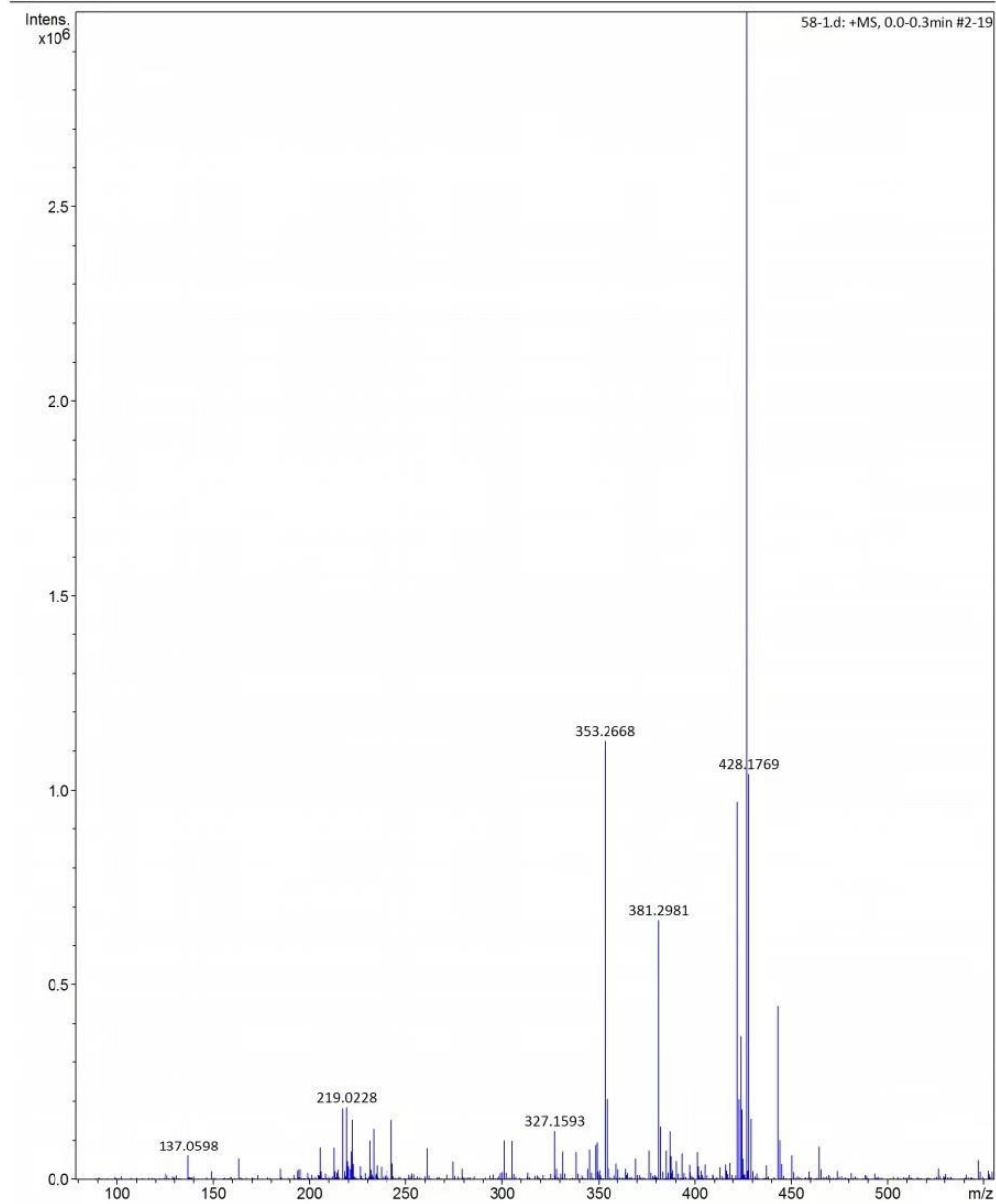
Generic Display Report

Analysis Info

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Comment

Acquisition Date 2022/5/31 22:07:14

Operator Demo User
Instrument maXis HD



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Figure S2: HR-ESI-MS spectrum of compound **1** (100-500 m/z)

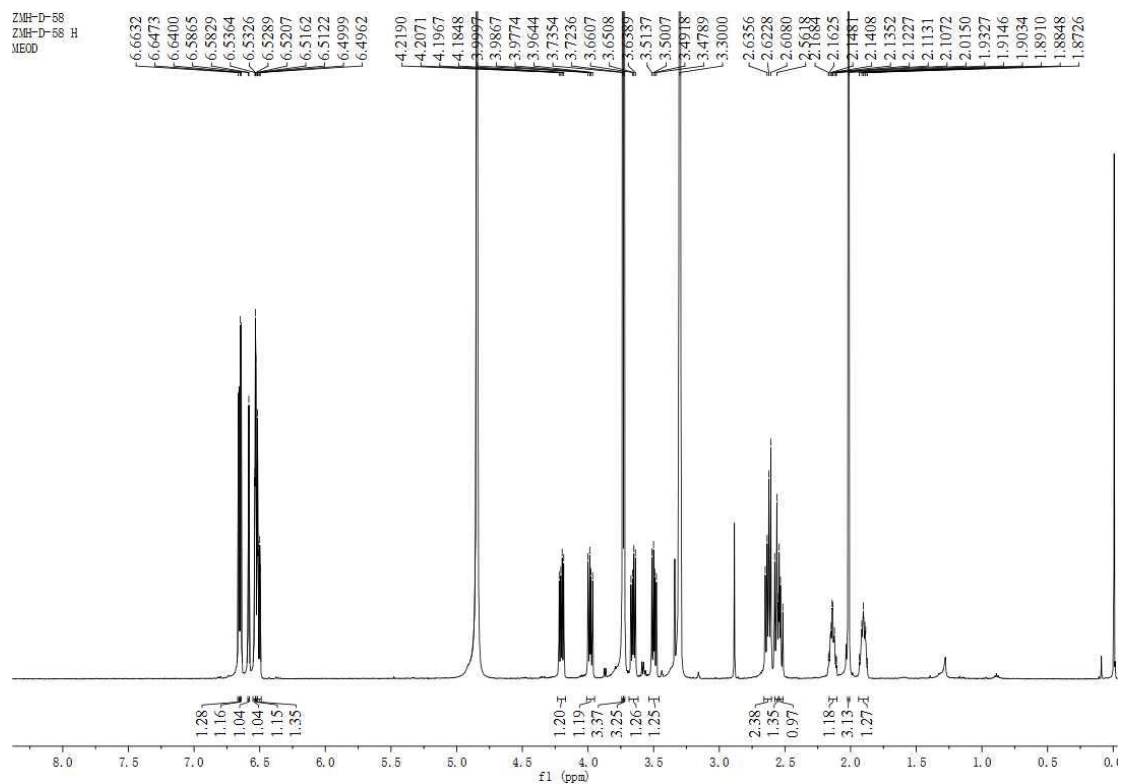


Figure S3: ^1H NMR spectrum (500MHz, CD_3OD) of **1**

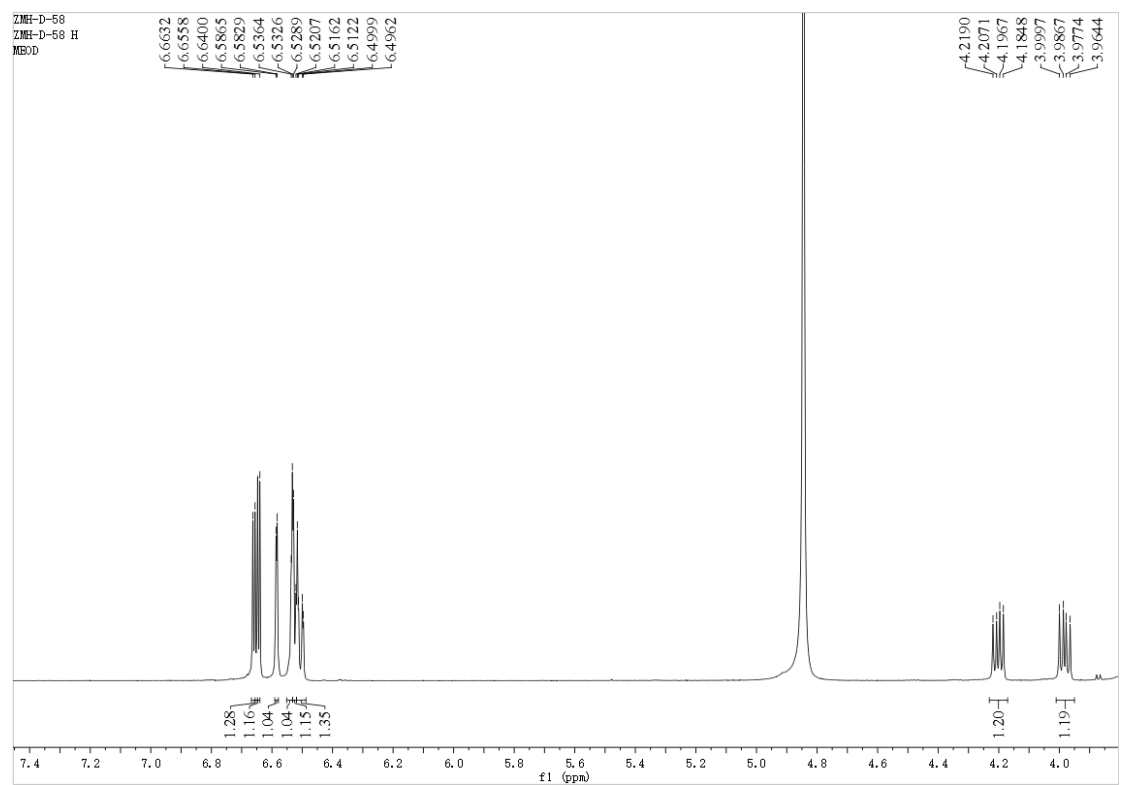


Figure S4: ^1H NMR spectrum (500MHz, CD_3OD) of **1** (From δ_{H} 3.9 ppm to δ_{H} 7.4 ppm)

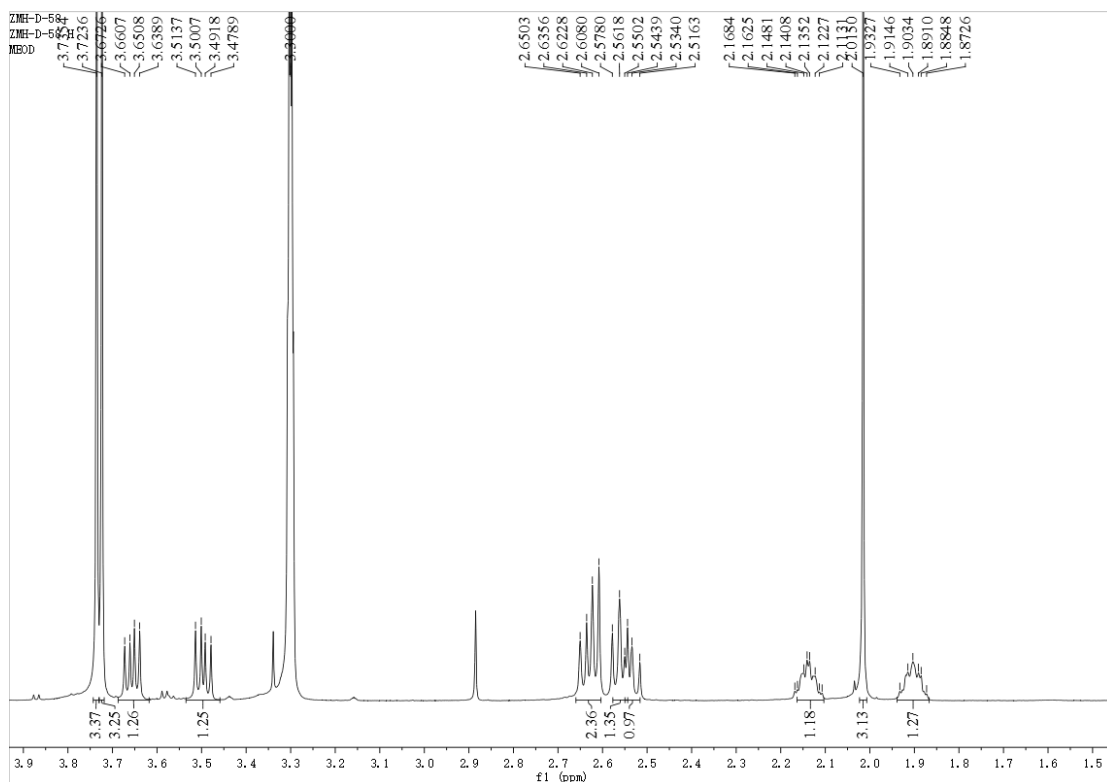


Figure S5: ^1H NMR spectrum (500MHz, CD_3OD) of **1** (From δ_{H} 1.5 ppm to δ_{H} 3.9 ppm)

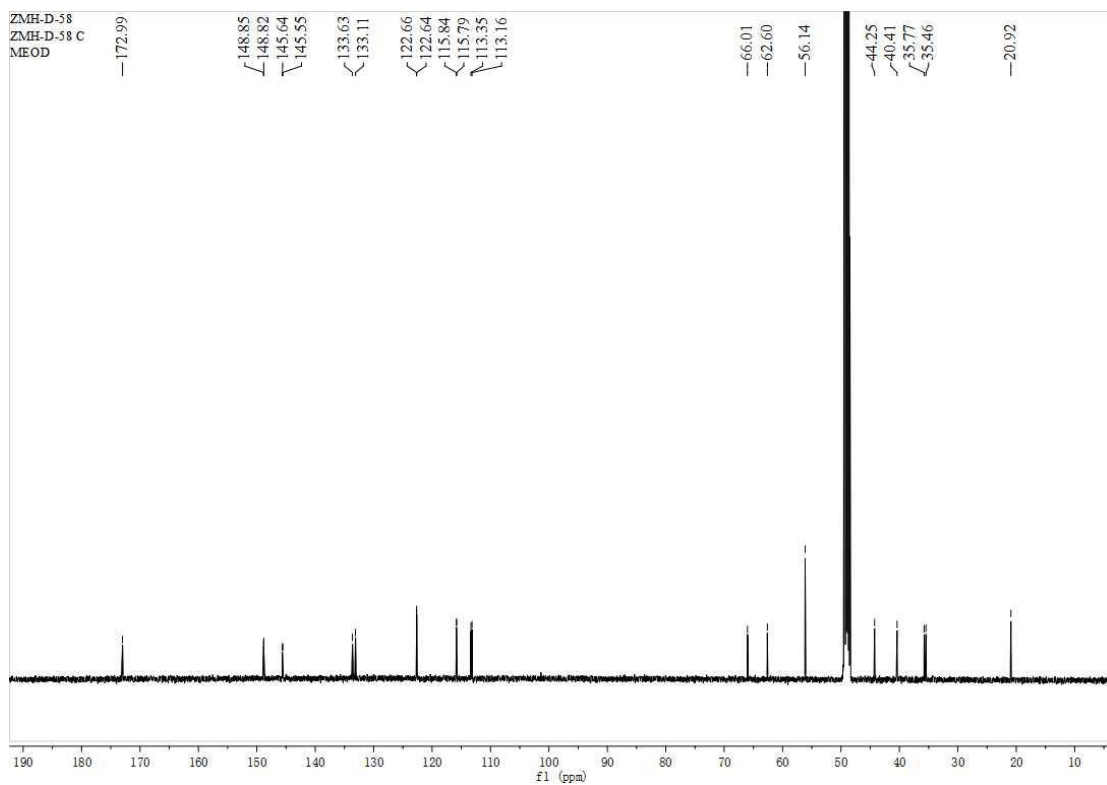


Figure S6: ^{13}C NMR spectrum (125MHz, CD_3OD) of **1**

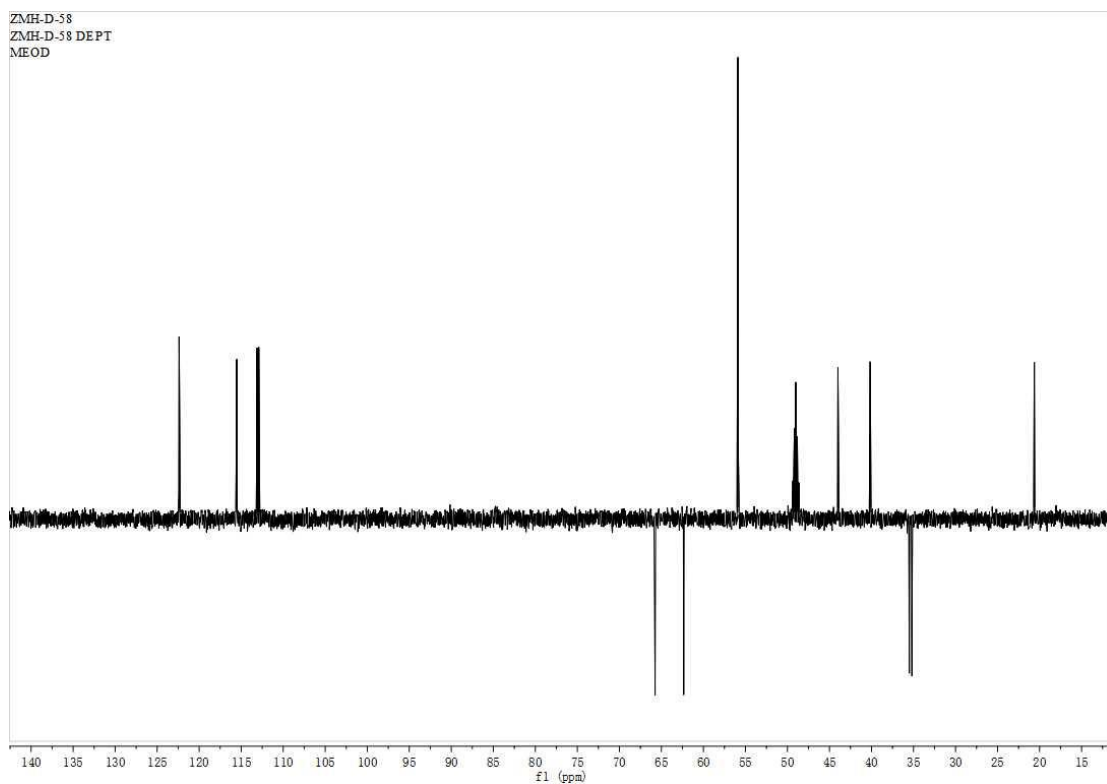


Figure S7: DEPT135 spectrum of **1**

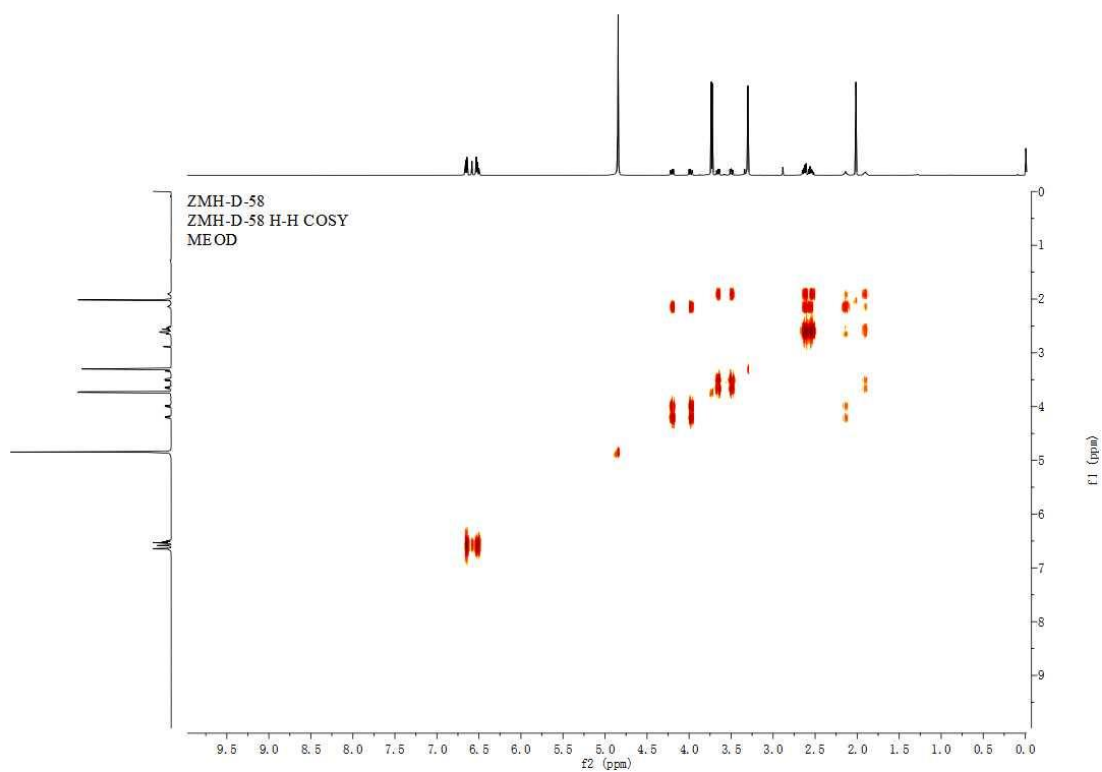


Figure S8: ^1H - ^1H COSY spectrum of **1**

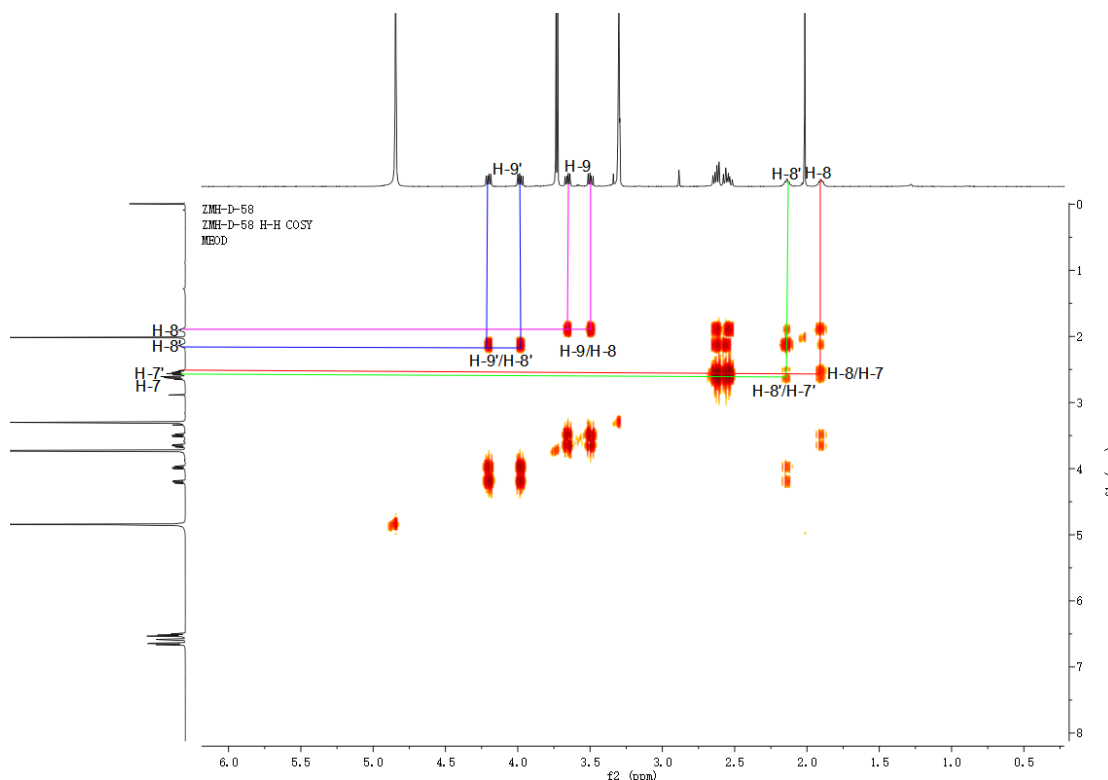


Figure S9: The enhanced ^1H - ^1H COSY spectrum of **1** (From δ_{H} 0.5 ppm to δ_{H} 6.0 ppm)

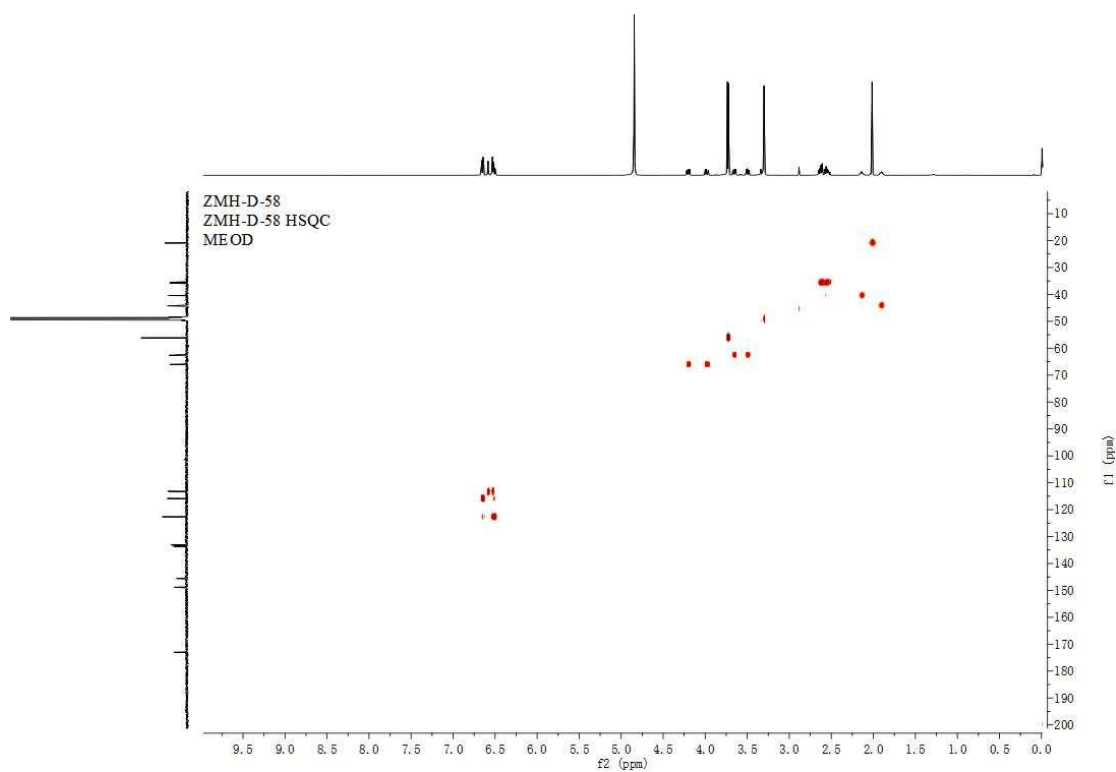


Figure S10: HSQC spectrum of **1**

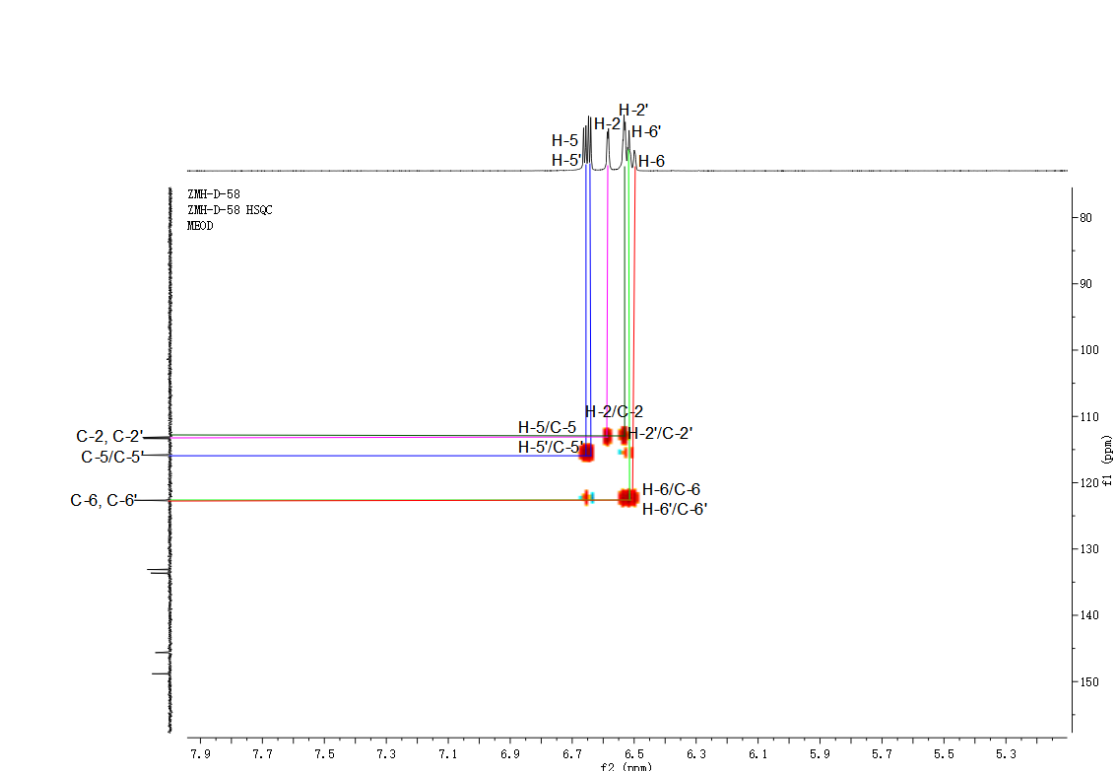


Figure S11: The enhanced HSQC spectrum of **1** (From δ_H 5.3 ppm to δ_H 7.9 ppm)

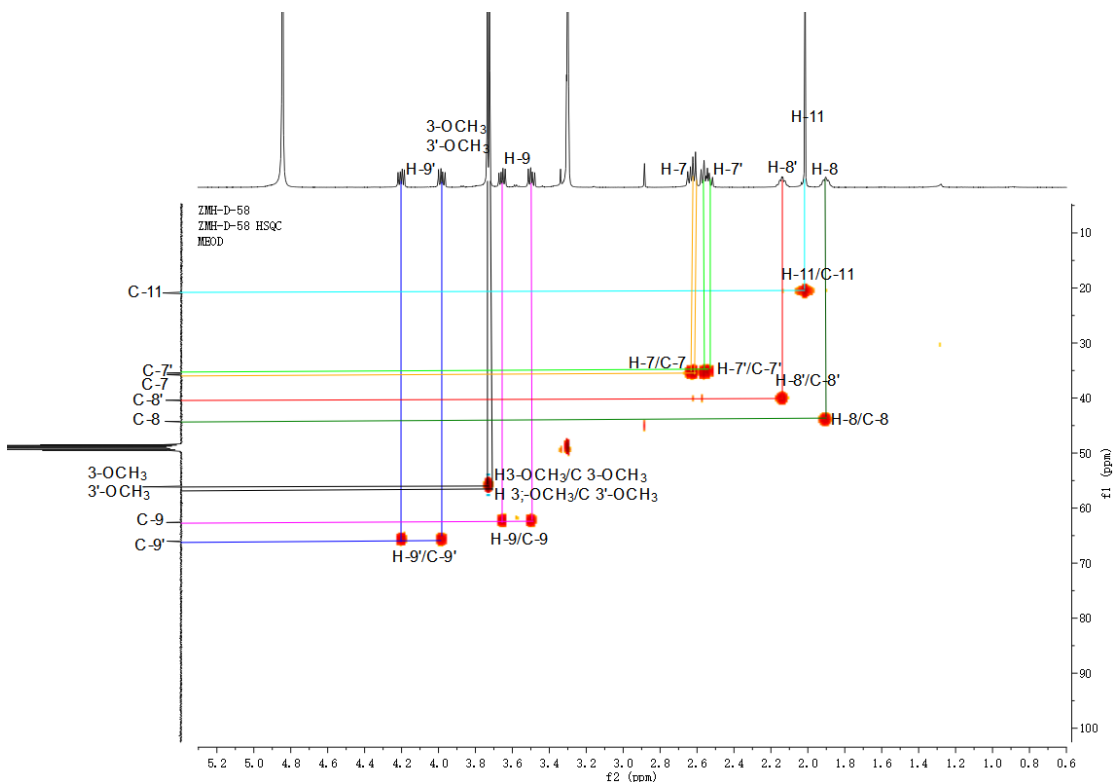


Figure S12: The enhanced HSQC spectrum of **1** (From δ_H 0.8 ppm to δ_H 5.2 ppm)

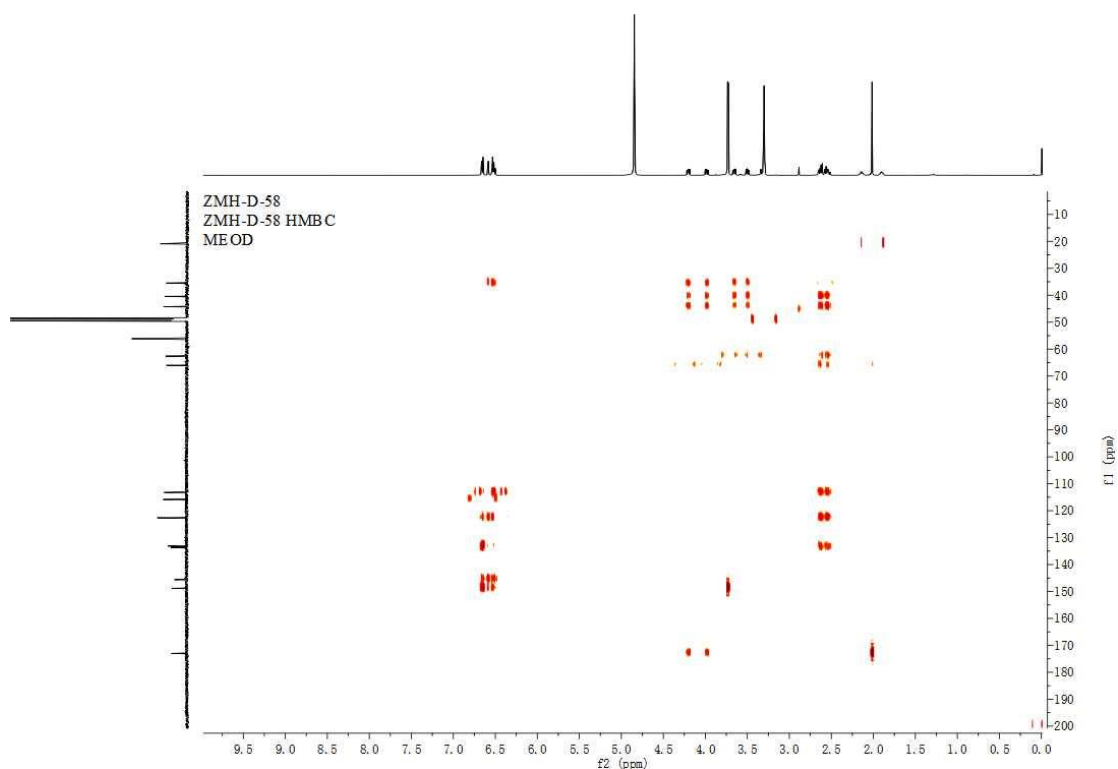


Figure S13: HMBC spectrum of **1**

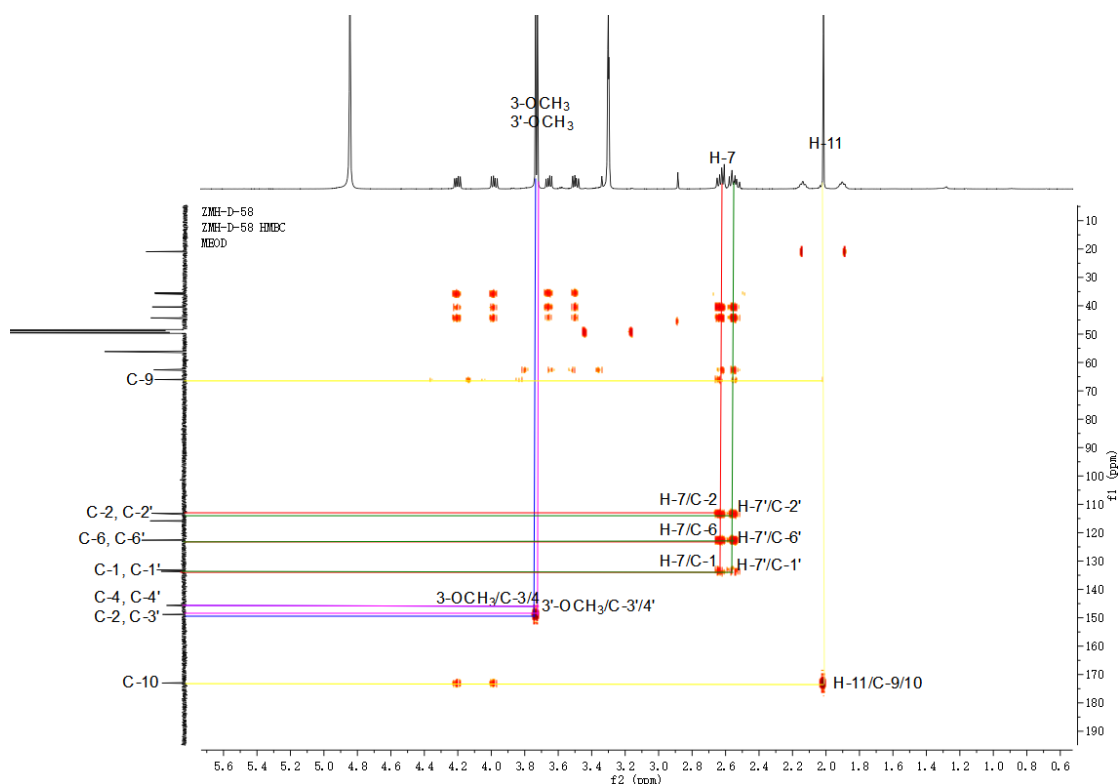


Figure S14: The enhanced HMBC spectrum of **1** (From δ_H 0.6 ppm to δ_H 5.6 ppm)

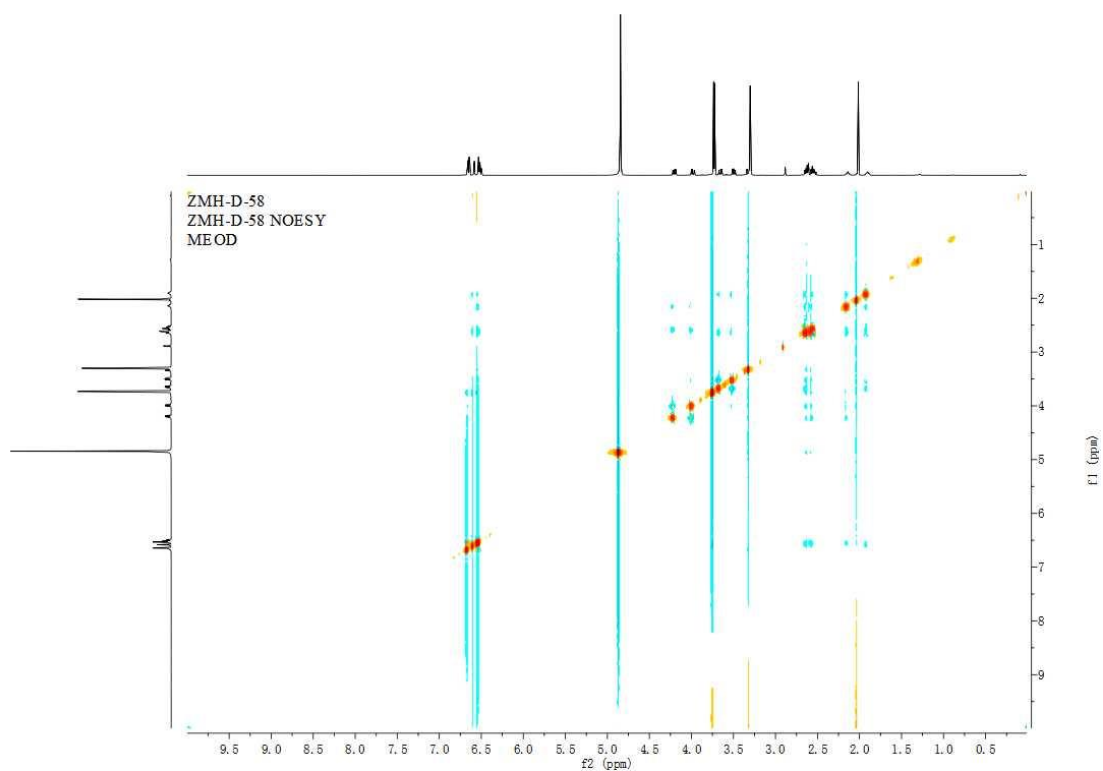
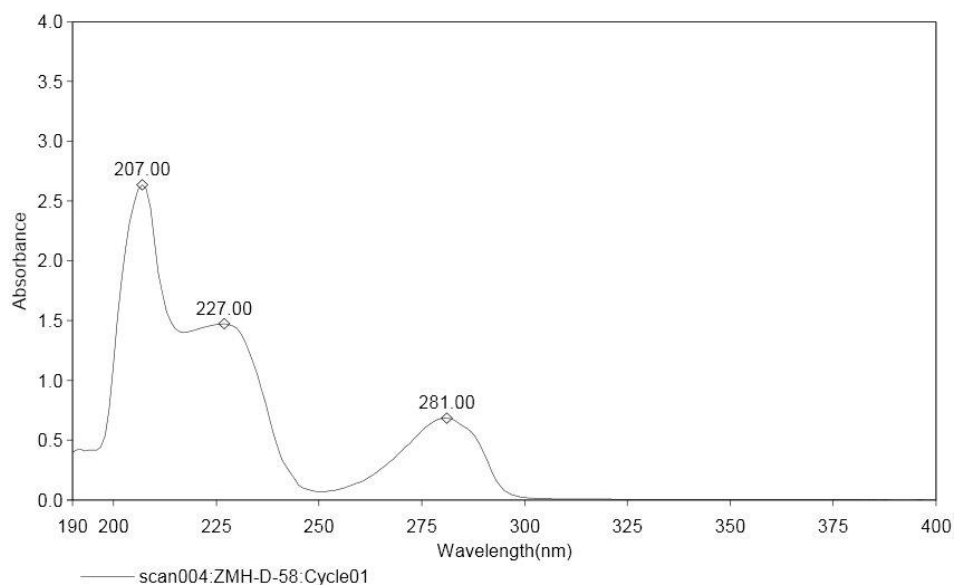


Figure S15: NOESY spectrum of **1**

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Operator Name (None Entered) Date of Report 2022/5/31
Department (None Entered) Time of Report 22:00:54下午
Organization (None Entered)
Information (None Entered)

Scan Graph



Results Table - scan004,ZMH-D-58,Cycle01

nm	A	Peak Pick Method
207.00	2.635	Find 8 Peaks Above -3.0000 A
227.00	1.472	Start Wavelength190.00 nm
281.00	.684	Stop Wavelength400.00 nm
		Sort By Wavelength
Sensitivity	Medium	

Figure S16: UV spectrum of 1

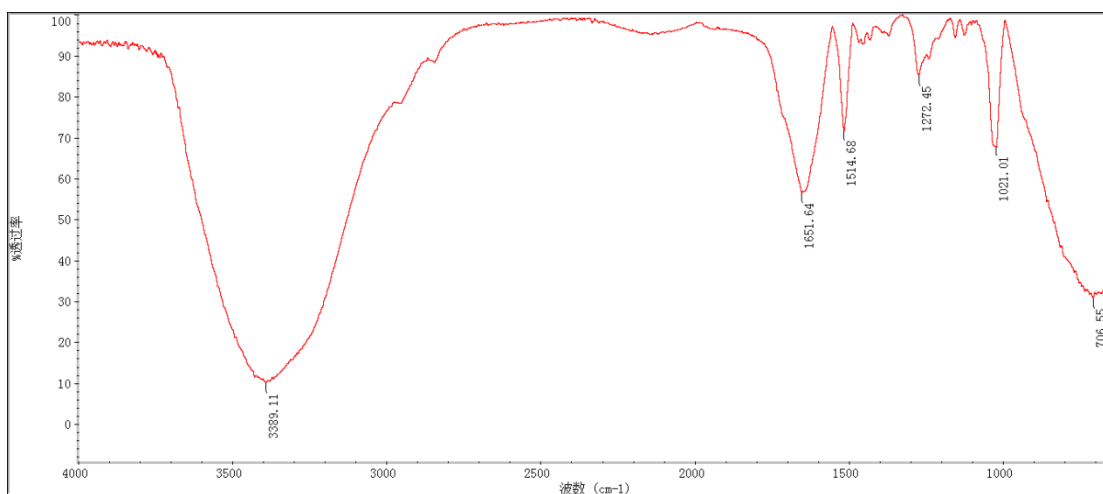


Figure S17: IR spectrum of 1
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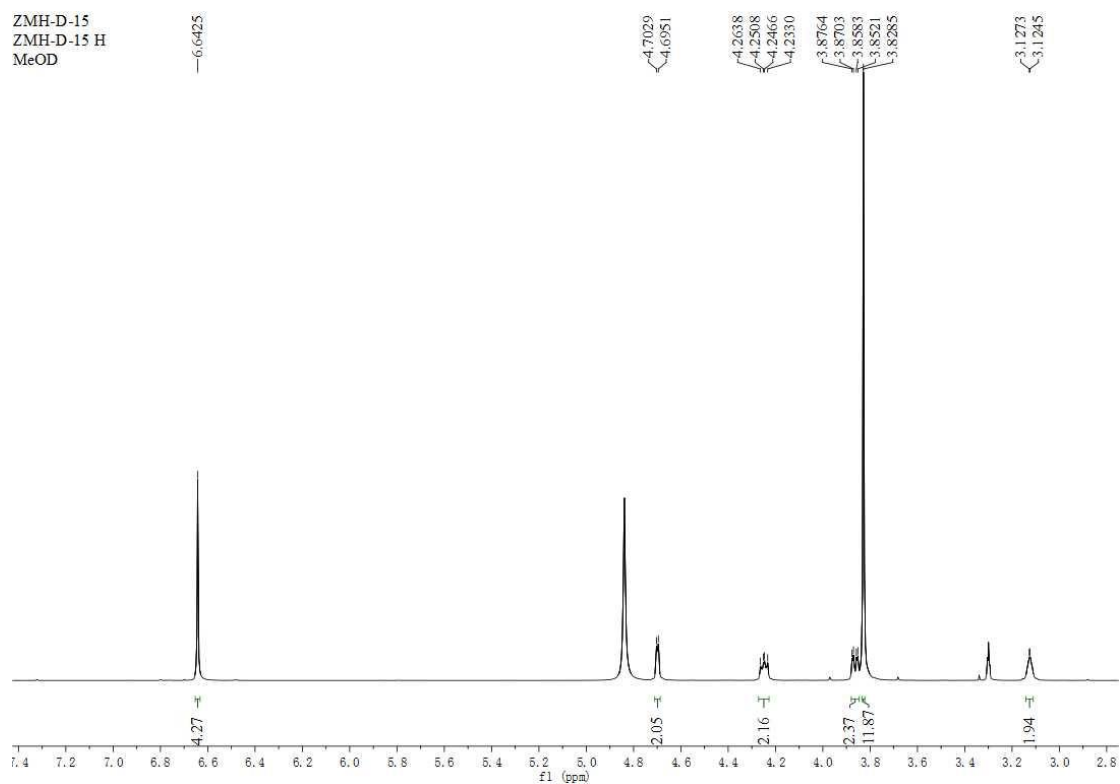


Figure S18: ^1H NMR spectrum (500MHz, CD_3OD) of **2**

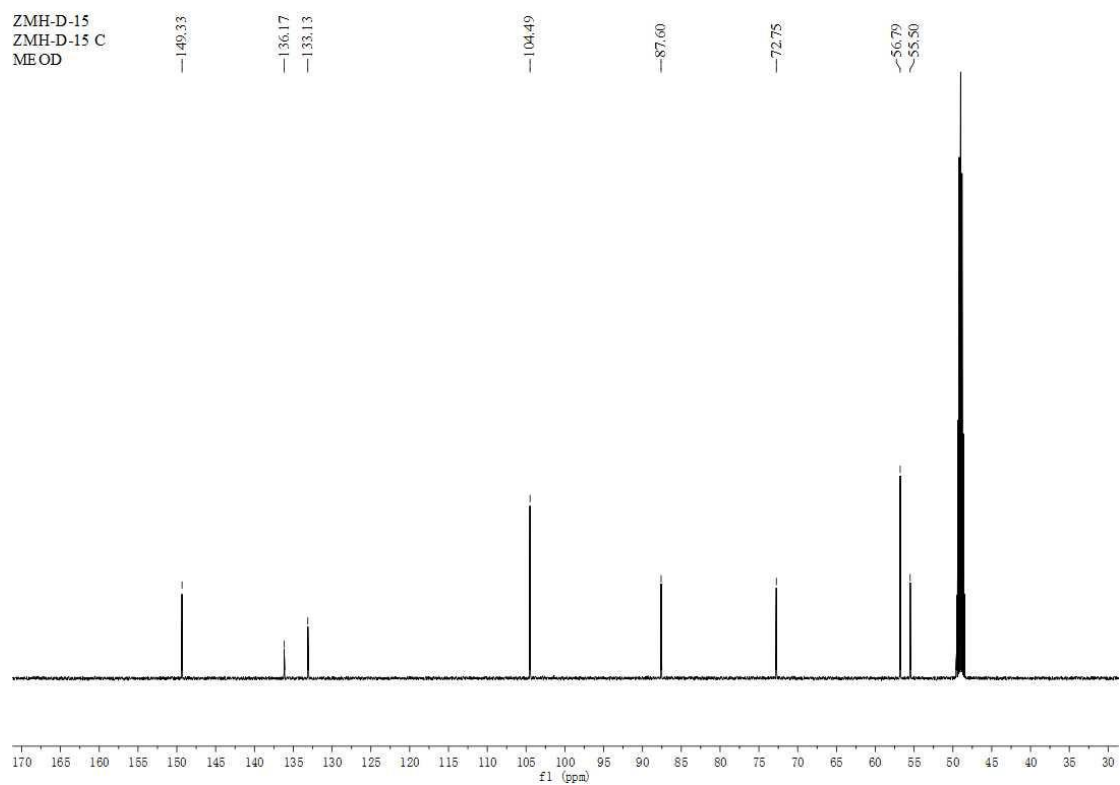


Figure S19: ^{13}C NMR spectrum (125MHz, CD_3OD) of **2**

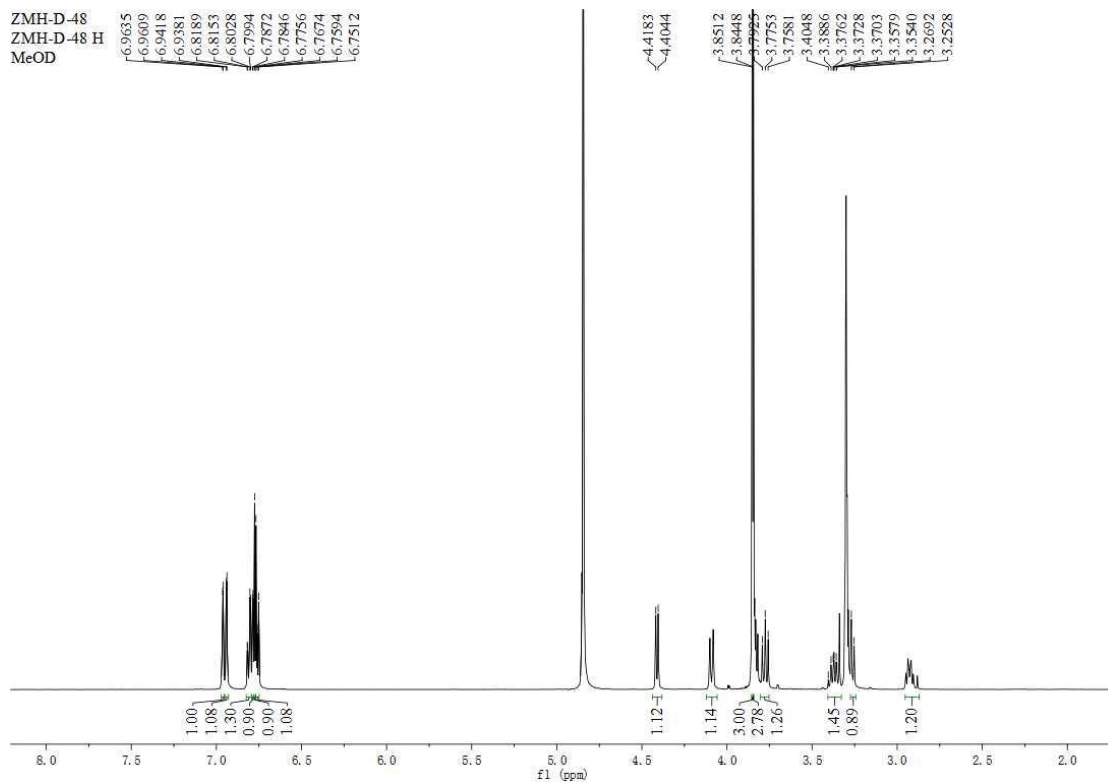


Figure S20: ^1H NMR spectrum (500MHz, CD_3OD) of **3**

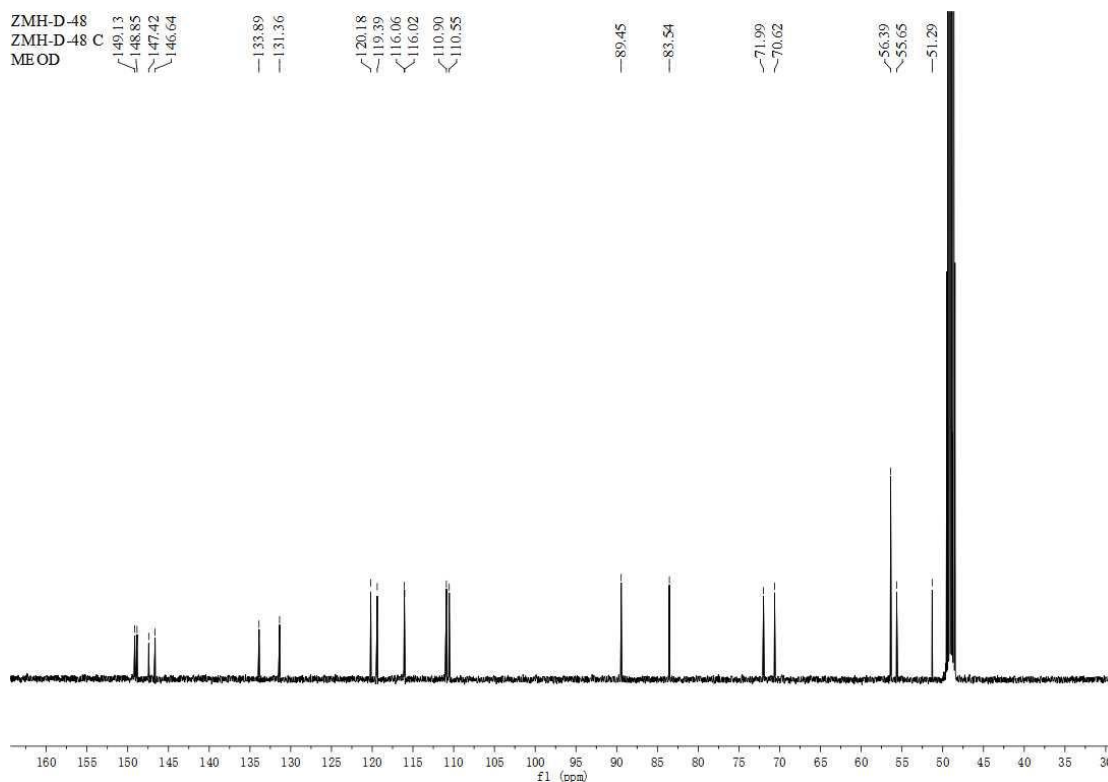


Figure S21: ^{13}C NMR spectrum (125MHz, CD_3OD) of **3**

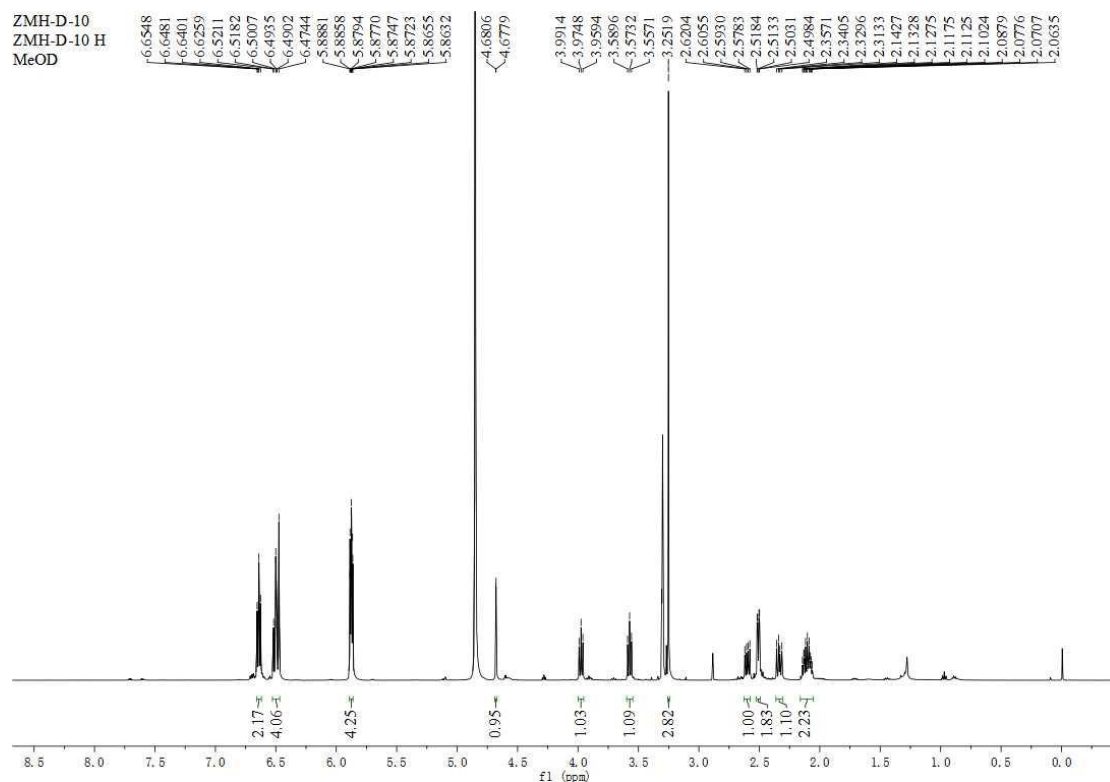


Figure S22: ^1H NMR spectrum (500MHz, CD_3OD) of **4**

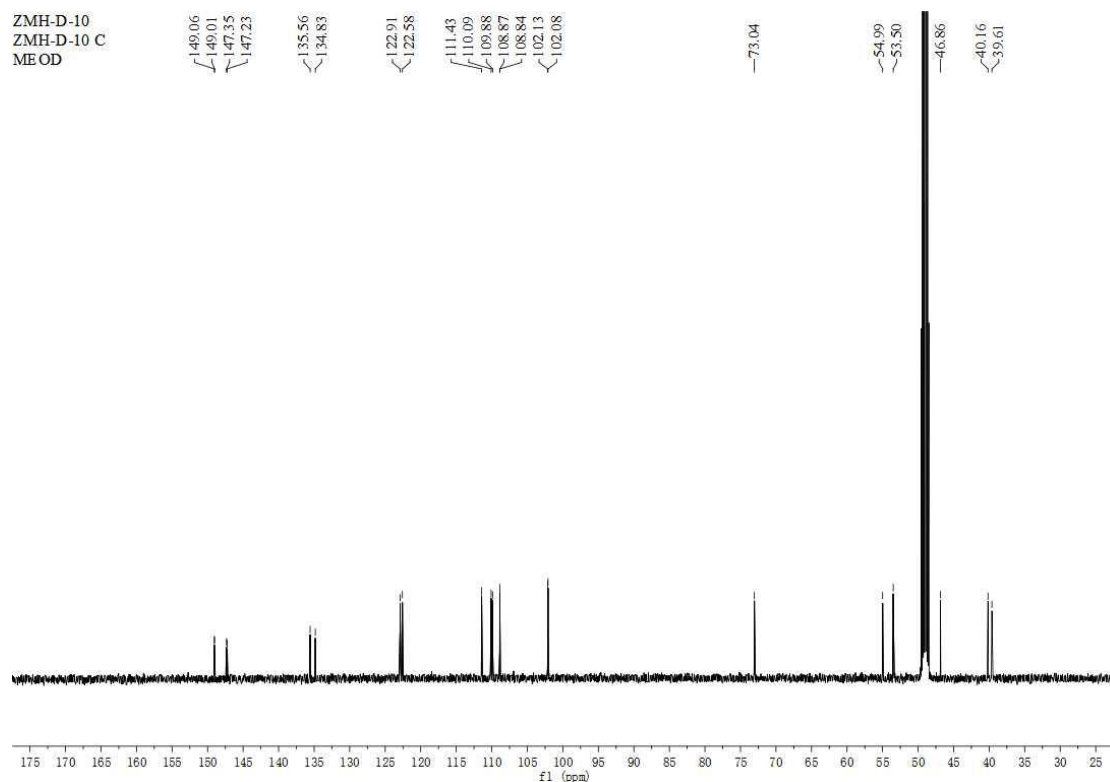


Figure S23: ^{13}C NMR spectrum (125MHz, CD_3OD) of **4**

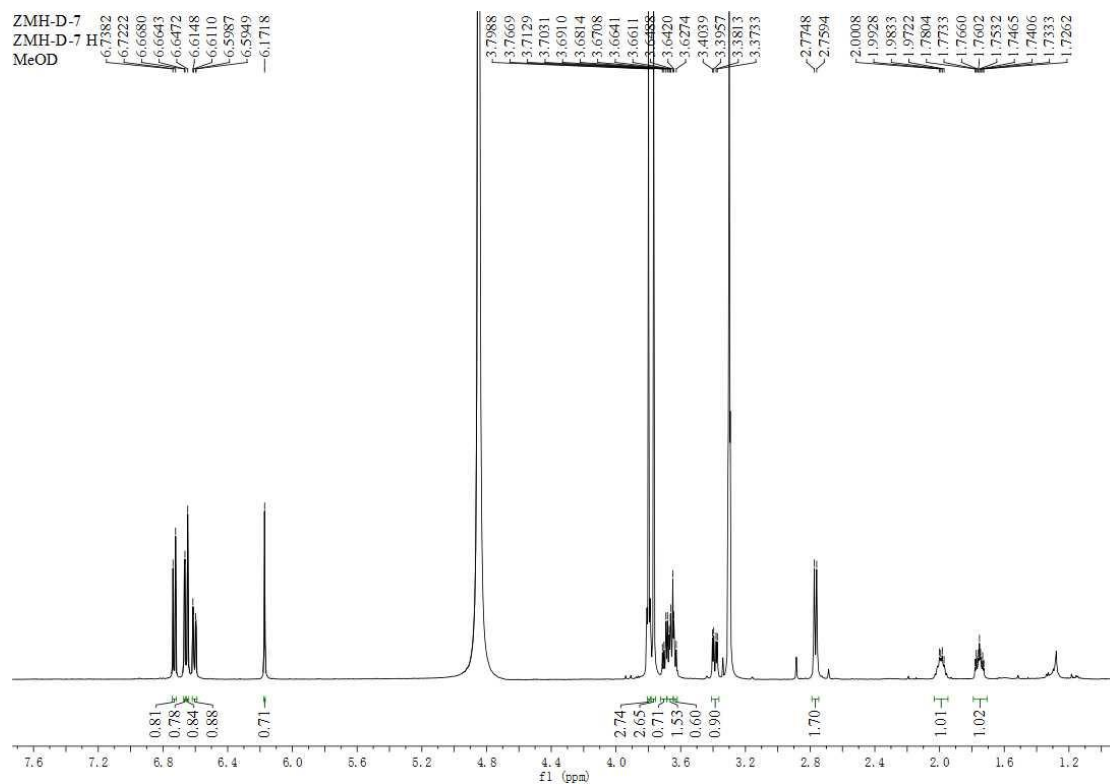


Figure S24: ^1H NMR spectrum (500MHz, CD_3OD) of **5**

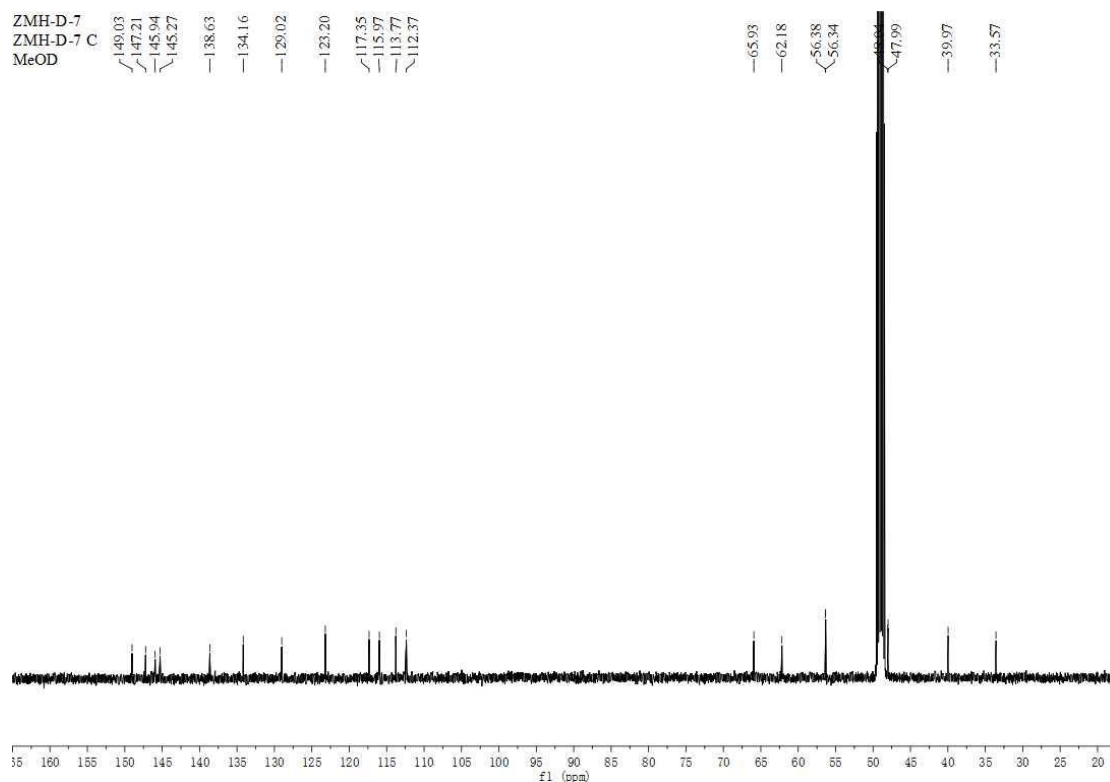


Figure S25: ^{13}C NMR spectrum (125MHz, CD_3OD) of **5**

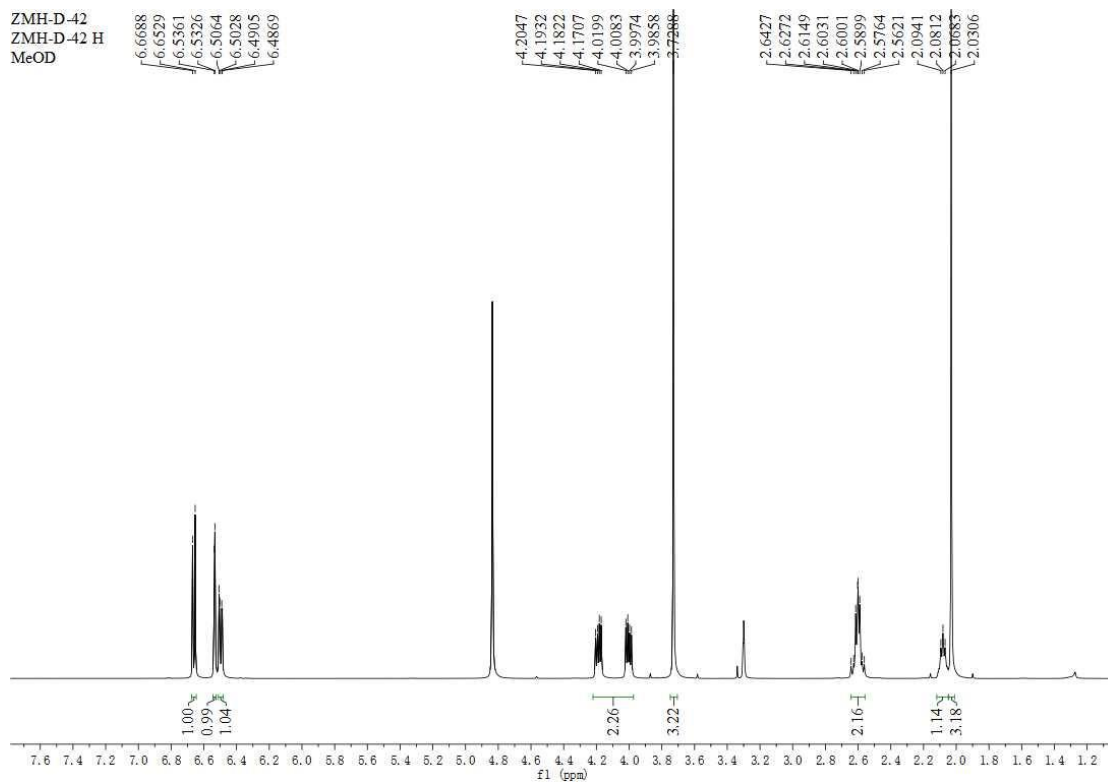


Figure S26: ^1H NMR spectrum (500MHz, CD_3OD) of **6**

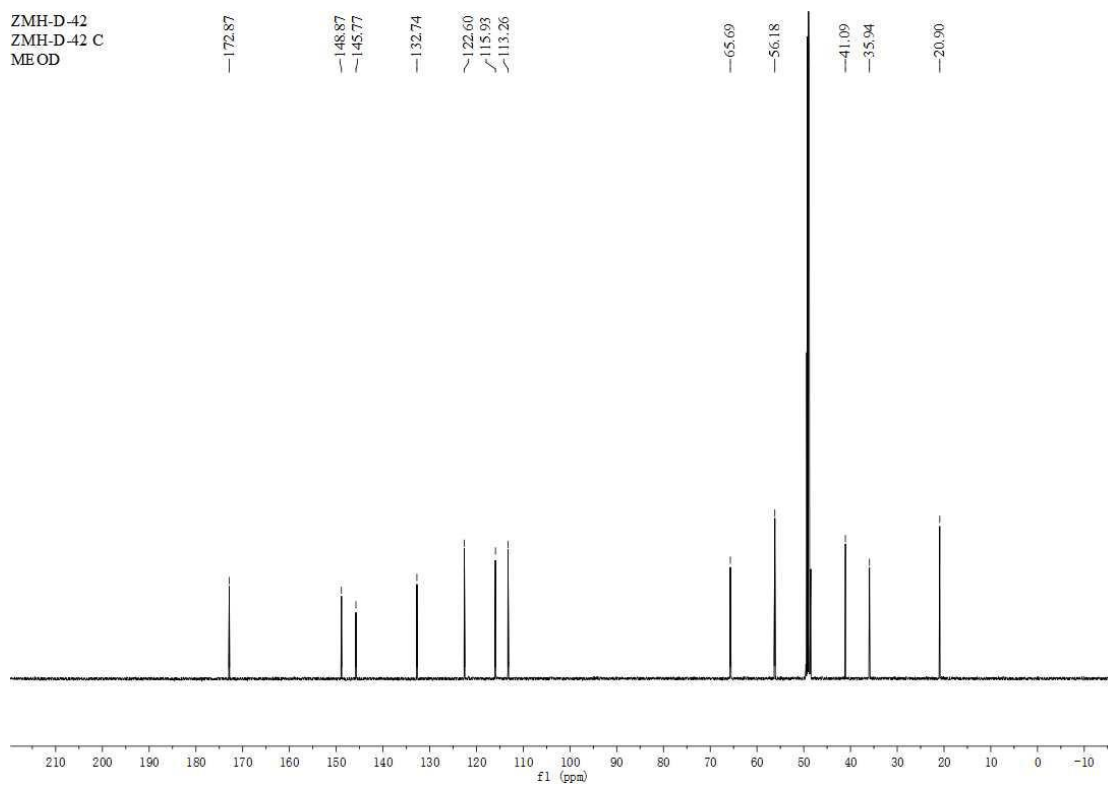


Figure S27: ^{13}C NMR spectrum (125MHz, CD_3OD) of **6**

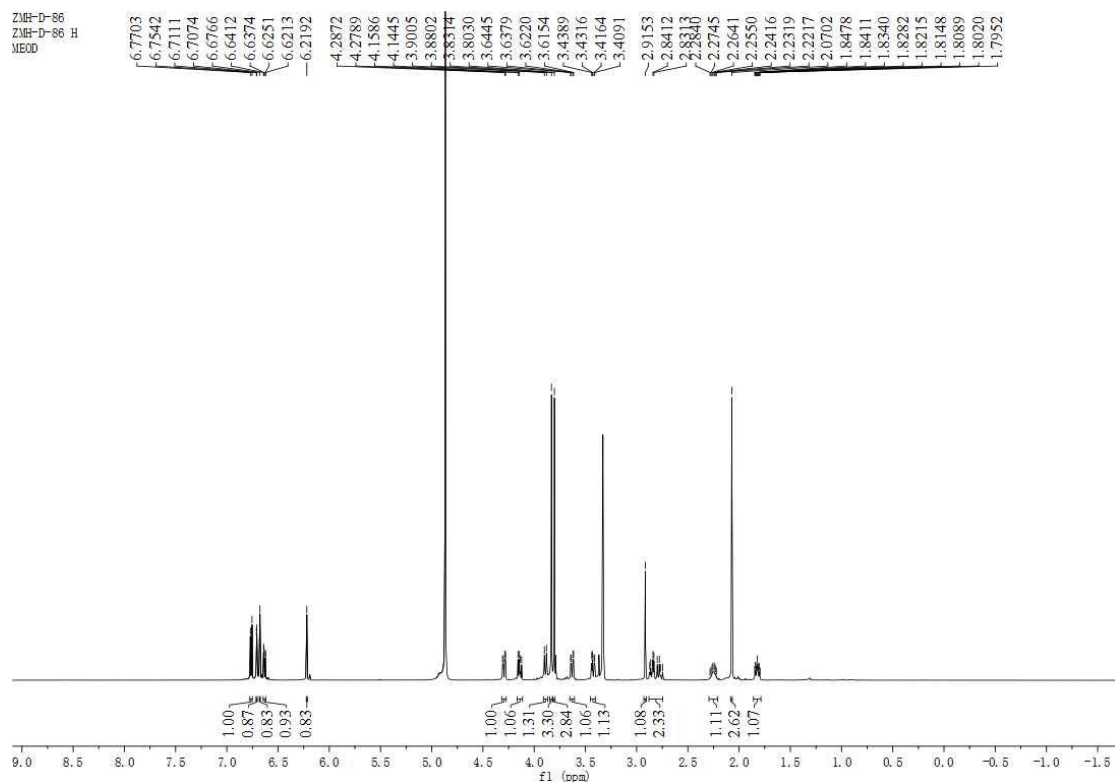


Figure S28: ^1H NMR spectrum (500MHz, CD_3OD) of 7

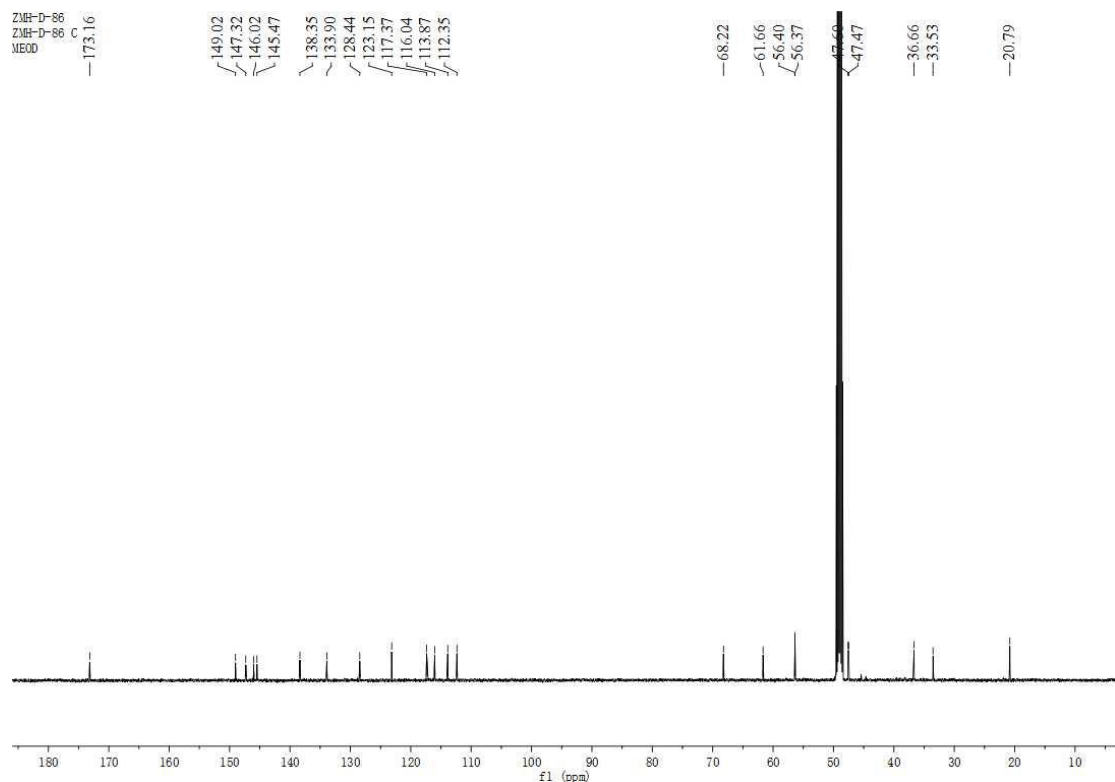


Figure S29: ^{13}C NMR spectrum (125MHz, CD_3OD) of 7

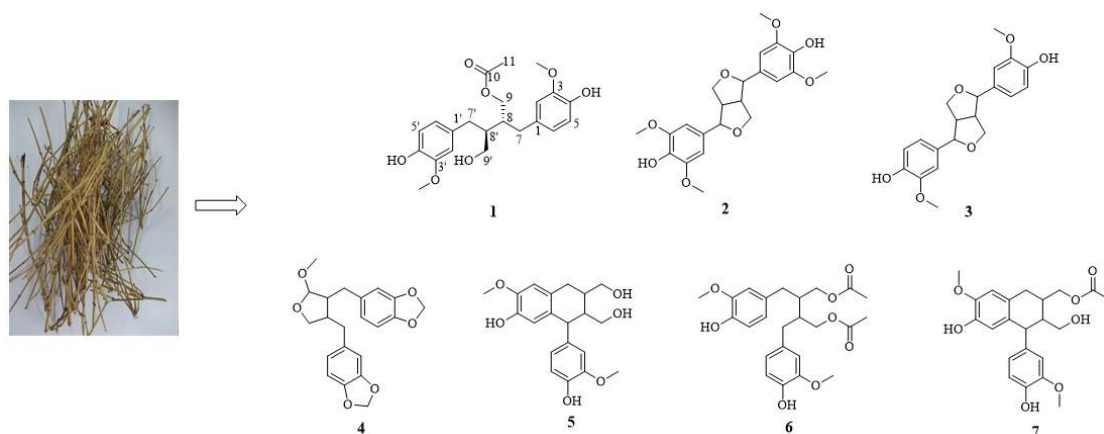


Figure S30: The structures of compounds **1–7**

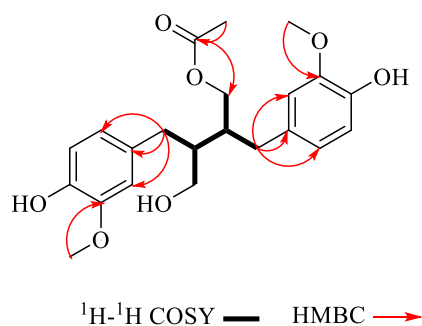


Figure S31: The key $^1\text{H}-^1\text{H}$ COSY, HMBC correlations of compounds **1**

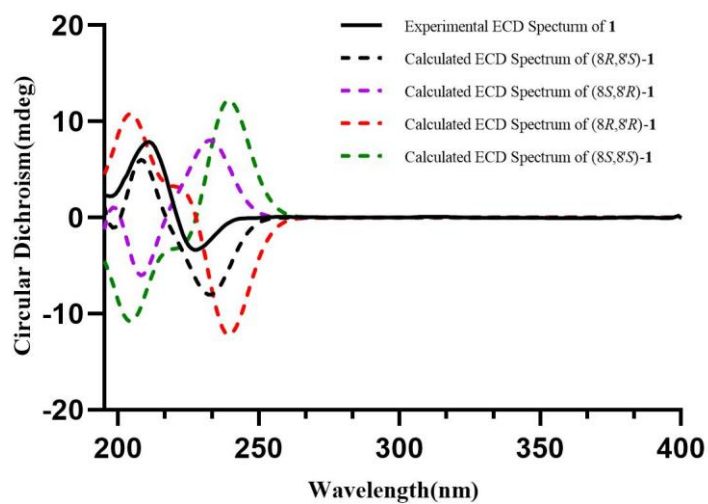


Figure S32: Experimental and calculated ECD spectra of compound **1**

Table 1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data for compound **1** (CD_3OD , δ in ppm, J in Hz)

Position	δ_{C}	δ_{H}
1	133.6	
2	113.4	6.58 (1H, <i>d</i> , 1.8)
3	148.9	
4	145.6	
5	115.8	6.65 (1H, <i>d</i> , 8.0)
6	122.7	6.51 (1H, <i>dd</i> , 8.0, 1.8)
7	35.8	2.64 (1H, <i>dd</i> , 13.8, 7.4) 2.62 (1H, <i>dd</i> , 13.8, 7.4)
8	44.3	1.90 (1H, <i>m</i>)
9	66.0	3.66 (1H, <i>dd</i> , 10.9, 5.9) 3.50 (1H, <i>dd</i> , 10.9, 6.5)
10	173.0	
11	20.9	2.02 (3H, <i>s</i>)
1'	133.1	
2'	113.2	6.53 (1H, <i>d</i> , 1.9)
3'	148.8	
4'	145.6	
5'	115.8	6.66 (1H, <i>d</i> , 7.9)
6'	122.6	6.52 (1H, <i>dd</i> , 7.9, 1.9)
7'	35.5	2.56 (1H, <i>dd</i> , 11.4, 5.6) 2.54 (1H, <i>dd</i> , 11.0, 6.0)
8'	40.4	2.14 (1H, <i>m</i>)
9'	62.6	4.20 (1H, <i>dd</i> , 11.2, 6.0) 3.98 (1H, <i>dd</i> , 11.2, 6.5)
3-OCH ₃	56.1	3.73 (3H, <i>s</i>)
3'-OCH ₃	56.1	3.72 (3H, <i>s</i>)

Figure S33: ^1H (500 MHz) and ^{13}C (125 MHz) NMR data for compound **1** (CD_3OD , δ in ppm, J in Hz)

Table 2. The effects of compounds 1–7 on BEAS-2B cell by TGF- β 1

Group	Dose (μ M)	cell viability (%)
CON	---	100.0 \pm 3.6**
TGF- β 1	1 ng/mL	90.7 \pm 1.9
1	10	97.9 \pm 3.6**
2	10	98.4 \pm 1.0**
3	10	94.4 \pm 2.3
4	10	96.0 \pm 1.1**
5	10	94.2 \pm 4.4
6	10	99.6 \pm 1.9**
7	10	94.4 \pm 2.2

(** $P < 0.001$ compared with the TGF- β 1 group)

Figure S34: The effects of compounds 1–7 on BEAS-2B cell by TGF- β 1

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Patent
Tags

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Markush
Molecular Formula
Property
Substance Identifier

REACTIONS
Reaction Structure

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Chemical Structure similarity

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Substances	Scores
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<input type="checkbox"/>	95-98
<input type="checkbox"/>	90-94
<input type="checkbox"/>	85-89
<input type="checkbox"/>	80-84
<input type="checkbox"/>	75-79
<input type="checkbox"/>	70-74
<input type="checkbox"/>	65-69
<input type="checkbox"/>	0-64 (least similar)

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SUBSTANCES

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Sort by: Similarity Scores

0 of 90 Substances Selected

Score	Substance	Chemical Structure	Key Physical Properties
Score: 99 3. 848844-77.9	C ₂₂ H ₃₁ O ₇ 1,4-Butanediol, 2,3-bis[(4-hydroxy-3-methoxyphenyl)methyl]-1-acetate, (2R,3R)	Absolute stereochemistry.	Key Physical Properties
Score: 98 2. 1612227-17.4	C ₂₂ H ₃₁ O ₈ Benzoinbutanal, 4-hydroxy-β-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-γ-methyl-, 1-acetate, (S,S)-	Rotation (-), Absolute stereochemistry.	Key Physical Properties
Score: 98 3. 2123479-60.5	C ₂₂ H ₃₁ O ₈ Benzoinbutanal, 4-hydroxy-β-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-γ-methyl-, 1-acetate, (S,S)-	Absolute stereochemistry.	Key Physical Properties
Score: 98 4. 2772946-50.4	C ₂₂ H ₃₁ O ₈ Benzoinbutanal, 4-hydroxy-β-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-γ-methyl-, 1-acetate, (S,S)-	Relative stereochemistry.	Key Physical Properties
Score: 97 5. 119030-71.6	C ₂₂ H ₃₁ O ₇ 1,4-Butanediol, 2-[[3,4-dimethoxyphenyl)methyl]-3-[(4-hydroxy-3-methoxyphenyl)methyl]-1-acetate, [(R*,R*)] (9CI)	Absolute stereochemistry.	Key Physical Properties
Score: 97 6. 119030-72.2	C ₂₂ H ₃₁ O ₇ 1,4-Butanediol, 2-[[3,4-dimethoxyphenyl)methyl]-3-[(4-hydroxy-3-methoxyphenyl)methyl]-1-acetate, (2R,3R) (9CI)	Absolute stereochemistry.	Key Physical Properties

Figure S35: The Scifinder similarity report for new compound 1

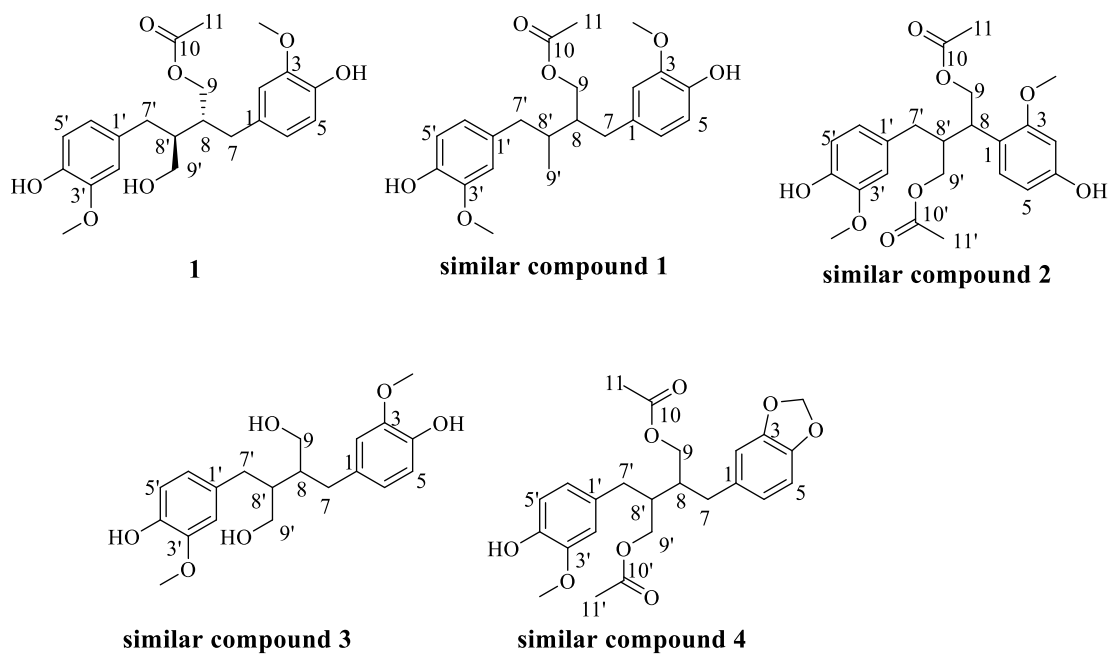


Figure S36: The structures similar to compound 1

Table S1: The ¹H NMR data for compound **1** and four similar compounds

NO	1 (CD ₃ OD)	similar compound 1 (CDCl ₃)	similar compound 2 (CDCl ₃)	similar compound 3 (Acetone- <i>d</i> ₆)	similar compound 4 (CDCl ₃)
1	-	-	-	-	-
2	6.58 (1H, <i>d</i> , 1.8)	6.47–6.48 (1H, <i>m</i>)	6.40 (1H, <i>d</i> , 2.0)	6.71 (1H, <i>d</i> , 1.6)	6.40–6.62 (1H, <i>m</i>)
3	-	-	-	-	-
4	-	-	-	-	-
5	6.65 (1H, <i>d</i> , 8.0)	6.79 (1H, <i>d</i> , 8.0)	6.70 (1H, <i>d</i> , 8.0)	6.68 (1H, <i>d</i> , 8.0)	6.81 (1H, <i>d</i> , 8.8)
6	6.51 (1H, <i>dd</i> , 8.0, 1.8)	6.55 (1H, <i>dd</i> , 8.0, 2.0)	6.50 (1H, <i>dd</i> , 8.0, 2.0)	6.60 (1H, <i>dd</i> , 1.6, 8.0)	6.40–6.62 (1H, <i>m</i>)
7	2.64 (1H, <i>dd</i> , 13.8, 7.4) 2.62 (1H, <i>dd</i> , 13.8, 7.4)	2.62 (1H, <i>dd</i> , 13.9, 6.5) 2.52 (1H, <i>dd</i> , 13.9, 8.2)	2.61 (2H, <i>d</i> , 7.2)	2.04 (2H, <i>t</i>)	2.61 (2H, <i>d</i> , 6.6)
8	1.90 (1H, <i>m</i>)	1.83 (1H, <i>dq</i> , 7.1, 3.1)	1.90–2.15 (1H, <i>m</i>)	1.90 (1H, <i>m</i>)	2.0–2.2 (1H, <i>m</i>)
9	3.66 (1H, <i>dd</i> , 10.9, 5.9) 3.50 (1H, <i>dd</i> , 10.9, 6.5)	4.19 (1H, <i>dd</i> , 11.2, 5.8) 4.00 (1H, <i>dd</i> , 11.2, 6.7)	4.23 (1H, <i>dd</i> , 11.4, 5.6) 3.95 (1H, <i>dd</i> , 11.4, 5.6)	3.66 (1H, <i>dd</i> , 11.2, 2.8) 3.52 (1H, <i>dd</i> , 11.2, 2.8)	4.17 (1H, <i>dd</i> , 11.2, 5.3) 4.00 (1H, <i>dd</i> , 11.2, 5.3)
10	-	-	-	-	-
11	2.02 (3H, <i>s</i>)	2.06 (3H, <i>s</i>)	2.06 (3H, <i>s</i>)	-	2.06 (3H, <i>s</i>)
1'	-	-	-	-	-
2'	6.53 (1H, <i>d</i> , 1.9)	6.47–6.48 (1H, <i>m</i>)	6.40 (1H, <i>d</i> , 2.0)	6.71 (1H, <i>d</i> , 1.6)	6.40–6.62 (1H, <i>m</i>)
3'	-	-	-	-	-
4'	-	-	-	-	-
5'	6.66 (1H, <i>d</i> , 7.9)	6.80 (1H, <i>d</i> , 7.9)	6.70 (1H, <i>d</i> , 8.0)	6.68 (1H, <i>d</i> , 8.0)	6.70 (1H, <i>d</i> , 8.4)
6'	6.52 (1H, <i>dd</i> , 7.9, 1.9)	6.57 (1H, <i>dd</i> , 7.9, 1.9)	6.50 (1H, <i>dd</i> , 8.0, 2.0)	6.60 (1H, <i>dd</i> , 1.6, 8.0)	6.40–6.62 (1H, <i>m</i>)
7'	2.56 (1H, <i>dd</i> , 11.4, 5.6) 2.54 (1H, <i>dd</i> , 11.0, 6.0)	2.61 (1H, <i>dd</i> , 13.7, 6.9) 2.40 (1H, <i>dd</i> , 13.7, 7.8)	2.61 (2H, <i>d</i> , 7.2)	2.04 (2H, <i>t</i>)	2.61 (2H, <i>d</i> , 6.6)
8'	2.14 (1H, <i>m</i>)	1.94 (1H, <i>m</i>)	1.90–2.15 (1H, <i>m</i>)	1.90 (1H, <i>m</i>)	2.0–2.2 (1H, <i>m</i>)
9'	4.20 (1H, <i>dd</i> , 11.2, 6.0) 3.98 (1H, <i>dd</i> , 11.2, 6.5)	0.91 (3H, <i>d</i> , 7.1)	4.23 (1H, <i>dd</i> , 11.4, 5.6) 3.95 (1H, <i>dd</i> , 11.4, 5.6)	3.66 (1H, <i>dd</i> , 11.2, 2.8) 3.52 (1H, <i>dd</i> , 11.2, 2.8)	4.17 (1H, <i>dd</i> , 11.2, 5.3) 4.00 (1H, <i>dd</i> , 11.2, 5.3)
10'	-	-	-	-	-
11'	-	-	2.06 (3H, <i>s</i>)	-	2.06 (3H, <i>s</i>)
3-OCH ₃	3.73 (3H, <i>s</i>)	3.79 (3H, <i>s</i>)	3.75 (3H, <i>s</i>)	3.75 (3H, <i>s</i>)	-
3'-OCH ₃	3.72 (3H, <i>s</i>)	3.78 (3H, <i>s</i>)	3.75 (3H, <i>s</i>)	3.75 (3H, <i>s</i>)	3.82 (3H, <i>s</i>)
4-OH	-	5.55 (1H, <i>s</i>)	5.40 (1H, <i>brs</i>)	-	5.50 (1H, <i>brs</i>)
4'-OH	-	5.53 (1H, <i>s</i>)	5.40 (1H, <i>brs</i>)	-	-
9-OH	-	-	-	3.31 (1H, <i>s</i>)	-
9'-OH	-	-	-	3.31 (1H, <i>s</i>)	-
-	-	-	-	-	5.92 (2H, <i>s</i>)
OCH ₂ O-	-	-	-	-	-

Table S2: The ^{13}C NMR data for compound **1** and four similar compounds

NO	1 (CD ₃ OD)	similar compound 1 (CDCl ₃)	similar compound 2 (CDCl ₃)	similar compound 3 (Acetone- <i>d</i> ₆)	similar compound 4 (CDCl ₃)
1	133.6	132.9	131.2	133.4	131.4
2	113.4	111.3	111.1	113.1	111.3
3	148.9	146.4	146.4	147.9	146.5
4	145.6	143.8	143.7	145.2	144.0
5	115.8	114.1	114.1	115.2	114.3
6	122.7	121.7	121.4	122.2	121.6
7	35.8	35.4	34.7	35.8	34.9
8	44.3	41.9	39.3	44.5	39.8
9	66.0	64.7	64.2	60.8	64.4
10	173.0	171.3	170.9	-	171.0
11	20.9	21.1	20.7	-	21.0
1'	133.1	132.2	131.2	133.4	133.5
2'	113.2	111.2	111.1	113.1	108.1
3'	148.8	146.3	146.4	147.9	147.7
4'	145.6	143.7	143.7	145.2	146.5
5'	115.8	114.0	114.1	115.2	109.2
6'	122.6	121.7	121.4	122.2	121.8
7'	35.5	35.0	34.7	35.8	34.9
8'	40.4	40.6	39.3	44.5	39.8
9'	62.6	15.2	64.2	60.8	64.4
10'	-	-	170.9	-	171.0
11'	-	-	20.7	-	21.0
3-OCH ₃	56.1	55.8	55.4	55.9	-
3'-OCH ₃	56.1	55.7	55.4	55.9	55.8
4-OH	-	-	-	-	-
4'-OH	-	-	-	-	-
9-OH	-	-	-	-	-
9'-OH	-	-	-	-	-
-	-	-	-	-	-
OCH ₂ O-	-	-	-	-	100.9