

Supporting Information

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A New Eremophilanolide from the Fresh Roots of

Rehmannia glutinosa

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Contents	Page
Figure S1: HR-ESI-MS spectrum of compound 1	3
Figure S2: ¹ H NMR spectrum (500MHz, CD ₃ OD) of 1	4
Figure S3: The enhanced ¹ H NMR spectrum (500MHz, CD ₃ OD) of 1	4
Figure S4: ¹³ C NMR spectrum (125MHz, CD ₃ OD) of 1	5
Figure S5: DEPT135 spectrum of 1	5
Figure S6: ¹ H- ¹ H COSY spectrum of 1	6
Figure S7: The enhanced ¹ H- ¹ H COSY spectrum of 1	7
Figure S8: HSQC spectrum of 1	8
Figure S9: The enhanced HSQC spectrum of 1	9
Figure S10: HMBC spectrum of 1	10
Figure S11: The enhanced HMBC spectrum of 1	11
Figure S12: NOESY spectrum of 1	12
Figure S13: The enhanced NOESY spectrum of 1	13
Figure S14: UV spectrum of 1	14
Figure S15: IR spectrum of 1	14
Figure S16: ¹ H NMR spectrum (500MHz, CD ₃ OD) of 2	15
Figure S17: ¹³ C NMR spectrum (125MHz, CD ₃ OD) of 2	15
Figure S18: ¹ H NMR spectrum (500MHz, CD ₃ OD) of 3	16
Figure S19: ¹³ C NMR spectrum (125MHz, CD ₃ OD) of 3	16
Figure S20: ¹ H NMR spectrum (500MHz, CD ₃ OD) of 4	17
Figure S21: ¹³ C NMR spectrum (125MHz, CD ₃ OD) of 4	17
Figure S22: ¹ H NMR spectrum (500MHz, CD ₃ OD) of 5	18

Figure S23: ^{13}C NMR spectrum (125MHz, CD_3OD) of 5	18
Figure S24: ^1H NMR spectrum (500MHz, CD_3OD) of 6	19
Figure S25: ^{13}C NMR spectrum (125MHz, CD_3OD) of 6	19
Figure S26: ^1H NMR spectrum (500MHz, CD_3OD) of 7	20
Figure S27: ^{13}C NMR spectrum (125MHz, CD_3OD) of 7	20
Figure S28: The Scifinder similarity report for new compound 1	21
Table 1: NMR data of compounds 1 and the similar compound	22
Table 2: ^1H NMR data of compounds 1–7	23
Table 3: ^{13}C NMR data of compounds 1–7	25

Analysis Info		Acquisition Date	2020/11/27 21:25:57
Analysis Name	\\ESI-PC\data-D\Data\GJHWMN\20201128\XDH2-5-10.d	Operator	Demo User
Method	tune_pos_standard_20141031.m	Instrument	maXis HD
Sample Name	XDH2-5-10		
Comment			

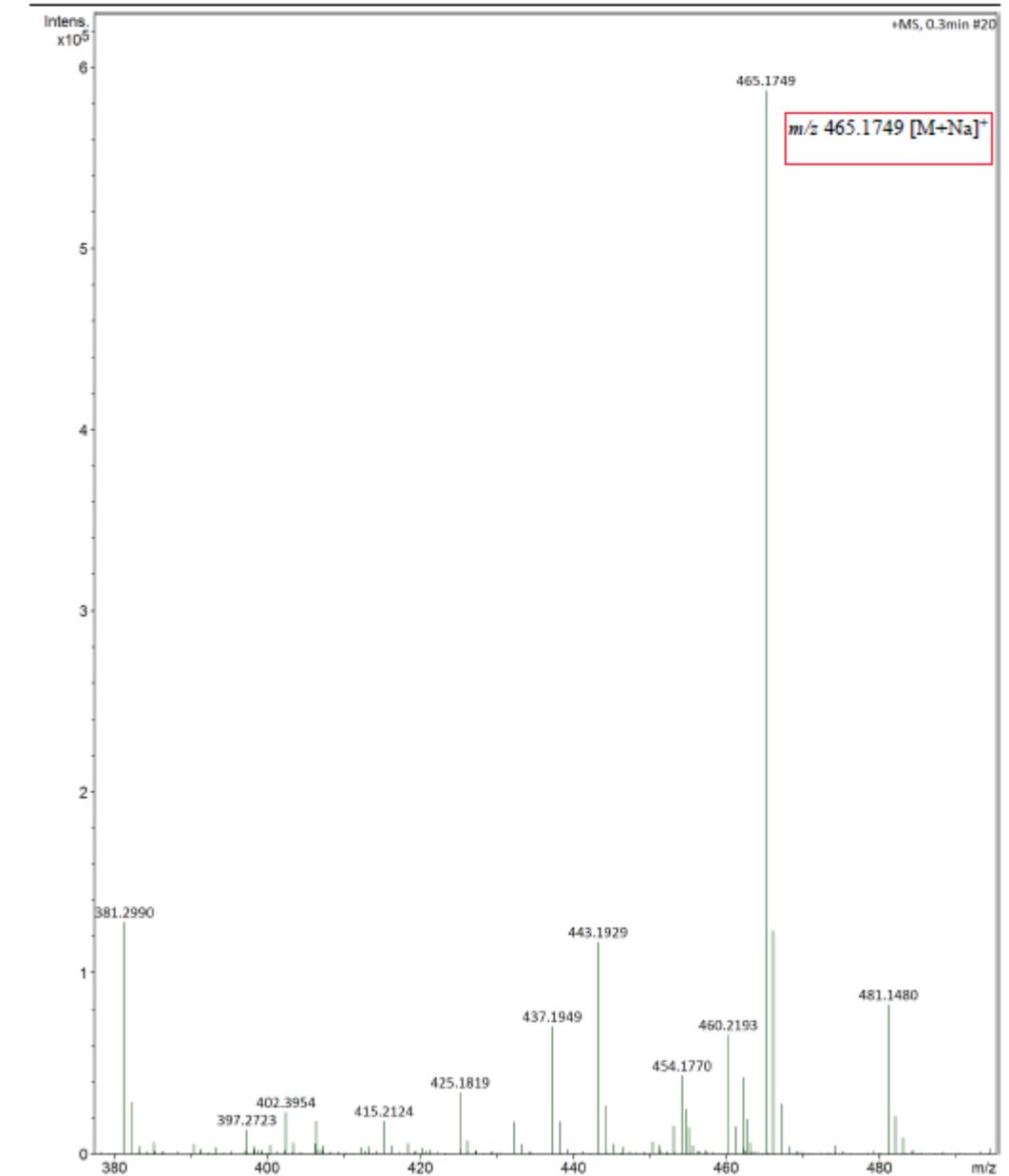


Figure S1: HR-ESI-MS spectrum of compound 1

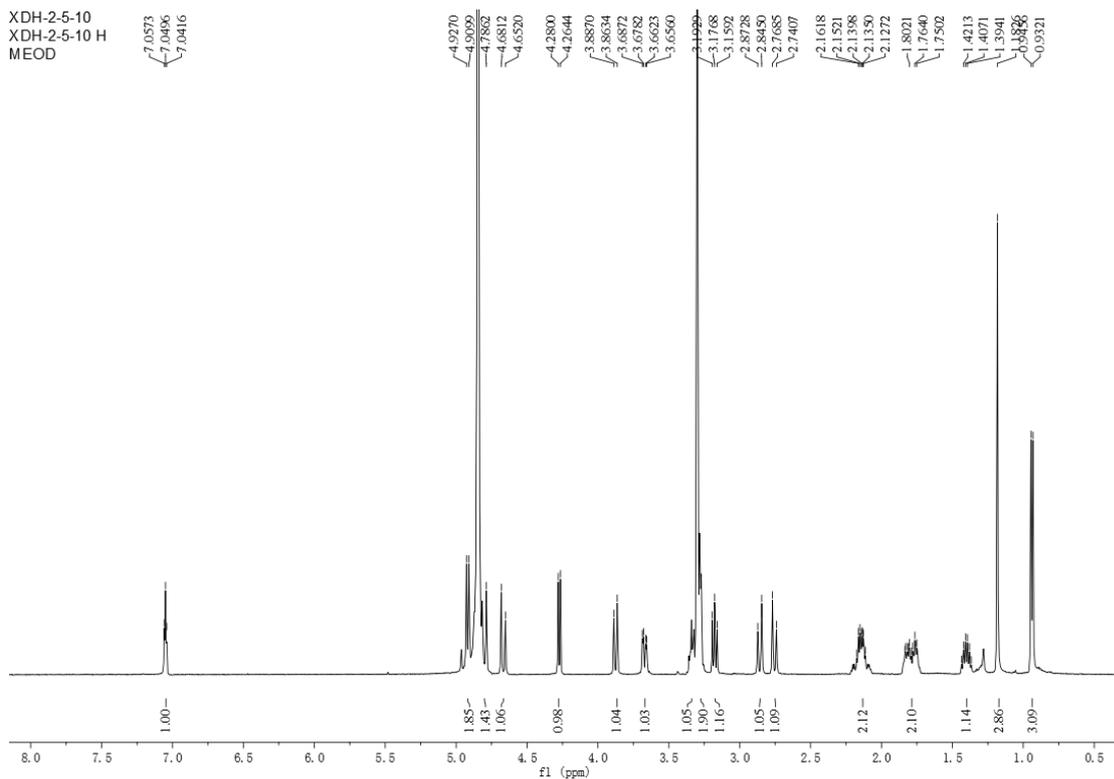


Figure S2: ^1H NMR spectrum (500MHz, CD_3OD) of **1**

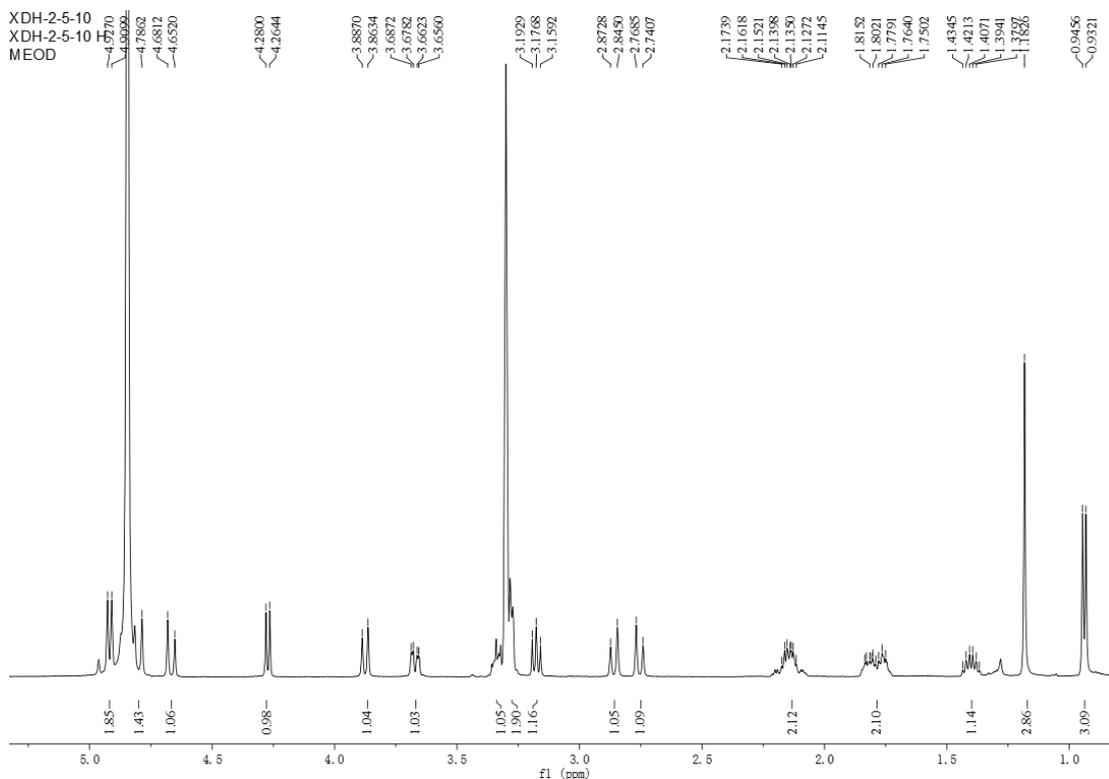


Figure S3: The enhanced ^1H NMR spectrum (500MHz, CD_3OD) of **1**
(From δ_{H} 0.8 ppm to δ_{H} 5.2 ppm)

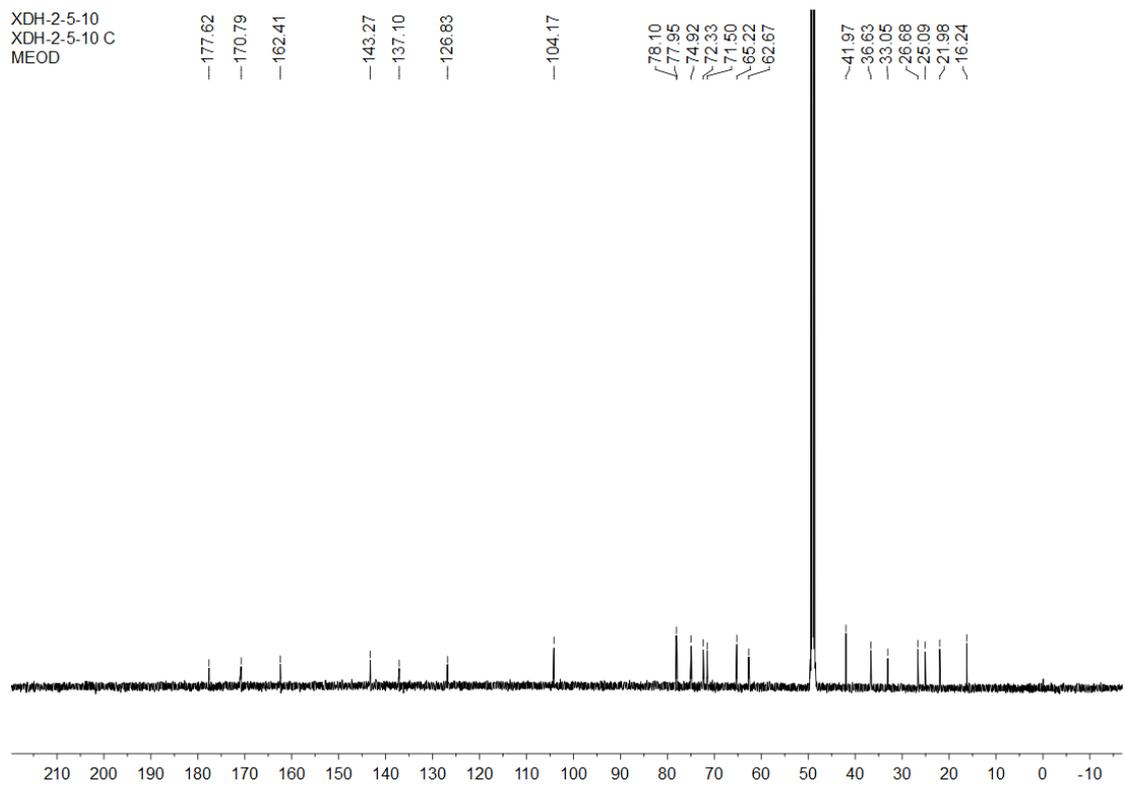


Figure S4: ^{13}C NMR spectrum (125MHz, CD_3OD) of **1**

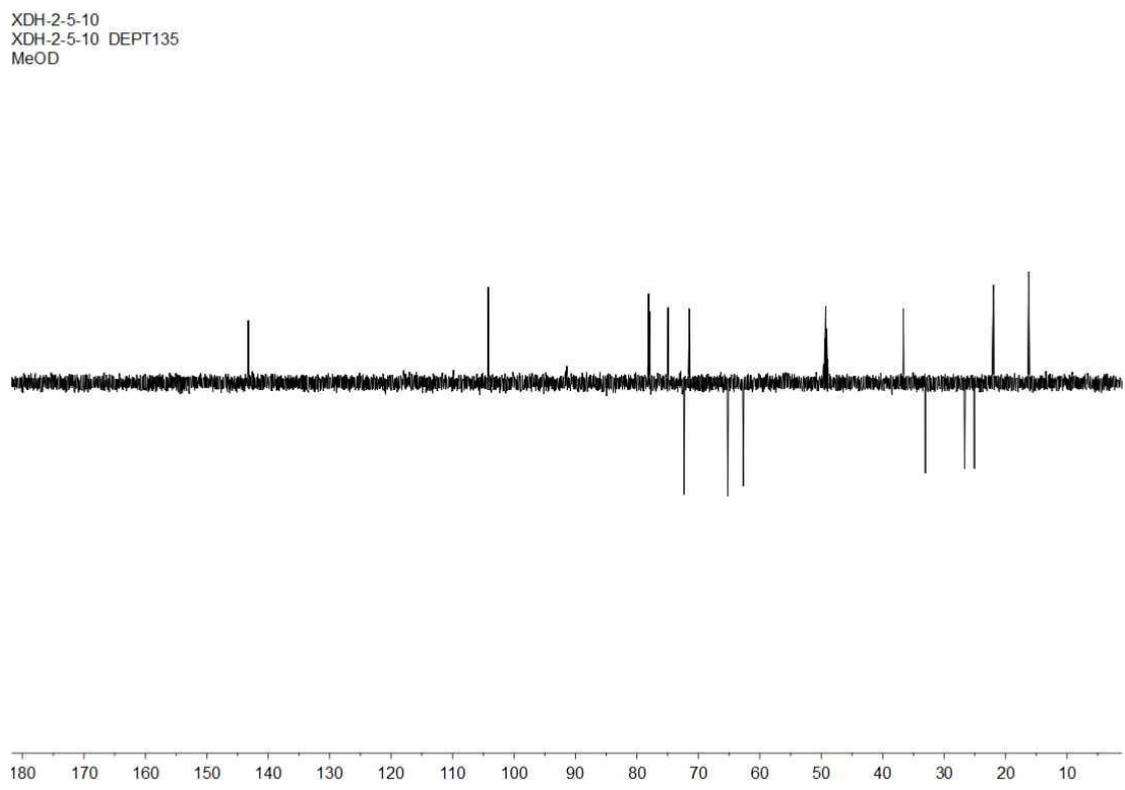


Figure S5: DEPT135 spectrum of **1**

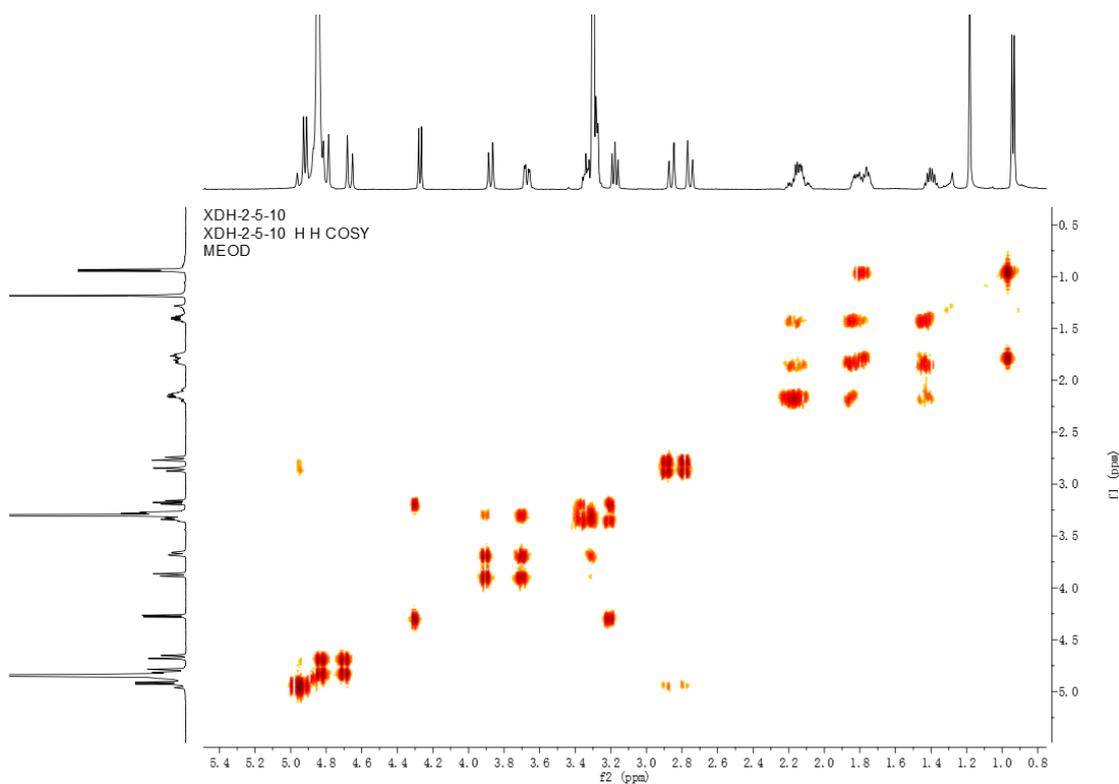


Figure S7: The enhanced ^1H - ^1H COSY spectrum of **1**(From δ_{H} 0.8 ppm to δ_{H} 5.2 ppm)

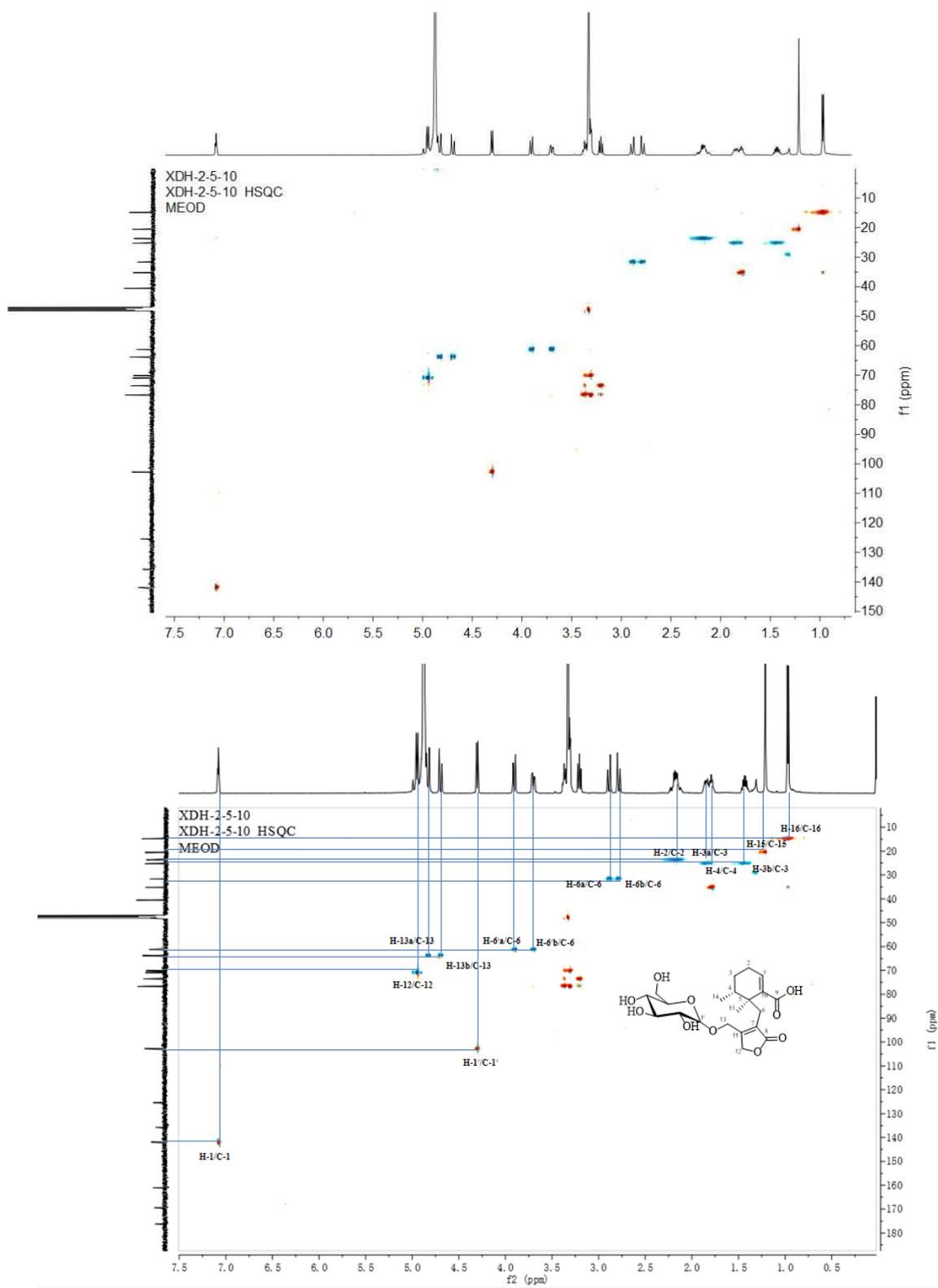


Figure S8:HSQC spectrum of **1**

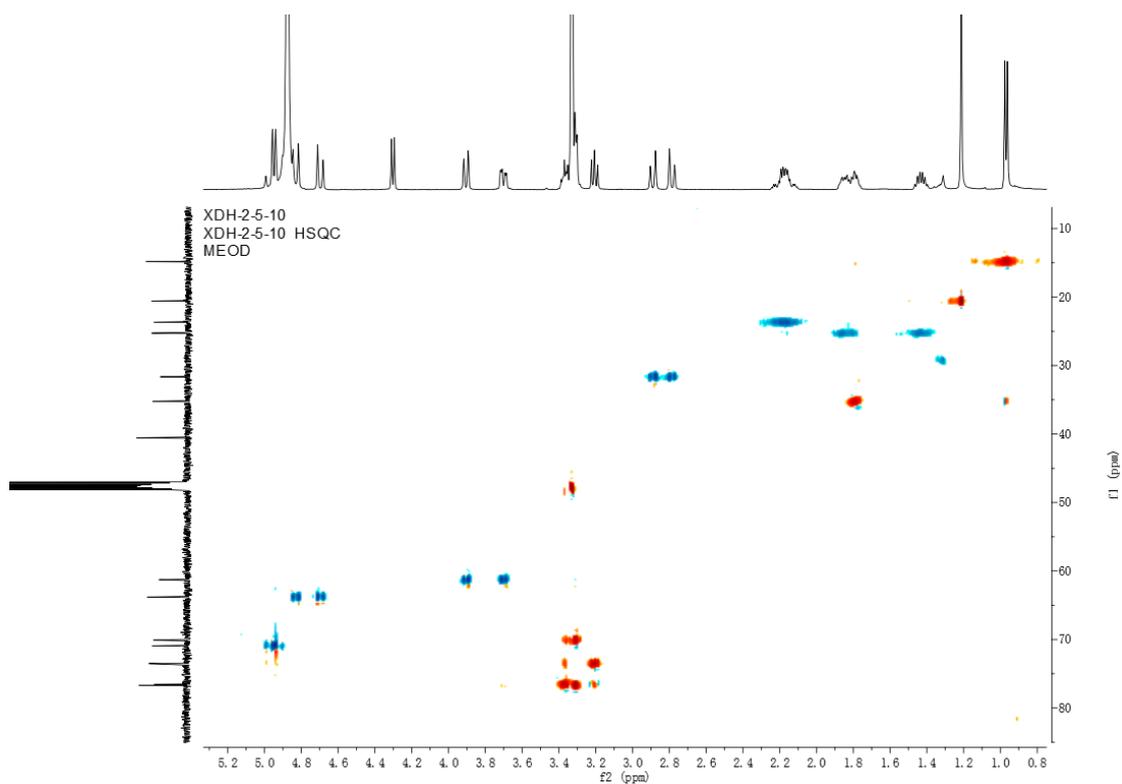


Figure S9: The enhanced HSQC spectrum of **1**(From δ_c 10 ppm to δ_c 90 ppm)

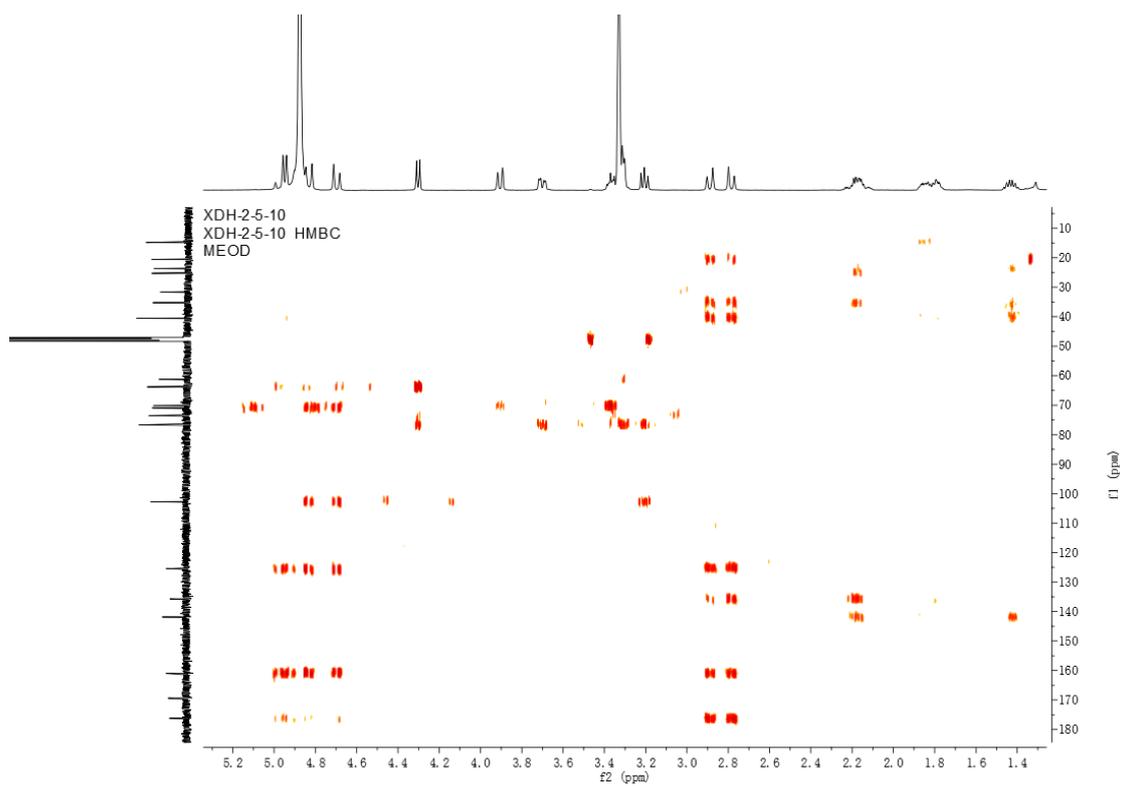


Figure S11: The enhanced HMBC spectrum of **1** (From δ_{H} 1.4 ppm to δ_{H} 5.2 ppm)

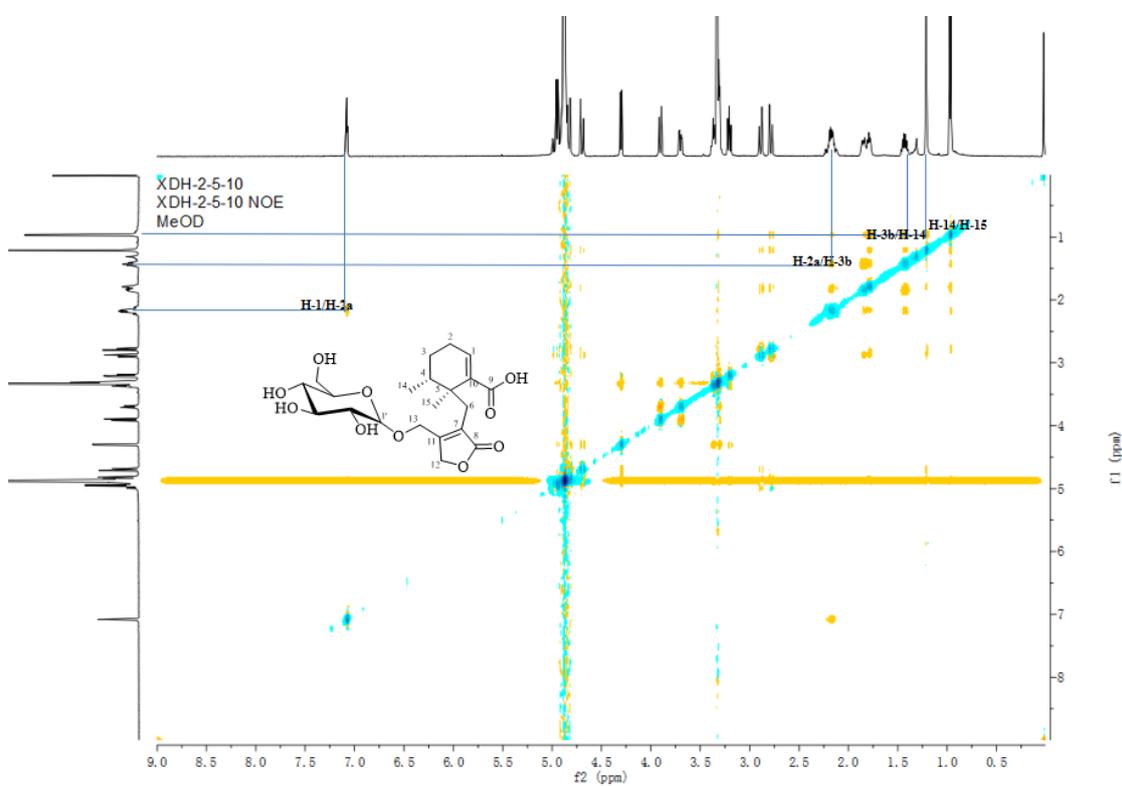
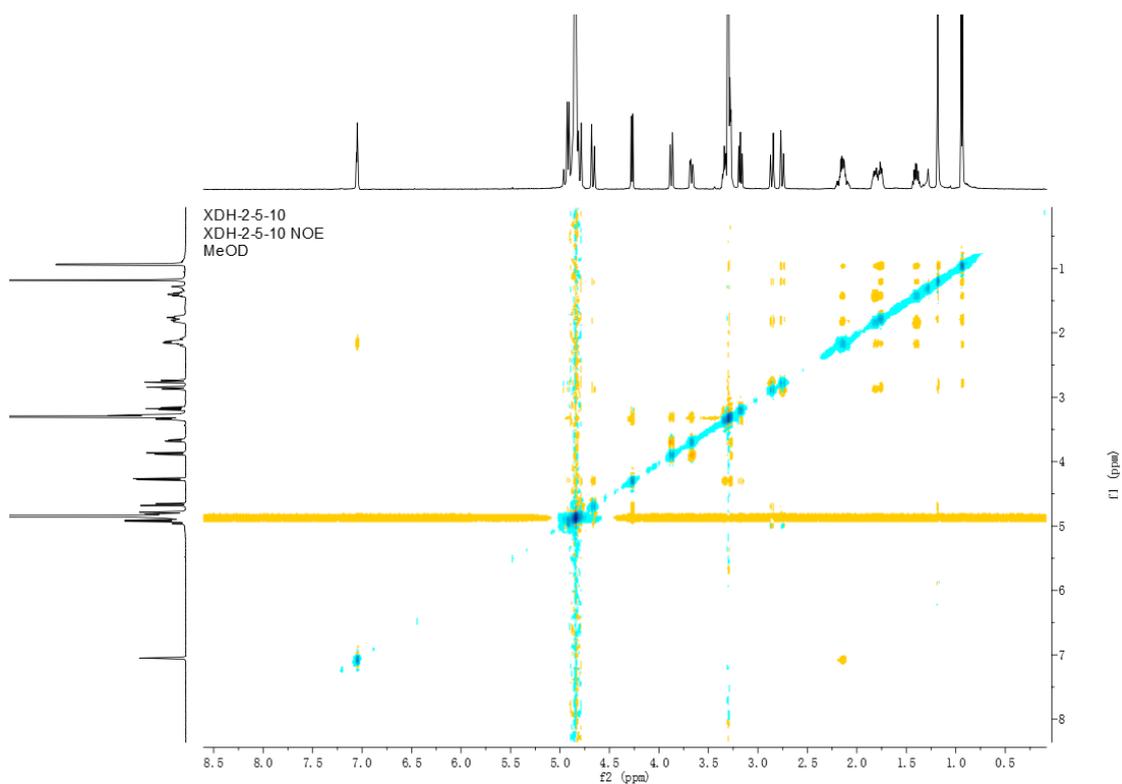


Figure S12: NOESY spectrum of 1

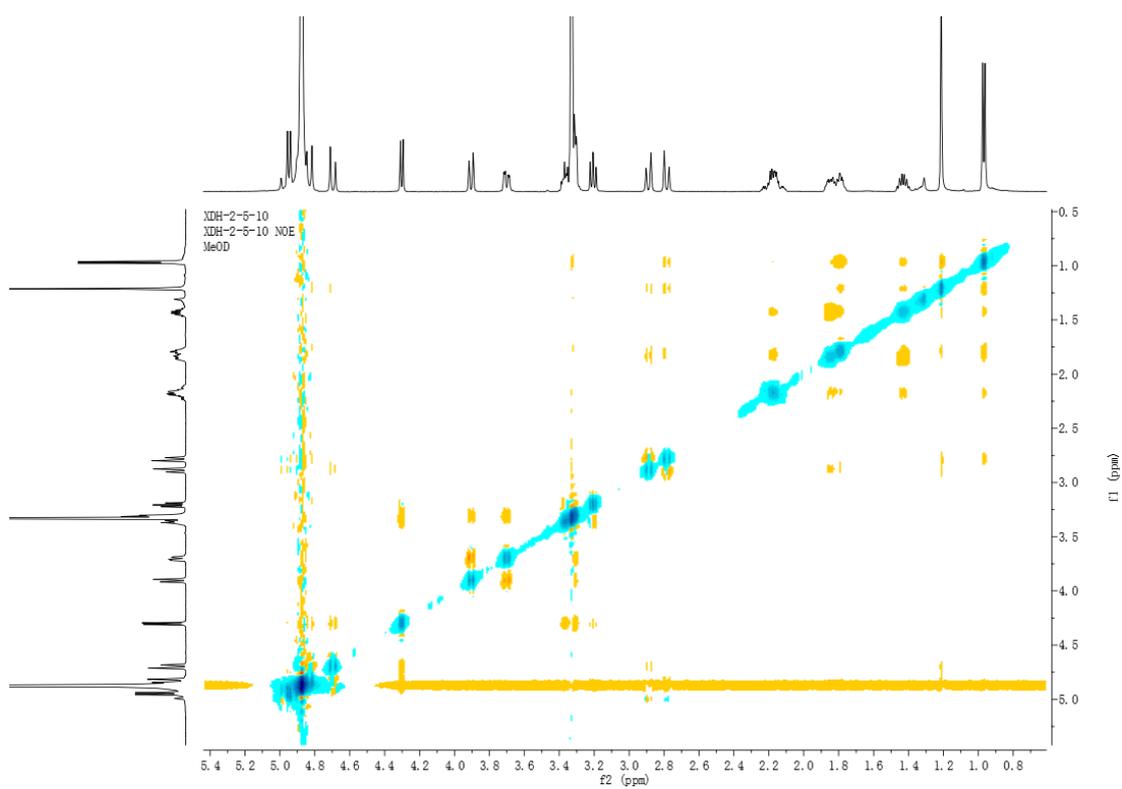


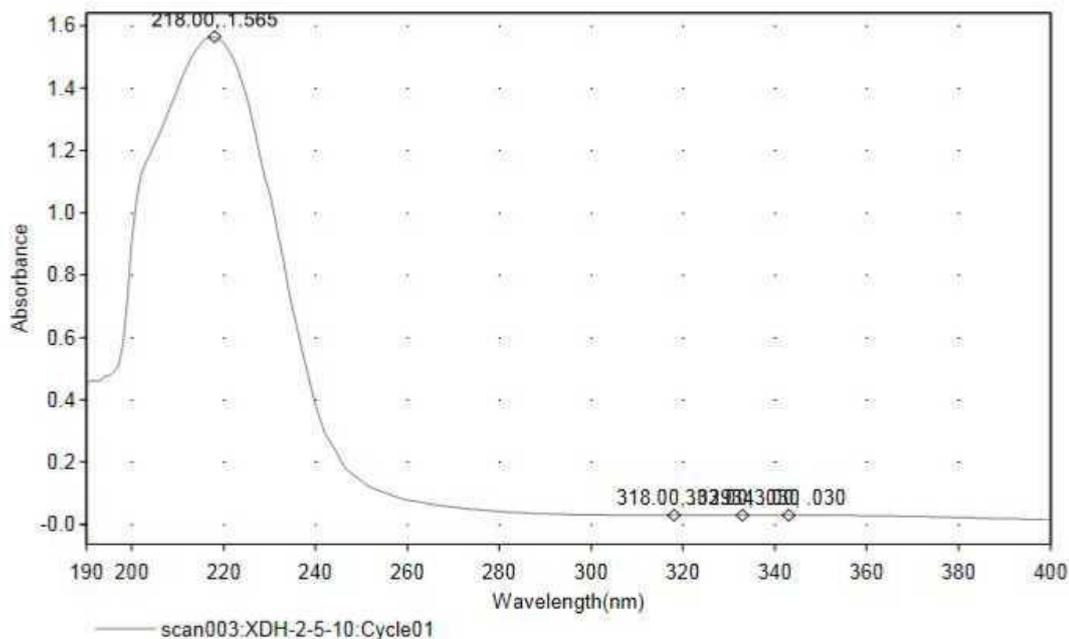
Figure S13: The enhanced NOESY spectrum of **1** (From δ_{H} 0.5 ppm to δ_{H} 5.0 ppm)

Thermo Scientific ~ VISIONpro SOFTWARE V4.41

Operator Name (None Entered)
 Department (None Entered)
 Organization (None Entered)
 Information (None Entered)

Date of Report 2020/12/24
 Time of Report 21:27:43下午

Scan Graph



Results Table - scan003, XDH-2-5-10, Cycle01

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333.00	.030	Stop Wavelength 400.00 nm
343.00	.030	Sort By Wavelength
Sensitivity	High	

Figure S14: UV spectrum of 1

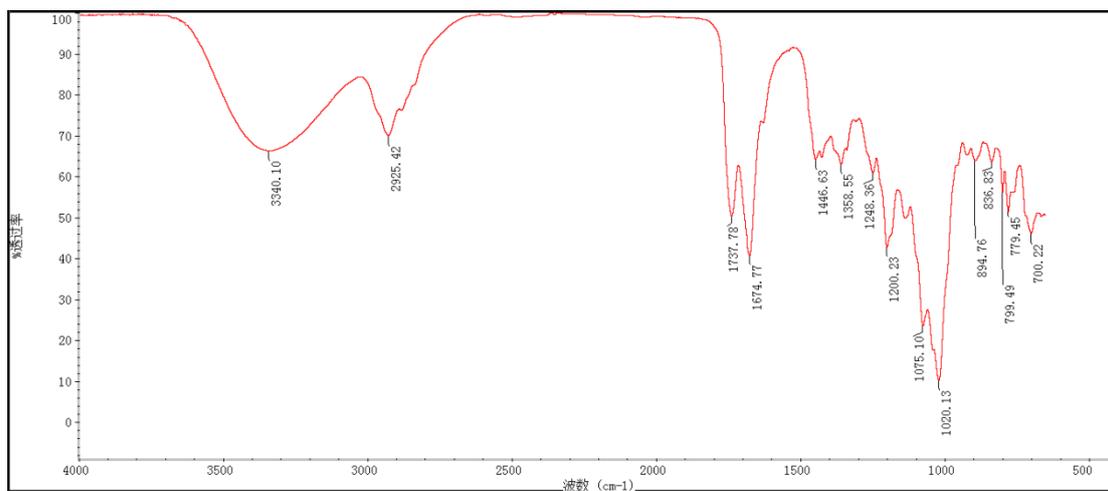


Figure S15: IR spectrum of 1

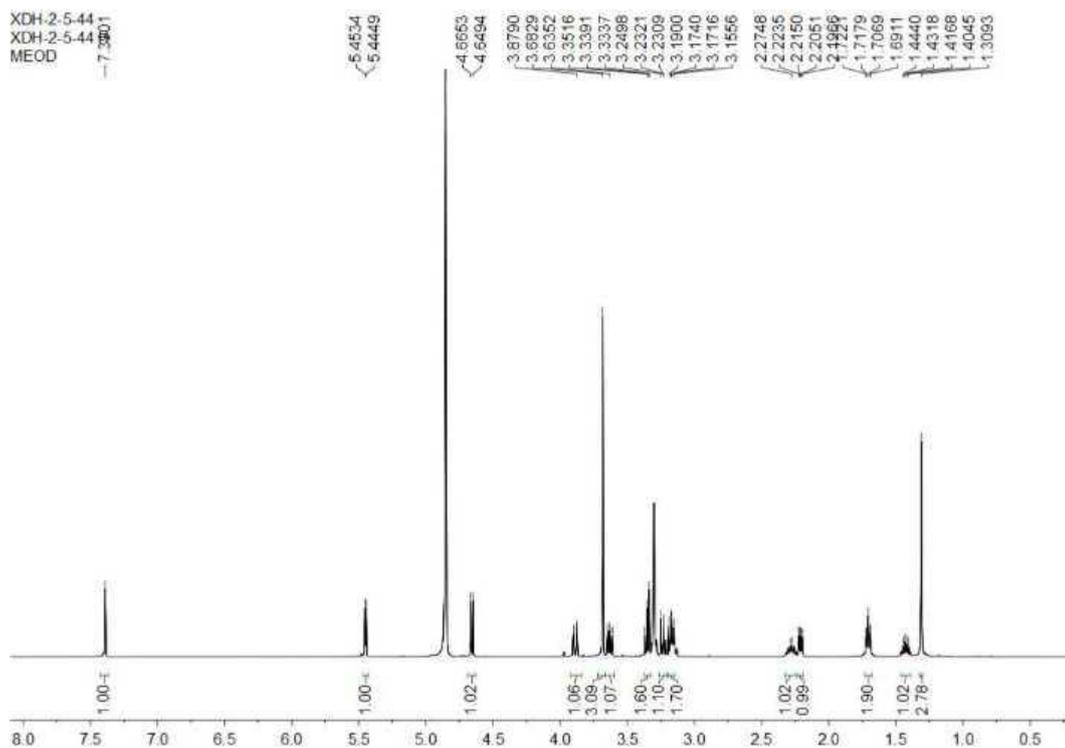


Figure S16: ^1H NMR spectrum (500MHz, CD_3OD) of **2**

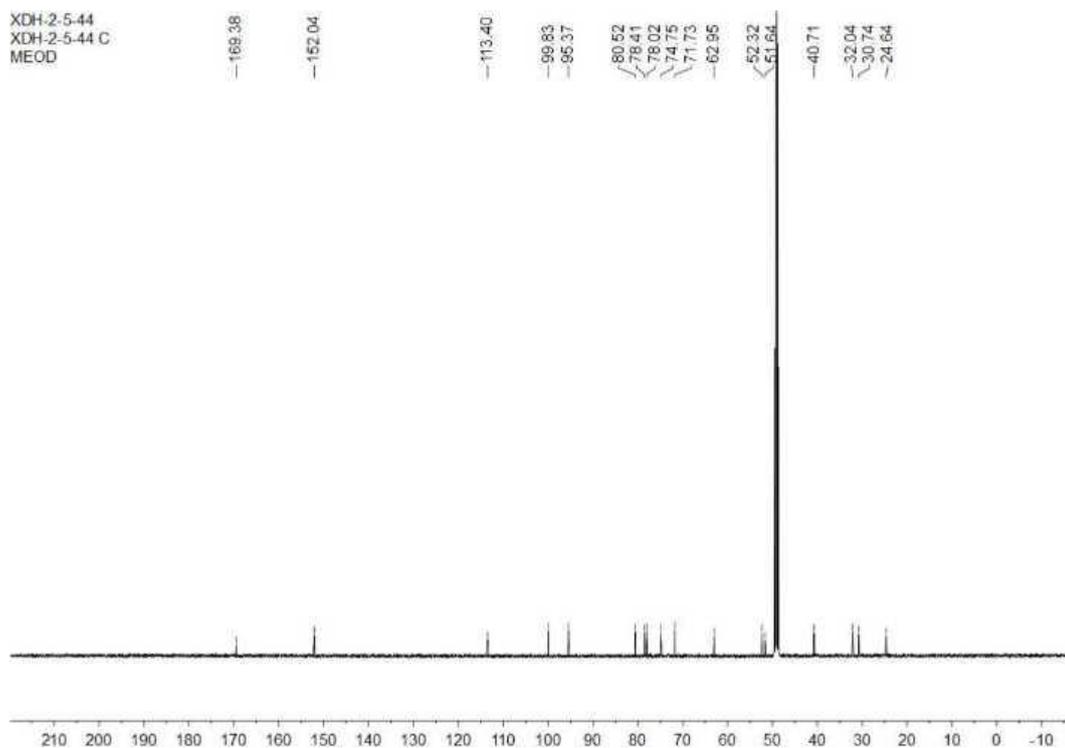


Figure S17: ^{13}C NMR spectrum (125MHz, CD_3OD) of **2**

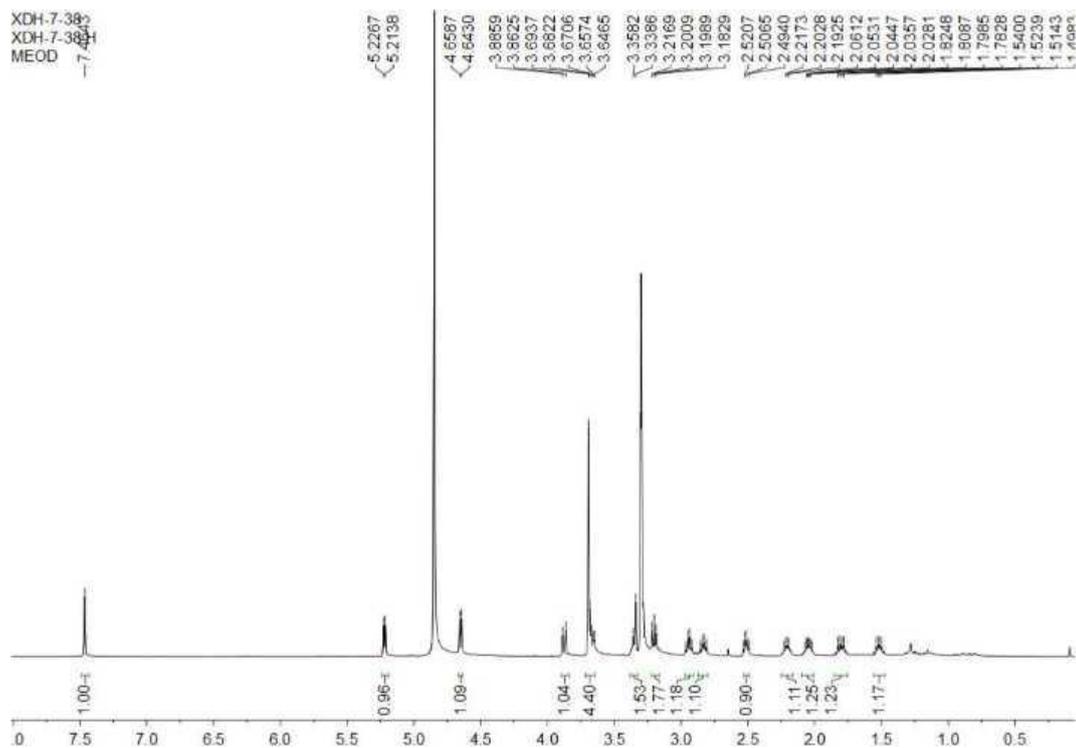


Figure S18: ^1H NMR spectrum (500MHz, CDCl_3) of **3**

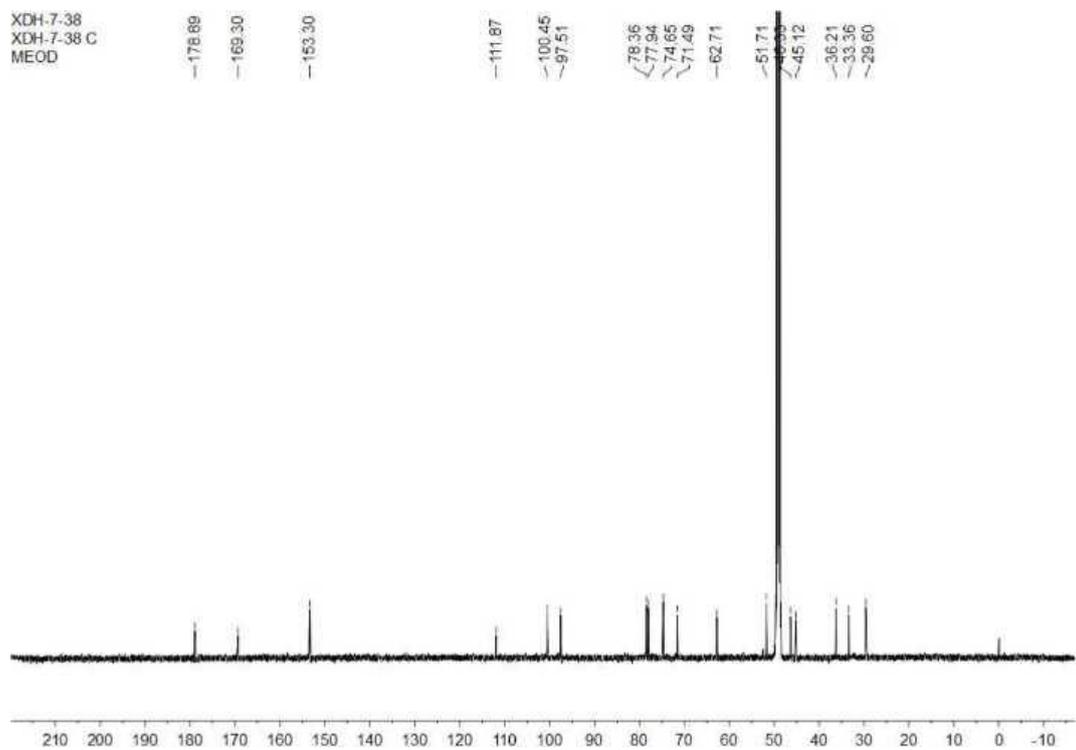


Figure S19: ^{13}C NMR spectrum (125MHz, CD_3OD) of **3**

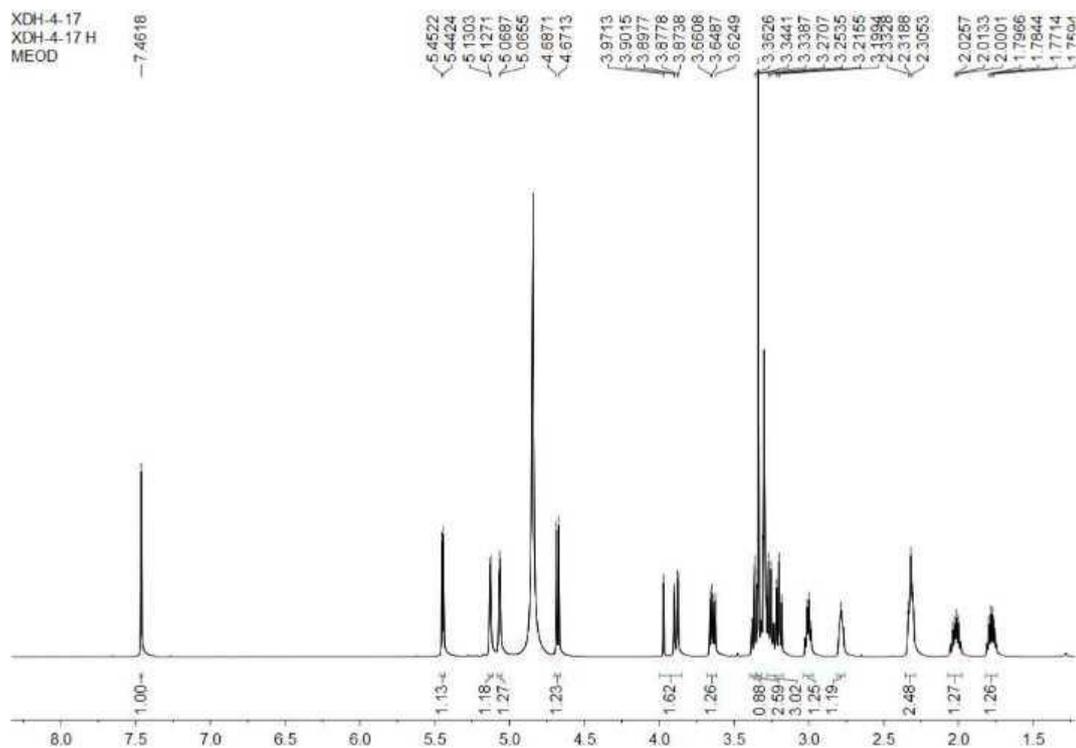


Figure S20: ^1H NMR spectrum (500MHz, CDCl_3) of **4**

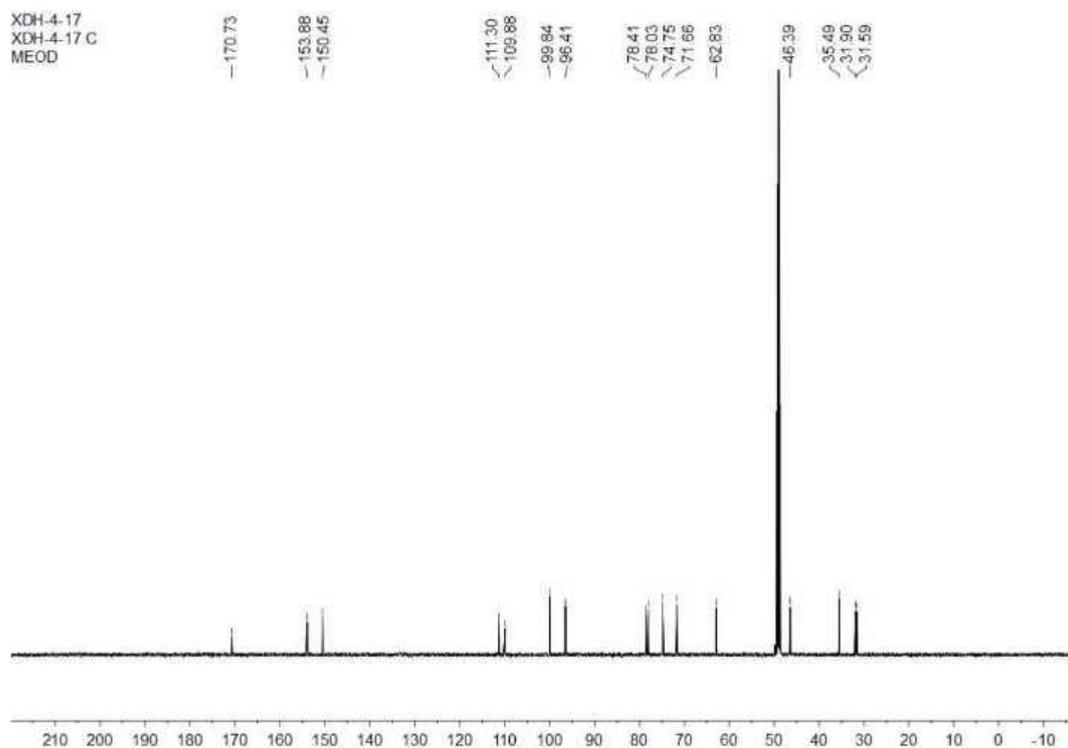


Figure S21: ^{13}C NMR spectrum (125MHz, CDCl_3) of **4**

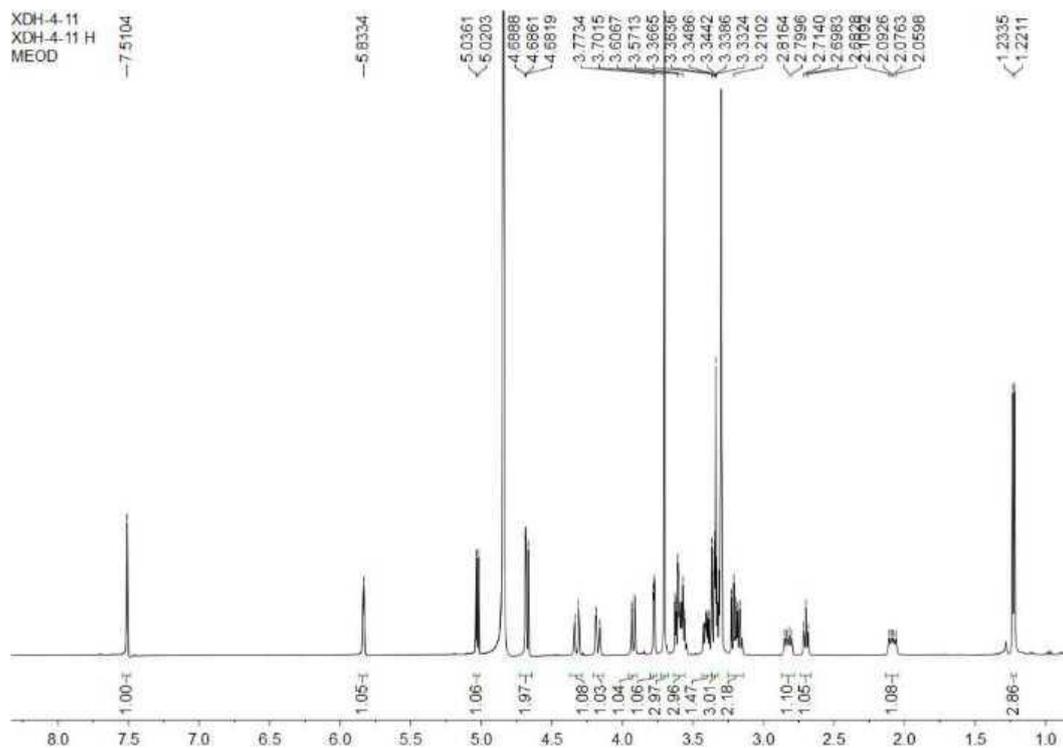


Figure S22: ^1H NMR spectrum (500MHz, CD_3OD) of **5**

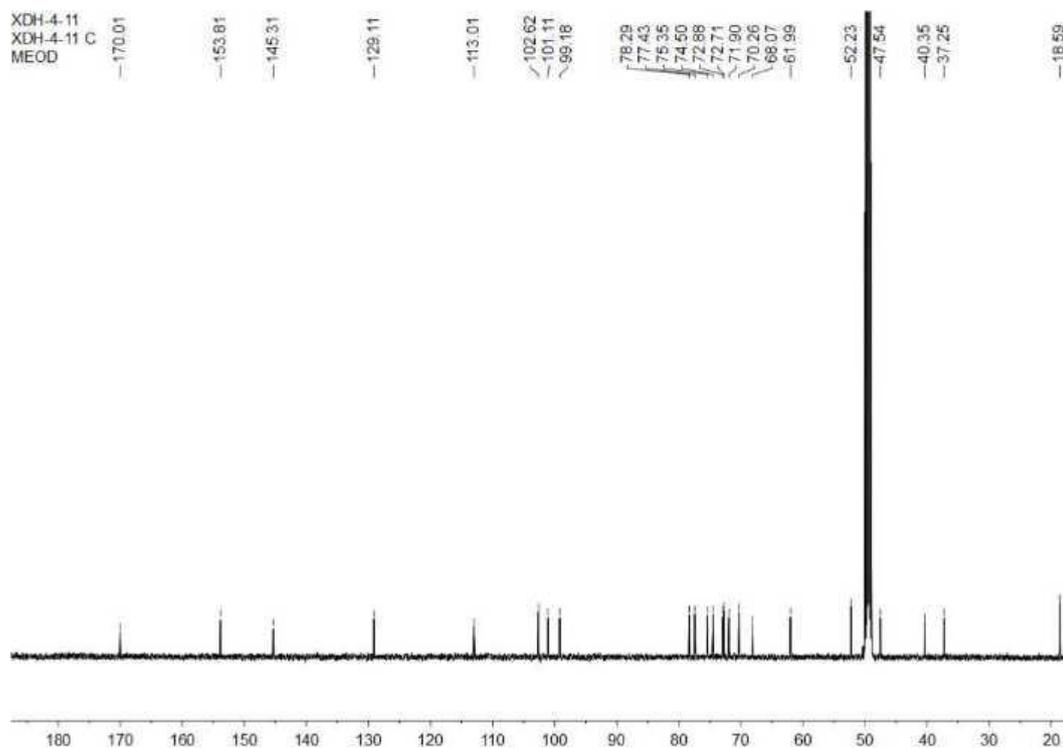


Figure S23: ^{13}C NMR spectrum (125MHz, CD_3OD) of **5**

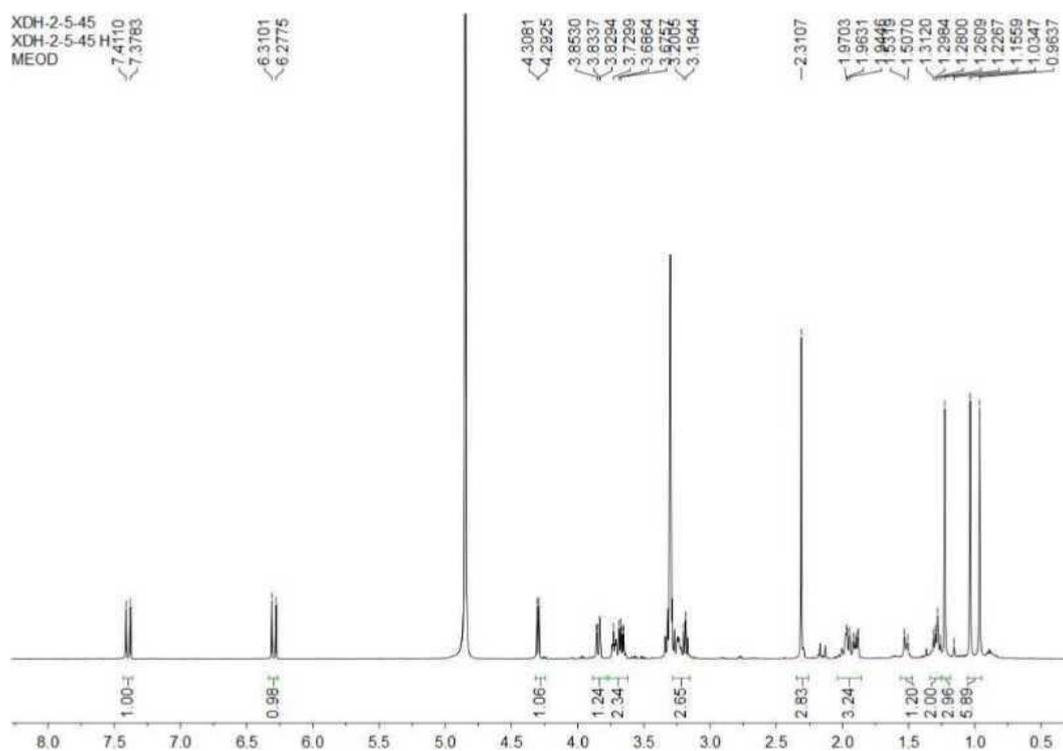


Figure S24: ^1H NMR spectrum (500MHz, CD_3OD) of **6**

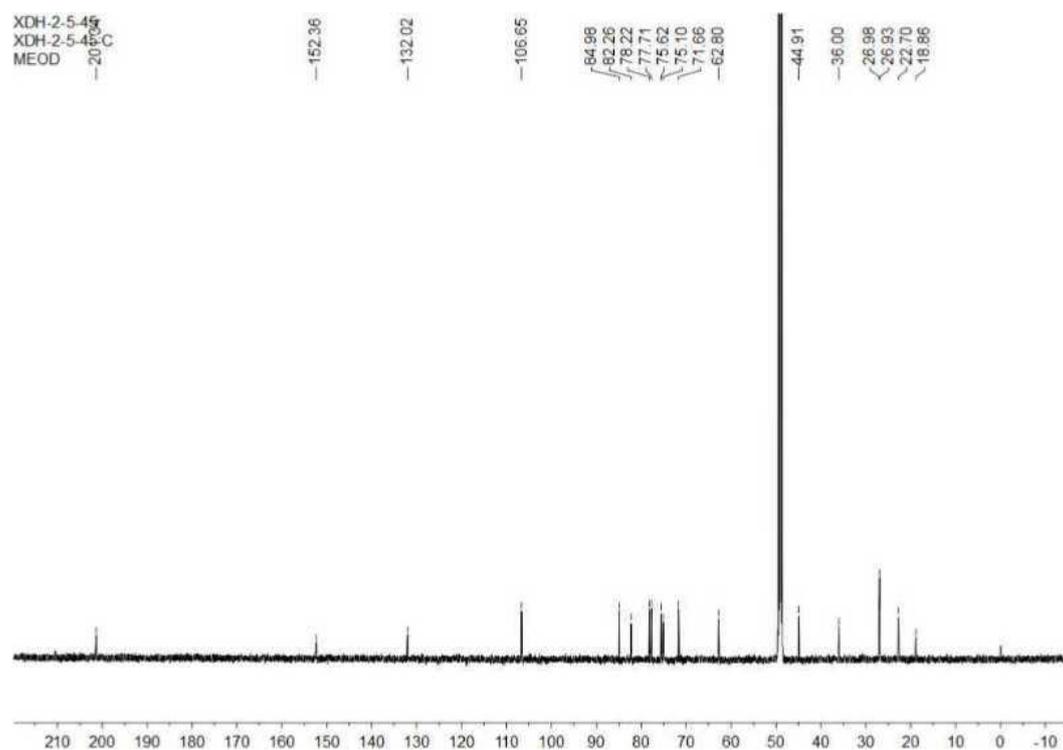


Figure S25: ^{13}C NMR spectrum (125MHz, CD_3OD) of **6**

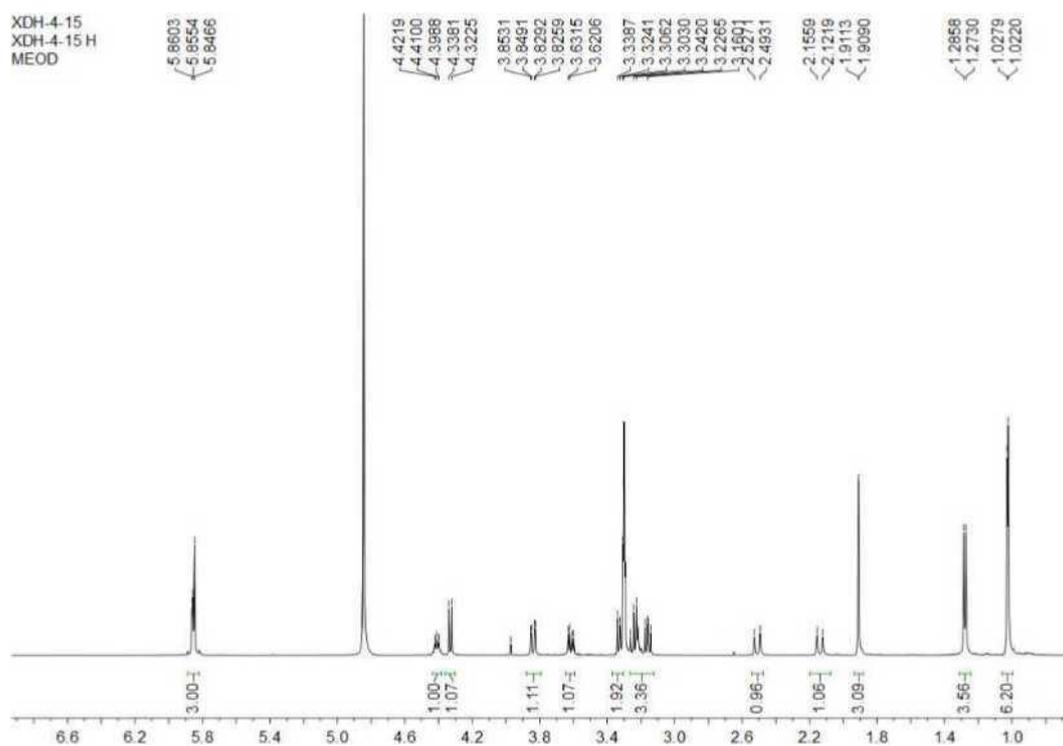


Figure S26: ^1H NMR spectrum (500MHz, CD_3OD) of **7**

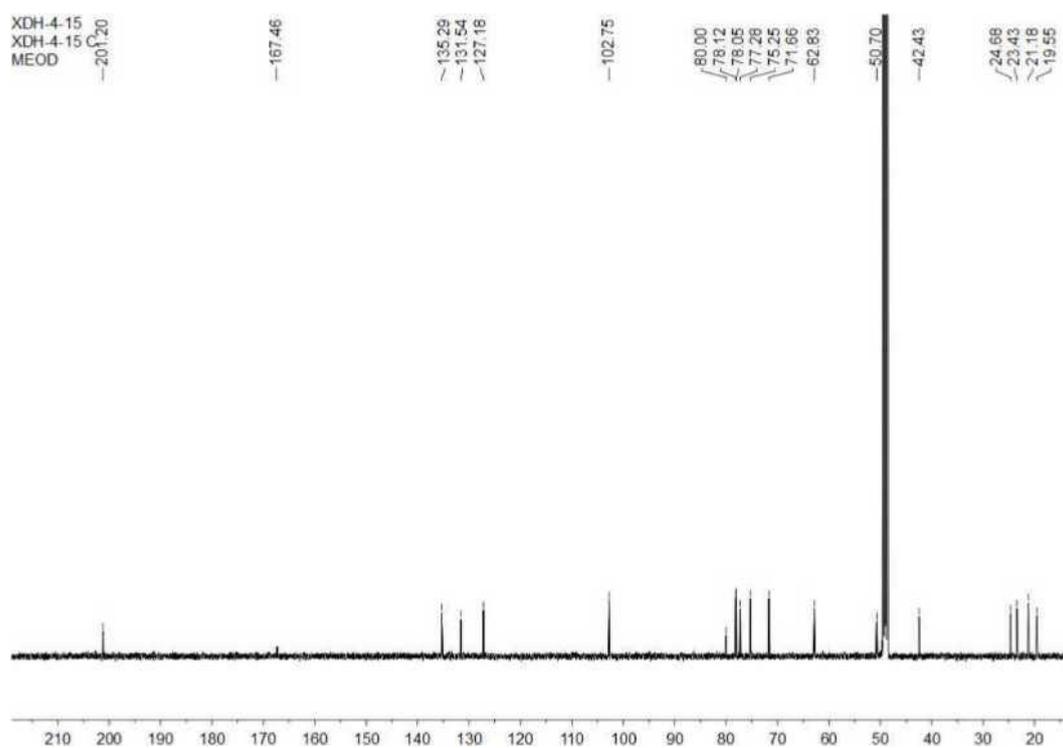


Figure S27: ^{13}C NMR spectrum (125MHz, CD_3OD) of **7**

Chemical Structure similarity > substances (3)

REFERENCES
 Research Topic
 Author Name
 Company Name
 Document Identifier
 Journal
 Patent
 Tag

SUBSTANCES
 Chemical Structure
 Molecule
 Molecular Formula
 Property
 Substance Identifier

REACTIONS
 Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor

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 Exact Structure
 Substructure
 Similarity

Show precision analysis

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Chemical Structure similarity

SUBSTANCES

Select All Deselect All

0 of 5 Similarity Candidates Selected

Similarity Range	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	0
80-84	3
75-79	50
70-74	603
65-69	4713
0-64 (least similar)	36664

Get Substances

Chemical Structure similarity > substances (3) Save Print Export

SUBSTANCES Get References Get Reactions Get Commercial Sources Tools

Create Export the Feature Alert Send to SciFinder Display Options

Sort by: [Similarity Score]

0 of 3 Substances Selected

Score	Substance
Score 80 1: 854494-90-1	 Absolute stereochemistry C ₁₀ H ₁₂ O ₄ 3,4-Dihydroxyphenylacetic acid [1,4,2,6,8,9,10,5,12]-(1,5-dihydro-2-oxo-3-furan-2-yl)-2-hydroxyethyl(decahydro-2-hydroxy-1,4-dimethyl-5-member-1-naphthalenyl)ethyl
Score 80 2: 854494-90-6	 Absolute stereochemistry C ₁₀ H ₁₂ O ₄ 3,4-Dihydroxyphenylacetic acid [1,4,2,6,8,9,10,5,12]-(1,5-dihydro-2-oxo-3-furan-2-yl)-2-hydroxyethyl(decahydro-2-hydroxy-1,4-dimethyl-5-member-1-naphthalenyl)ethyl
Score 80 3: 128824-30-3	 Absolute stereochemistry C ₁₀ H ₁₂ O ₄ 3,4-Dihydroxyphenylacetic acid [1,4,2,6,8,9,10,5,12]-(2,5-dihydro-2-oxo-3-furan-2-yl)-2-hydroxyethyl(decahydro-2-hydroxy-1,4-dimethyl-5-member-1-naphthalenyl)ethyl

Figure S28: The Scifinder similarity report for new compound 1

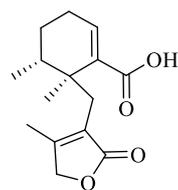
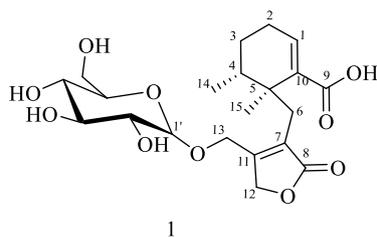


Table 1 : NMR data of compounds **1** and the similar compound

No	1^a	4,5,11-trimethyl-8,9-seco-1(10),7(11)-eremophiladien-8,12-olid-9-oic acid^b		
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	7.04 (1H, t, $J = 3.9$ Hz)	143.3	7.19 (1H, brs)	144.1
2	2.15 (2H, t, $J = 4.9$ Hz)	25.1	2.18 (2H, brs)	24.2
3	1.80 (1H, overlap)	26.7	1.90 (1H, m, H-3'b)	25.3
	1.40 (1H, m)		1.43 (1H, m, H-3b)	
4	1.76 (1H, overlap)	36.6	1.80 (1H, m)	35.1
5	-	41.9		40.8
6	2.85 (1H, d, $J = 13.9$ Hz)	33.1	2.84 (1H, d, $J = 13.7$ Hz)	31.7
	2.75 (1H, d, $J = 13.9$ Hz)		2.74 (1H, d, $J = 13.7$ Hz)	
7		126.8		125.4
8		177.6		175.5
9		170.8		175.5
10		137.1		135.4
11		162.4		159.5
12	4.91 (2H, d, $J = 8.6$ Hz)	72.3	4.63 (2H, brs)	72.5
13	4.78 (1H, d, $J = 14.6$ Hz)	65.2	2.06 (3H, s)	13.2
	4.67 (1H, d, $J = 14.6$ Hz)			
14	0.93 (3H, d, $J = 6.8$ Hz)	16.2	0.93 (3H, d, $J = 6.8$ Hz)	15.7
15	1.18 (3H, s)	21.9	0.94 (3H, s)	21.3
1'	4.27 (1H, d, $J = 7.8$ Hz)	104.2		
2'	3.18 (1H, overlap)	74.8		
3'	3.33 (1H, overlap)	77.9		
4'	3.27 (1H, overlap)	71.5		
5'	3.28 (1H, overlap)	78.1		
6'	3.86 (1H, d, $J = 11.8$ Hz)	62.7		
	3.67 (1H, m)			

^a Recorded δ in ppm, J in Hz, in CD₃OD. ^b Recorded in CDCl₃.

Table 2 : ¹H NMR data of compounds **1–7** (δ in ppm, J in Hz, in CD₃OD at 500 MHz)

No	1	2	3	4	5	6	7
1	7.04 (1H, t, $J = 3.9$ Hz)	5.54 (1H, d, $J = 4.3$ Hz)	5.21 (1H, d, $J = 6.4$ Hz)	5.44 (1H, d, $J = 4.9$ Hz)	5.15 (1H, d, $J = 7.6$ Hz)		
2	2.15 (2H, t, $J = 4.9$ Hz)					3.72 (2H, m)	2.50 (1H, d, $J = 17.0$ Hz) 2.14 (1H, d, $J = 17.0$ Hz)
3	1.80 (1H, overlap) 1.40 (1H, m)	7.39 (1H, s)	7.46 (1H, brs)	7.46 (1H, brs)	7.51 (1H, brs)	1.95 (1H, m) 1.52 (1H, m)	
4	1.76 (1H, overlap)					1.97 (1H, m) 1.88 (1H, m)	5.84 (1H, brs)
5	-	3.17 (1H, m)	3.20 (1H, m)	3.20 (1H, m)	3.21 (1H, m)		
6	2.85 (1H, d, $J = 13.9$ Hz) 2.75 (1H, d, $J = 13.9$ Hz)	2.25 (1H, m) 1.43 (1H, m)	2.21 (1H, m) 1.52 (1H, m)	2.21 (1H, m) 1.52 (1H, m)	2.80 (1H, m) 2.08 (1H, m)		
7		1.71 (1H, m)	2.06 (1H, m) 1.80 (1H, m)	2.06 (1H, m) 1.80 (1H, m)	5.83 (1H, s)	7.40 (1H, d, $J = 16.4$ Hz)	5.85 (1H, d, $J = 2.5$ Hz)
8			2.94 (1H, m)	2.94 (1H, m)		6.30 (1H, d, $J = 16.4$ Hz)	5.85 (1H, d, $J = 2.5$ Hz)
9		2.20 (1H, m)	2.52 (1H, t, $J = 7.6$ Hz)	2.52 (1H, t, $J = 7.6$ Hz)	2.69 (1H, t, $J = 7.8$ Hz)		4.41 (1H, t, $J = 6.0$ Hz)
10		1.30 (3H, s)		5.12 (1H, d, $J = 1.6$ Hz) 5.06 (1H, d, $J = 1.6$ Hz)	4.32 (1H, d, $J = 4.3$ Hz) 4.16 (1H, d, $J = 4.3$ Hz)	2.31 (3H, s)	1.28 (3H, d, $J = 6.4$ Hz)
11						1.22 (3H, s)	1.03 (3H, s)
12	4.91 (2H, d, $J = 8.6$ Hz)	3.68 (3H, s)	3.69 (3H, s)		3.70 (3H, s)	0.96 (3H, s)	1.02 (3H, s)
13	4.78 (1H, d, $J = 14.6$ Hz) 4.67 (1H, d, $J = 14.6$ Hz)					1.03 (3H, s)	1.91 (3H, s)
14	0.93 (3H, d, $J = 6.8$ Hz)						
15	1.18 (3H, s)						
1'	4.27 (1H, d, $J = 7.8$ Hz)	4.65 (1H, d, $J = 8.0$ Hz)	4.65 (1H, d, $J = 7.9$ Hz)	4.67 (1H, d, $J = 7.9$ Hz)	4.68 (1H, brs)	4.30 (1H, d, $J = 7.7$ Hz)	4.32 (2H, d, $J = 7.8$ Hz)
2'	3.18 (1H, overlap)	3.17 (1H, overlap)	3.19 (1H, overlap)	3.21 (1H, overlap)	3.19 (1H, overlap)	3.19 (1H, overlap)	3.20 (1H, overlap)

3'	3.33 (1H, overlap)	3.34 (1H, overlap)	3.33 (1H, overlap)	3.35 (1H, overlap)	3.3-3.4 (1H, overlap)	3.33 (1H, overlap)	3.33 (1H, overlap)
4'	3.27 (1H, overlap)	3.23 (1H, overlap)	3.23 (1H, overlap)	3.26 (1H, overlap)	3.3-3.4 (1H, overlap)	3.23 (1H, overlap)	3.24 (1H, overlap)
5'	3.28 (1H, overlap)	3.24 (1H, overlap)	3.24 (1H, overlap)	3.27 (1H, overlap)	3.58(1H, overlap)	3.24 (1H, overlap)	3.25 (1H, overlap)
6'	3.86 (1H, d, $J = 11.8$ Hz)	3.87(1H, overlap)	3.87 (1H, d, $J = 11.8$ Hz)	3.88 (1H, d, $J = 11.9$ Hz)	3.92 (1H, dd, $J = 1.8, 11.3$ Hz)	3.84 (1H, dd, $J = 2.1, 11.9$ Hz)	3.83 (1H, dd, $J = 2.0, 12.0$ Hz)
	3.67 (1H, m)	3.67 (1H, overlap)	3.67 (1H, overlap)	3.65(1H, t, $J = 6.1$ Hz)	3.77 (1H, overlap)	3.67 (1H, overlap)	3.62 (1H, d, $J = 5.5$ Hz)
1"					4.68 (1H, brs)		
2"					3.3-3.4 (1H, overlap)		
3"					3.3-3.4 (1H, overlap)		
4"					3.21(1H, overlap)		
5"					3.62 (1H, overlap)		
6"					1.23 (3H, d, $J = 5.5$ Hz)		

Table 3 : ^{13}C NMR data of compounds **1–7** (δ in ppm, in CD_3OD at 125 MHz)

No	1	2	3	4	5	6	7
1	143.3	95.4	97.5	96.4	99.2	44.9	42.4
2	25.1					75.6	50.7
3	26.7	152.0	153.3	153.9	153.8	27.0	201.2
4	36.6	113.4	111.9	111.3	113.0	36.0	127.2
5	41.9	32.0	36.2	35.5	37.3	84.9	167.5
6	33.1	30.7	33.4	31.9	40.3	82.3	80.0
7	126.8	40.7	29.6	31.6	129.1	152.4	131.5
8	177.6	80.5	46.3	150.5	145.3	132.0	135.3
9	170.8	52.3	45.1	46.4	47.5	201.3	77.3
10	137.1	24.6	178.7	109.9	61.9	26.9	21.2
11	162.4	169.4	169.3	170.3	170.0	18.8	23.4
12	72.3	51.6	51.7		52.2	22.7	24.7
13	65.2					26.9	19.6
14	16.2						
15	21.9						
1'	104.2	99.8	100.5	99.8	101.1	106.6	102.7
2'	74.8	74.7	74.7	74.7	75.3	75.1	75.2
3'	77.9	78.4	78.5	78.4	78.3	78.2	78.1
4'	71.5	71.7	71.4	71.7	72.7	71.7	71.7
5'	78.1	78.0	77.9	78.0	77.4	77.7	78.0
6'	62.7	62.9	62.7	62.8	68.1	62.8	62.8
1''					102.6		
2''					71.9		
3''					74.5		
4''					70.4		
5''					72.9		
6''					18.6		