Supporting Information

Rec. Nat. Prod. 16:5 (2022) 509-514

A New Eremophilanolide from the Fresh Roots of *Rehmannia glutinosa*

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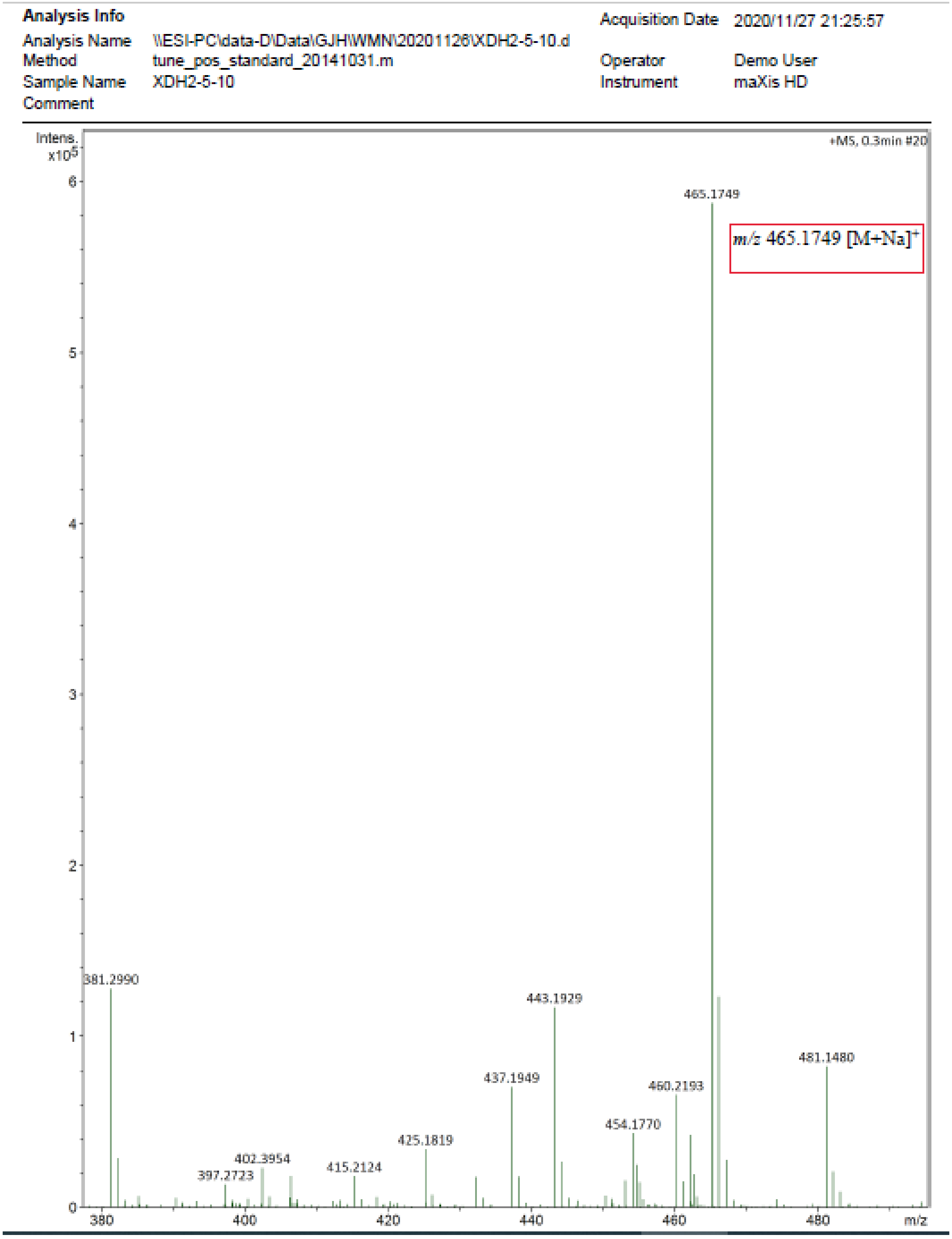


Figure S1: HR-ESI-MS spectrum of compound **1**

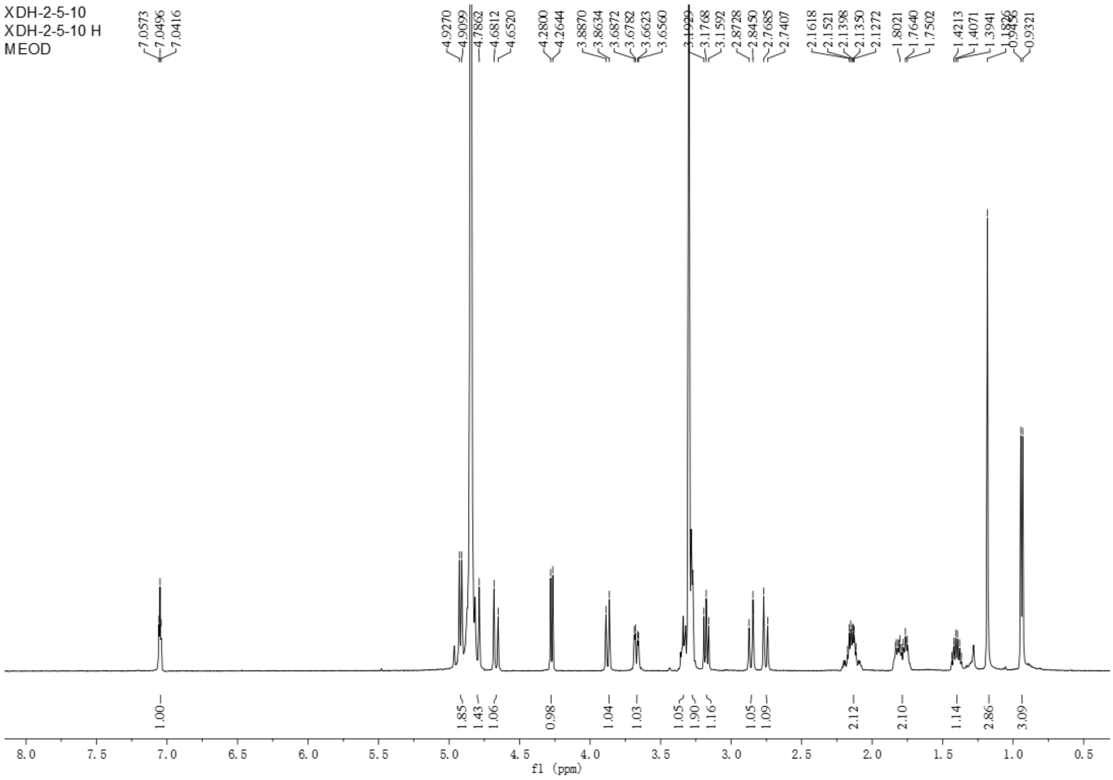


Figure S2: ^{1}H NMR spectrum (500MHz, CD_3OD) of **1**

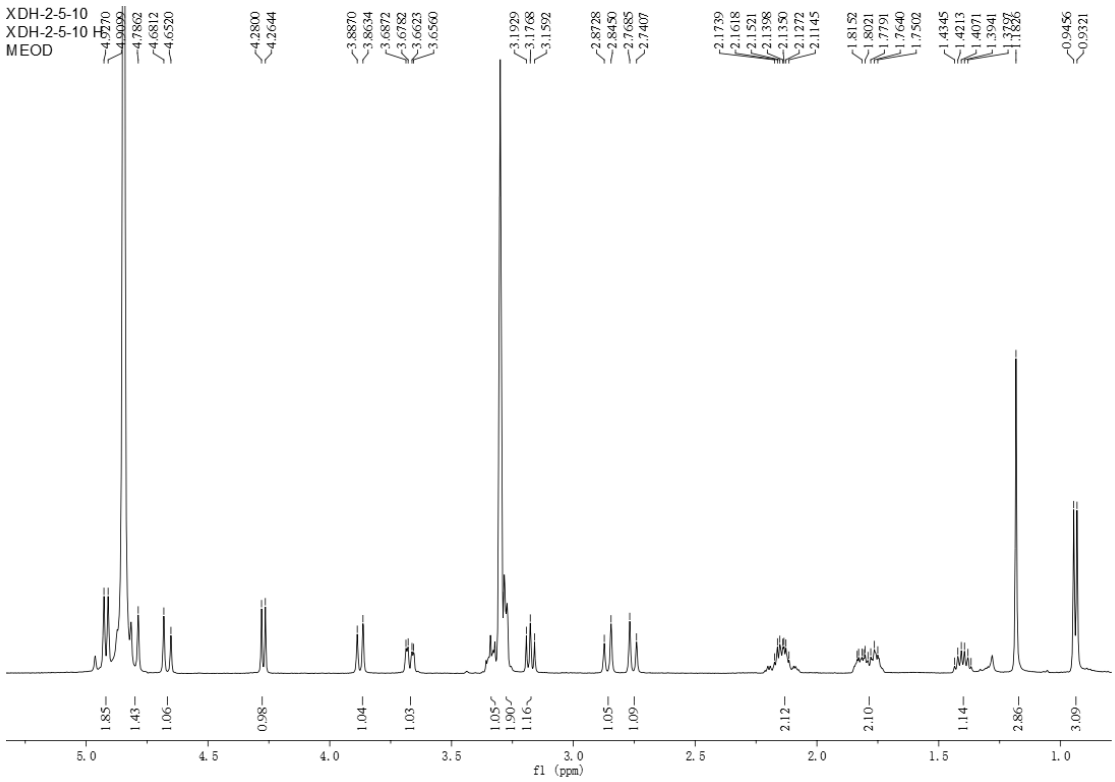


Figure S3: The enhanced ^{1}H NMR spectrum (500MHz, CD_3OD) of **1**

(From δ_H 0.8 ppm to δ_H 5.2 ppm)

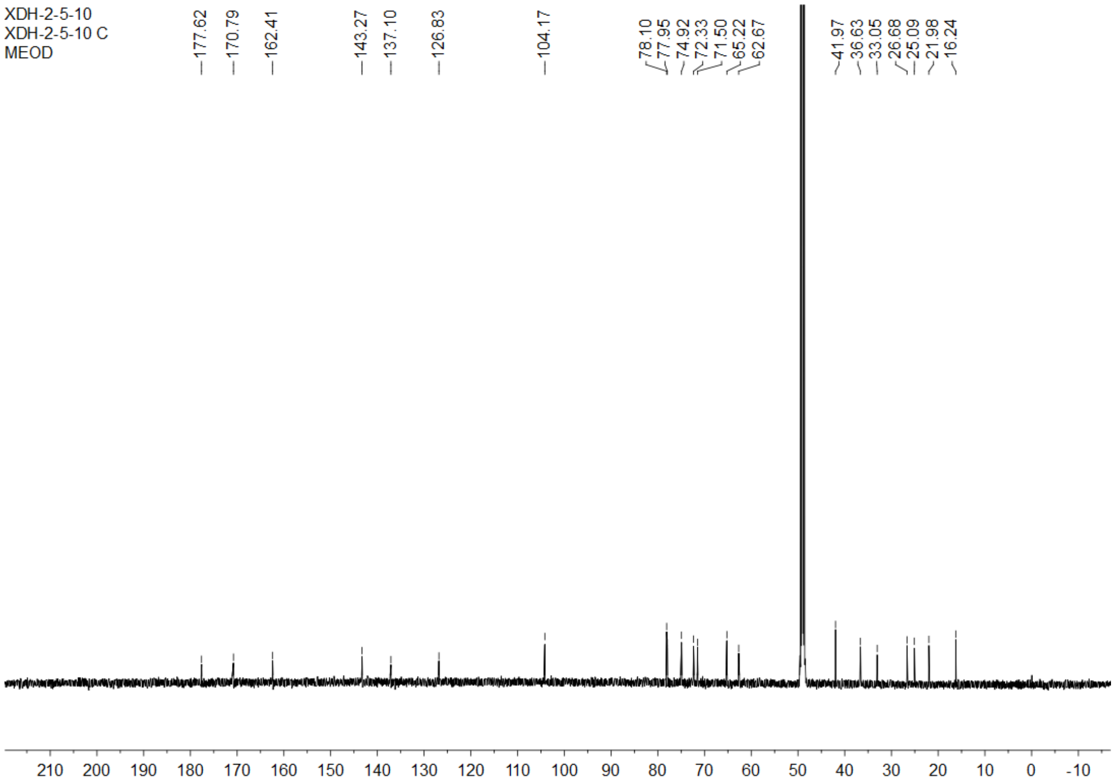


Figure S4: [13]C NMR spectrum (125MHz, CD_3OD) of **1**

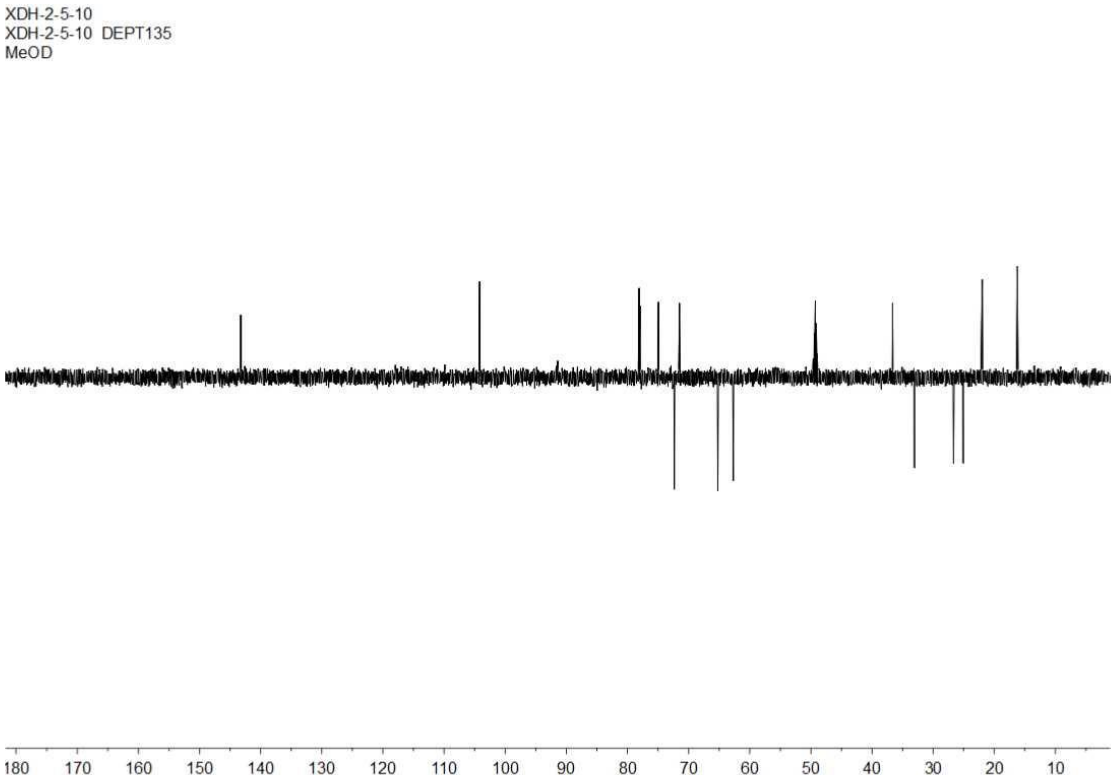


Figure S5: DEPT135 spectrum of **1**

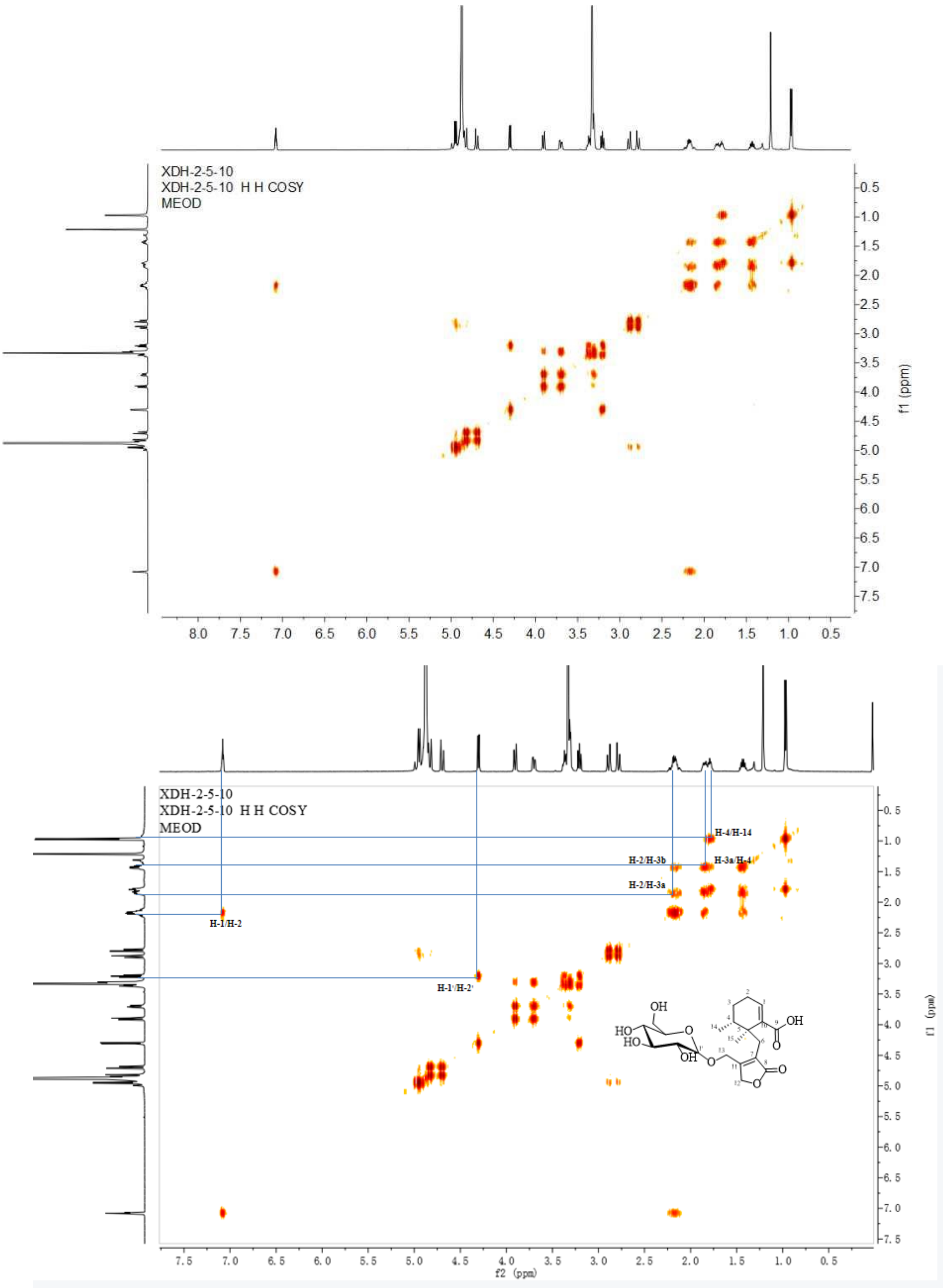


Figure S6: ^{1}H-^{1}H COSY spectrum of **1**

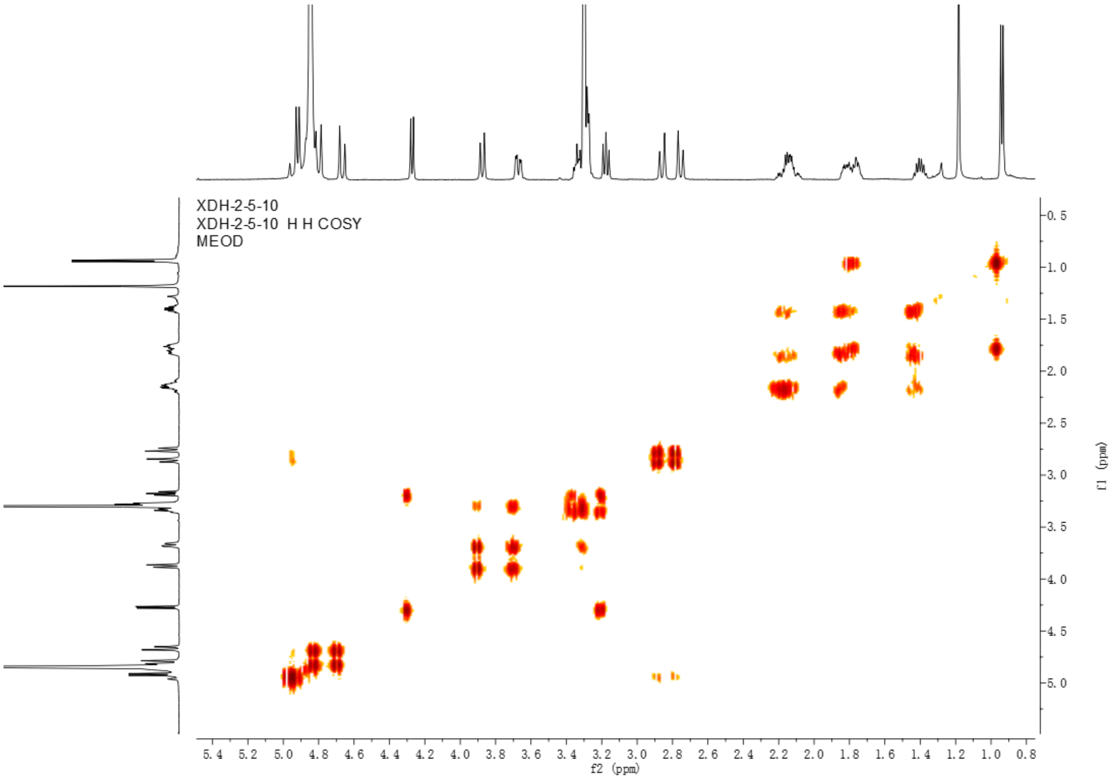


Figure S7: The enhanced ^{1}H-^{1}H COSY spectrum of **1**(From δ_H 0.8 ppm to δ_H 5.2 ppm)

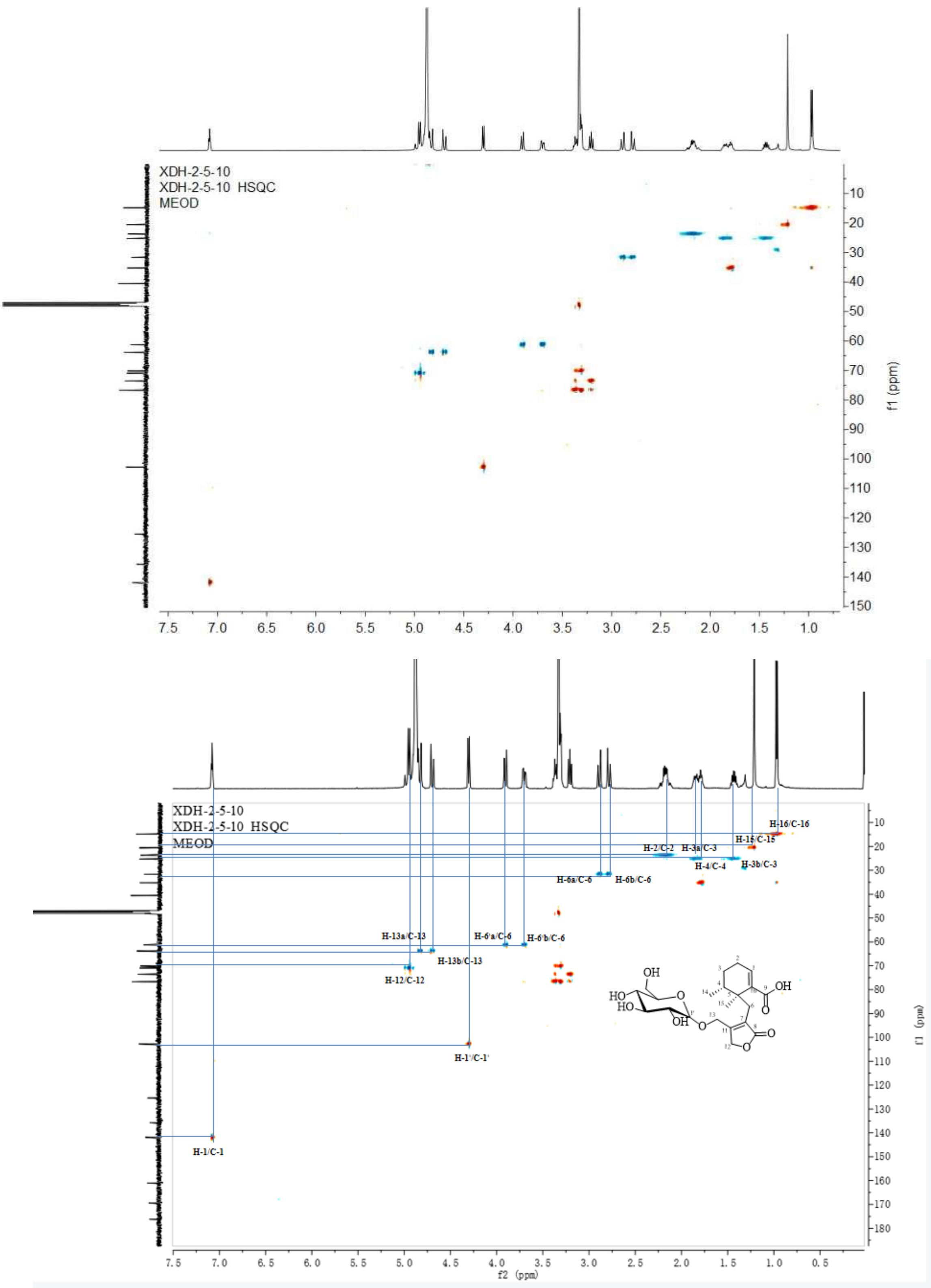


Figure S8:HSQC spectrum of **1**

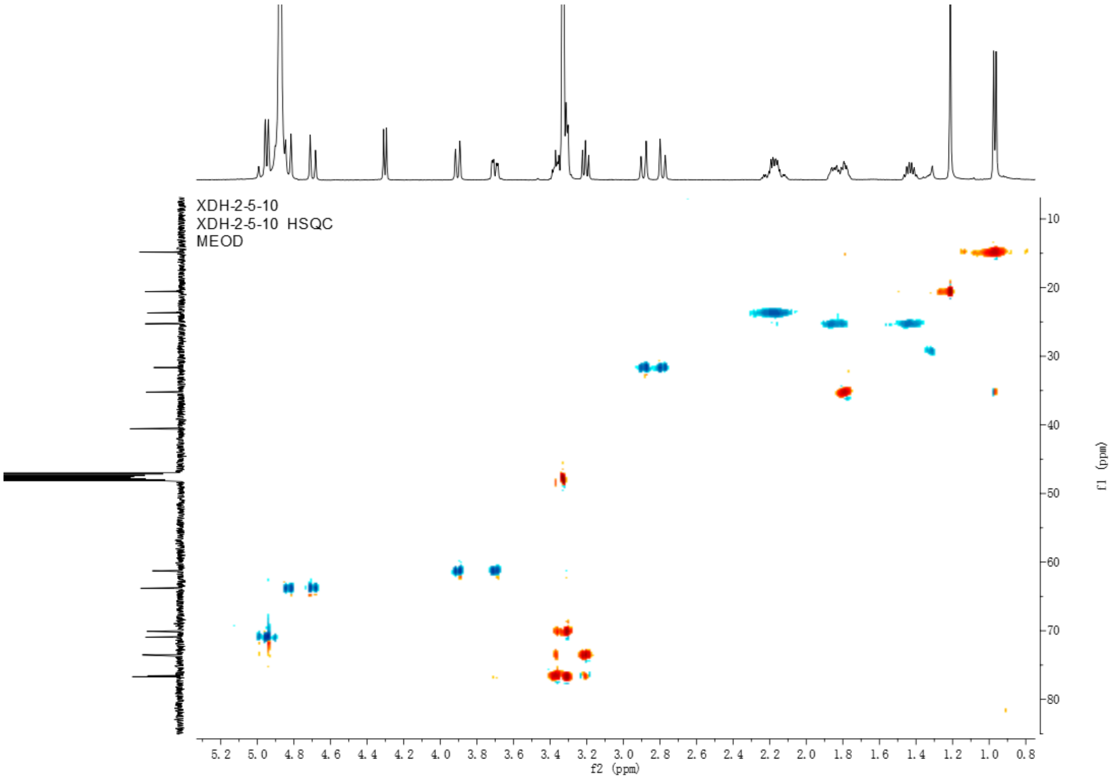
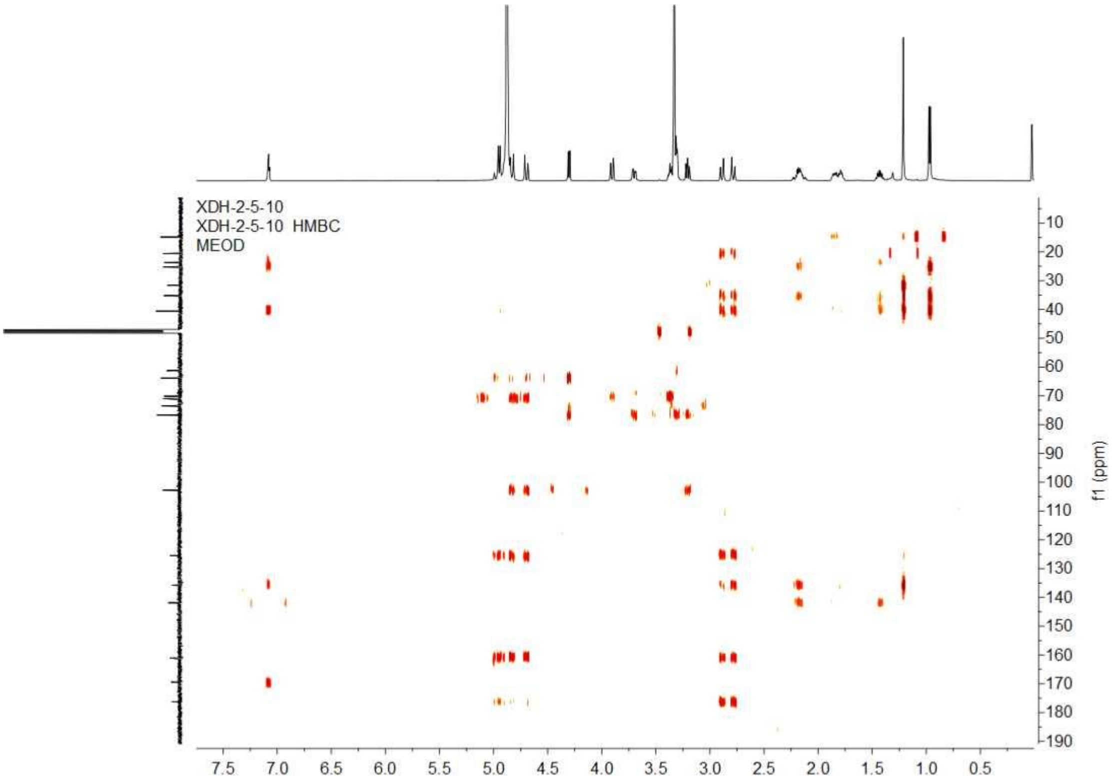


Figure S9: The enhanced HSQC spectrum of **1**(From δ_C 10 ppm to δ_C 90 ppm)



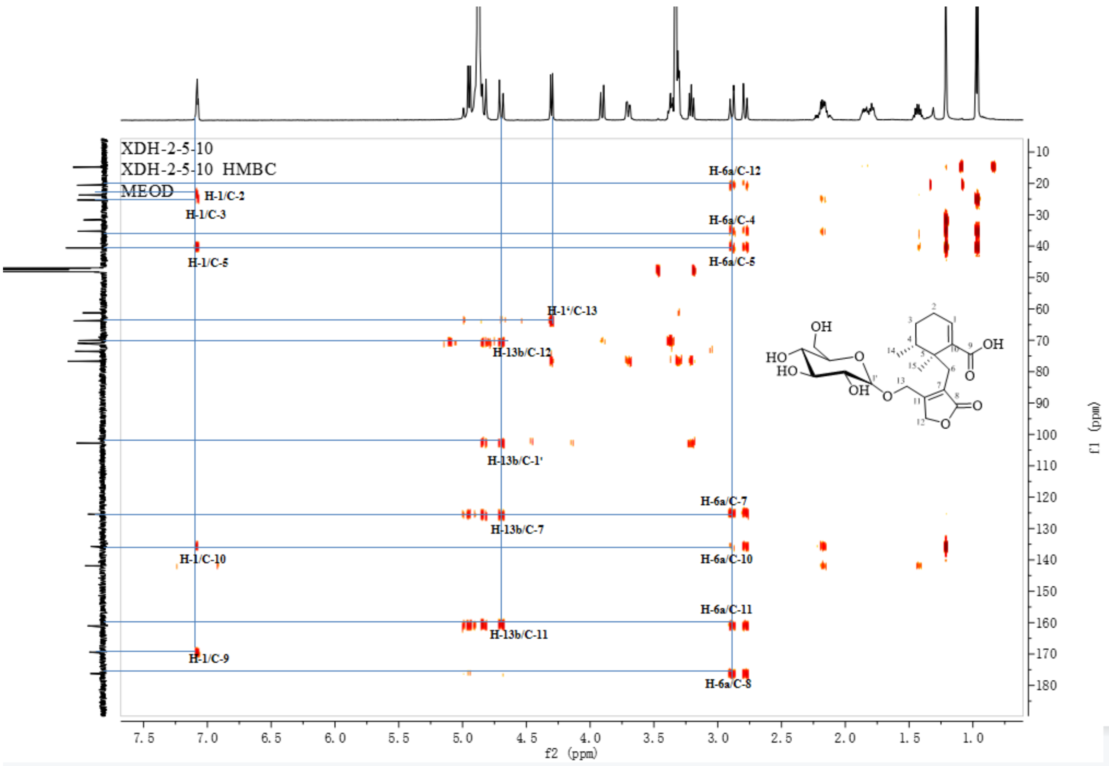


Figure S10: HMBC spectrum of **1**

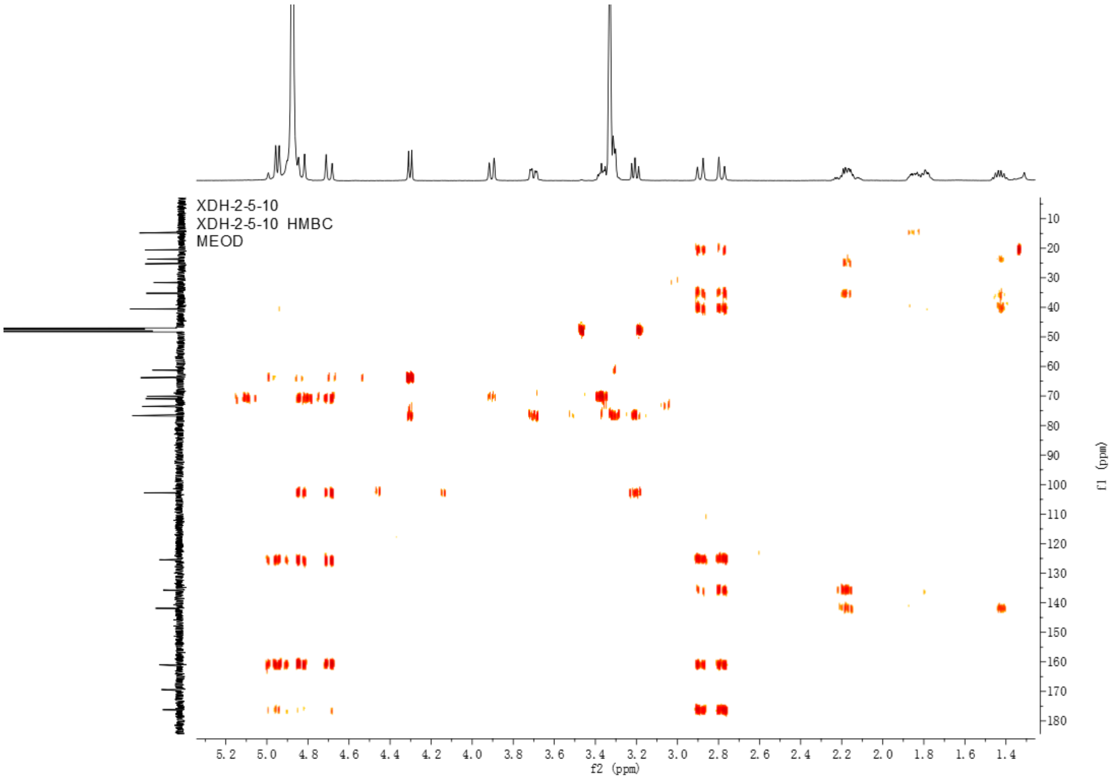
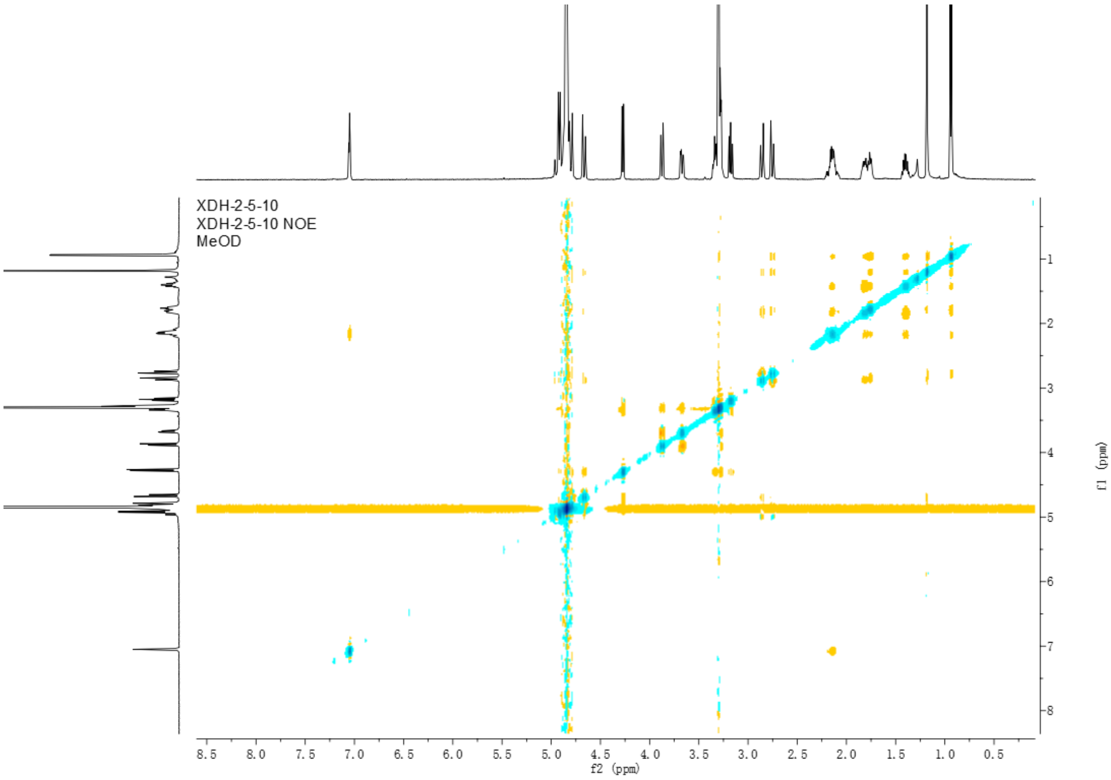


Figure S11: The enhanced HMBC spectrum of **1**(From δ_H 1.4 ppm to δ_H 5.2 ppm)



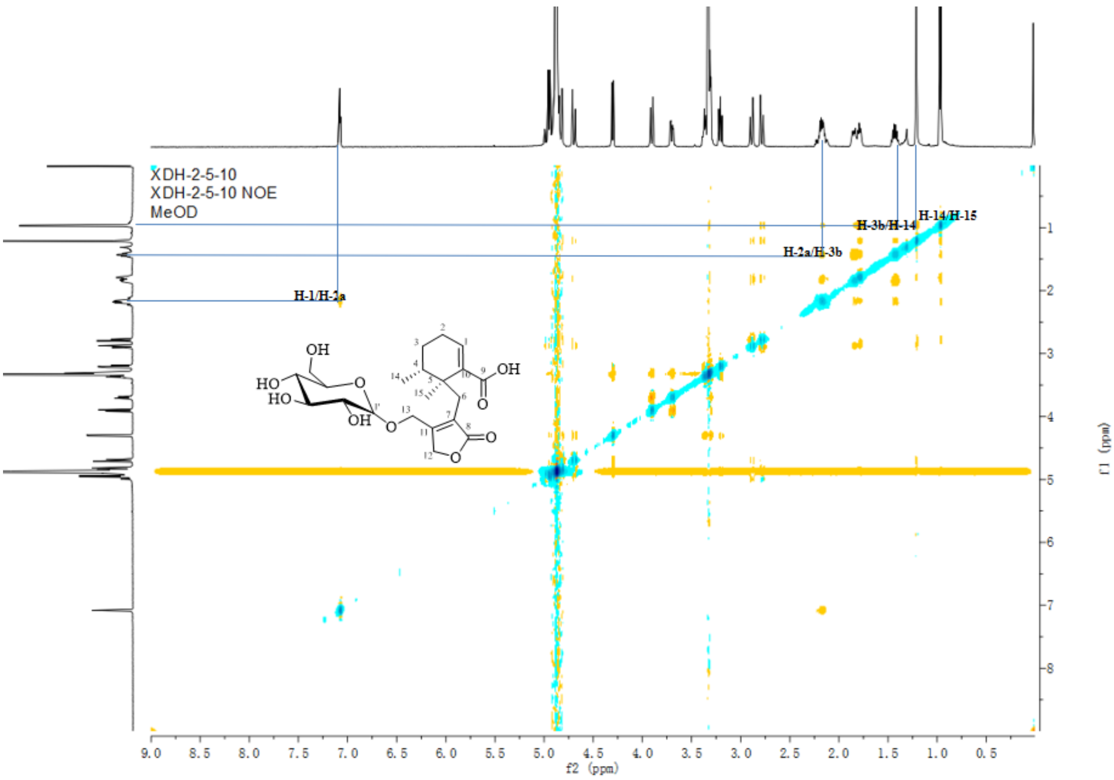


Figure S12: NOESY spectrum of **1**

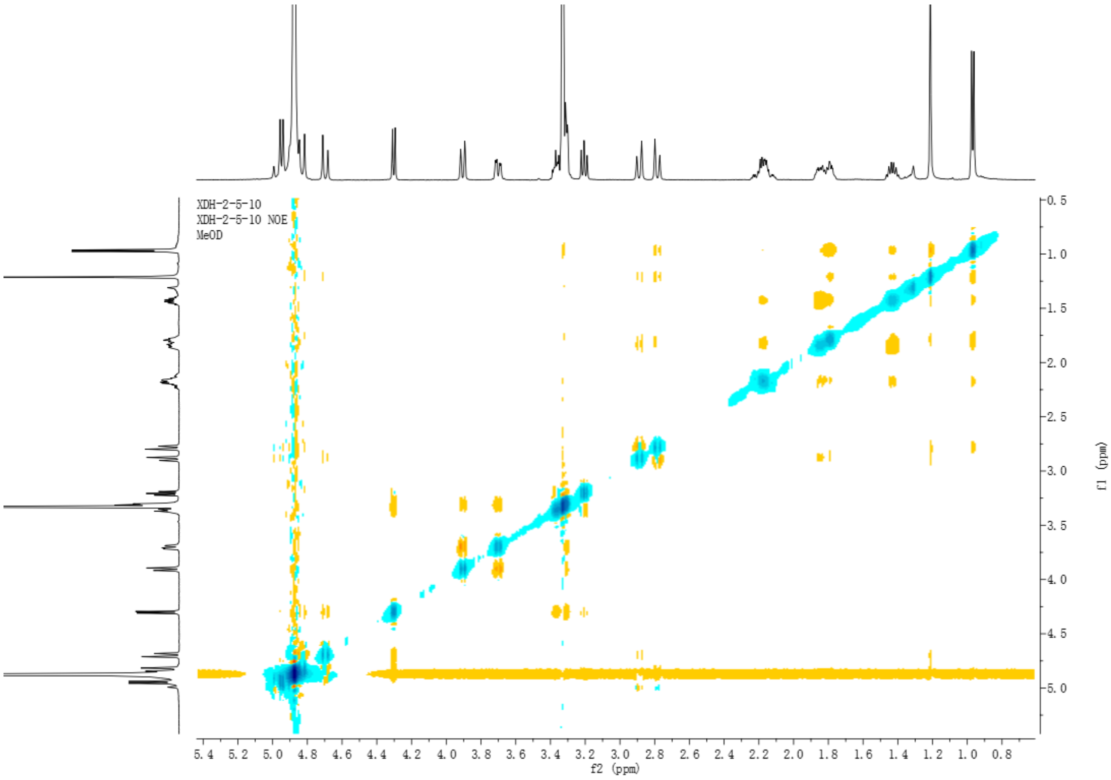


Figure S13: The enhanced NOESY spectrum of **1** (From δ_H 0.5 ppm to δ_H 5.0 ppm)

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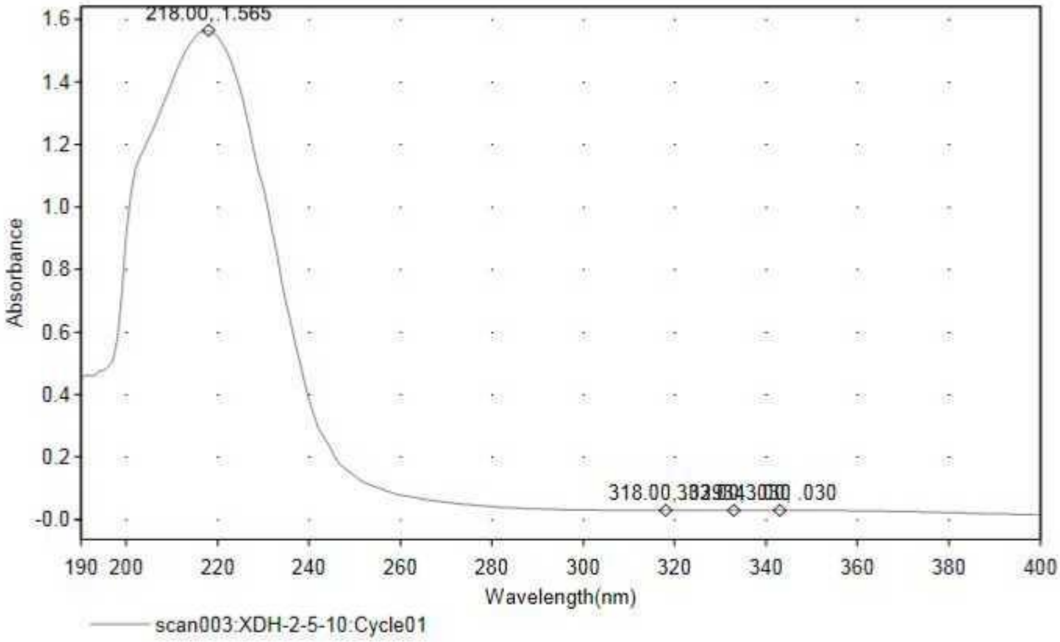
Operator Name	(None Entered)	Date of Report	2020/12/24
Department	(None Entered)	Time of Report	21:27:43下午
Organization	(None Entered)		
Information	(None Entered)		

Scan Graph



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

nm	A	Peak Pick Method
218.00	1.565	Find 8 Peaks Above -3.0000 A
318.00	.029	Start Wavelength190.00 nm
333.00	.030	Stop Wavelength400.00 nm
343.00	.030	Sort By Wavelength
Sensitivity	High	

Figure S14:UV spectrum of **1**

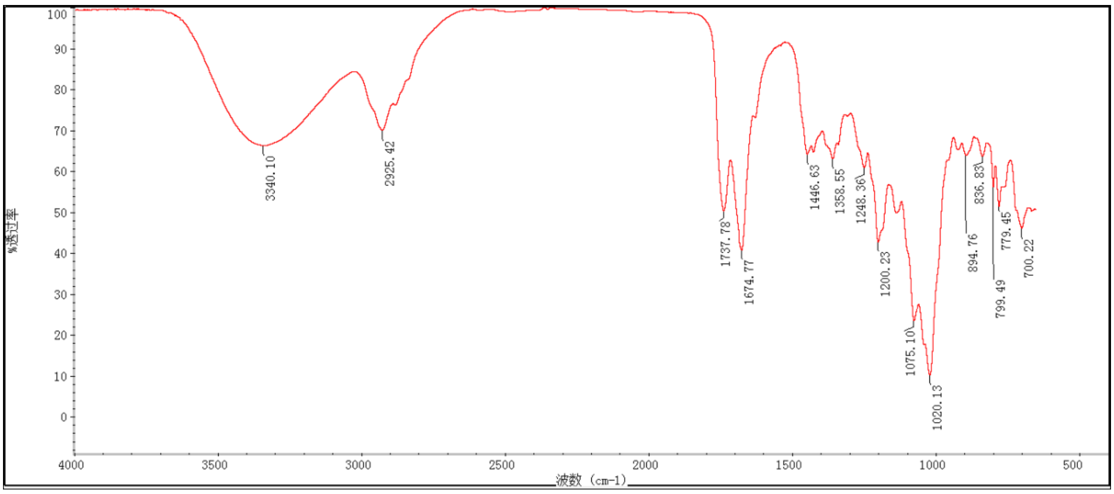


Figure S15: IR spectrum of **1**

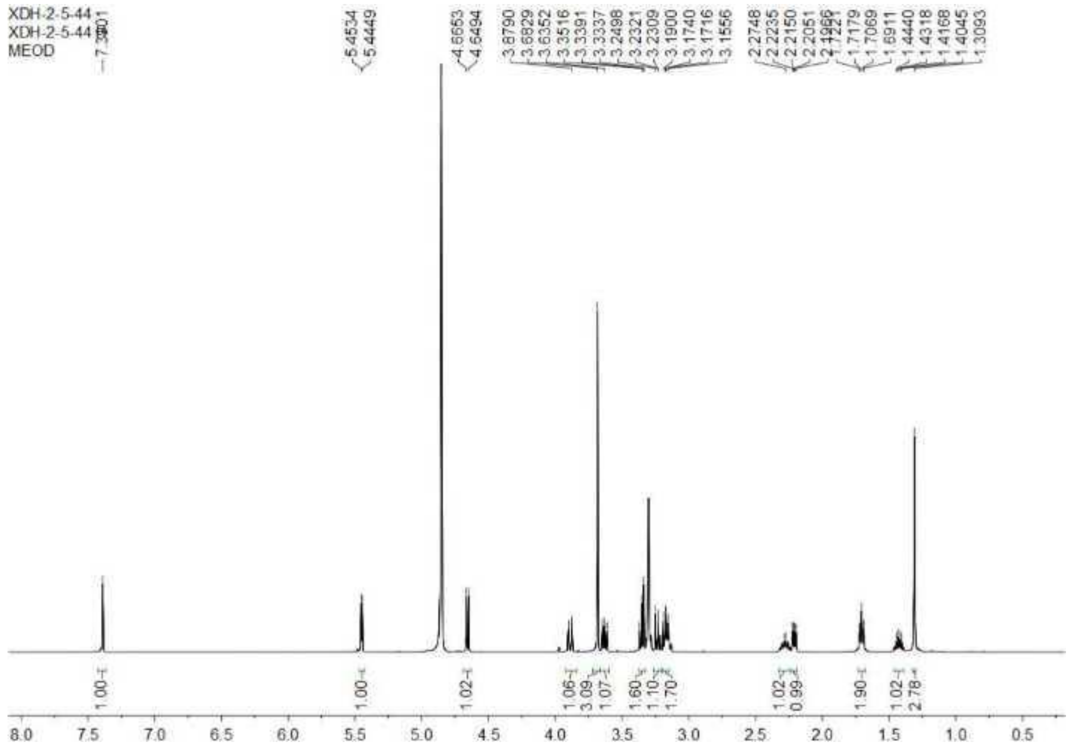


Figure S16: ^{1}H NMR spectrum (500MHz, CD_3OD) of **2**

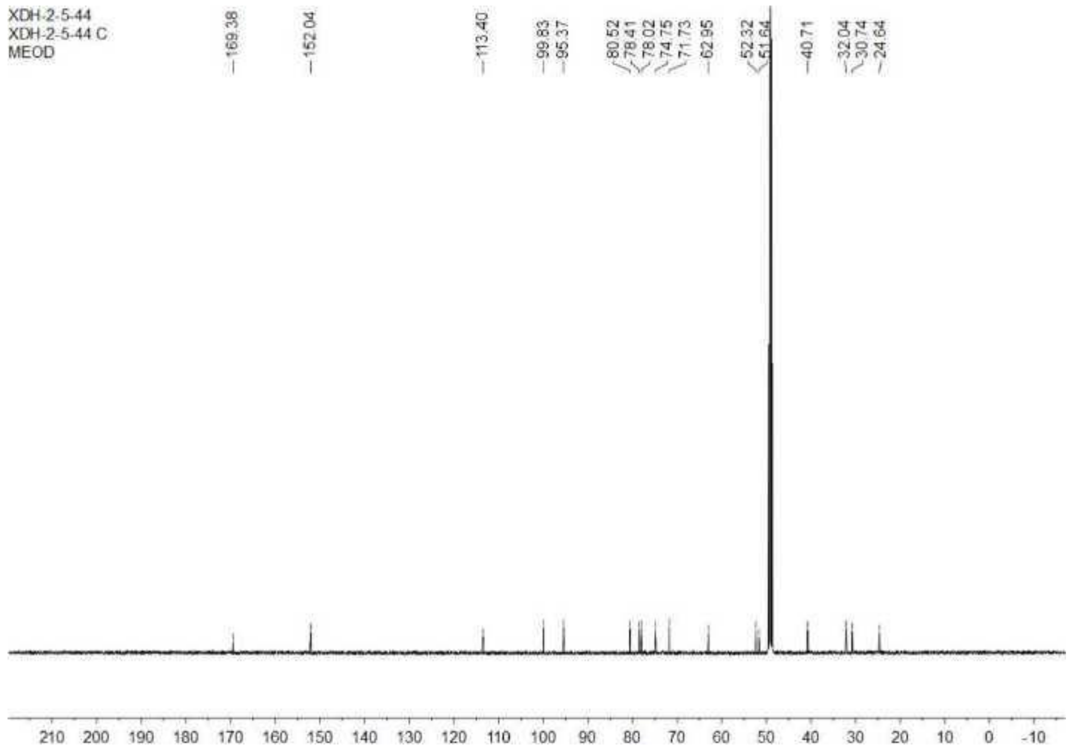


Figure S17:^{13}C NMR spectrum (125MHz, CD_3OD) of **2**

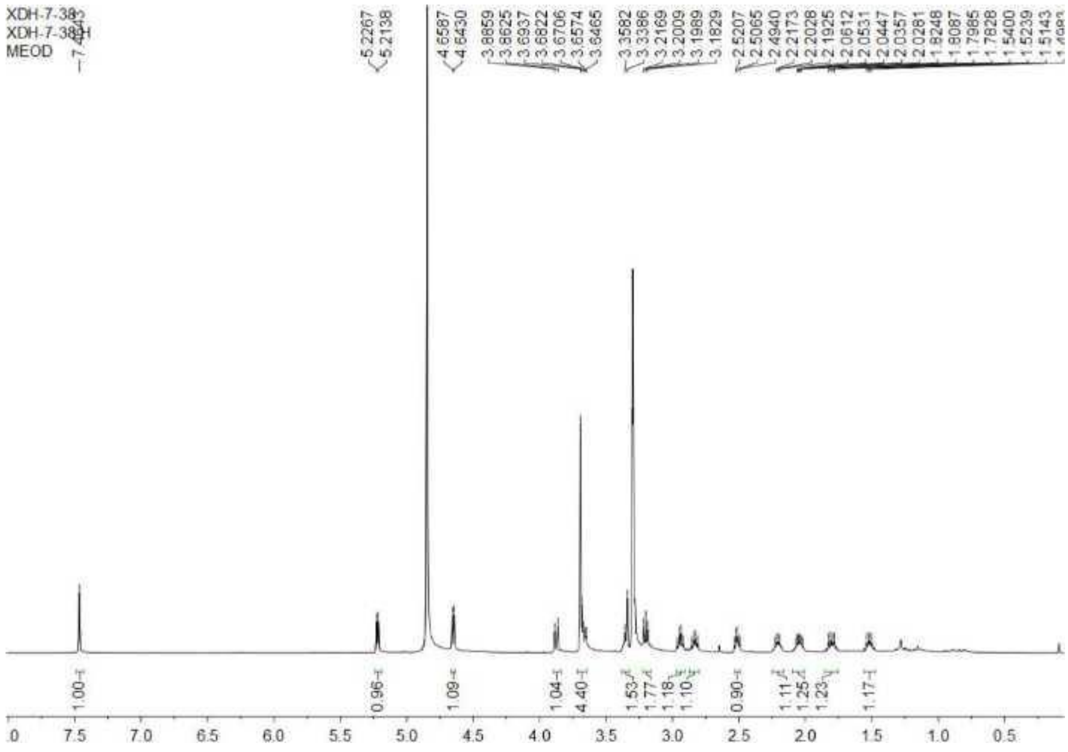


Figure S18: ^{1}H NMR spectrum (500MHz, $CDCl_3$) of **3**

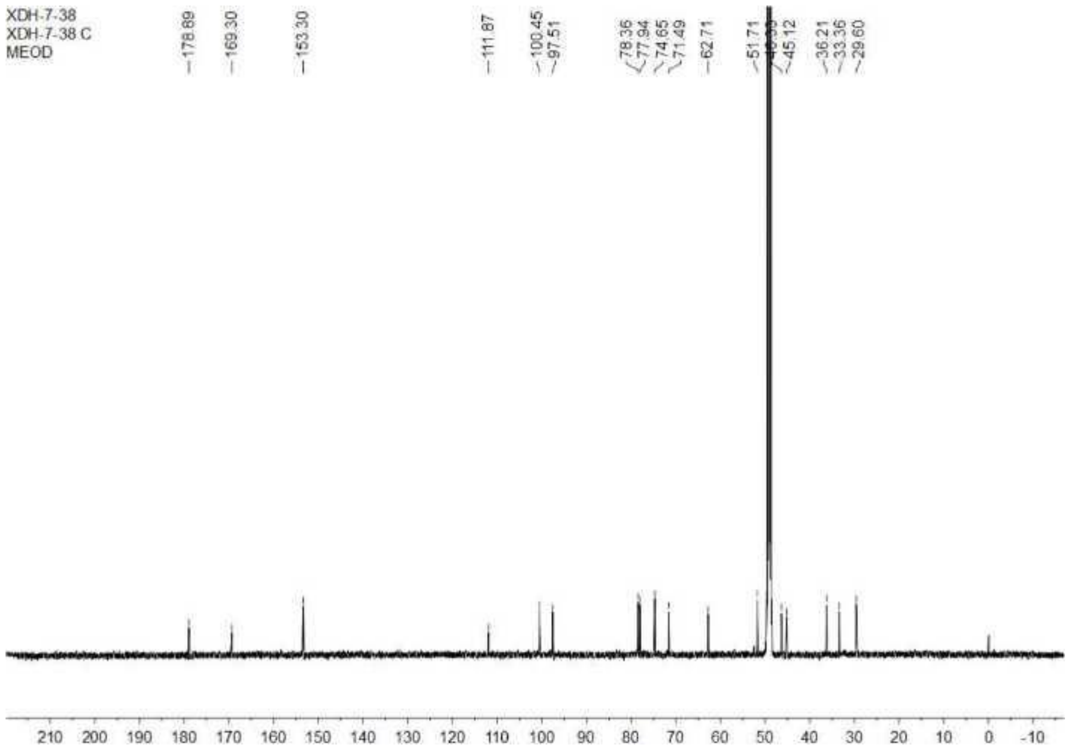


Figure S19: ^{13}C NMR spectrum (125MHz, CD_3OD) of **3**

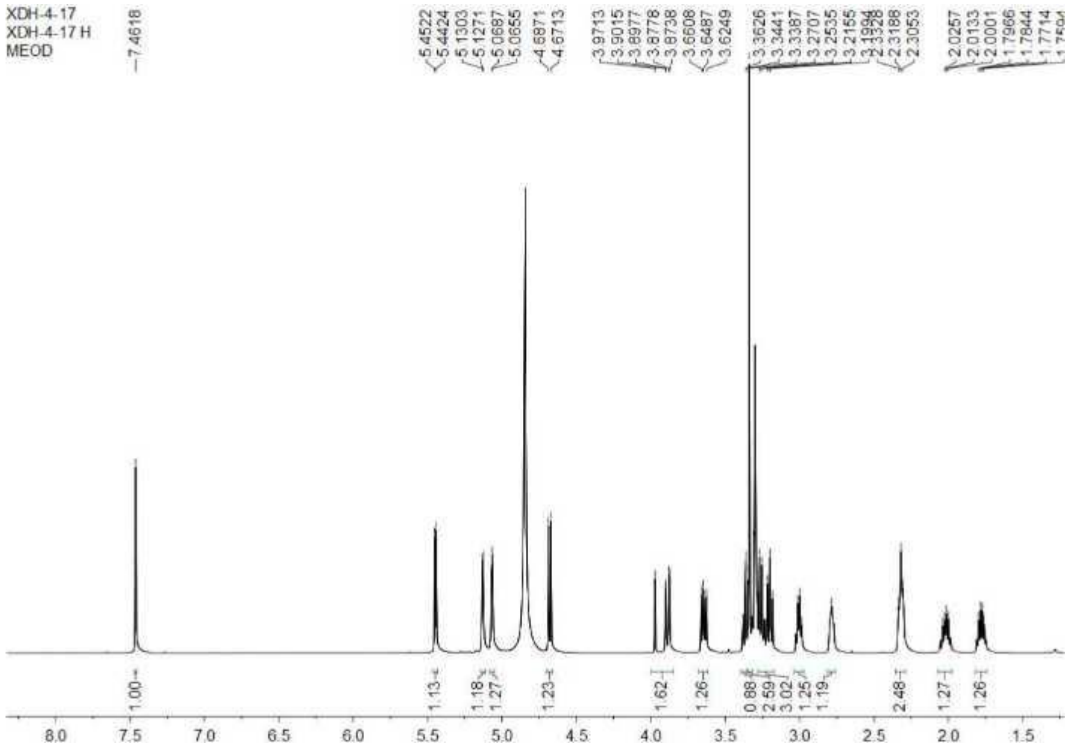


Figure S20: ^{1}H NMR spectrum (500MHz, $CDCl_3$) of **4**

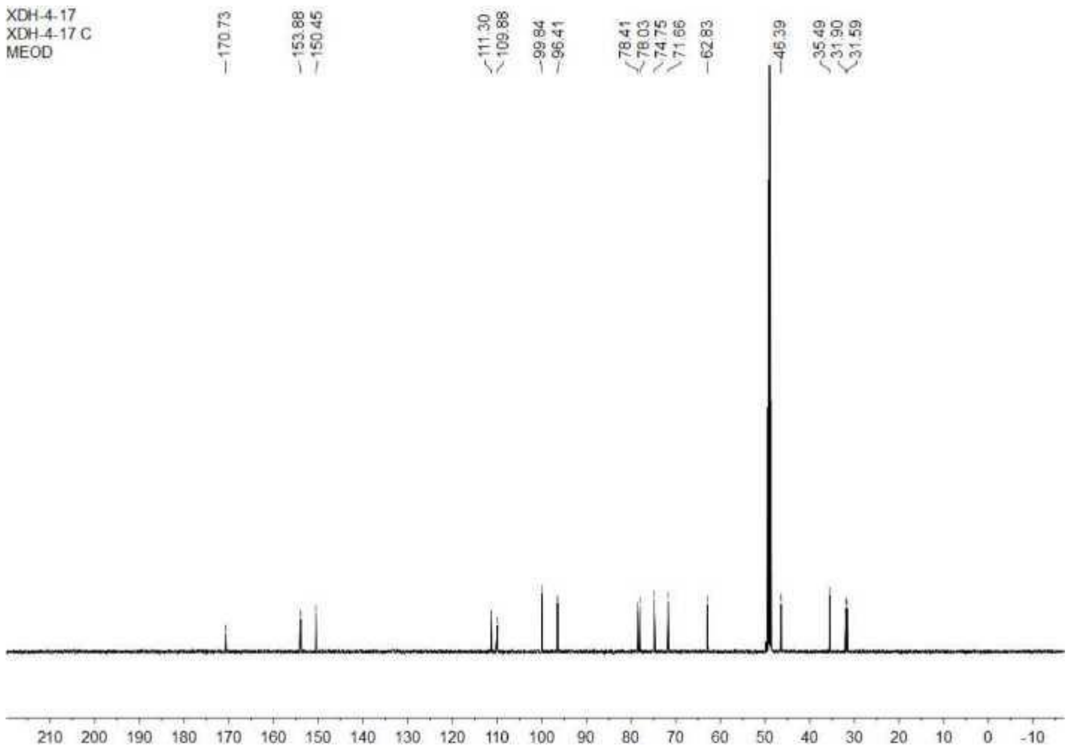


Figure S21: ^{13}C NMR spectrum (125MHz,$CDCl_3$) of **4**

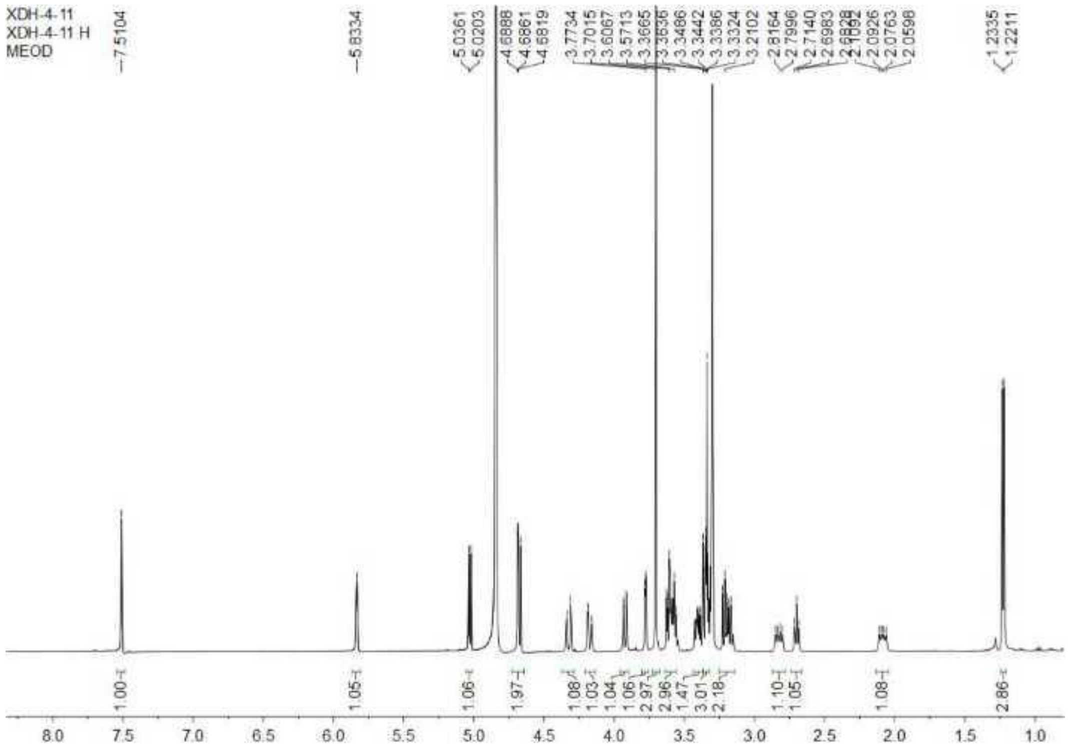


Figure S22:[1]H NMR spectrum (500MHz, CD_3OD) of **5**

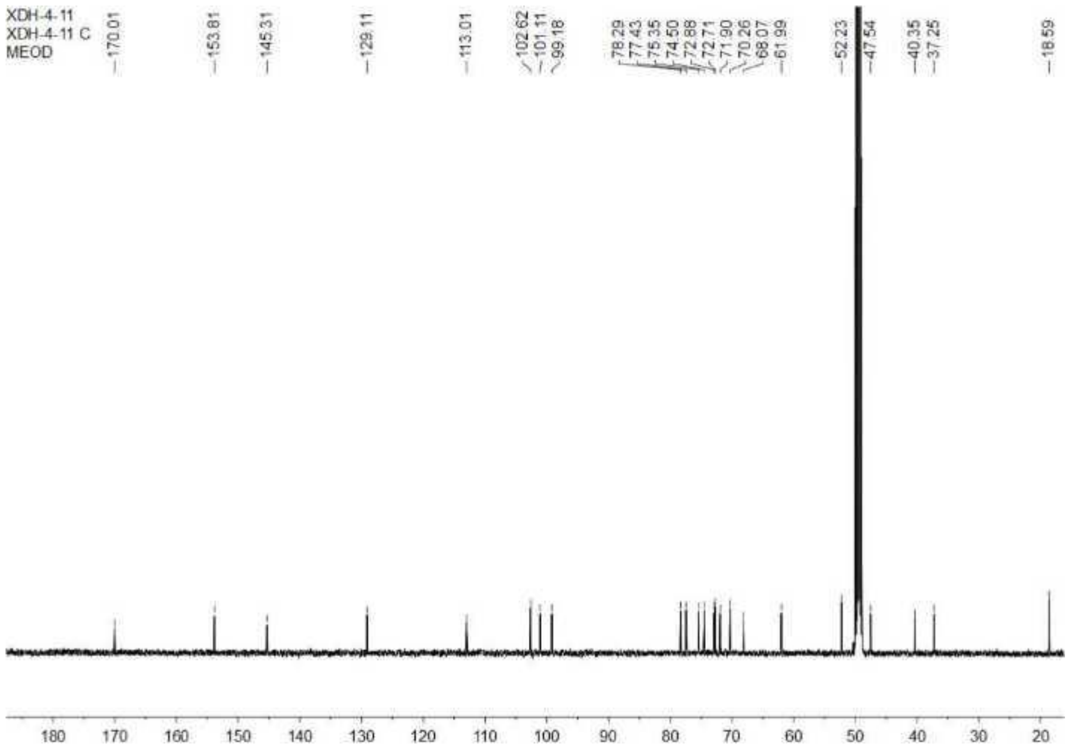


Figure S23: ^{13}C NMR spectrum (125MHz, CD_3OD) of **5**

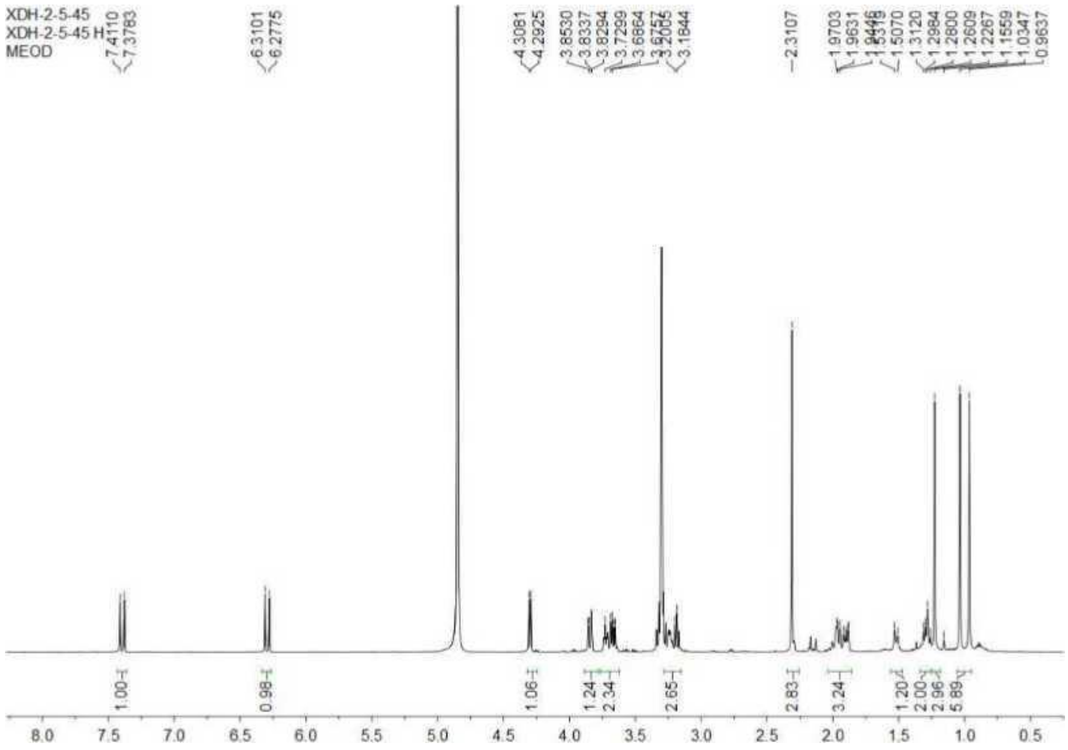


Figure S24: ^{1}H NMR spectrum (500MHz, CD_3OD) of **6**

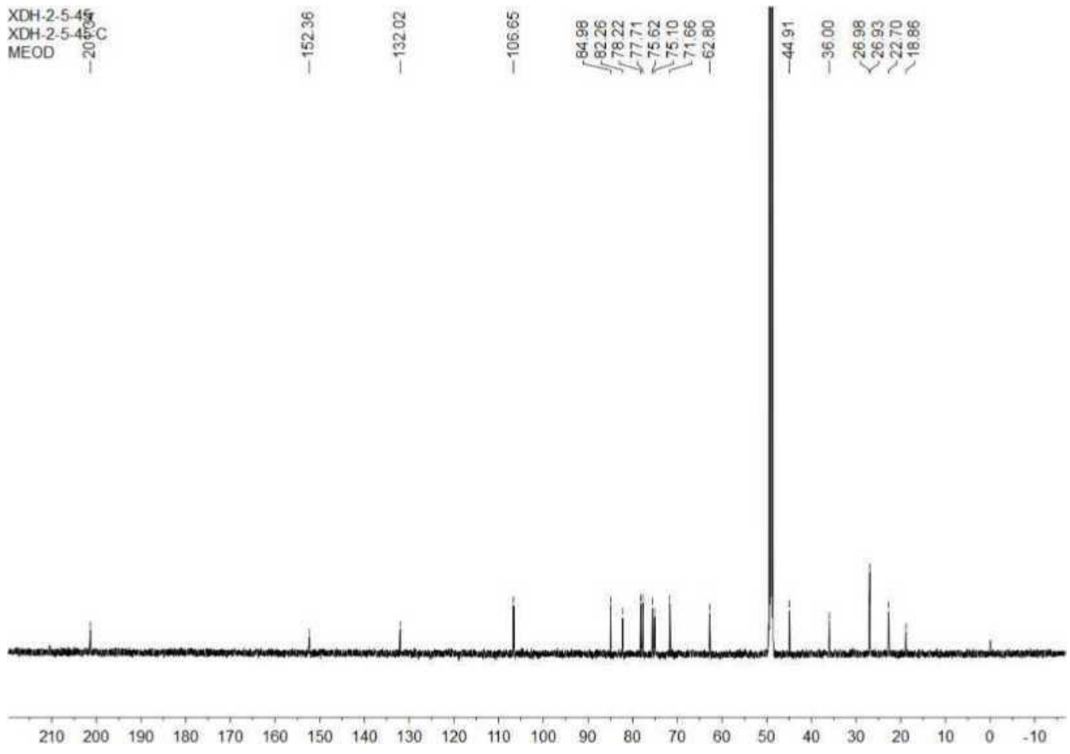


Figure S25: ^{13}C NMR spectrum (125MHz, CD_3OD) of **6**

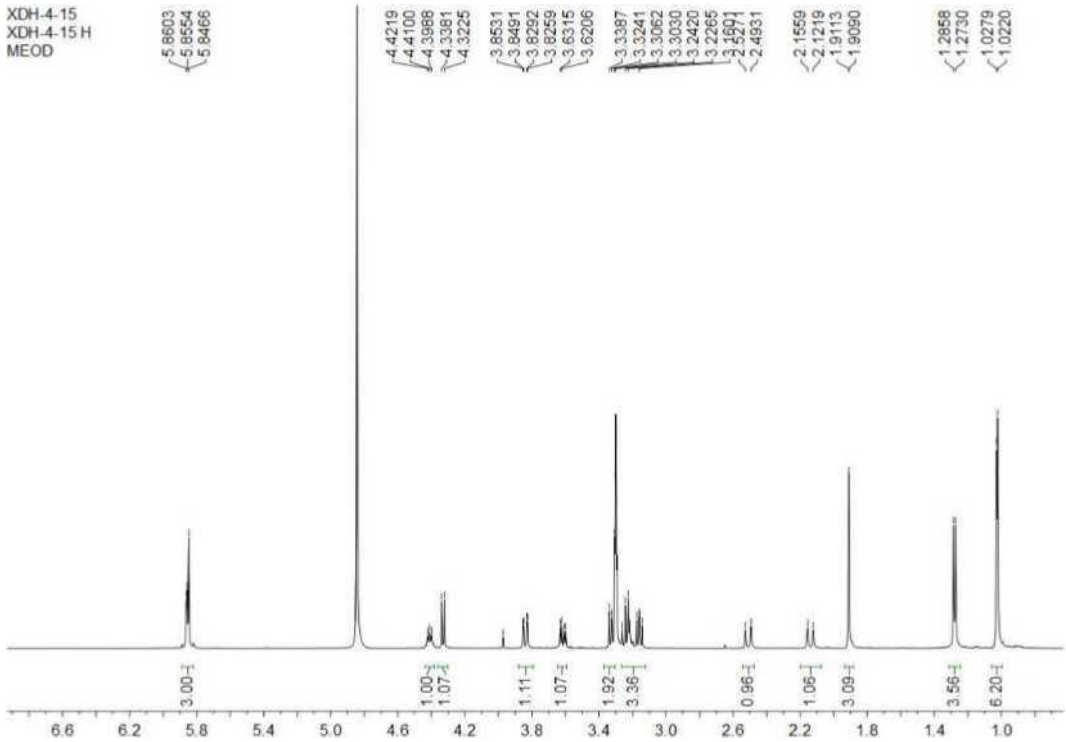


Figure S26: ^{1}H NMR spectrum (500MHz, CD_3OD) of **7**

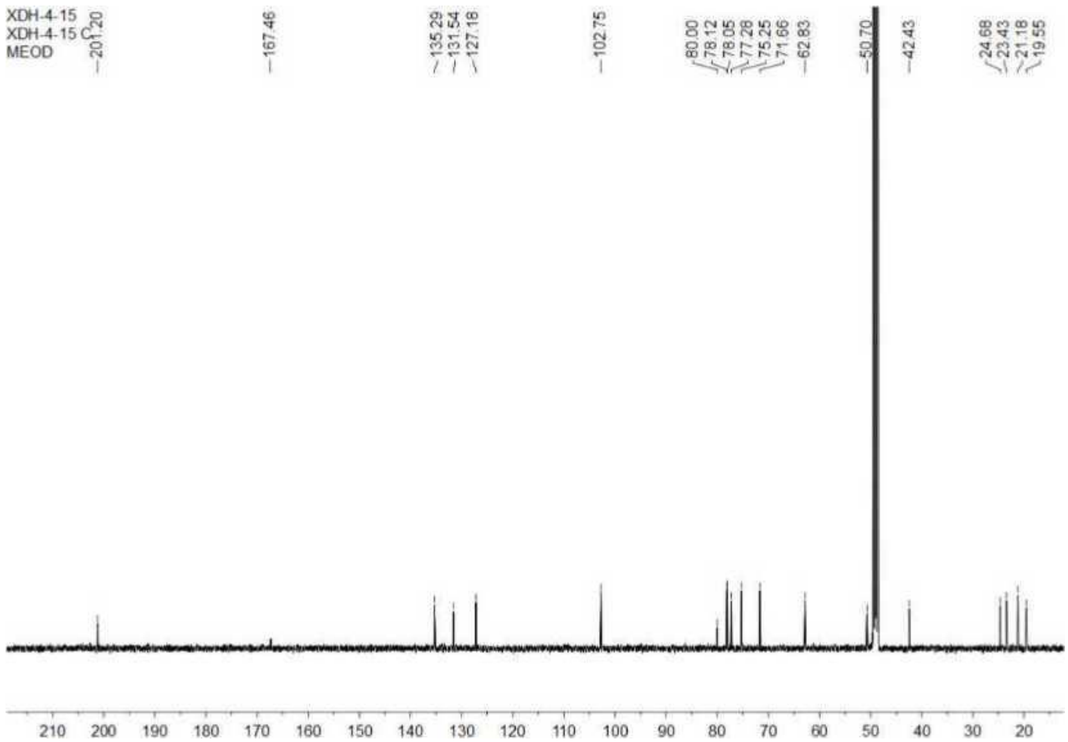


Figure S27:^{13}C NMR spectrum (125MHz, CD_3OD) of **7**

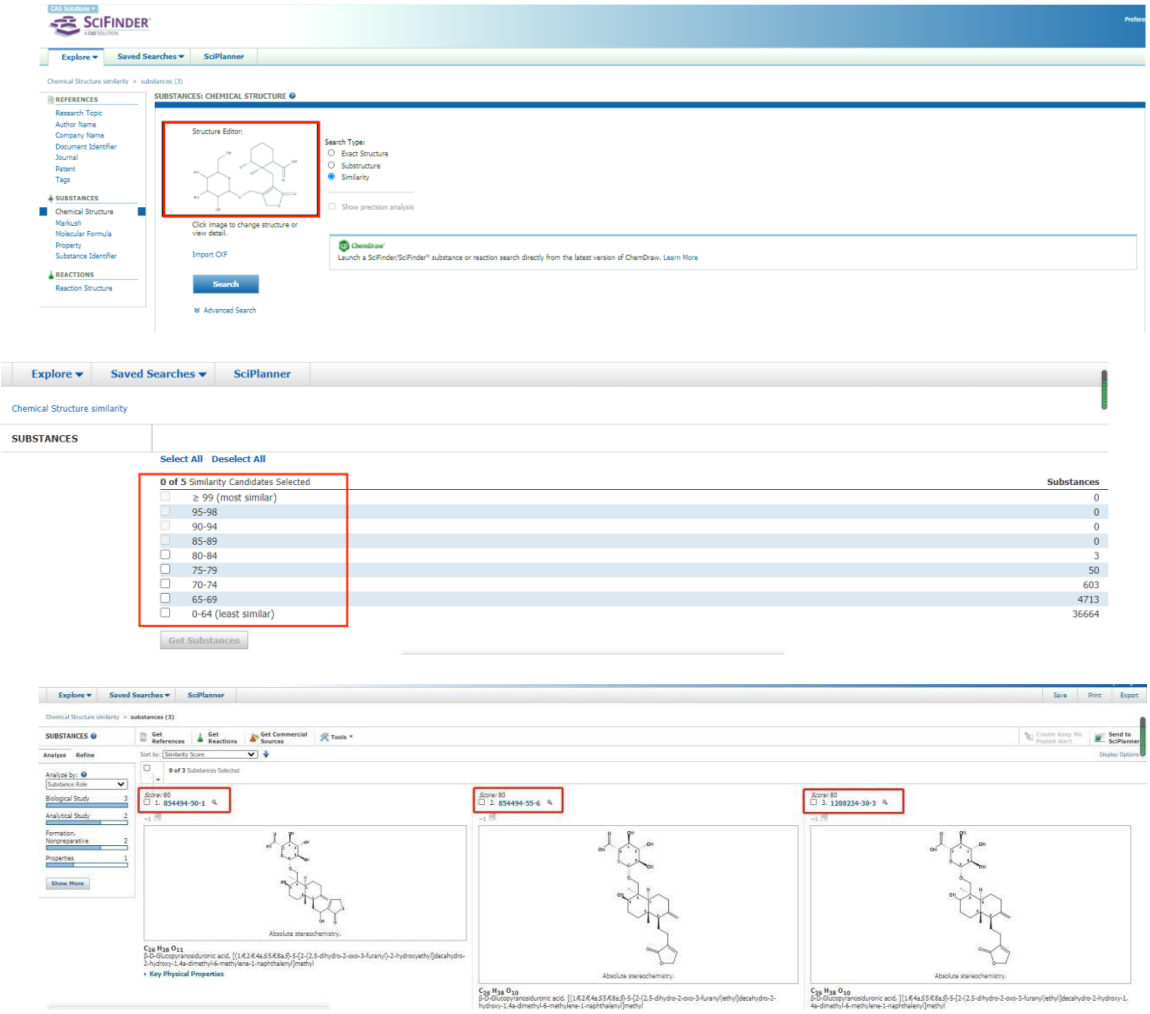
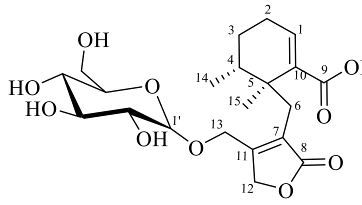
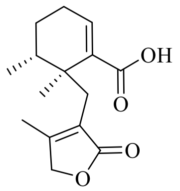


Figure S28: The Scifinder similarity report for new compound **1**



1



4,5,11-trimethyl-8,9-seco-1(10),7(11)-eremophiladien -8,12-olid-9-oic acid

Table1 : 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) 1.40 (1H, m)	26.7	1.90 (1H, m, H-3'b) 1.43 (1H, m, H-3b)	25.3
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) 2.75 (1H, d, J = 13.9 Hz)	33.1	2.84 (1H, d, J = 13.7 Hz) 2.74 (1H, d, J = 13.7 Hz)	31.7
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) 4.67 (1H, d, J = 14.6 Hz)	65.2	2.06 (3H, s)	13.2
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) 3.67 (1H, m)	62.7		

[a] Recorded δ in ppm, J in Hz, in CD_3OD. [b] Recorded in $CDCl_3$.

Table 2 : ^{1}H NMR data of compounds **1−7** (δ in ppm, J in Hz, in CD_3OD 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)	7.39 (1H, s)	7.46 (1H, brs)	7.46 (1H, brs)	7.51 (1H, brs)	1.95 (1H, m)	
	1.40 (1H, m)					1.52 (1H, m)	
4	1.76 (1H, overlap)					1.97 (1H, m)	5.84 (1H, brs)
						1.88 (1H, m)	
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)	2.25 (1H, m)	2.21 (1H, m)	2.21 (1H, m)	2.80 (1H, m)		
	2.75 (1H, d, J = 13.9 Hz)	1.43(1H, m)	1.52 (1H, m)	1.52 (1H, m)	2.08 (1H, m)		
7		1.71 (1H, m)	2.06 (1H, m)	2.06 (1H, m)	5.83 (1H, s)	7.40 (1H, d, J = 16.4 Hz)	5.85 (1H, d, J = 2.5 Hz)
			1.80 (1H, m)	1.80 (1H, m)			
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)	4.32 (1H, d, J = 4.3 Hz)	2.31 (3H, s)	1.28 (3H, d, J = 6.4 Hz)
				5.06 (1H, d, J = 1.6 Hz)	4.16 (1H, d, J = 4.3 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)					1.03 (3H, s)	1.91 (3H, s)
	4.67 (1H, d, J = 14.6 Hz)						
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) 3.67 (1H, m)	3.87(1H, overlap) 3.67 (1H, overlap)	3.87 (1H, d, *J* = 11.8 Hz) 3.67 (1H, overlap)	3.88 (1H, d, *J* = 11.9 Hz) 3.65(1H, t, *J* = 6.1 Hz)	3.92 (1H, dd, *J* = 1.8, 11.3 Hz) 3.77 (1H, overlap)	3.84 (1H, dd, *J* = 2.1, 11.9 Hz) 3.67 (1H, overlap)	3.83 (1H, dd, *J* = 2.0, 12.0 Hz) 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		