Supporting Information

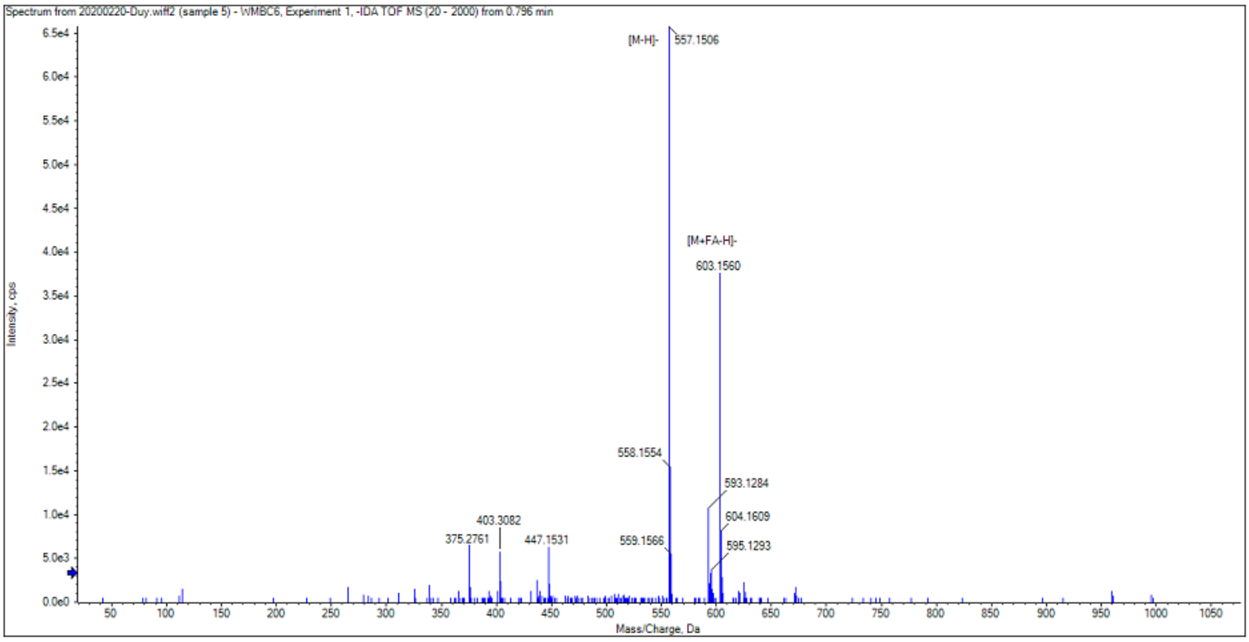
Rec. Nat. Prod. X:X (202X) XX-XX

A New Iridoid Glucoside from the Stems of *Myoporum bontioides* A. Gray Growing in Vietnam

Tran Thi Minh*, Nguyen Thi Viet Thanh and Vu Dinh Hoang

[1]*School of Chemical Engineering, Hanoi University of Science and Technology, Hanoi 112456, Vietnam*

Table of Contents	Page



Hit	Formula	m/z	RDB	ppm	MS Rank	MSMS ppm	MSMS Rank	Found
1	C24H30O15	603.15667	10.0	1.4	1			NA/NA

Figure S1: HR-ESI Mass Spectrum of Myobontioside E (**1**)

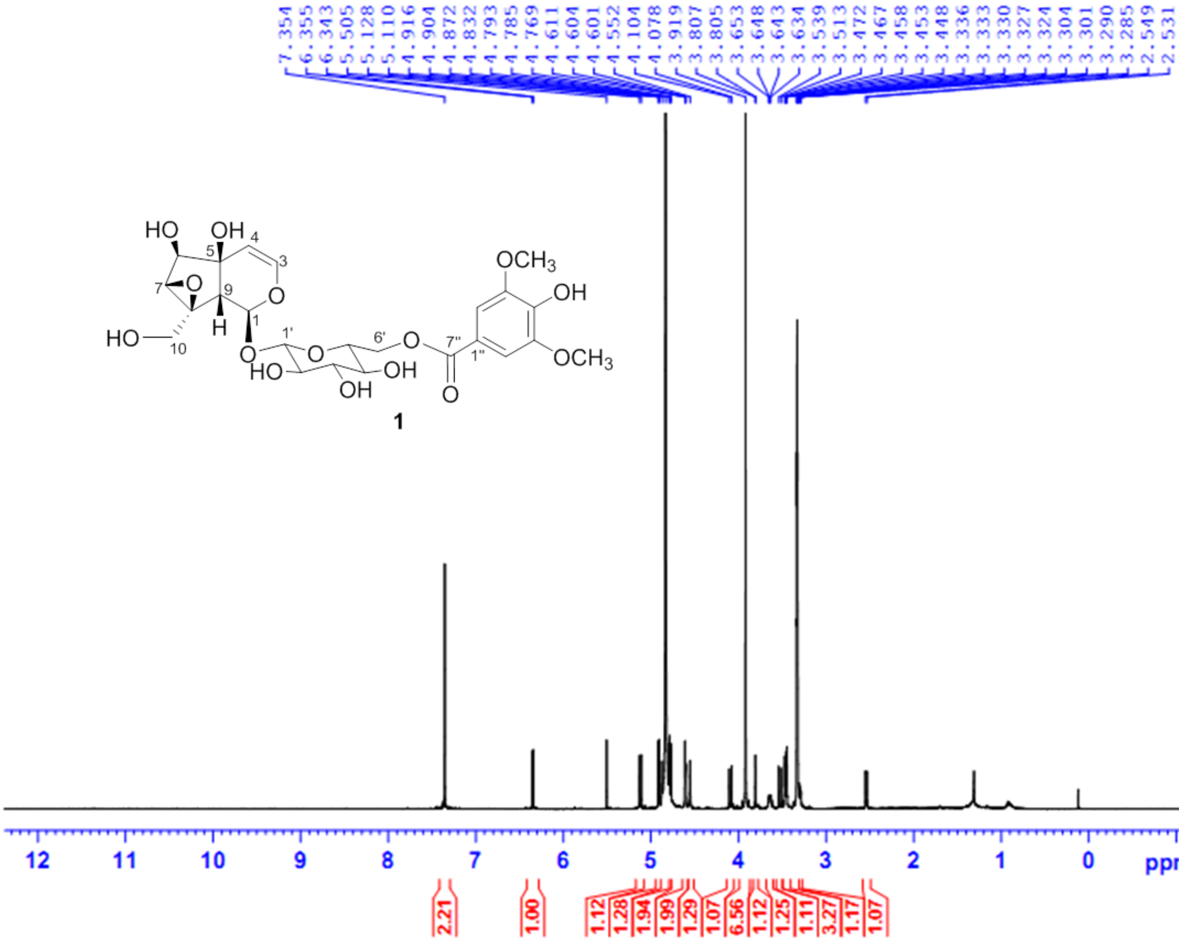


Figure S2: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Myobontioside E (**1**)

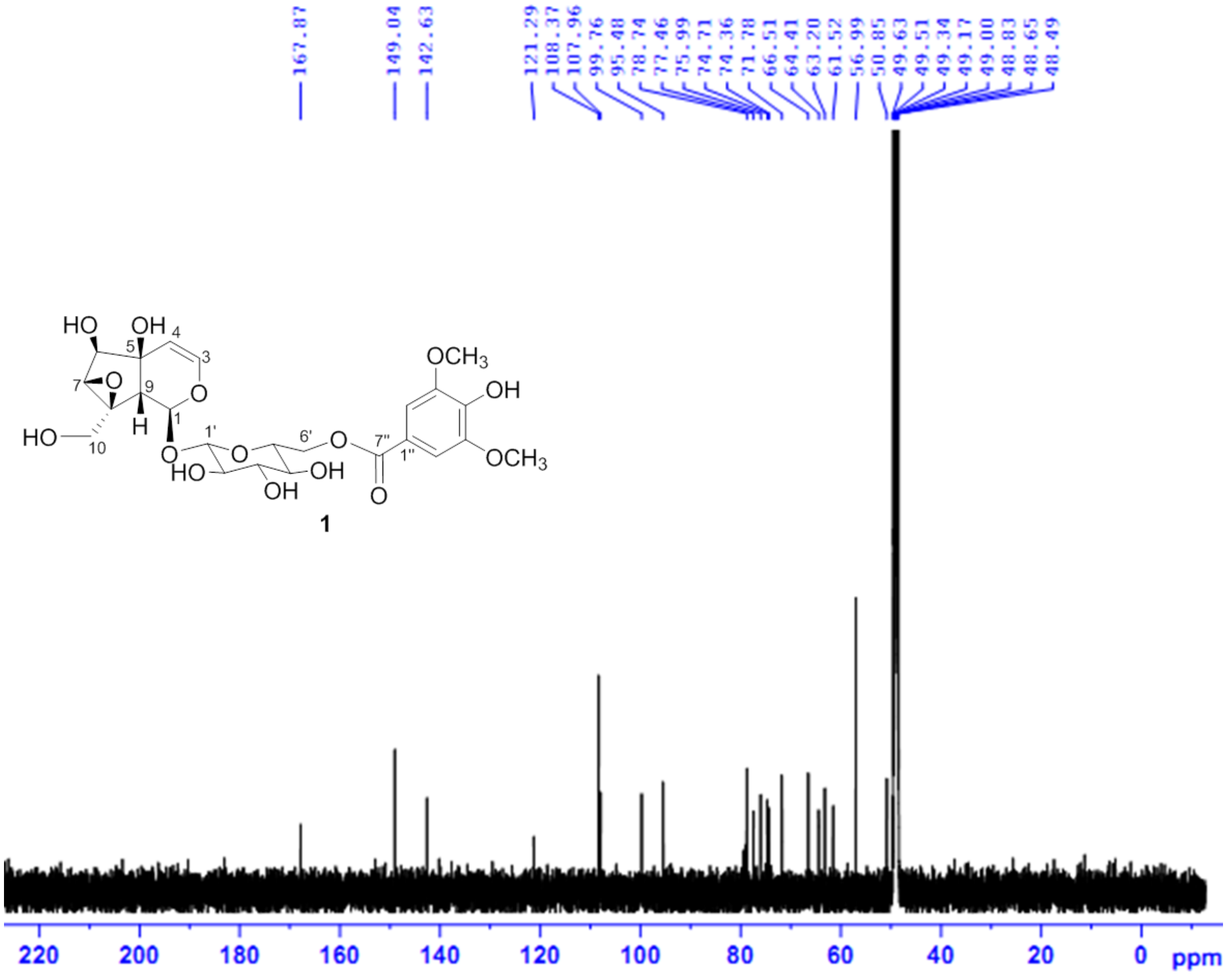


Figure S3: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Myobontioside E (**1**)

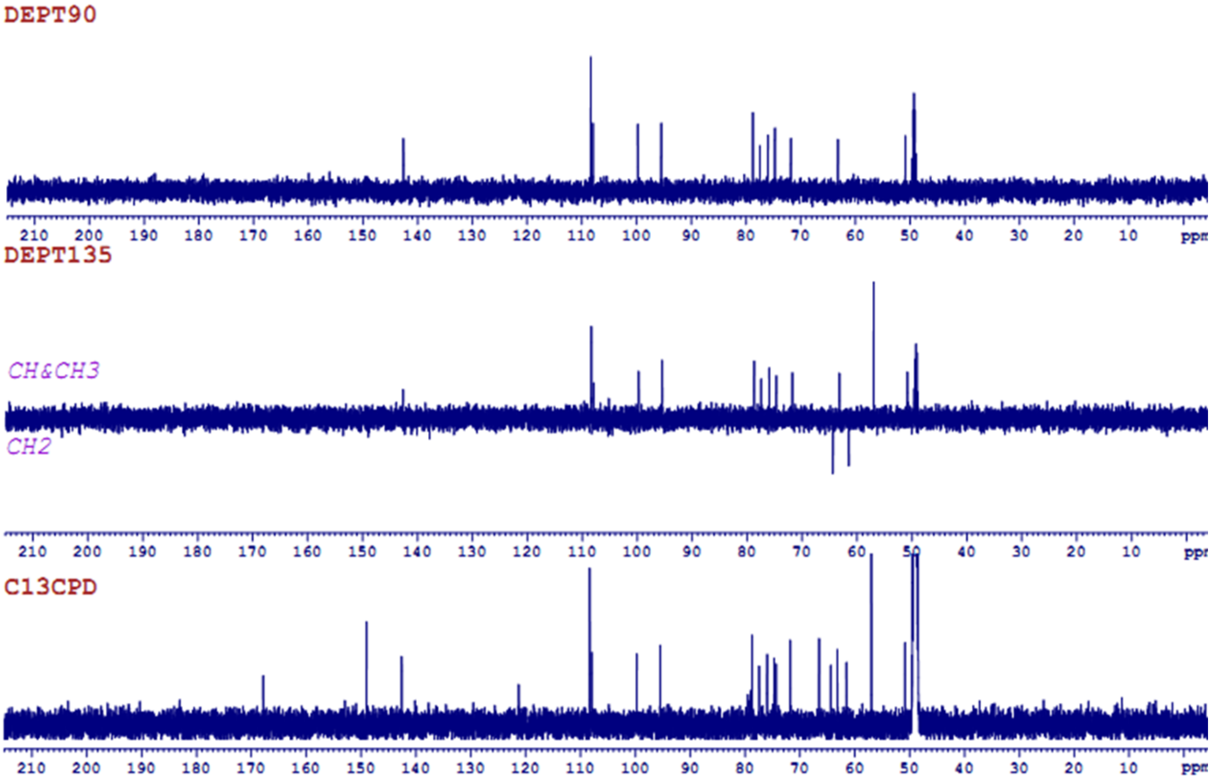


Figure S4: DEPT90 and 135 (125 MHz, CD_3OD) Spectrum of Myobontioside E (**1**)

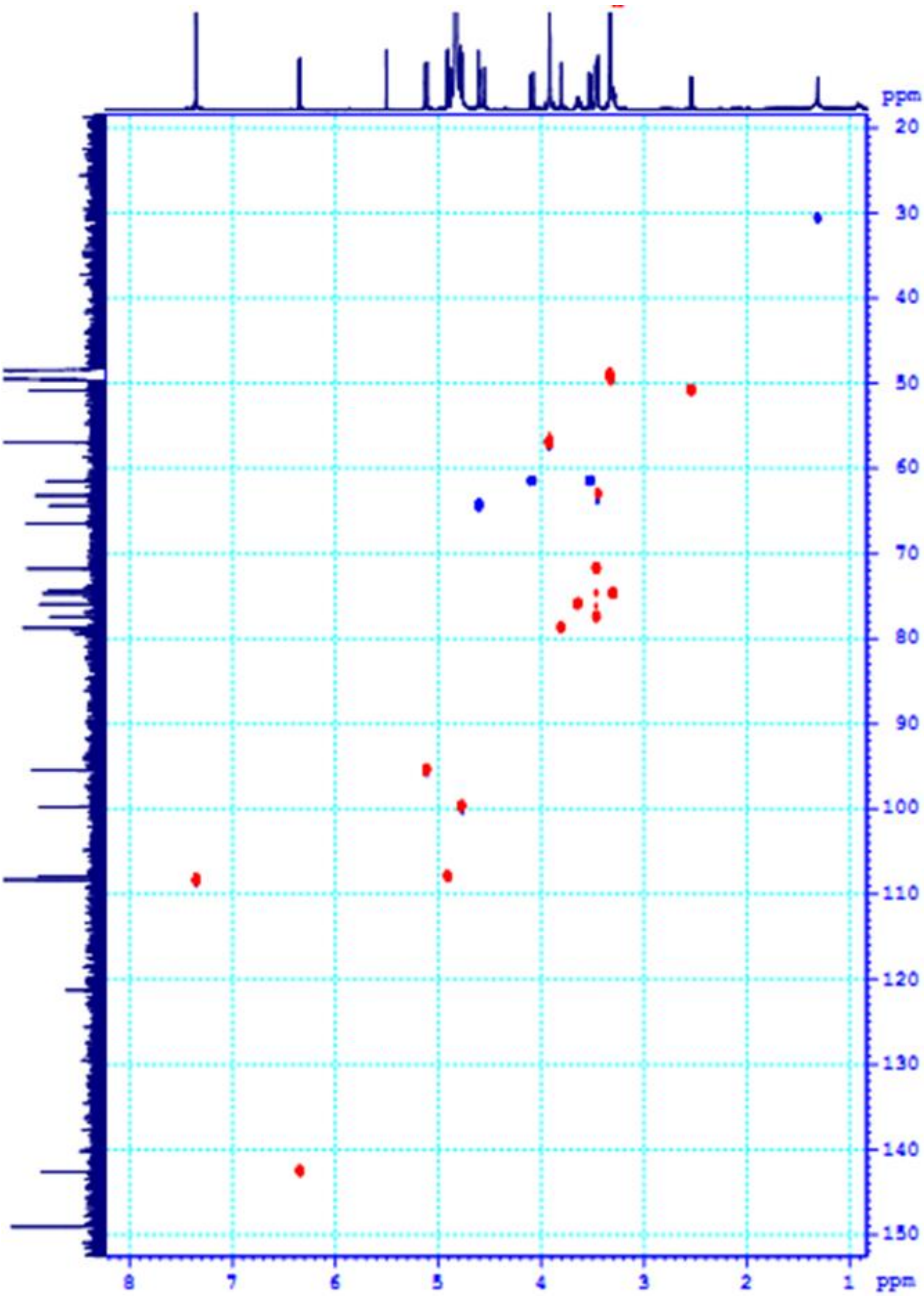


Figure S5: HSQC Spectrum of Myobontioside E (**1**)

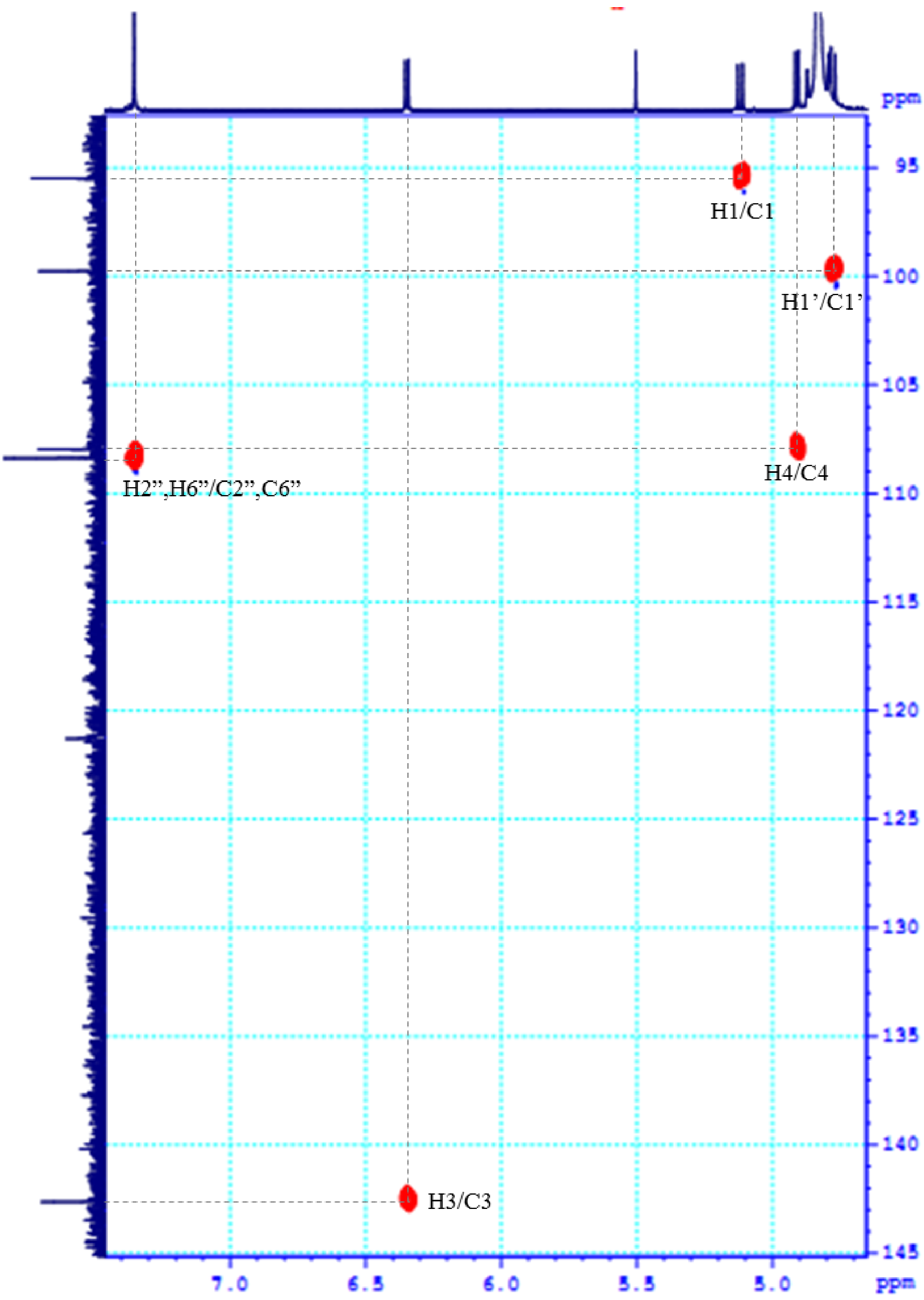


Figure S6: HSQC Spectrum of Myobontioside E (**1**) (From δ_C 95 ppm to δ_C 145 ppm)

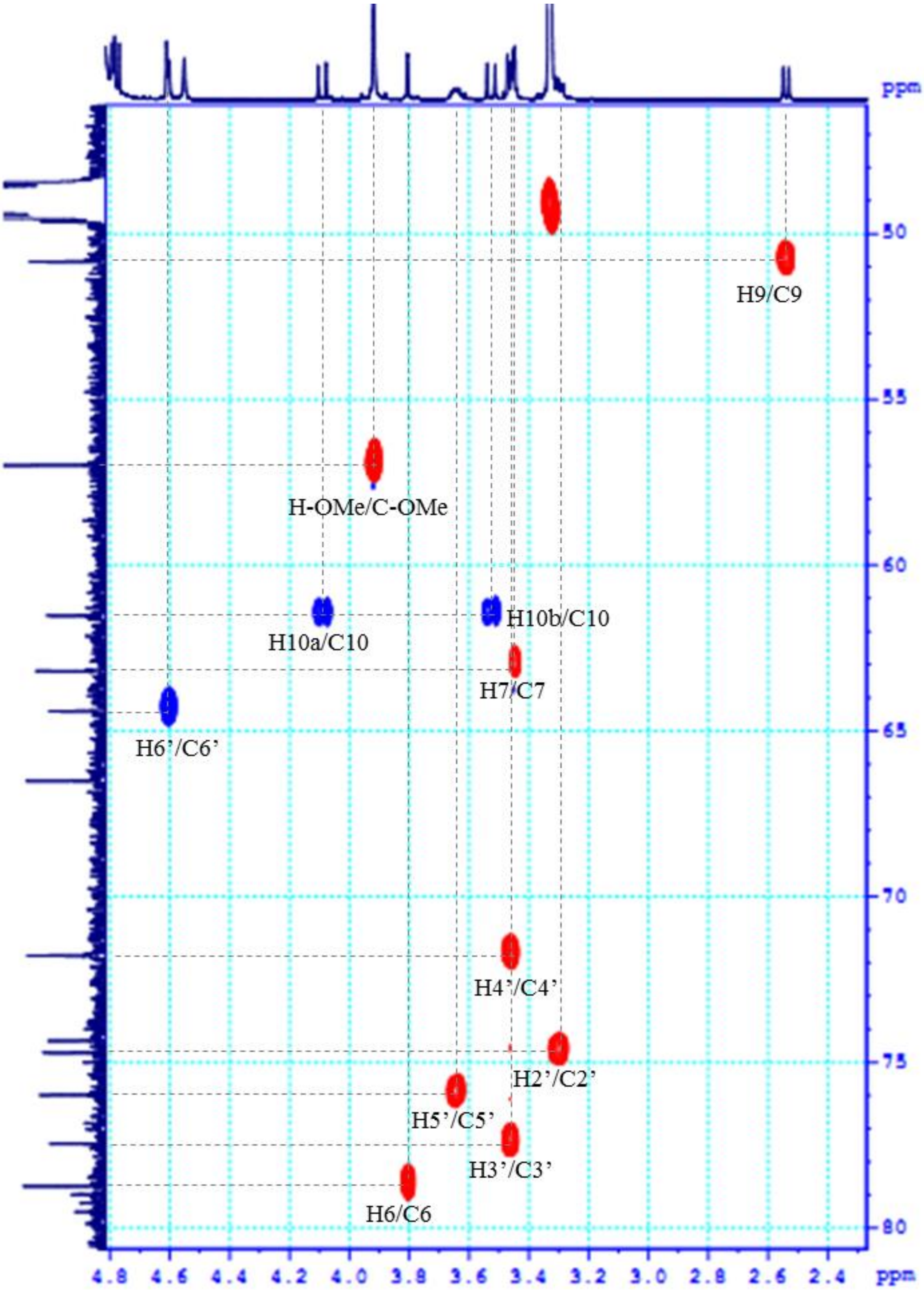


Figure S7: HSQC Spectrum of Myobontioside E (**1**) (From δ_C 45 ppm to δ_C 80 ppm)

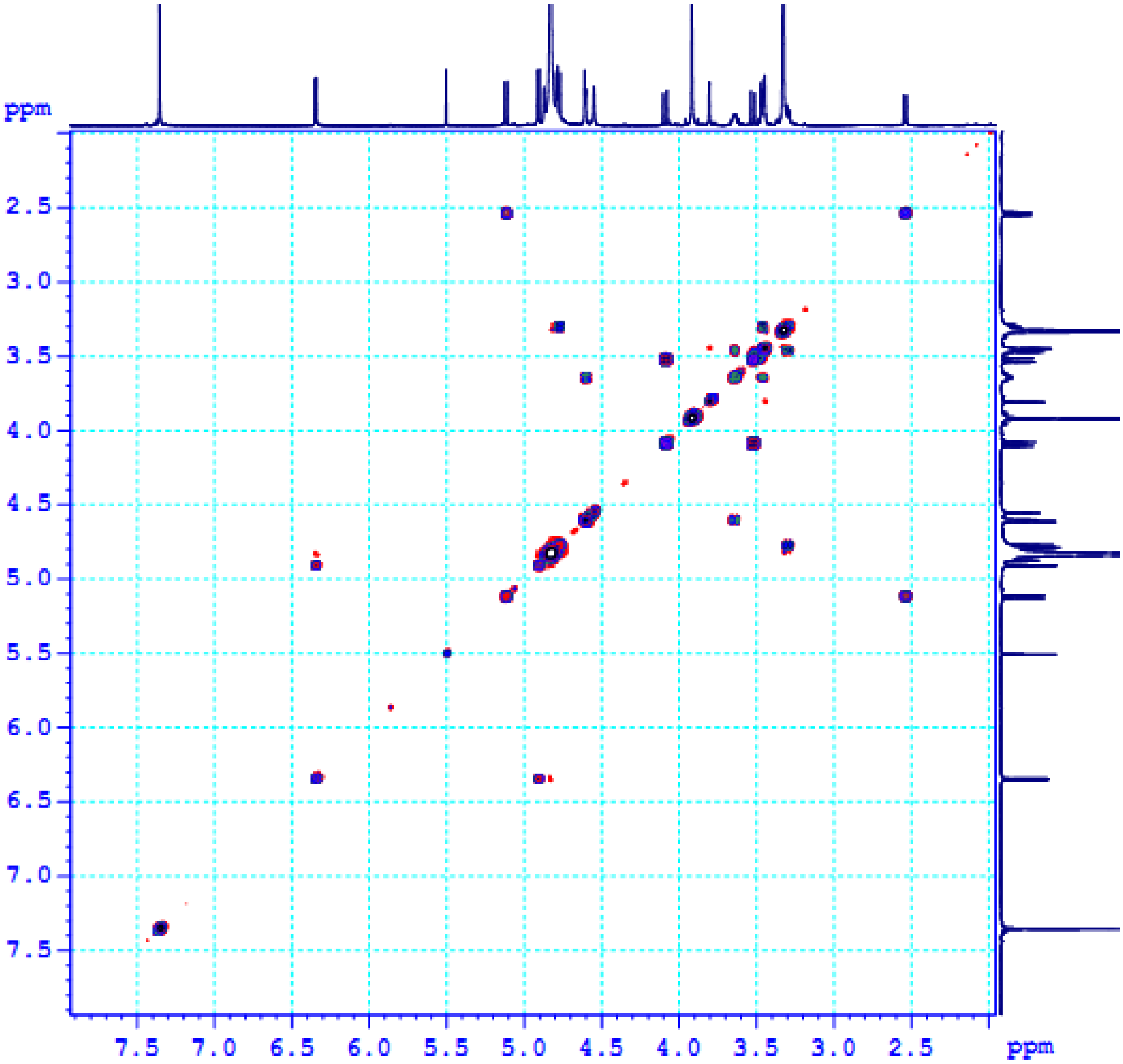


Figure S8: ^1H-^1H COSY Spectrum of Myobontioside E (**1**)

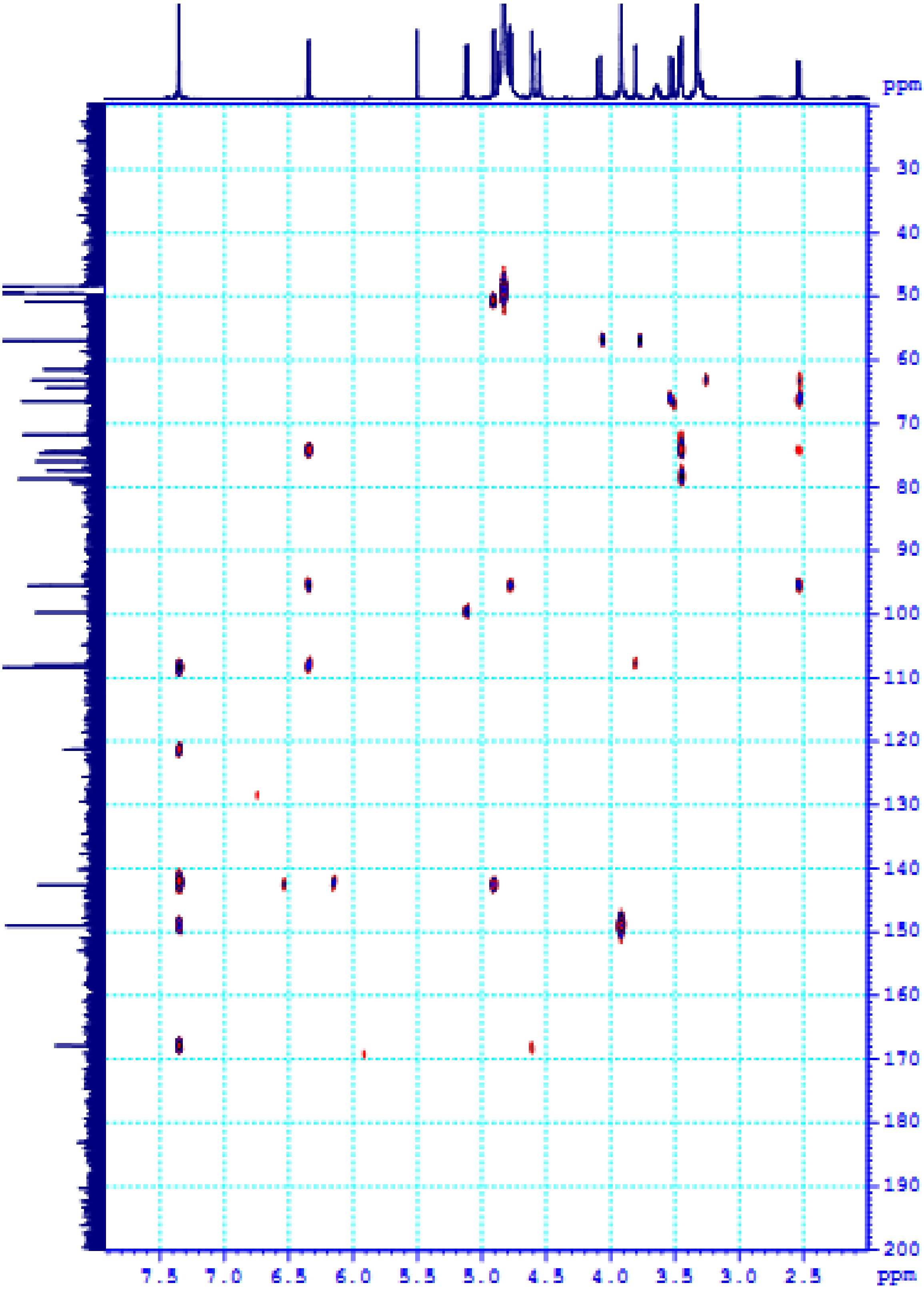


Figure S9: HMBC Spectrum of Myobontioside E (**1**)

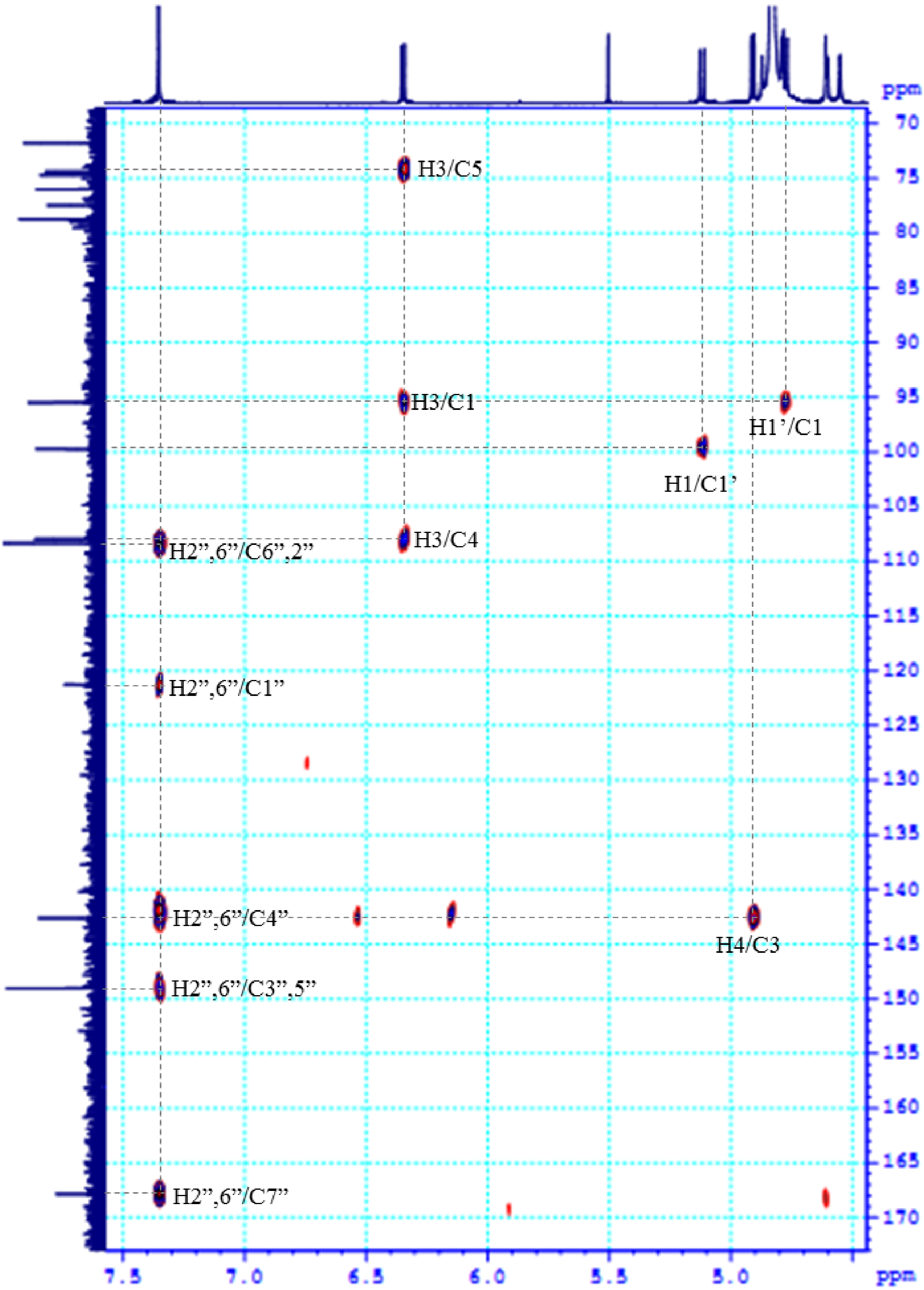


Figure S10: HMBC Spectrum of Myobontioside E (**1**) **(**From δ_C 70 ppm to δ_C 170 ppm)

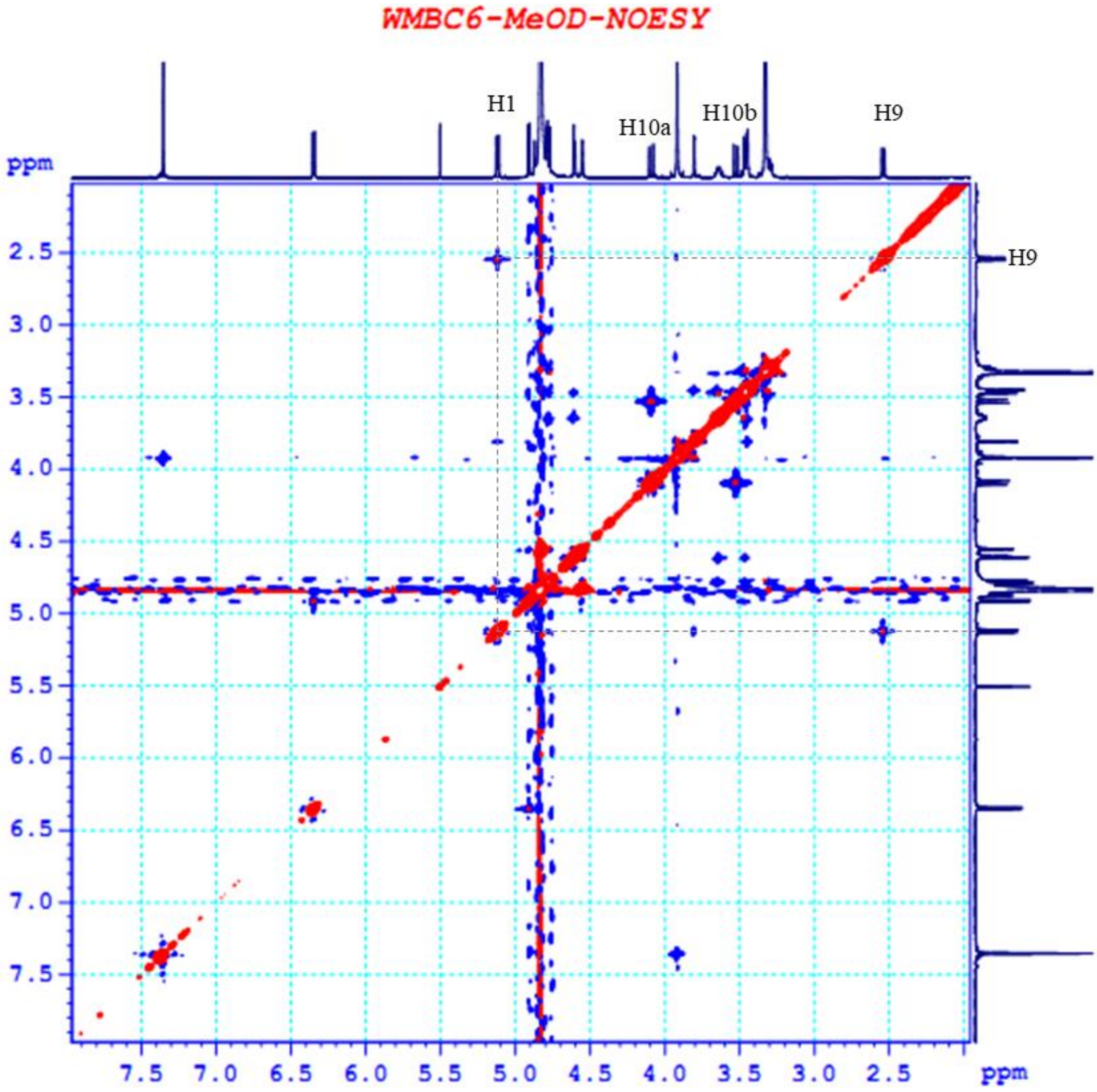


Figure S11: NOESY Spectrum of Myobontioside E (**1**)

Myopochlorin (2): ESI-MS (positive): *m/z* = 273 [M + 2H_2O + H]$^+$ ($C_9H_{14}O_5{}^{35}Cl$), 275 [M + 2H_2O + H]$^+$ ($C_9H_{14}O_5{}^{37}Cl$); ^{1}H NMR (500 MHz, CD_3COCD_3) δ: 5.40 (1H, d, *J* = 5.5 Hz, H-1), 4.56 (1H, dd, *J* = 1.5, 10.5 Hz, H-7), 4.41 (1H, d, *J* = 10.0 Hz, H-10a), 3.78 (1H, dd, *J* = 7.5, 10.5 Hz, H-6), 3.72 (1H, td, *J* = 2.0, 12.0 Hz, H-3a), 3.62 (1H, ddd, *J* = 2.5, 5.5, 12.0 Hz, H-3b), 3.42 (1H, dd, *J* = 1.5, 10.0 Hz, H-10b), 2.20 (1H, d, *J* = 6.0 Hz, H-9), 1.86 (1H, dt, *J* = 2.0, 13.5 Hz, H-4a), 1.61 (1H, td, *J* = 5.5, 13.5 Hz, H-4b); ^{13}C NMR (125 Hz, CD_3COCD_3) data (Table S2).

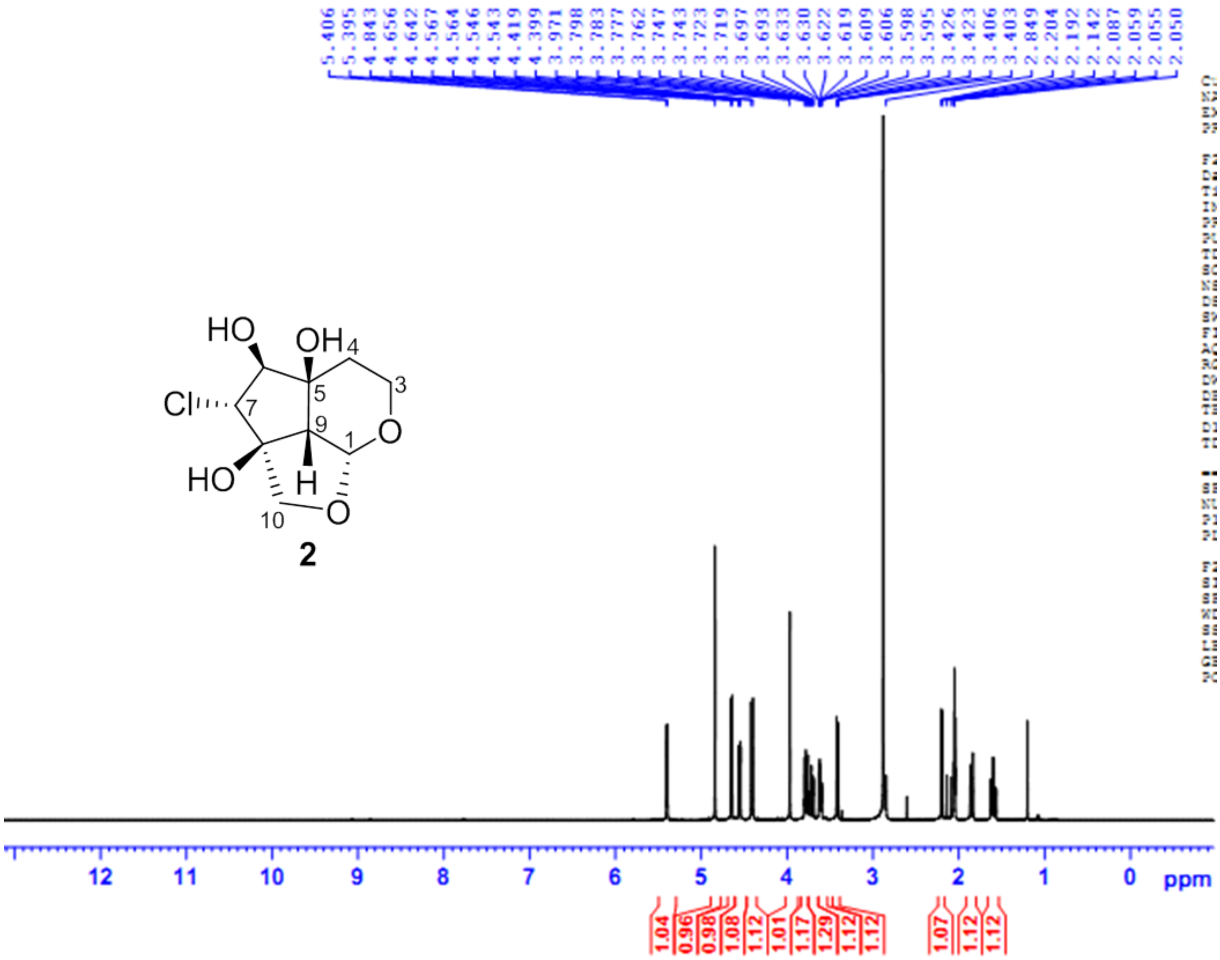


Figure S12: ^{1}H-NMR (500 MHz, CD_3COCD_3) Spectrum of Myopochlorin (**2**)

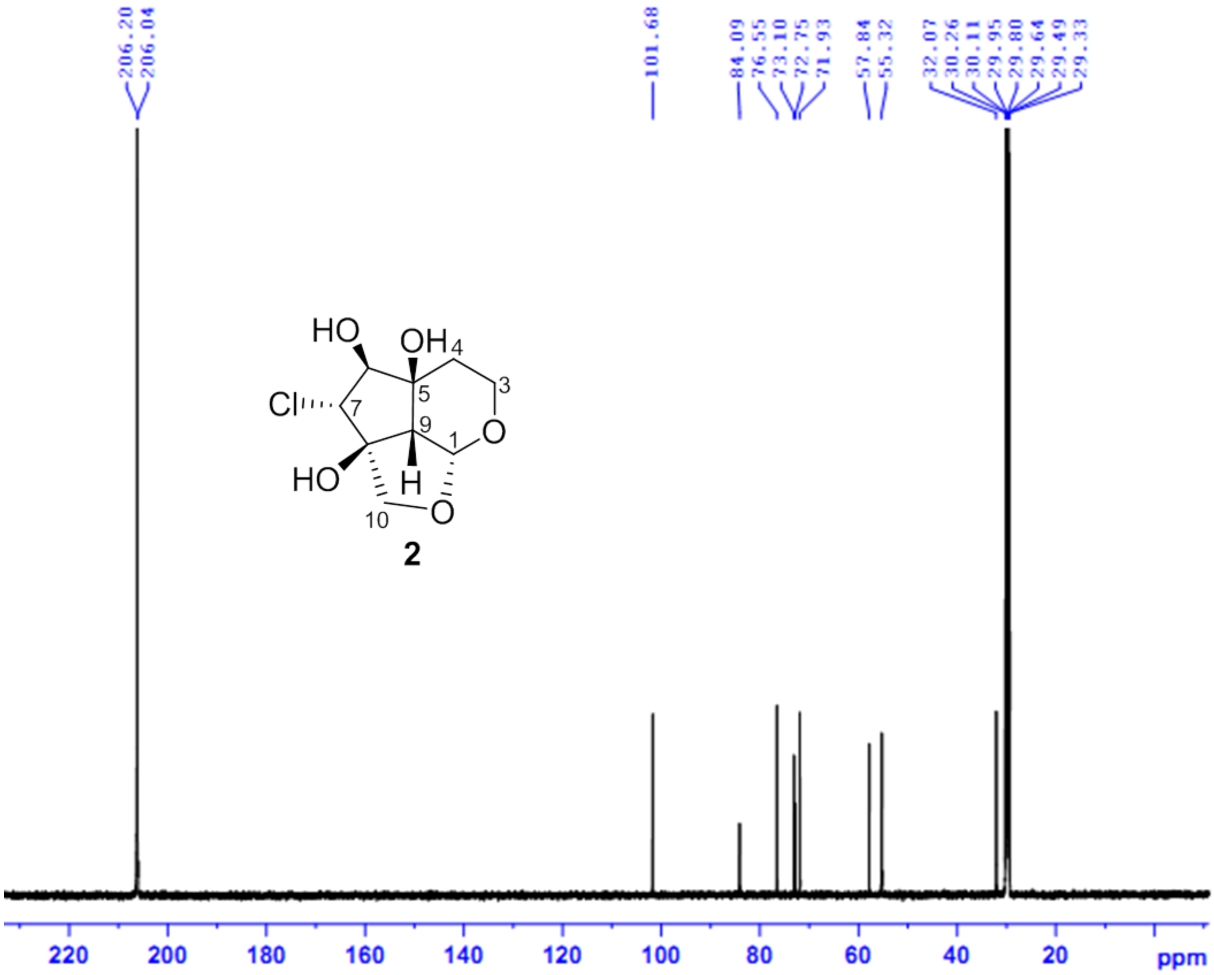


Figure S13: ^{13}C-NMR (125 MHz, CD_3COCD_3) Spectrum of Myopochlorin (**2**)

3-hydroxymyopochlorin (3): ESI-MS (positive): *m/z* = 253 $[M+H]^+$ ($C_9H_{14}O_6{}^{35}Cl$), 255 $[M+H]^+$ ($C_9H_{14}O_6{}^{37}Cl$); ^1H NMR (500 MHz, CD_3OD) δ: 5.6 (1H, d, *J* = 6.0 Hz, H-1), 5.14 (1H, dd, *J* = 3.5, 9.0 Hz, H-3), 4.50 (1H, d, *J* = 10.5 Hz, H-7), 4.35 (1H, d, *J* = 10.5 Hz, H-10a), 3.63 (1H, d, *J* = 10.5 Hz, H-6), 3.54 (1H, d, *J* = 10.5 Hz, H-10b), 2.24 (1H, d, *J* = 6.0 Hz, H-9), 2.21 (1H, dd, *J* = 3.5, 9.0 Hz, H-4a), 1.46 (1H, dd, *J* = 9.0, 13.0 Hz, H-4b); ^{13}C NMR (125MHz, CD_3OD) data (table S2).

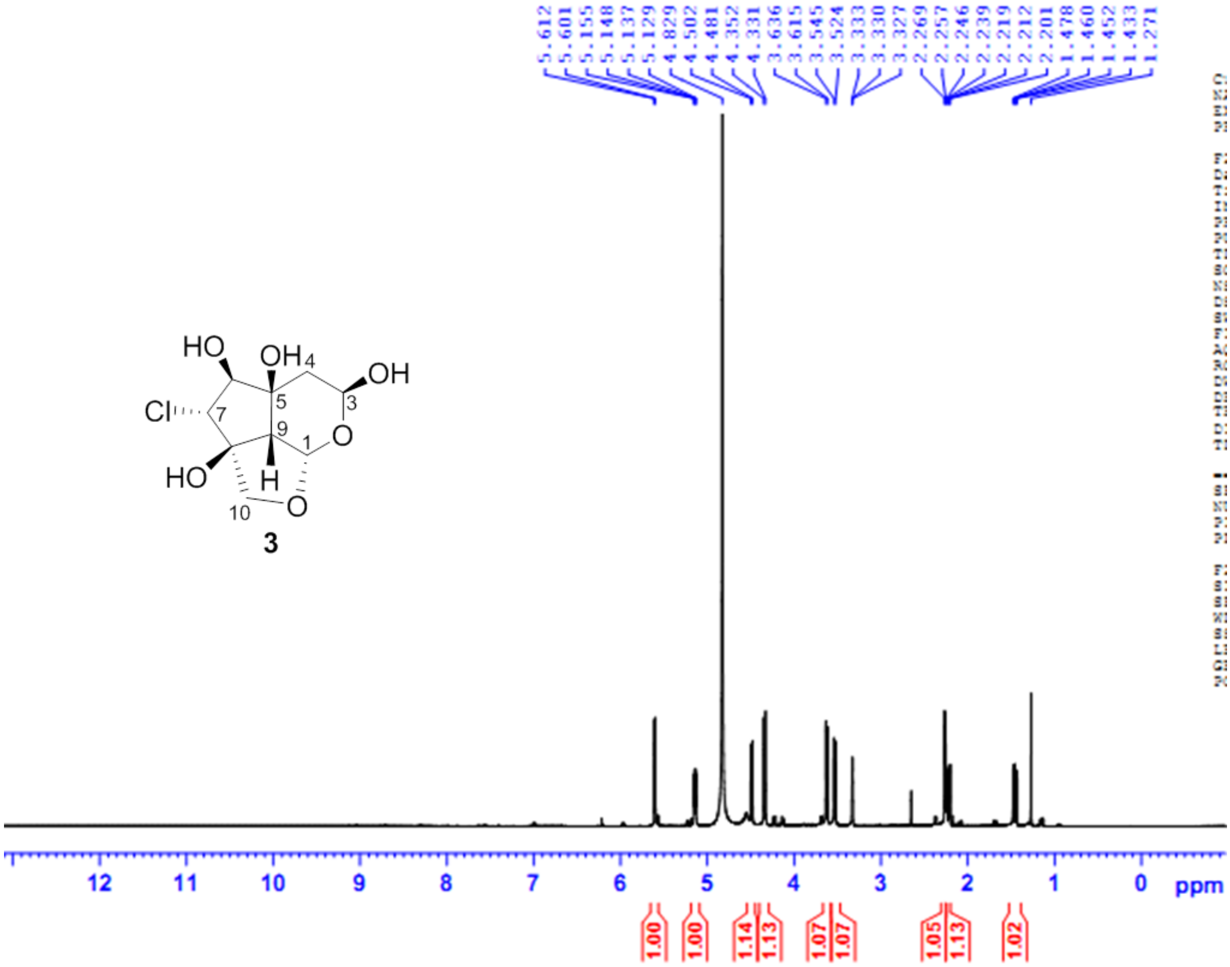


Figure S14: ^1H-NMR (500 MHz, CD_3OD) Spectrum of 3-hydroxymyopochlorin (**3**)

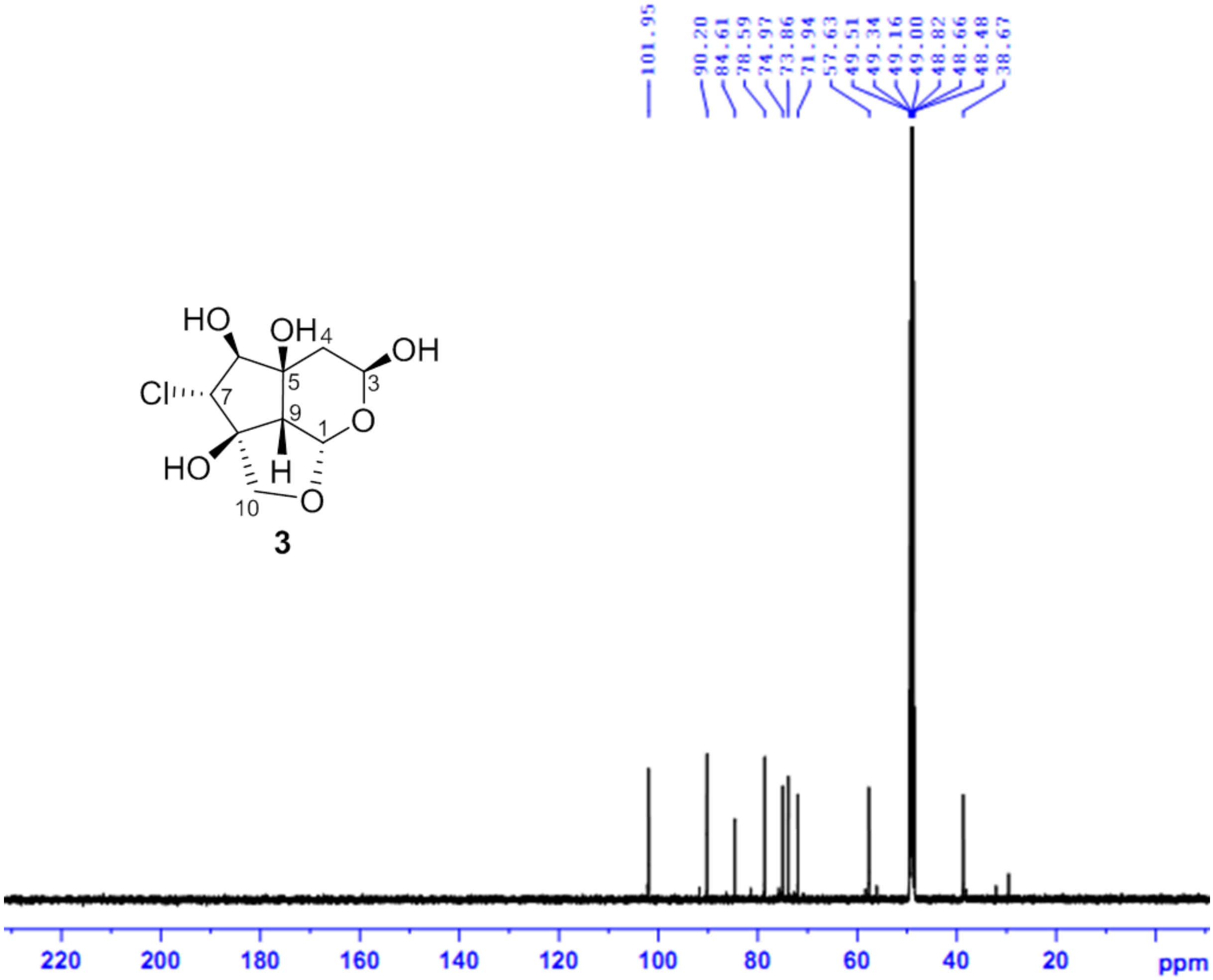


Figure S15: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of 3-hydroxymyopochlorin (**3**)

8-*epi*-loganic acid (4): ^{1}H NMR (500 MHz, CD$_3$OD) δ: 7.31 (1H, s, H-3), 5.49 (1H, d, *J* = 4.0 Hz, H-1), 4.67 (1H, d, *J* = 7.5 Hz, H-1'), 3.93 (1H, dd, *J* = 2.0, 12.0 Hz, H-6'a), 3.83 (1H, d, *J* = 5.5 Hz, H-7), 3.67 (1H, dd, *J* = 6.0, 12.0 Hz, H-6'b), 3.30-3.36 (3H, m, H-3', 4', 5'), 3.22 (1H, m, H-2'), 3.08 (1H, d, *J* = 6.0 Hz, H-5), 2.60 (1H, m, H-9), 2.13 (1H, m, H-8), 2.06 (1H, m, H-6a), 1.90 (1H, m, H-6b), 1.07 (3H, d, *J* = 7.5 Hz, H$_3$-10); ^{13}C NMR (125MHz, CD$_3$OD) data (Table S2).

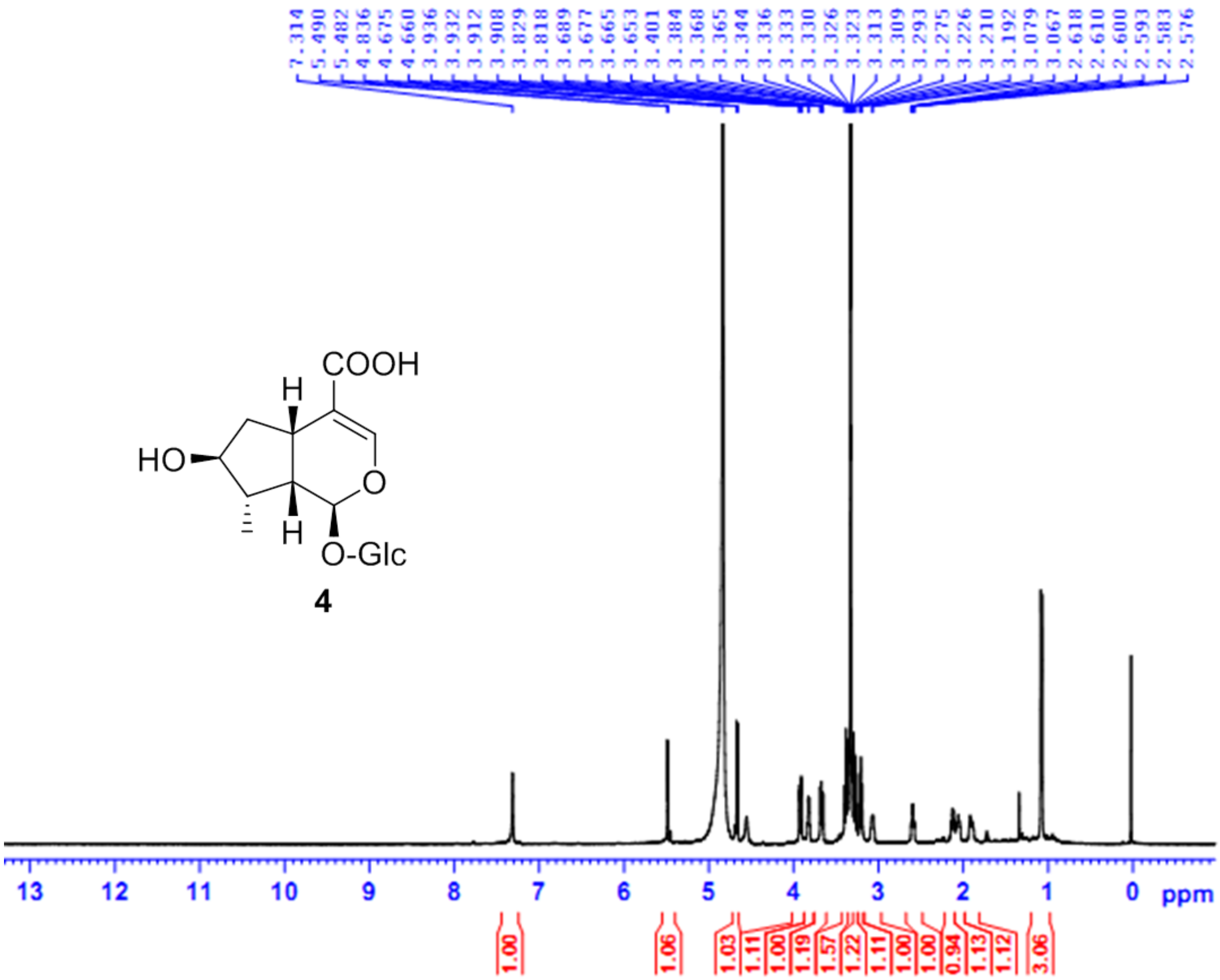


Figure S16: ^{1}H-NMR (500 MHz, CD$_3$OD) Spectrum of 8-*epi*-loganic acid **(4)**

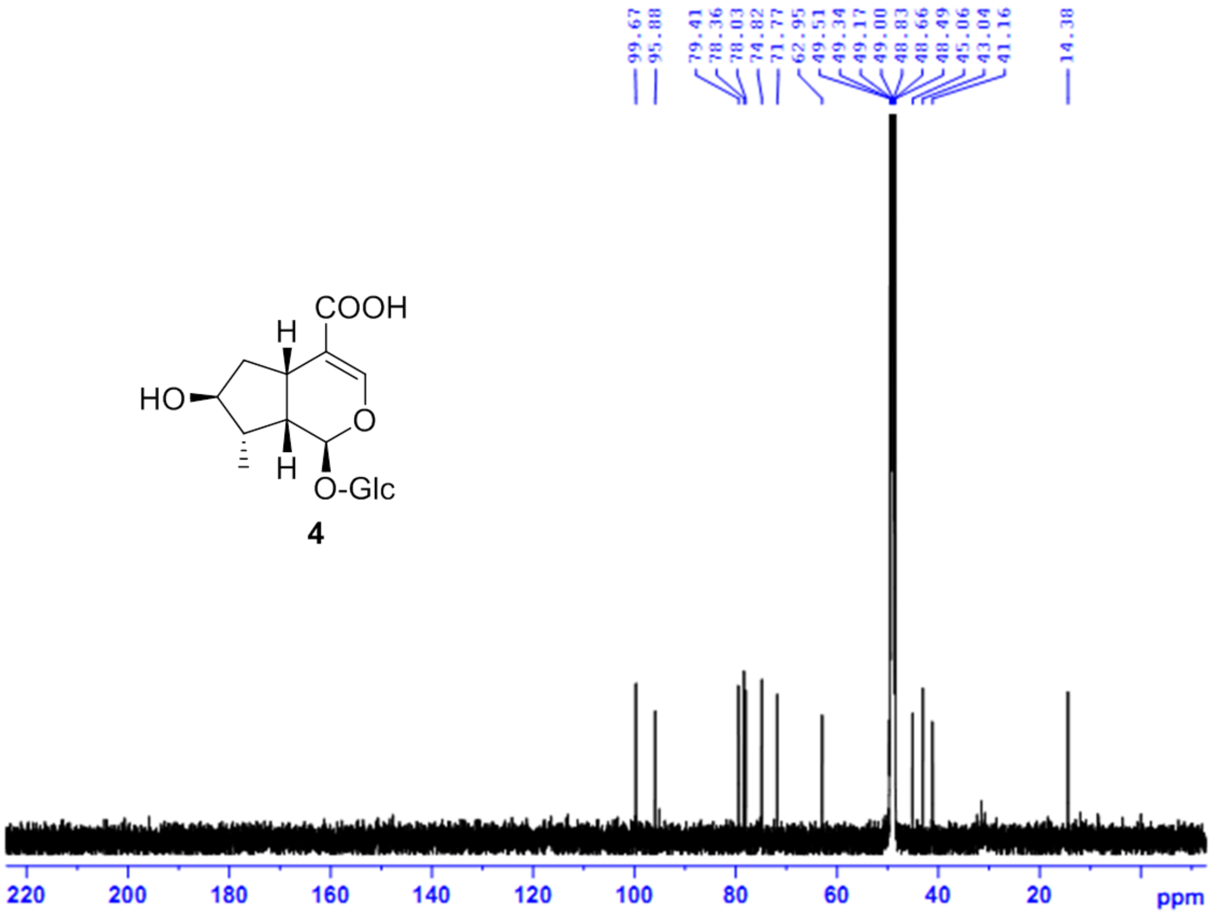


Figure S17: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of 8-*epi*-loganic acid **(4)**

Ajugol (5): ^{1}H NMR (500 MHz, CD_3OD) δ: 6.18 (1H, dd, *J* = 2.0, 6.0 Hz, H-3), 5.48 (1H, d, *J* = 1.5 Hz, H-1), 4.88 (1H, dd, *J* = 3.0, 6.0 Hz, H-4), 4.67 (1H, d, *J* = 8.0 Hz, H-1'), 3.94 (1H, m, H-6), 3.89 (1H, m, H-6'a), 3.68 (1H, dd, *J* = 6.0, 12.0 Hz, H-6'b), 3.41 (1H, m, H-3'), 3.32 (2H, m, H-4', 5'), 3.22 (1H, dd, *J* = 8.0, 9.0 Hz, H-2'), 2.75 (1H, m, H-5), 2.57 (1H, dd, *J* = 1.5, 9.5 Hz, H-9), 2.06 (1H, dd, *J* = 5.5, 13.5 Hz, H-7a), 1.82 (1H, dd, *J* = 4.5, 13.5 Hz, H-7b), 1.33 (3H, s, H_3-10); ^{13}C NMR (125MHz, CD_3OD) data (Table S2).

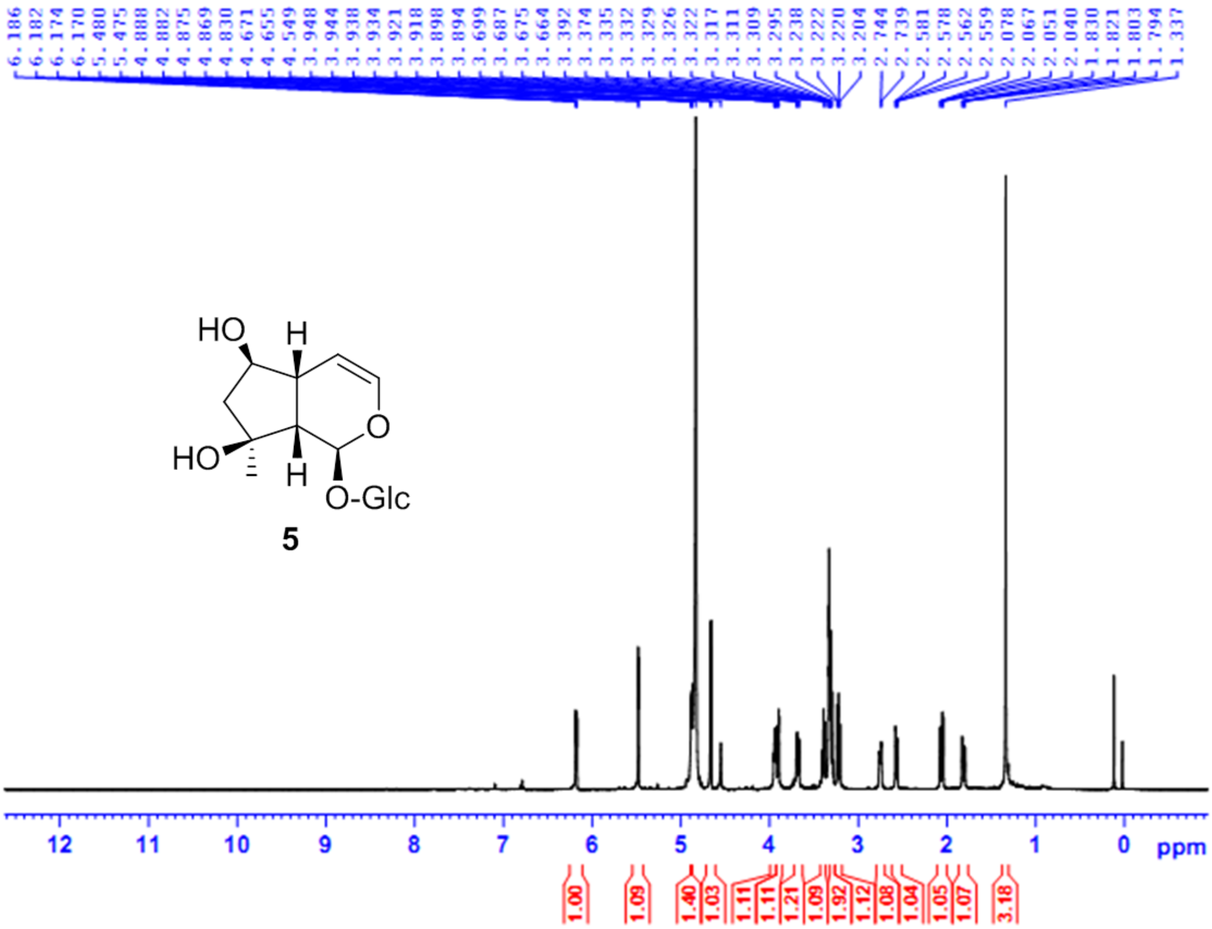


Figure S18: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Ajugol **(5)**

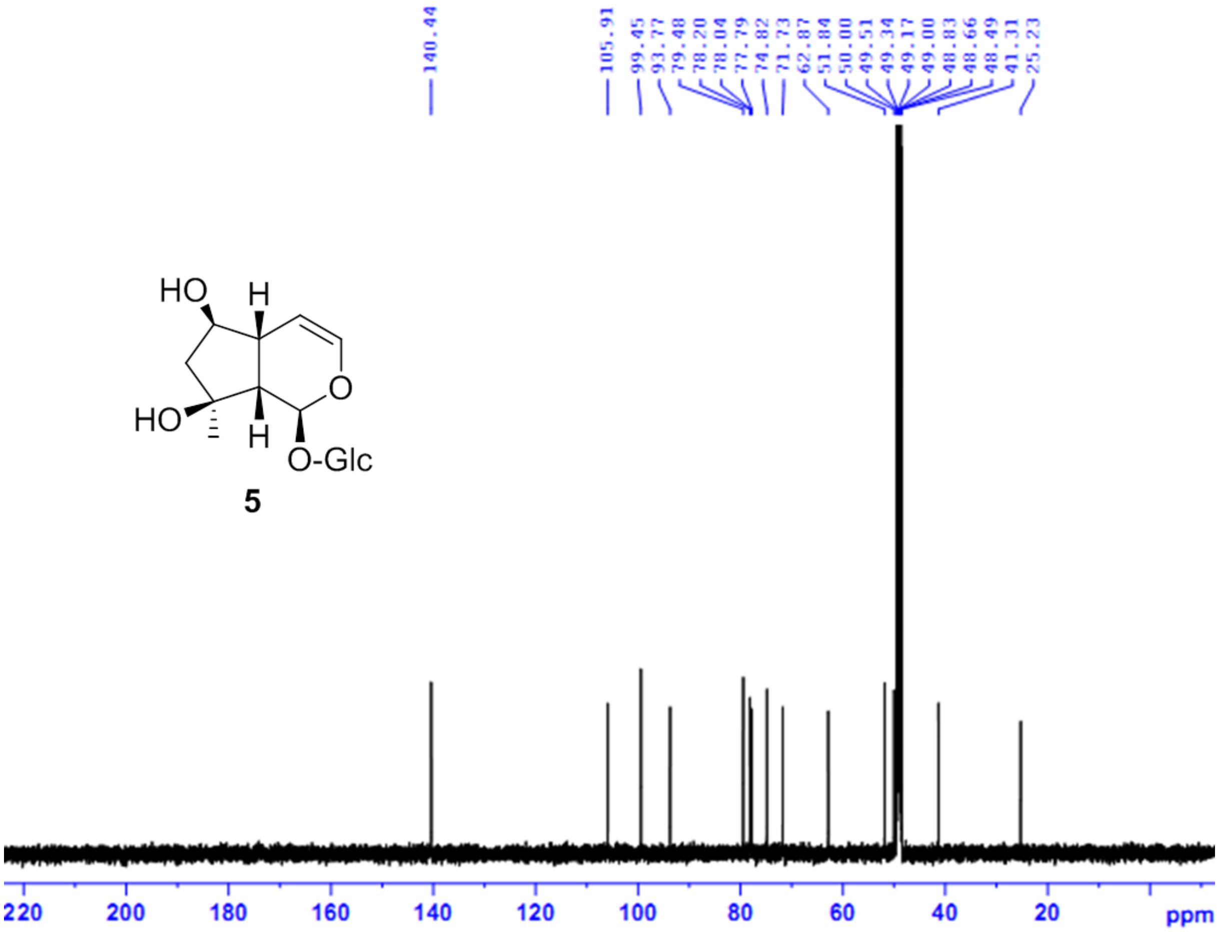


Figure S19: [13]C-NMR (125 MHz, CD_3OD) Spectrum of Ajugol **(5)**

8-*O*-acetylharpagide (6): ESI-MS (positive): *m/z* = 429 $[M+Na]^+$ ($C_{17}H_{26}O_{11}Na$); ^{1}H NMR (500 MHz, DMSO-d_6) δ: 6.36 (1H, d, J = 6.0 Hz, H-3), 5.87 (1H, d, J = 1.5 Hz, H-1), 4.88 (1H, dd, J = 1.5, 6.0 Hz, H-4), 4.39 (1H, d, J = 8.0 Hz, H-1'), 3.70 (1H, dd, J = 6.0, 12.0 Hz, H-6'a), 3.57 (1H, t, J = 4.5 Hz, H-6α), 3.48 (1H, d, J = 12.0 Hz, H-6'b), 2.65 (1H, brs, H-9), 2.08 (1H, d, J = 15.0 Hz, H-7β), 1.93 (3H, s, 8-OAc), 1.80 (1H, dd, J = 4.5, 15.0 Hz, H-7α), 1.36 (3H, s, H_3-10); ^{13}C NMR (125MHz, DMSO-d_6) data (Table S2).

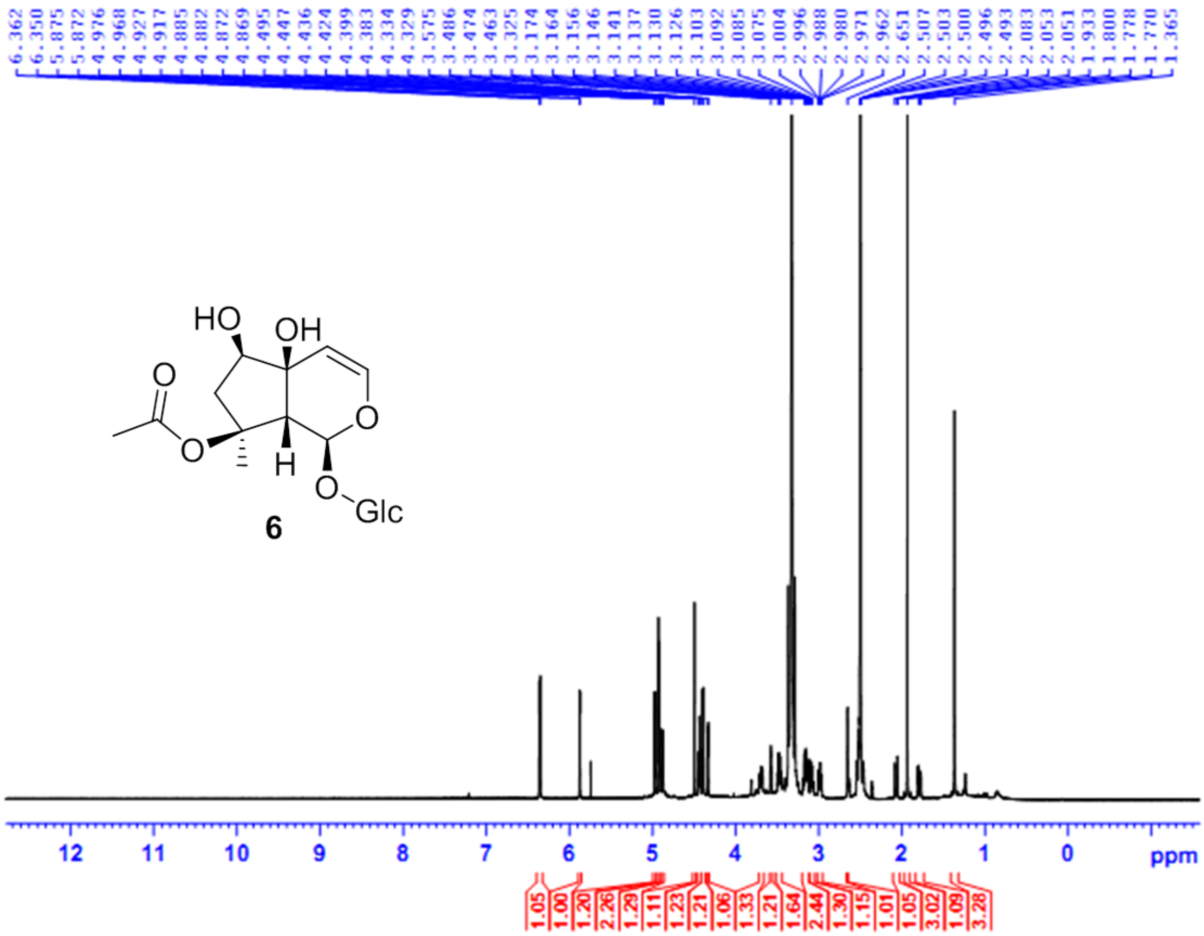


Figure S20: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of 8-*O*-acetylharpagide (**6**)

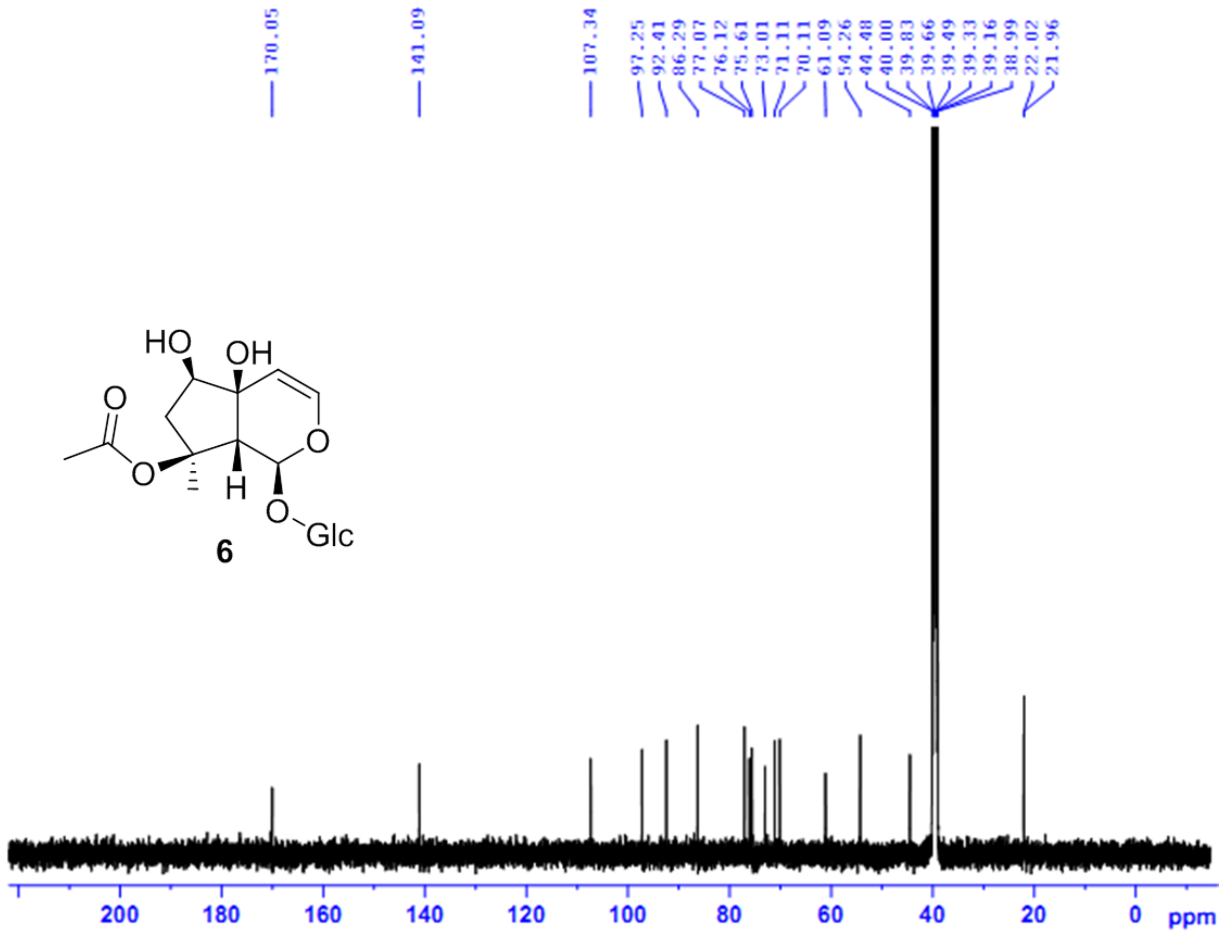


Figure S21: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of 8-*O*-acetylharpagide (**6**)

Harpagide (7): ESI-MS (negative): *m/z* = 363 [M-H]$^-$ ($C_{15}H_{23}O_{10}$); ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ: 6.26 (1H, d, *J* = 6.5 Hz, H-3), 5.55 (1H, d, *J* = 1.5 Hz, H-1), 4.89 (1H, dd, *J* = 1.5, 6.5 Hz, H-4), 4.39 (1H, d, *J* = 7.5 Hz, H-1'), 3.69 (1H, dd, *J* = 5.0, 10.0 Hz, H-6'a), 3.54 (1H, d, *J* = 5.0 Hz, H-6), 3.47 (1H, d, *J* = 10.0 Hz, H-6'b), 3.16-2.98 (4H, m, H-2', 3', 4', 5'), 2.35 (1H, brs, H-9), 1.72 (1H, dd, *J* = 5.0, 13.0 Hz, H-7a), 1.63 (1H, dd, *J* = 5.0, 13.0 Hz, H-7b), 1.08 (3H, s, H_3-10); ^{13}C NMR (125 MHz, DMSO-*d*$_6$) data (Table S2)

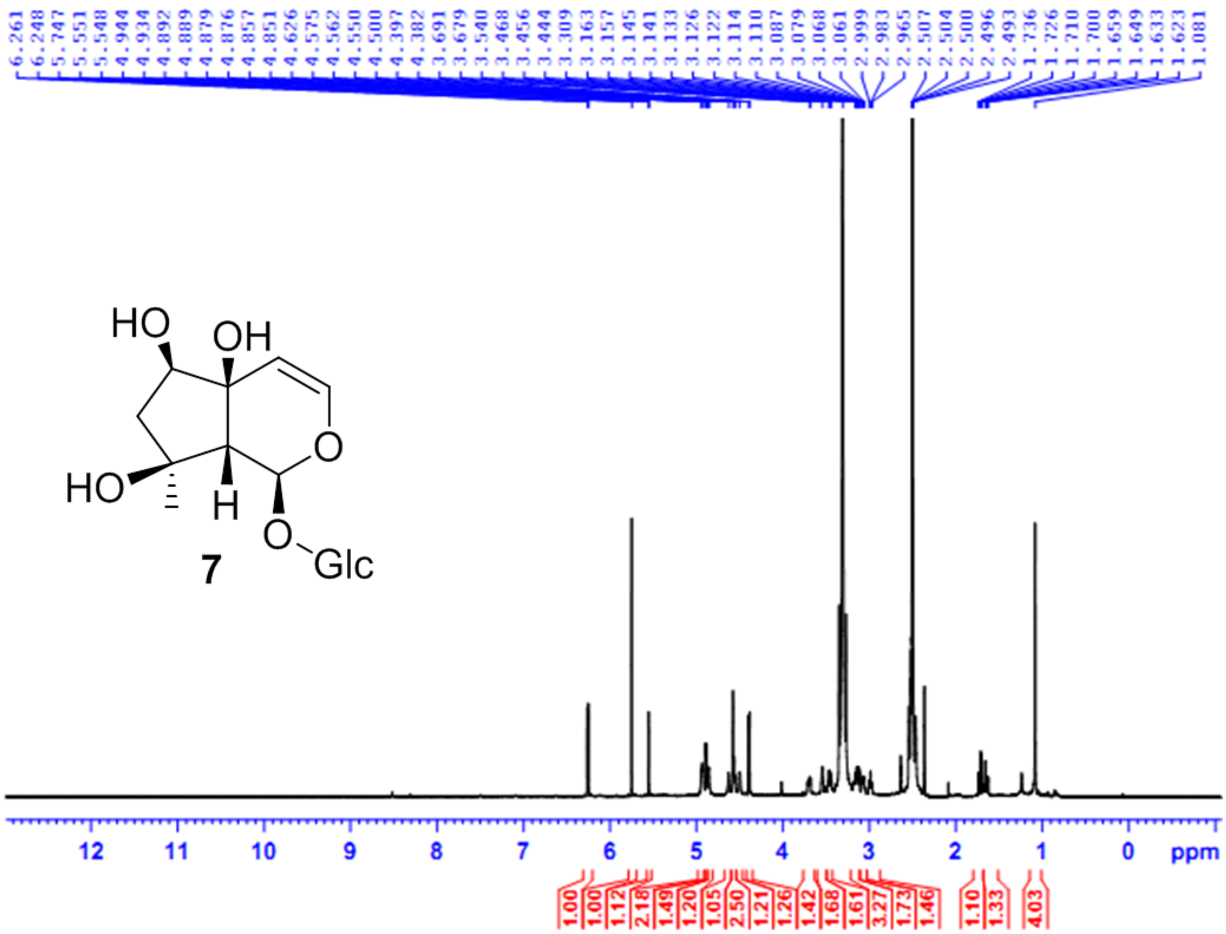


Figure S22: ^{1}H-NMR (500 MHz, DMSO-*d*$_6$) Spectrum of Harpagide (**7**)

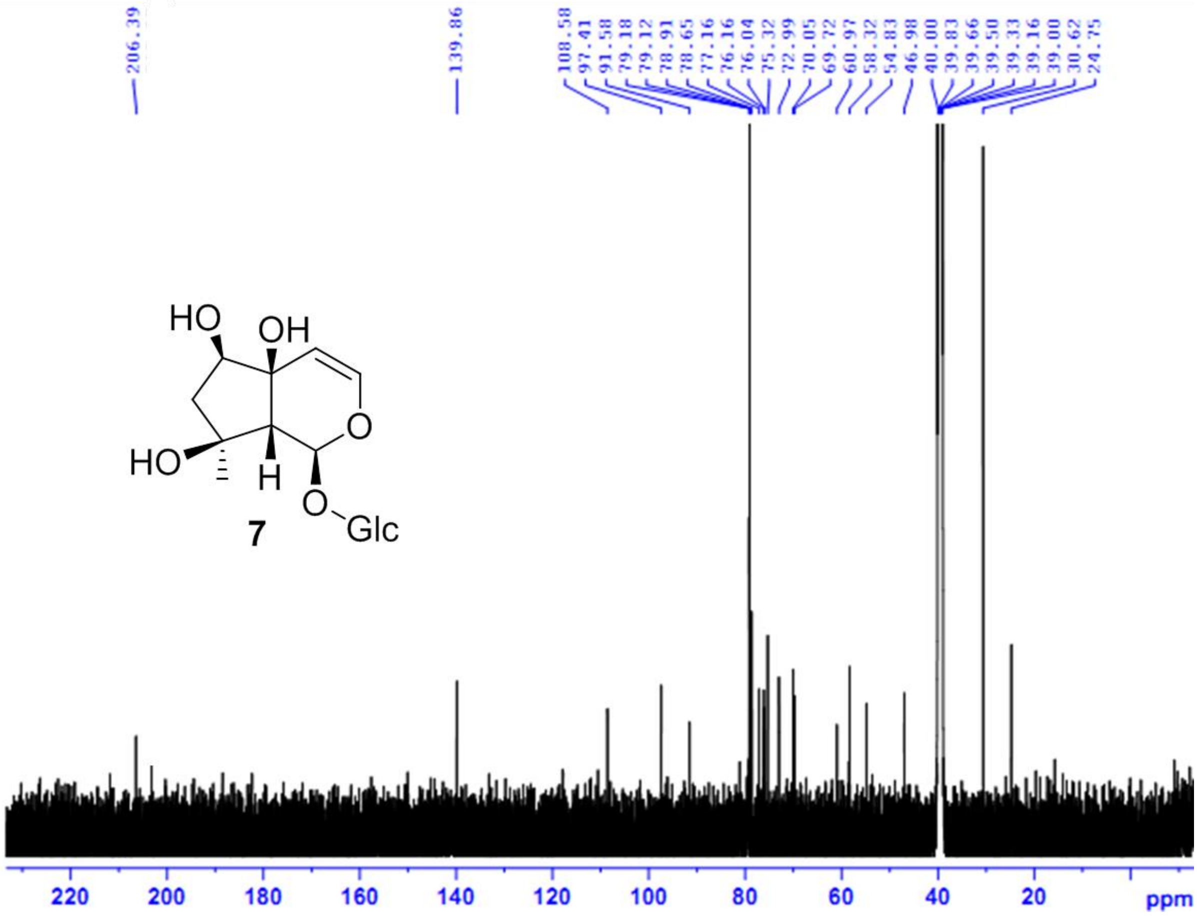


Figure S23: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of Harpagide (**7**)

***Cis*-melilotoside (8):** [1]H NMR (500 MHz, CD_3OD) and [13]C NMR (125 MHz, CD_3OD) data (Table S3)

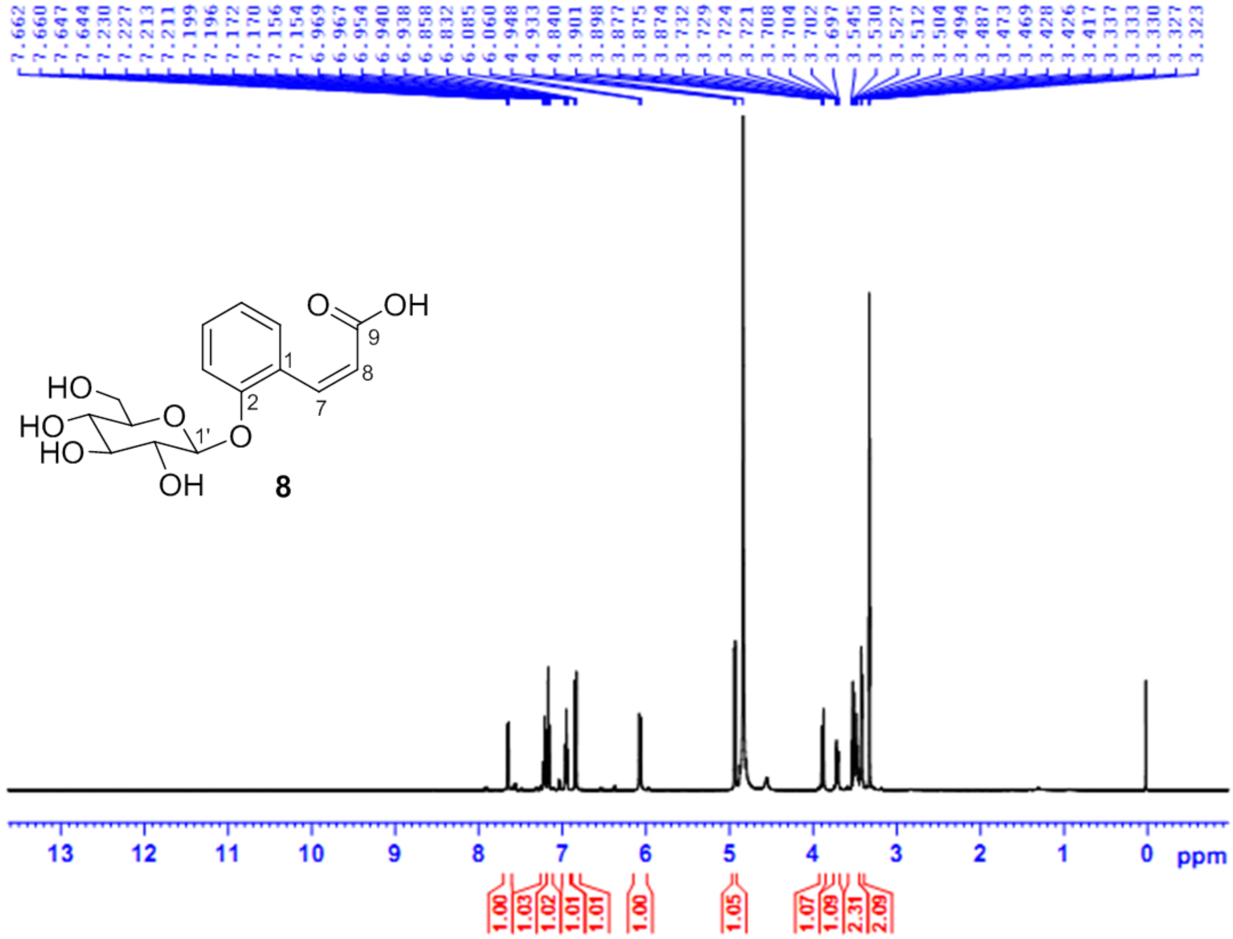


Figure S24: [1]H-NMR (500 MHz, CD_3OD) Spectrum of *Cis*-melilotoside (**8**)

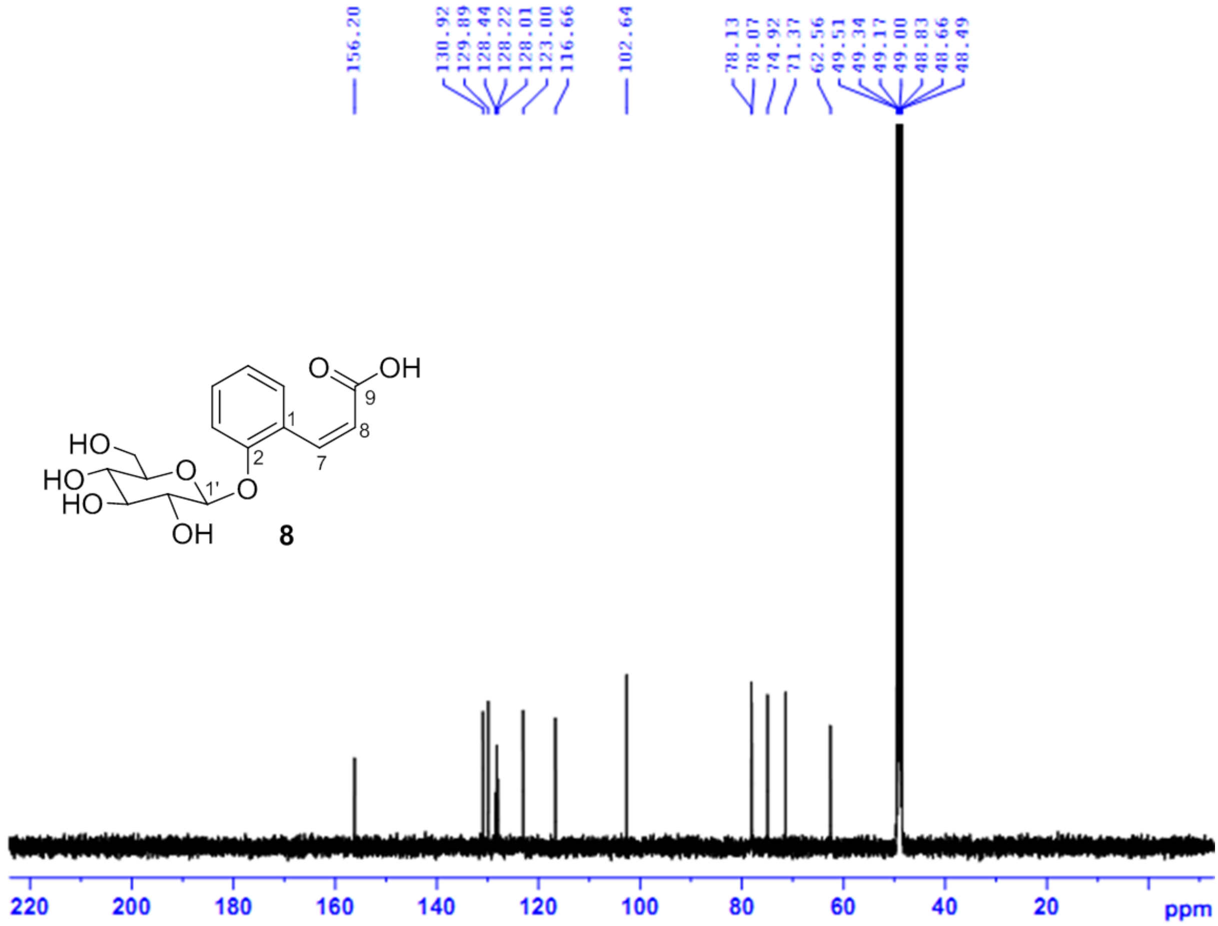


Figure S25: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of *Cis*-melilotoside (**8**)

***Trans*-melilotoside (9)**: [1]H NMR (500 MHz, CD_3OD) and [13]C NMR (125 MHz, CD_3OD) data (Table S3)

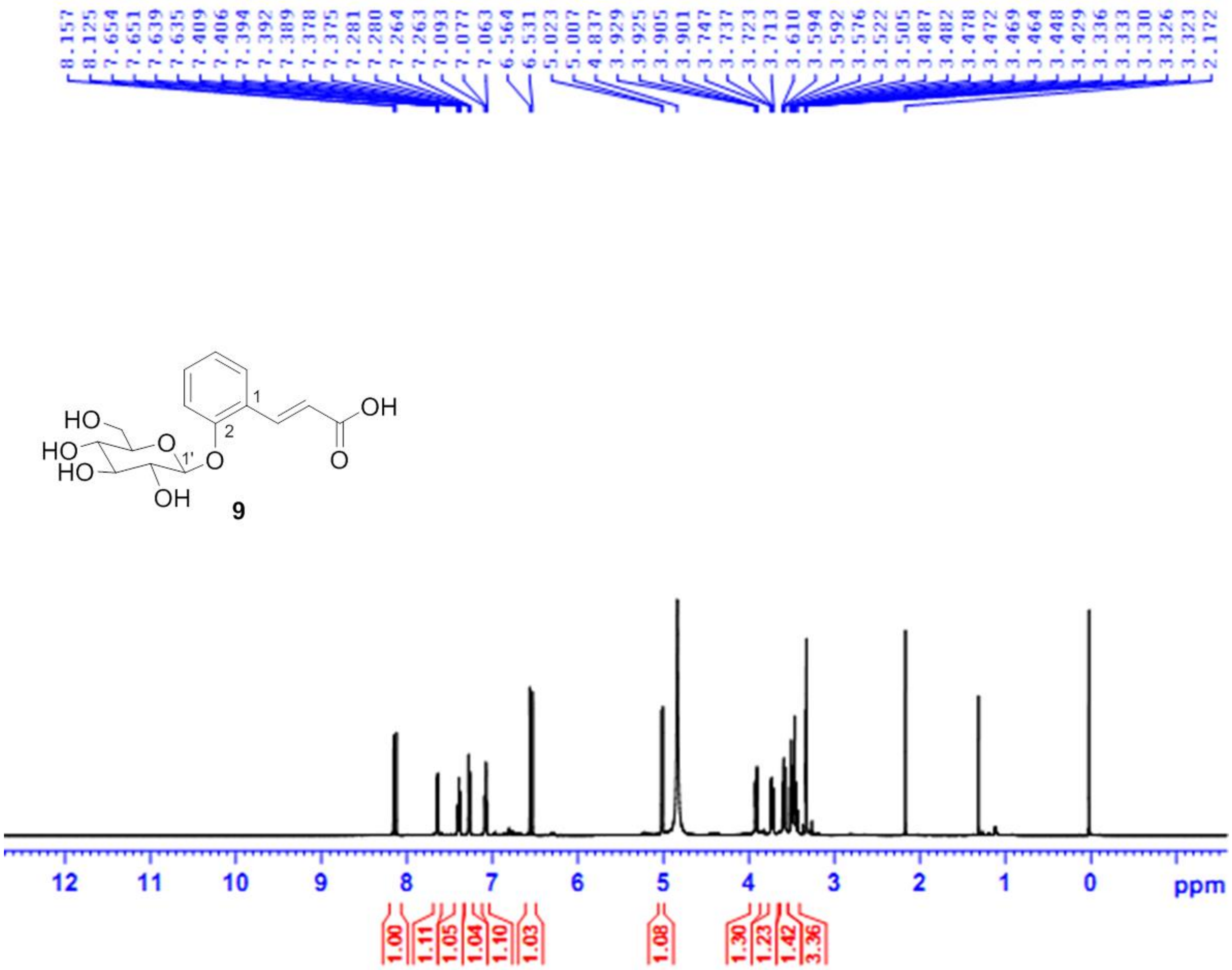


Figure S26: [1]H-NMR (500 MHz, CD_3OD) Spectrum of *Trans*-melilotoside (**9**)

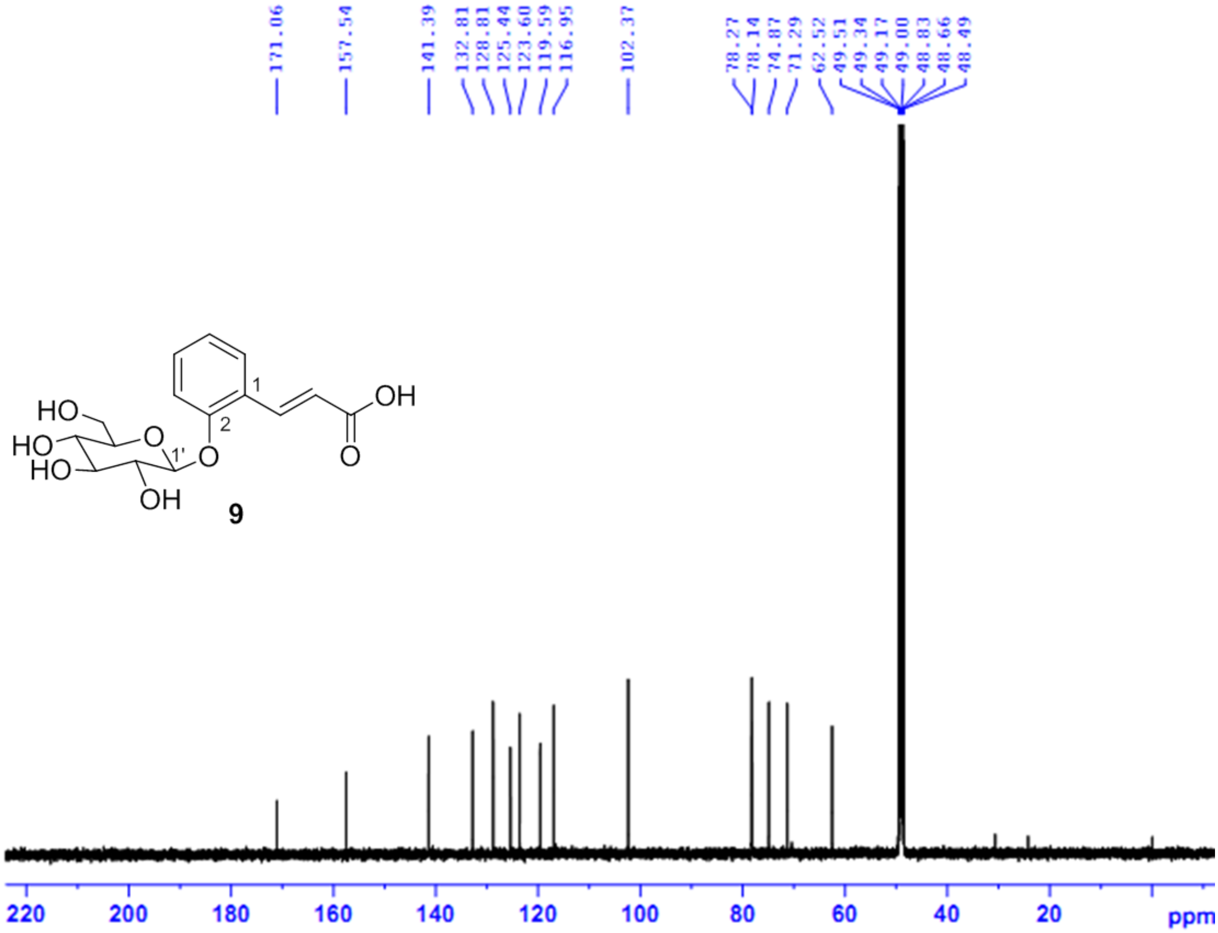


Figure S27: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of *Trans*-melilotoside (**9**)

Octane-1-en-3-ol-3-*O*-β-D-glucopyranosyl(1→2)-β-D-glucopyranoside (10): ^{1}H NMR (500 MHz, CD_3OD) and ^{13}C NMR (125 MHz, CD_3OD) data (Table S4)

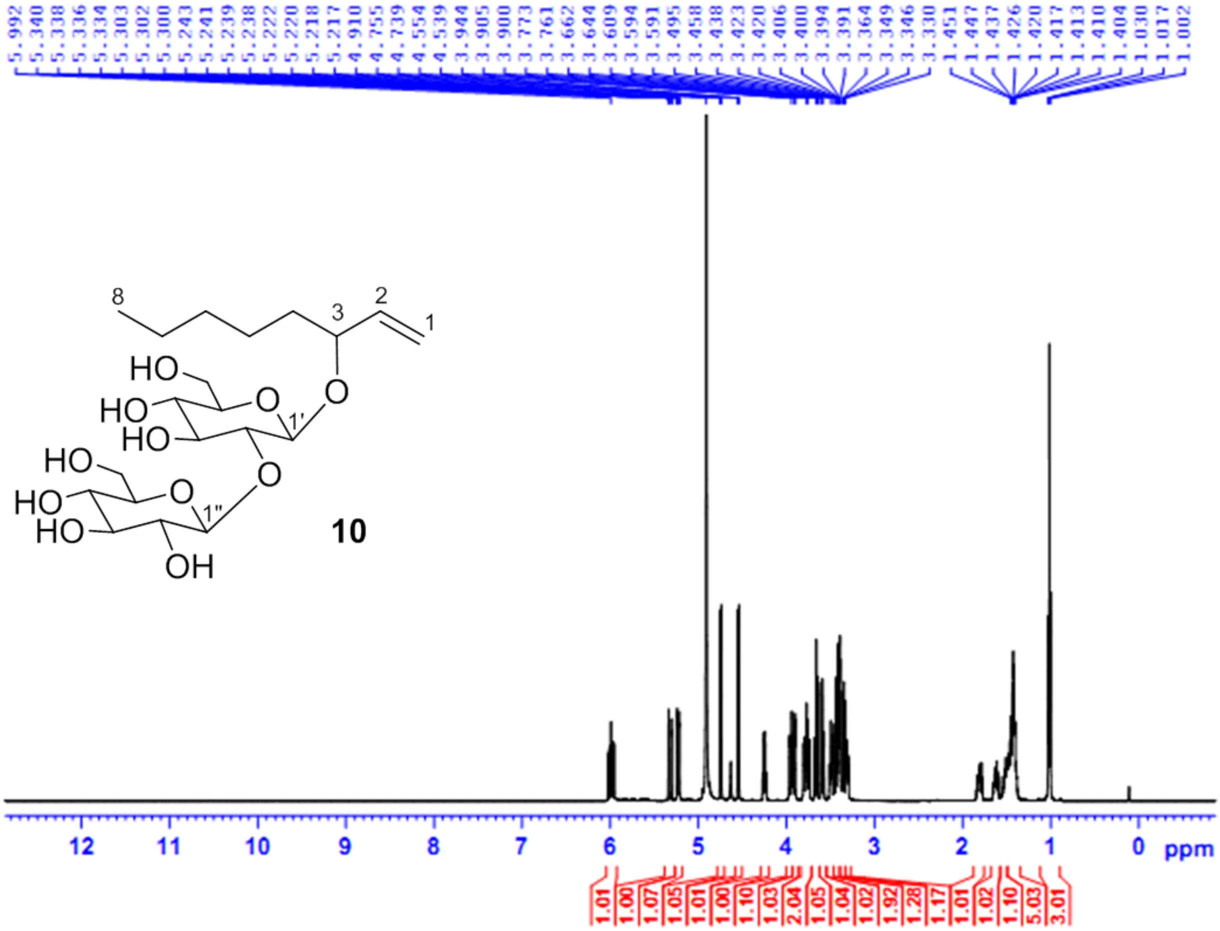


Figure S28: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Compound **10**

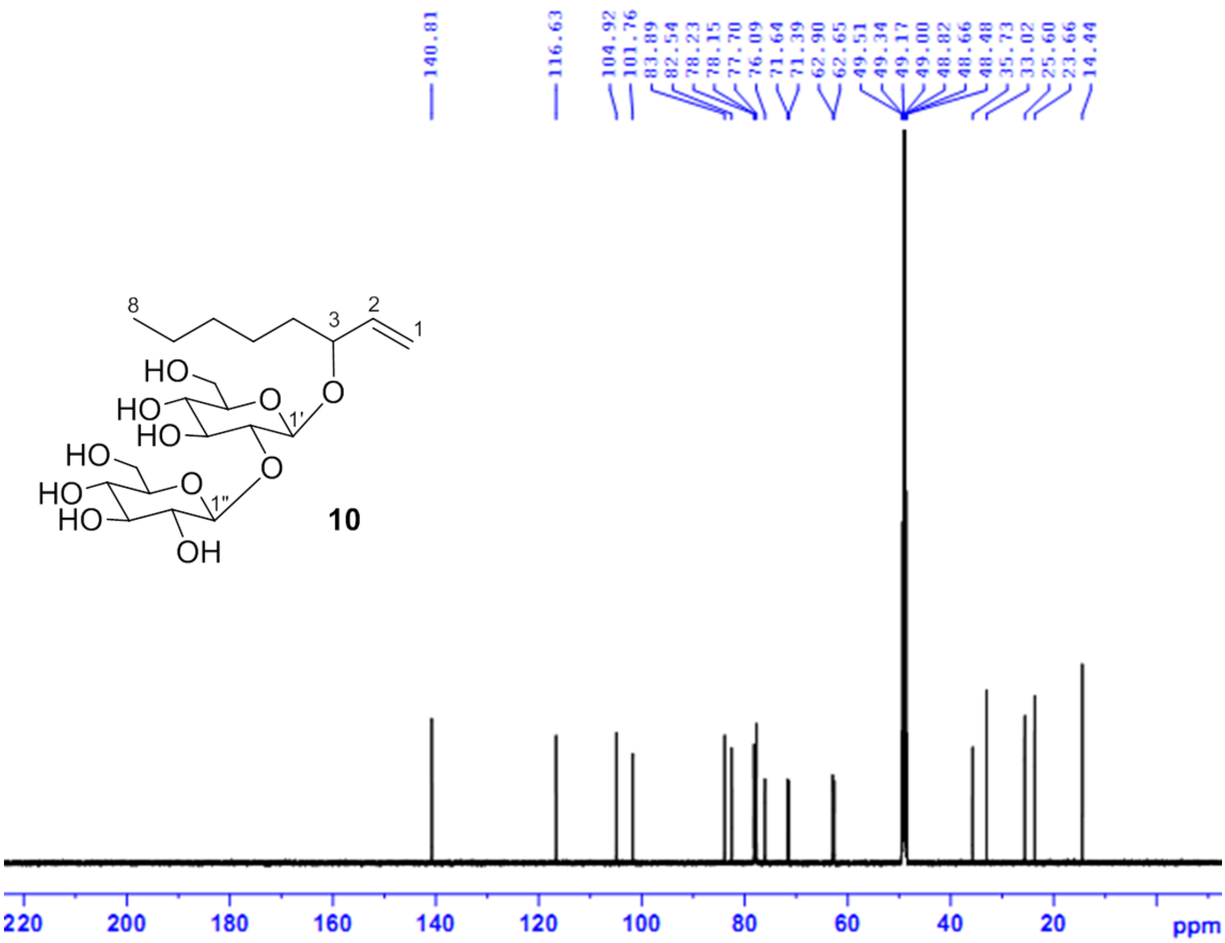


Figure S29: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Compound **10**

Ebracteatoside B (11): [1]H NMR (500 MHz, CD_3OD) and [13]C NMR (125 MHz, CD_3OD) data (Table S4)

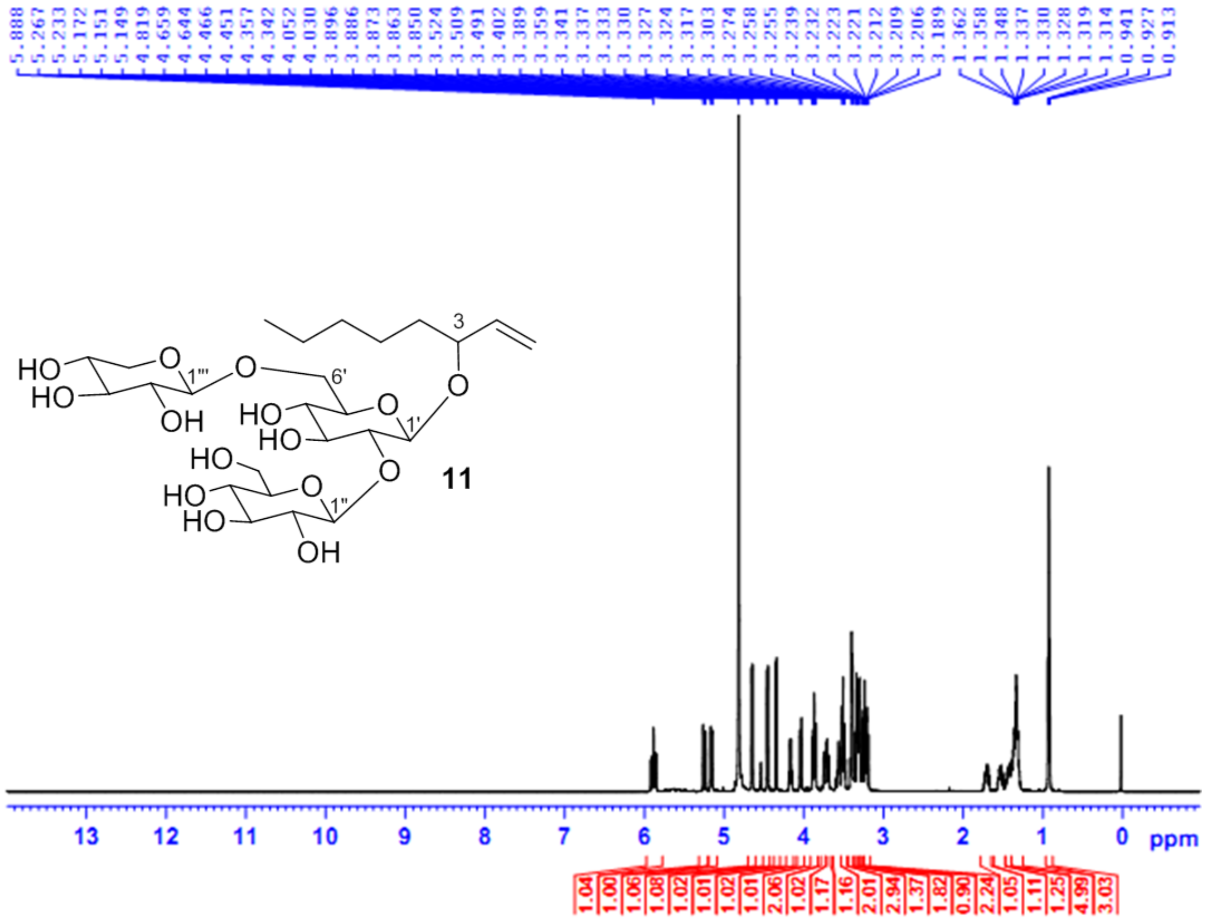


Figure S30: [1]H-NMR (500 MHz, CD_3OD) Spectrum of Ebracteatoside B (**11**)

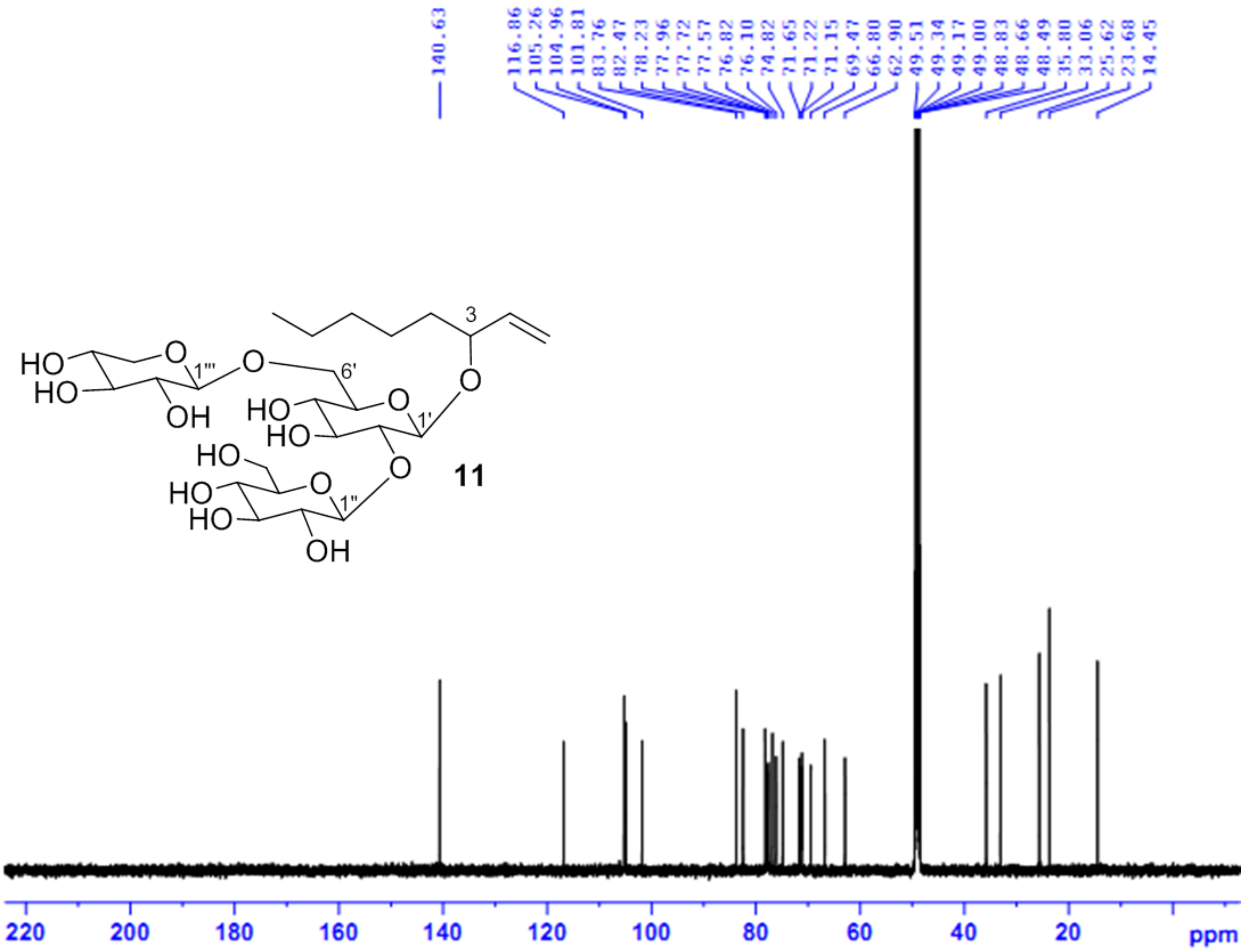


Figure S31: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Ebracteatoside B (**11**)

Lariciresinol-9-*O*-β-D-glucopyranoside (12): ^{1}H NMR (500 MHz, CD_3OD) δ: 6.95 (1H, d, *J* = 2.0 Hz, H-2), 6.82 (1H, d, *J* = 2.0 Hz, H-2'), 6.81 (1H, dd, *J* = 2.0, 8.0 Hz, H-6), 6.78 (1H, d, *J* = 8.0 Hz, H-5), 6.73 (1H, d, *J* = 8.0 Hz, H-5'), 6.68 (1H, dd, *J* = 2.0, 8.0 Hz, H-6'), 4.87 (1H, d, *J* = 6.5 Hz, H-7), 4.32 (1H, d, *J* = 7.5 Hz, H-1"), 4.07 (1H, dd, *J* = 6.5, 10.0 Hz, H-9a), 4.01 (1H, dd, *J* = 6.5, 8.5 Hz, H-9'a), 3.90 (1H, m, H-6"a), 3.87 (3H, s, 3-OCH_3), 3.85 (3H, s, 3'-OCH_3), 3.79 (1H, dd, *J* = 7.5, 10.0 Hz, H-9b), 3.76 (1H, dd, *J* = 6.5, 8.5 Hz, H-9'b), 3.70 (1H, dd, *J* = 5.5, 12.0 Hz, H-6"b), 3.38 (1H, m, H-3"), 3.30 (2H, m, H-4", 5"), 3.24 (1H, dd, *J* = 8.0, 9.0 Hz, H-2"), 2.94 (1H, dd, *J* = 5.0, 13.5 Hz, H-7'a), 2.79 (1H, m, H-8'), 2.55 (1H, m, H-7'b), 2.51 (1H, m, H-8); ^{13}C NMR (125 MHz, CD_3OD) δ: 149.0 (C-3), 148.9 (C-3'),147.0 (C-4), 145.8 (C-4'), 135.6 (C-1), 133.7 (C-1'), 122,3 (C-6'), 119.8 (C-6), 116.1 (C-5'), 116.0 (C-5), 113.5 (C-2'), 110.8 (C-2), 104.7 (C-1"), 84.2 (C-7), 78.2 (C-3"), 78.0 (C-5"), 75.2 (C-2"), 73.6 (C-9'), 71.7(C-4"), 68.5 (C-9), 62.7 (C-6"), 56.4 (3, 3'-OCH_3), 51.7 (C-8), 43.9 (C-8'), 33.9 (C-7').

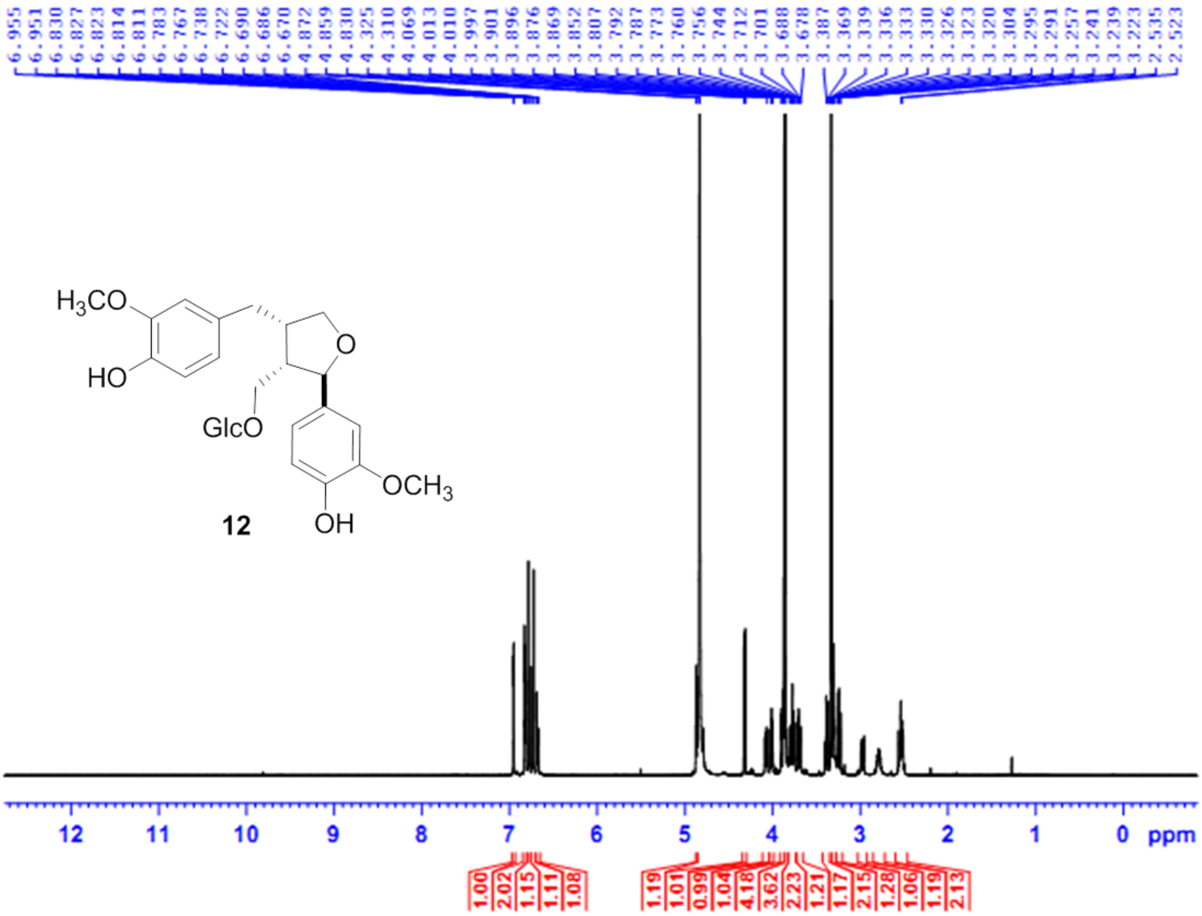


Figure S32: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Lariciresinol-9-*O*-β-D-glucopyranoside (**12**)

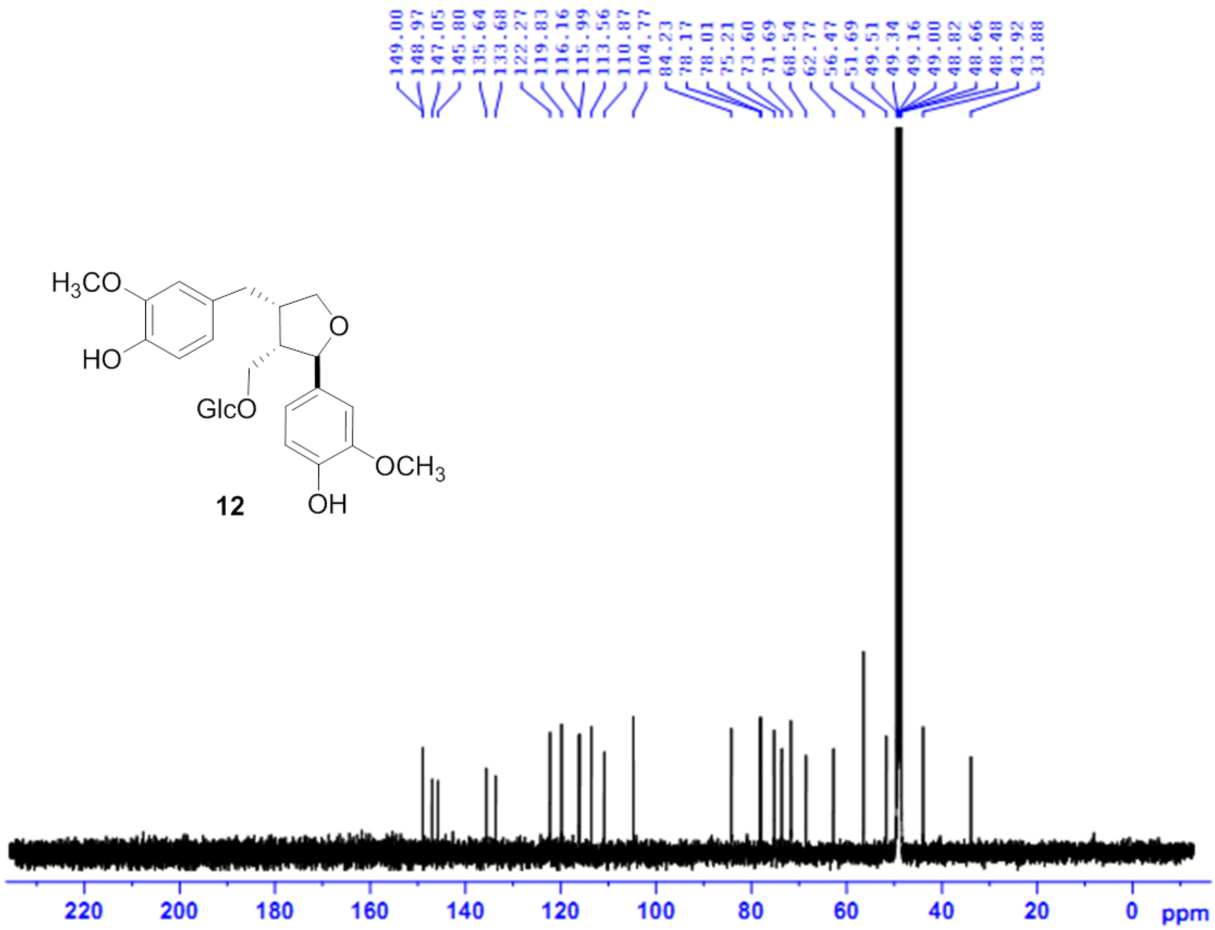


Figure S33: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Lariciresinol-9-*O*-β-D-glucopyranoside (**12**)

Ginsenoside Rg1 (13): ^{1}H NMR (500 MHz, CD_3OD) and ^{13}C NMR (125 MHz, CD_3OD) data (Table S5).

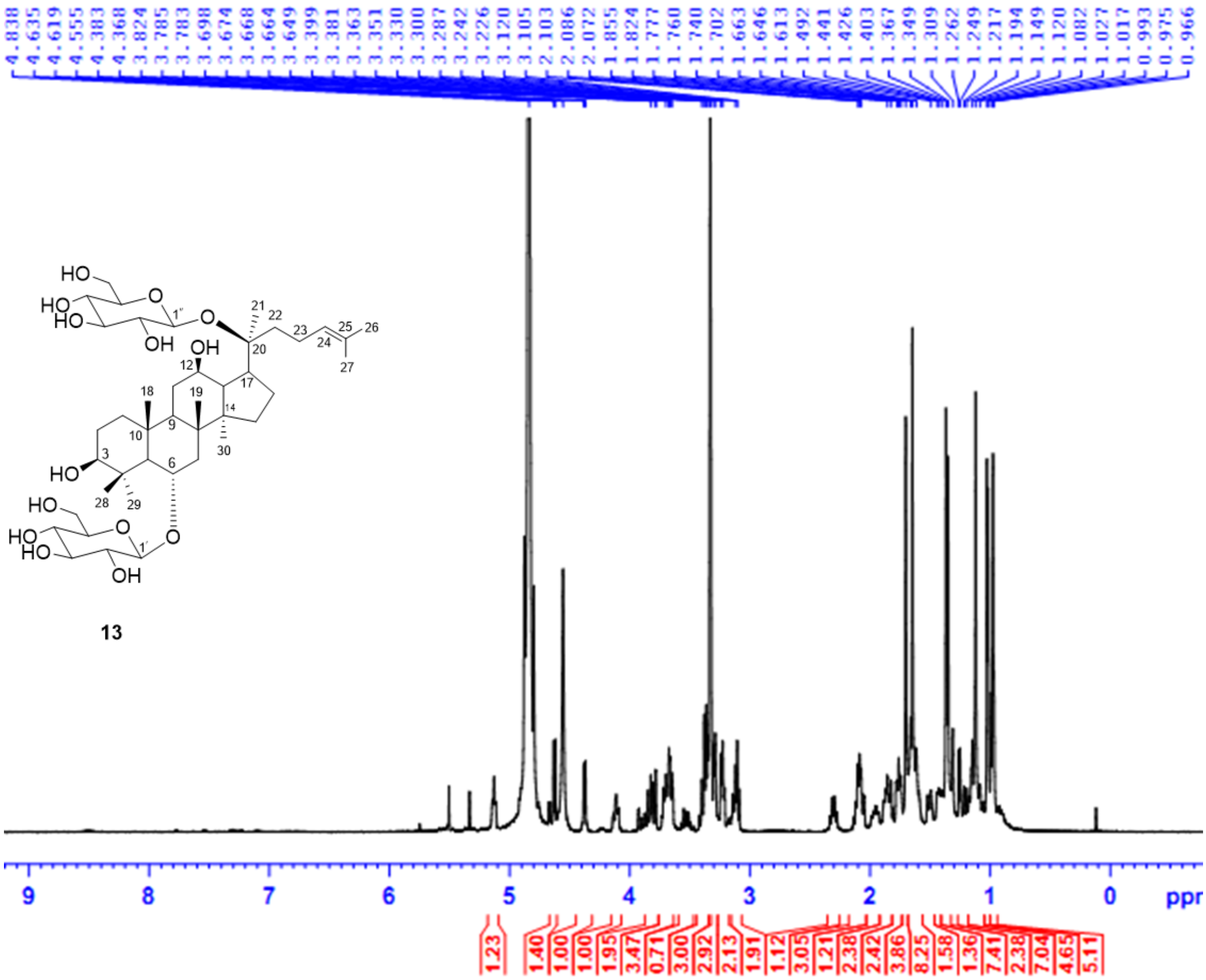


Figure S34: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Ginsenoside Rg1 (**13**)

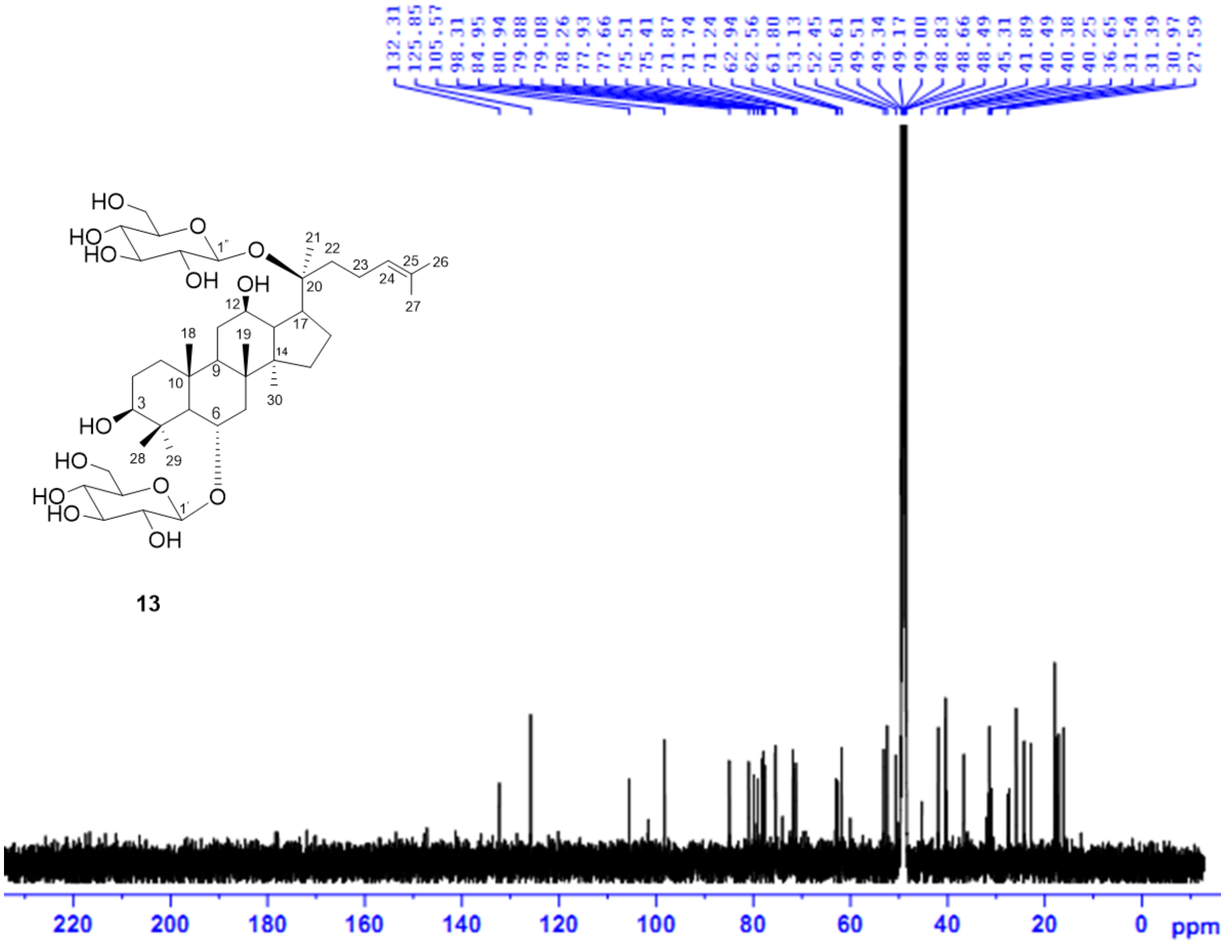


Figure S35: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Ginsenoside Rg1 (**13**)

Notoginsenoside-R1 (14): HR ESI-MS: *m/z* 987.5132 [M + MeOH + Na]+ (calcd. for $C_{48}H_{84}O_{19}Na$, 987.51592); ^{1}H NMR (500 MHz, CD_3OD) and ^{13}C NMR (125 MHz, CD_3OD) data (Table S5).

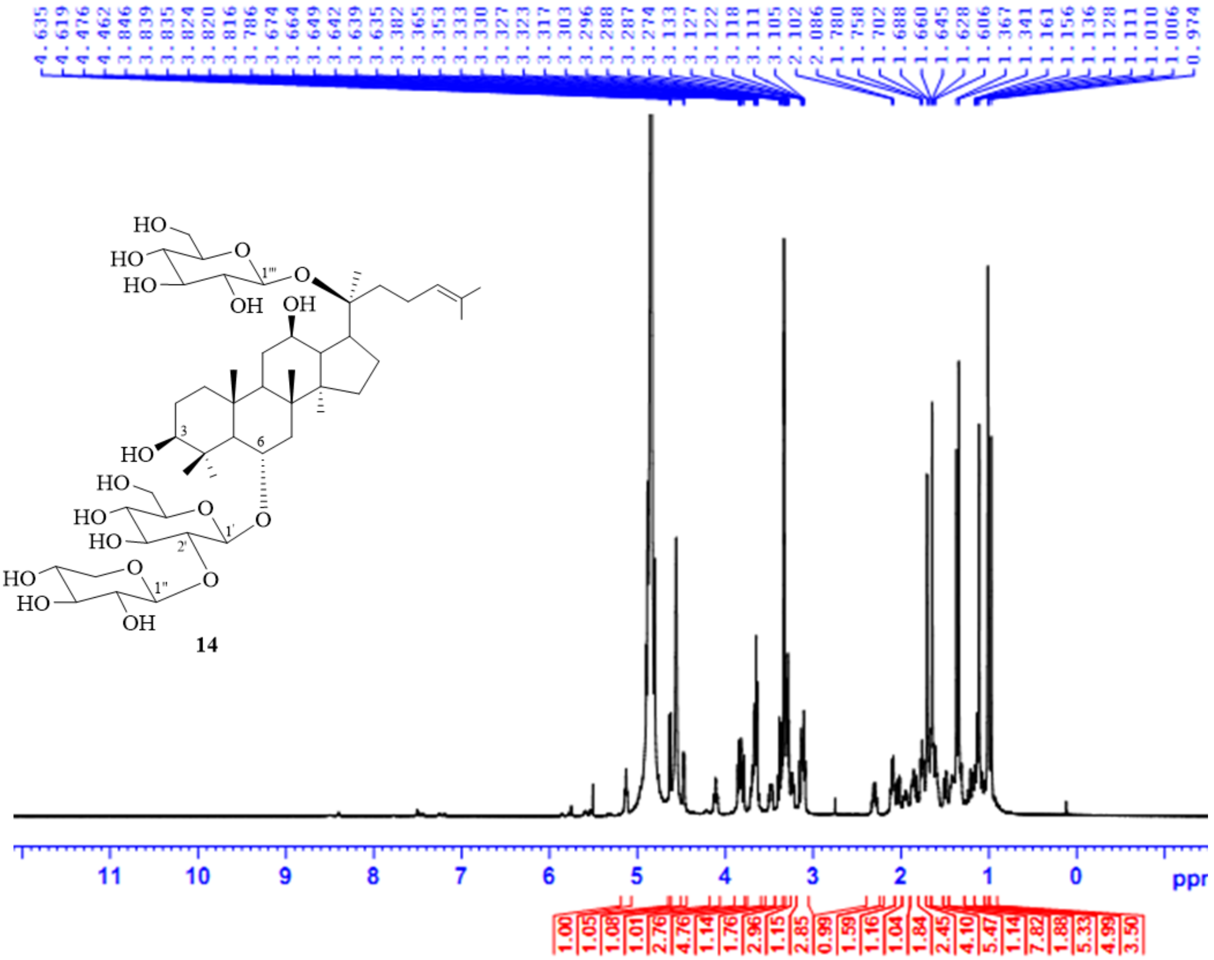


Figure S36: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Notoginsenoside-R1 (**14**)

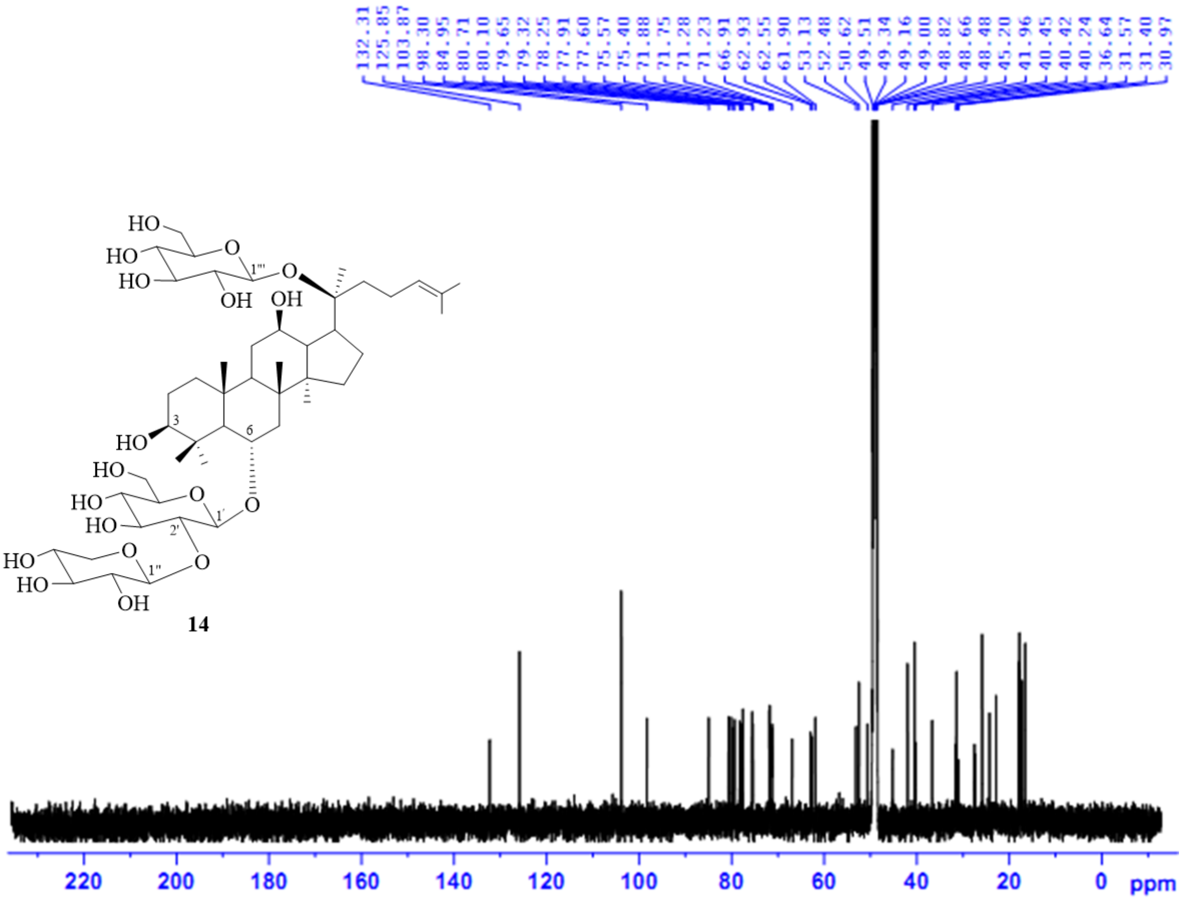


Figure S37: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Notoginsenoside-R1 (**14**)

Ginsenoside Rb1 (15): [1]H NMR (500 MHz, CD_3OD) and [13]C NMR (125 MHz, CD_3OD) data (Table S5).

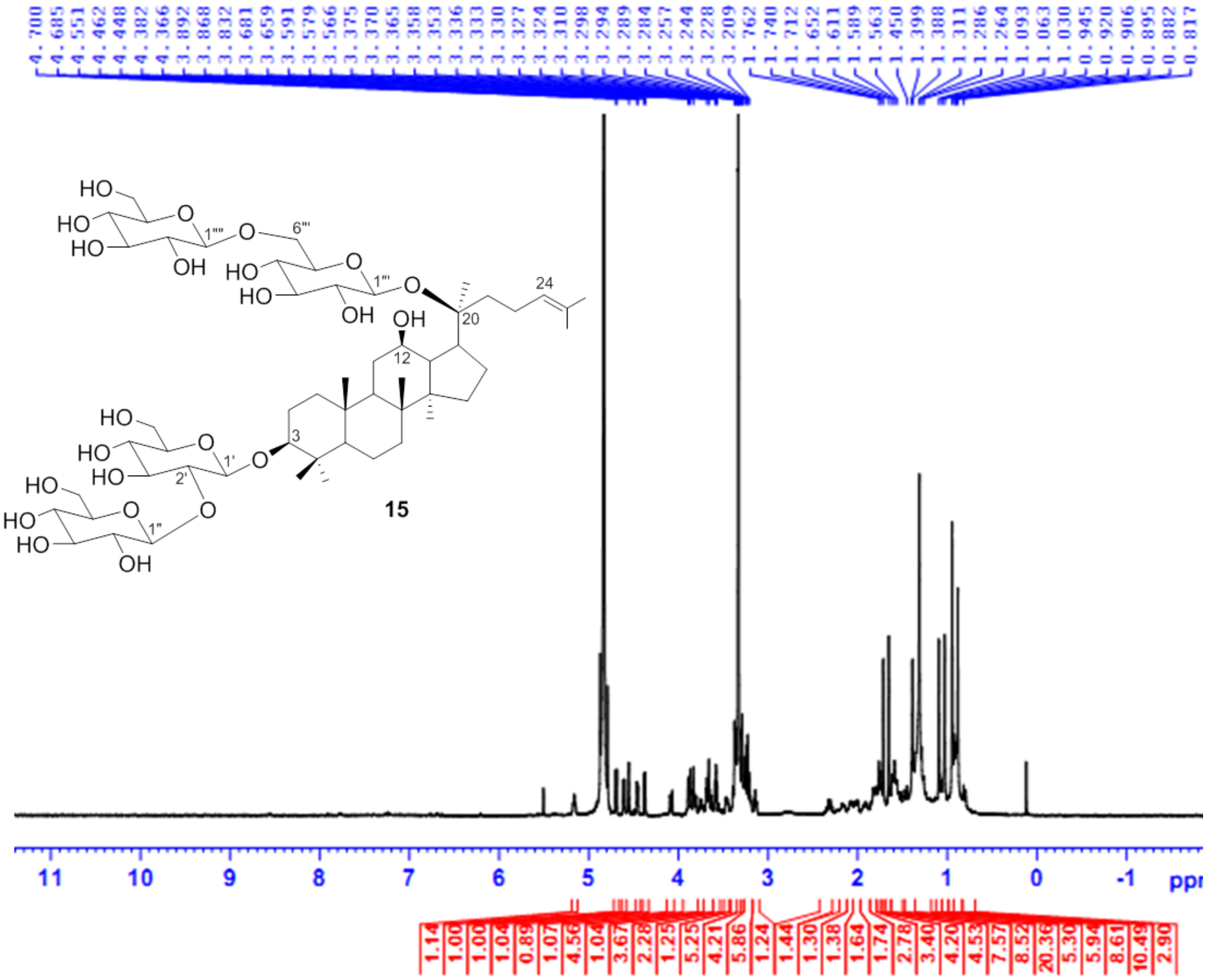


Figure S38: [1]H-NMR (500 MHz, CD_3OD) Spectrum of Ginsenoside Rb1 (**15**)

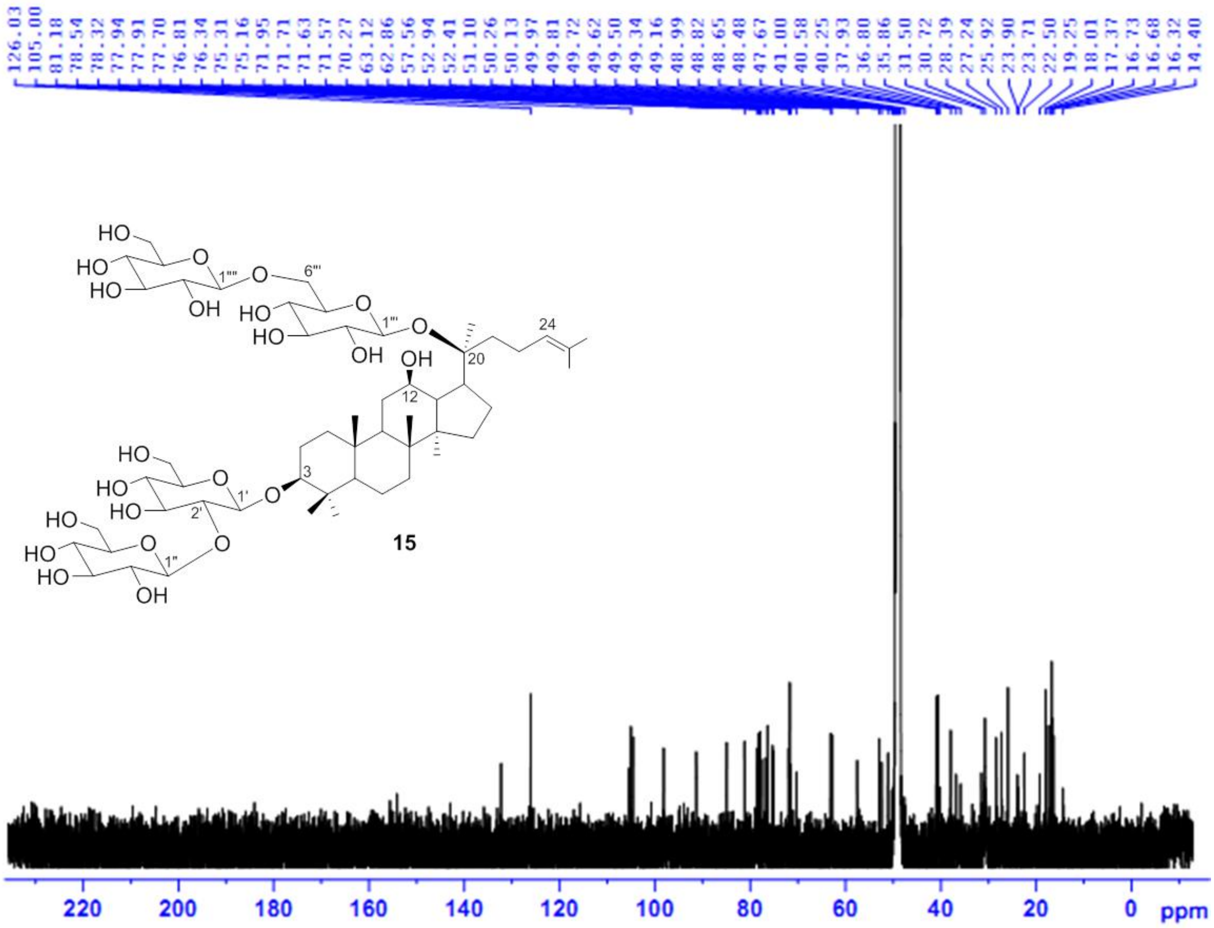
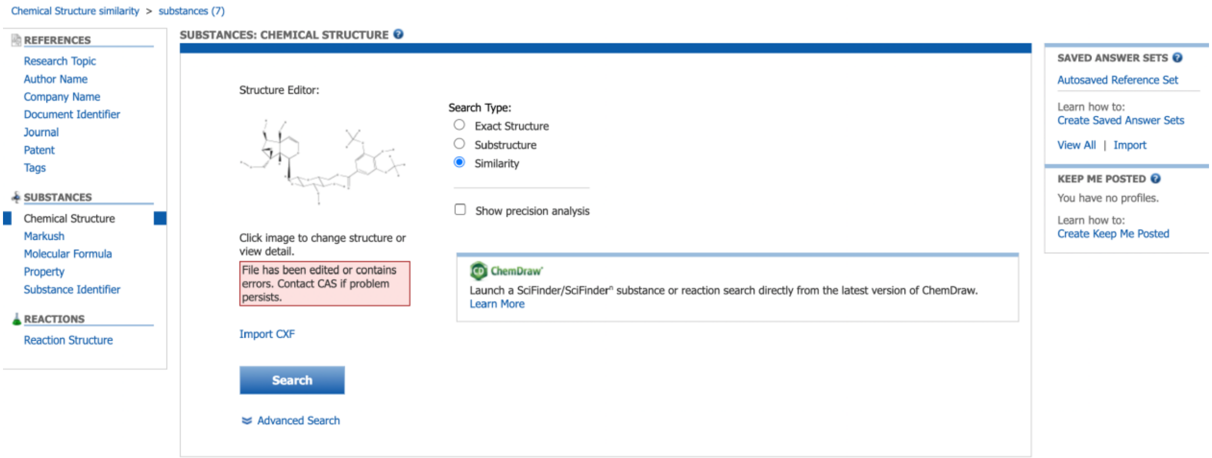
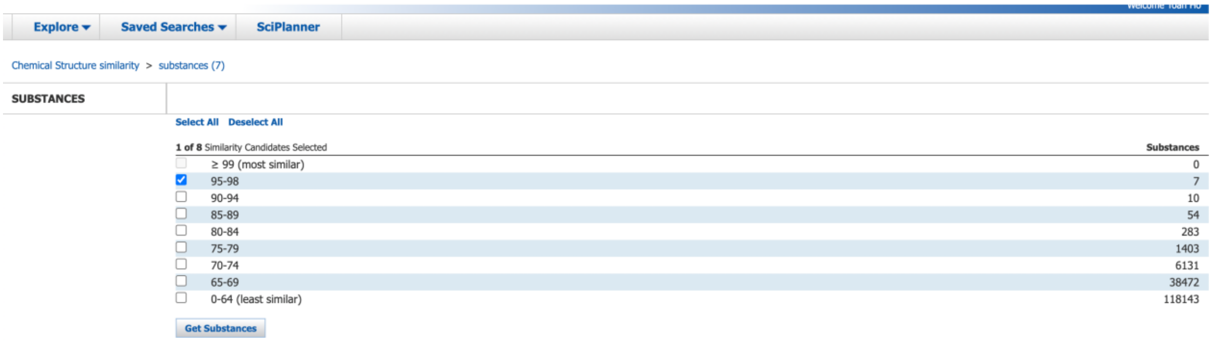
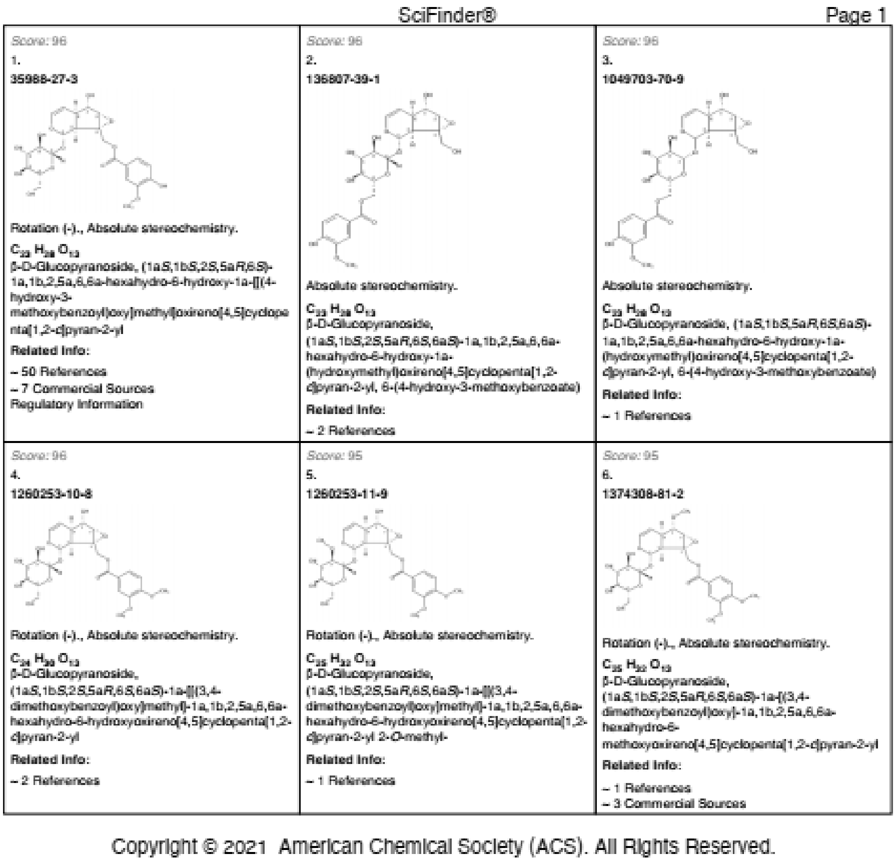


Figure S39: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Ginsenoside Rb1 (**15**)







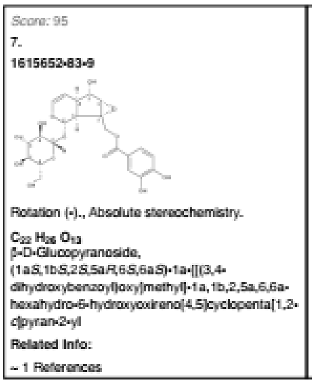
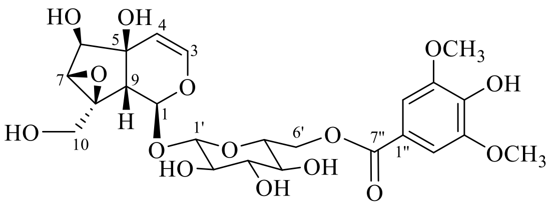
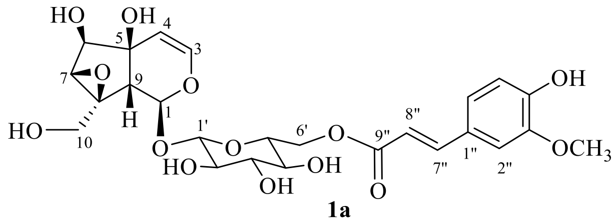


Figure S40: SciFinder Search Results of Compound **1**



1

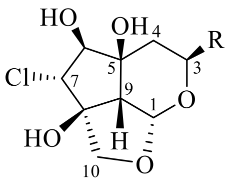


1a

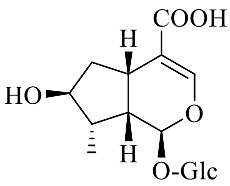
Table S1. ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) data for compounds **1** and **1a** in CD_3OD

Position	**1**		**1a**	
	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	95.5 (CH)	5.13 (1H, *d*, *J* = 9.0)	95.5 (CH)	5.22 (1H, *d*, *J* = 8.0)
2	-	-	-	-
3	142.6 (CH)	6.35 (1H, *d*, *J* = 6.0)	142.8 (CH)	6.35 (1H, *d*, *J* = 6.0)
4	108.0 (CH)	4.92 (1H, *d*, *J* = 6.0)	108.0 (CH)	4.89 (1H, *d*, *J* = 6.0)
5	74.4 (C)	-	74.5 (C)	-
6	78.7 (CH)	3.81 (1H, *d*, *J* = 1.0)	78.7 (CH)	3.95 (1H, d, *J* = 1.0)
7	63.2 (CH)	3.45 (1H, *m*)	63.4 (CH)	3.53 (1H, d, *J* = 1.0)
8	66.5 (C)	-	66.8 (C)	-
9	50.9 (CH)	2.55 (1H, *d*, *J* = 9.0)	51.0 (CH)	2.55 (1H, *d*, *J* = 8.0)
10	61.5 (CH_2)	4.10 (1H, *d*, *J* = 13.0)	61.6 (CH_2)	4.13 (1H, *d*, *J* = 13.0)
		3.54 (1H, *d*, *J* = 13.0)		3.61 (1H, *d*, *J* = 13.0)
Glc-1′	99.8 (CH)	4.78 (1H, *d*, *J* = 8.0)	100.0 (CH)	4.73 (1H, *d*, *J* = 8.0)
2′	74.7 (CH)	3.30 (1H, *dd*, *J* = 9.0, 8.0)	74.7 (CH)	3.28 (1H, *dd*, *J* = 9.0, 8.0)
3′	77.5 (CH)	3.45 (1H, *m*)	77.6 (CH)	3.53 (1H, *m*)
4′	71.8 (CH)	3.45 (1H, *m*)	71.7 (CH)	3.40 (1H, *m*)
5′	76.0 (CH)	3.64 (1H, *m*)	76.1 (CH)	3.40 (1H, *m*)
6′	64.4 (CH_2)	4.60 (2H, *m*)	64.1 (CH_2)	4.50 (1H, *dd*, *J* = 12.0, 2.0)
				4.43 (1H, *dd*, *J* = 12.0, 6.0)
Acyl-1″	121.3 (C)	-	128.7 (C)	
2″	108.4 (CH)	7.35 (1H, *s*)	112.0 (CH)	7.20 (1H, *d*, *J* = 2.0)
3″	149.0 (C)	-	149.2 (C)	-
4″	142.6 (C)	-	151.1 (C)	-
5″	149.0 (C)	-	116.6 (CH)	6.82 (1H, *d*,*J* = 8.0)
6″	108.4 (CH)	7.35 (1H, *s*)	124.3 (CH)	7.09 (1H, *dd*, *J* = 8.0, 2.0)
7″	167.9 (C)	-	147.2 (CH)	7.63 (1H, *d*, *J* = 16.0)
8″	-	-	115.4 (CH)	6.38 (1H, *d*, *J* = 16.0)
9″	-	-	168.9 (C)	-
3″-OCH_3	57.0 (CH_3)	3.92 (3H, *s*)	56.6 (CH_3)	3.90 (3H, s)
5″-OCH_3	57.0 (CH_3)	3.92 (3H, *s*)	-	

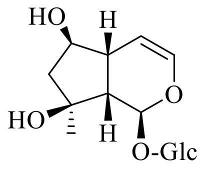
1a: Myobontioside B [M. Kanemoto, K. Matsunami, H. Otsuka, T. Shinzato, C. Ishigaki, Y. Takeda (2008). Chlorine-containing iridoid and iridoid glucoside and other glucosides from leaves of *Myoporum bontioides*, *Phytochemistry*, **69**, 2517-2522.]



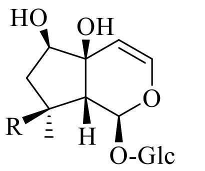
2: R = H
3: R = OH



4



5

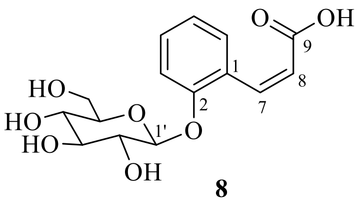


6: R = $OCOCH_3$
7: R = OH

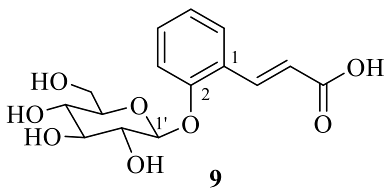
Table S2. ^{13}C NMR (125 MHz) data for compounds 2-7

Position	**2**[a]	**3**[b]	**4**[b]	**5**[b]	**6**[c]	**7**[c]
1	101.7	102.0	95.6	93.8	92.4	91.6
3	57.8	90.2	150.0	140.4	141.1	139.8
4	32.1	38.7	-	105.9	107.3	108.5
5	72.8	75.0	31.7	41.3	71.1	69.7
6	76.6	78.6	41.1	77.8	75.6	76.1
7	73.1	71.9	79.4	50.0	44.5	46.9
8	84.1	84.6	45.0	79.5	86.1	75.3
9	55.3	57.6	43.0	51.8	54.2	58.3
10	71.9	73.9	14.3	25.2	22.0	24.7
1′			99.0	99.4	97.1	97.4
2′			74.8	74.8	73.0	72.9
3′			78.3	78.2	77.1	77.1
4′			71.8	71.7	70.1	70.0
5′			78.0	78.0	76.1	76.0
6′			62.9	62.6	61.1	60.9
4-COOH			-			
8-$OCOCH_3$					170.1	
					21.9	

a Recorded in CD_3COCD_3, **b** in CD_3OD, **c** in DMSO-d_6



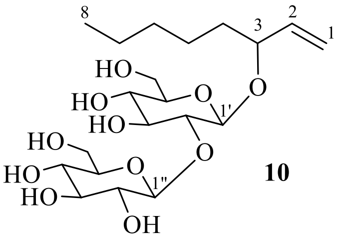
8



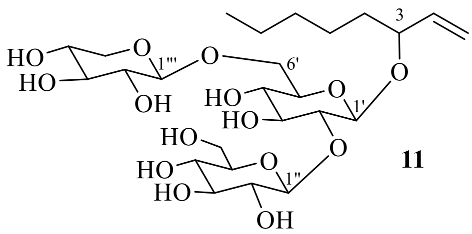
9

Table S3. [1]H NMR (500 MHz) and [13]C NMR (125 MHz) data for compounds **8** and **9** in CD_3OD

Position	**8**		**9**	
	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	128.2 (C)	-	125.4	-
2	156.2 (C)	-	157.5	-
3	116.6 (CH)	7.17 (1H, *dd*, *J* = 1.0, 8.0)	116.9	7.28 (1H, *d*, *J* = 8.0)
4	129.9 (CH)	7.21 (1H, *td*, *J* = 1.0, 8.0)	132.8	7.39 (1H, *td*, *J* = 1.5, 8.0)
5	123.0 (CH)	6.95 (1H, *td*, *J* = 1.0, 8.0)	123.6	7.07 (1H, *t*, *J* = 8.0)
6	130.9 (CH)	7.66 (1H, *dd*, *J* = 1.0, 8.0)	128.8	7.65 (1H, *dd*, *J* = 1.5, 8.0)
7	128.0 (CH)	6.85 (1H, *d*, *J* = 12.5)	141.4	8.15 (1H, *d*, *J* = 16.0)
8	128.4 (CH)	6.08 (1H, *d*, *J* = 12.5)	119.6	6.56 (1H, *d*, *J* = 16.0)
9	177.5 (C)	-	171.0	-
1′	102.6 (CH)	4.94 (1H, *d*, *J* = 7.5)	102.4	5.02 (1H, *d*, *J* = 8.0)
2′	74.9 (CH)	3.42-3.52 (4H, *m*)	74.8	3.44-3.59 (4H, *m*)
3′	78.1 (CH)		78.2	
4′	71.3 (CH)		71.3	
5′	78.0 (CH)		78.1	
6′	62.5 (CH_2)	3.90 (1H, *dd*, *J* = 1.5, 12.0)	62.5	3.92 (1H, *dd*, *J* = 2.0, 12.0)
		3.72 (1H, *m*)		3.73 (1H, *dd*, *J* = 5.0, 12.0)



10

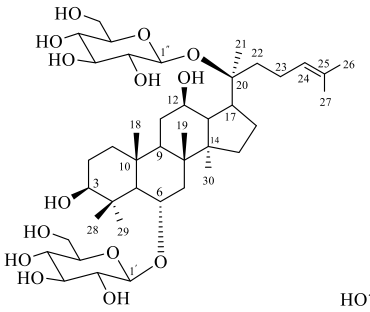


11

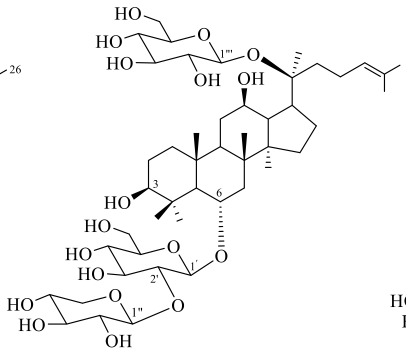
Table S4. [1]H NMR (500 MHz) and [13]C NMR (125 MHz) data for compounds **10** and **11** in CD_3OD

Position	**10**		**11**	
	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	116.1 (CH_2)	5.33 (1H, *brd*, *J* = 17.5)	116.8	5.26 (1H, *brd*, *J* = 17.0)
		5.24 (1H, *brd*, *J* = 10.5)		5.17 (1H, *brd*, *J* = 10.5)
2	140.8 (CH)	5.99 (1H, *ddd*, *J* = 7.0, 10.5, 17.5)	140.6	5.90 (1H, *ddd*, *J* = 6.5, 10.5, 17.0)
3	83.9 (CH)	4.25 (1H, *q*, *J* = 7.0)	83.7	4.17 (1H, *q*, *J* = 6.5)
4	35.7 (CH_2)	1.81 (1H, *m*), 1.62 (1H, *m*)	35.8	1.70 (1H, *m*), 1.53 (1H, *m*)
5	25.6 (CH_2)	1.48 (6H, *m*)	25.6	1.37 (6H, *m*)
6	33.0 (CH_2)		33.0	
7	23.6 (CH_2)		23.7	
8	14.4 (CH_3)	1.01 (3H, *t*, *J* = 6.5)	14.4	0.92 (3H, *t*, *J* = 6.5)
Glc-1′	101.7 (CH)	4.55 (1H, *d*, *J* = 8.0)	101.8	4.46 (1H, *d*, *J* = 7.5)
2′	82.5 (CH)	3.59 (1H, *dd*, *J* = 8.0, 9.0)	82.4	3.51 (1H, *m*)
3′	78.1 (CH)	3.66 (1H, *d*, *J* = 9.0)	77.9*	
4′	71.6* (CH)	3.41 (1H, *m*)	71.1*	
5′	77.7 (CH)	3.49 (1H, *m*)	77.5*	
6′	62.9* (CH_2)	3.96 (1H, *brd*, *J* =12.0)	69.4	4.05 (1H, *d*, *J* = 11.0)
		3.79 (1H, *m*)		3.74 (1H, *m*)
Glc-1″	104.9 (CH)	4.75 (1H, *d*, *J* = 8.0)	104.9	4.65 (1H, *d*, *J* = 7.5)
2″	76.1(CH)	3.34 (1H, *m*)	76.1	
3″	78.2 (CH)	3.43 (1H, *m*)	78.2	
4″	71.4* (CH)	3.41 (1H, *m*)	71.2*	
5″	77.7 (CH)	3.49 (1H, *m*)	77.7*	
6″	62.6* (CH_2)	3.92 (1H, *dd*, *J* = 2.0, 11.5)	62.9	3.88 (1H, *m*), 3.74 (1H, *m*)
		3.76 (1H, *m*)		
Xyl-1‴			105.2	4.35 (1H, *d*, *J* = 7.5)
2‴			74.8	
3‴			77.5*	
4‴			71.6	
5‴			66.8	3.88 (1H, *m*), 3.20 (1H, *m*)

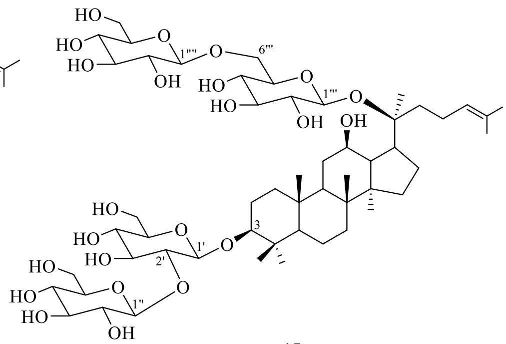
* Assignments may be interchanged in each column



13



14



15

Table S5. ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) data for compounds **13-15** in CD_3OD

C	**13**		**14**		**15**	
	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	40.2	1.76 (1H, *m*), 1.08 (1H, *m*)	40.2	1.74 (1H, *m*), 1.07 (1H, *m*)	40.2	1.76 (1H, *m*), 1.06 (1H, *m*)
2	27.6	1.66 (1H, *m*), 1.61 (1H, *m*)	27.5	1.64 (2H, *m*)	27.2	2.01 (1H, *m*), 1.76 (1H, *m*)
3	79.9	3.13 (1H, *m*)	79.6	3.66 (1H, *m*)	91.3	3.20 (1H, *m*)
4	40.5	-	40.5	-	40.6	-
5	61.8	1.15 (1H, *m*)	61.9	1.13 (1H, *m*)	57.6	0.81 (1H, *m*)
6	80.9	4.13 (1H, *td*, *J* = 3.0, 10.5)	80.7	4.11(1H, *td*, *J* = 3.0, 10.5)	19.2	1.61 (1H, *m*), 1.58 (1H, *m*)
7	45.3	2.05 (1H, *m*), 1.66 (1H, *m*)	45.2	1.68 (1H, *m*), 2.03 (1H, *m*)	35.8	1.56 (1H, *m*), 1.26 (1H, *m*)
8	41.9	-	41.9	-	41.0	-
9	50.6	1.49 (1H, *m*)	50.6	1.50 (1H, *m*)	51.1	1.47 (1H, *m*)
10	40.4	-	40.4	-	37.9	-
11	30.9	1.59 (1H, *m*), 1.15 (1H, *m*)	30.9	1.85 (1H, *m*), 1.18 (1H, *m*)	30.7	1.82 (1H, *m*), 1.26 (1H, *m*)
12	71.7	3.66 (1H, *m*)	71.7	3.65 (1H, *m*)	71.7	3.74 (1H, *m*)
13	49.5	1.76 (1H, *m*)	49.5	1.77 (1H, *m*)	49.8	1.76 (1H, *m*)
14	52.4	-	52.5	-	52.4	-
15	31.5	1.65 (1H, *m*), 1.15 (1H, *m*)	31.5	1.64 (1H, *m*), 1.18 (1H, *m*)	31.5	1.61 (1H, *m*), 1.06 (1H, *m*)
16	27.2	1.95 (1H, *m*), 1.42 (1H, *m*)	27.2	1.95 (1H, *m*), 1.42 (1H, *m*)	27.2	2.01 (1H, *m*), 1.76 (1H, *m*)
17	53.1	2.31 (1H, *m*)	53.1	2.31 (1H, *m*)	52.9	2.32 (1H, *m*)
18	17.6	1.12 (3H, *s*)	17.6	1.11 (3H, *s*)	16.3	1.03 (3H, *s*)
19	17.8	1.01 (3H, *s*)	17.8	1.01 (3H, *s*)	16.7	0.94 (3H, *s*)
20	84.9	-	84.9	-	85.0	-
21	22.8	1.36 (3H, *s*)	22.8	1.36 (3H, *s*)	22.5	1.33 (3H, *s*)
22	36.6	1.97 (1H, *m*), 1.66 (1H, *m*)	36.6	1.84 (1H, *m*), 1.66 (1H, *m*)	36.8	1.82 (1H, *m*), 1.58 (1H, *m*)
23	24.2	2.11 (2H, *m*)	24.2	2.10 (2H, *q*, *J* = 8.0)	23.9	2.15 (1H, *m*), 2.07 (1H, *m*)
24	125.8	5.13 (1H, *t*, *J* = 7.0)	125.8	5.12 (1H, *t*, *J* = 7.0)	126.0	5.16 (1H, *t*, *J* = 7.0)
25	132.3	-	132.3	-	132.0	-
26	25.8	1.70 (3H, *s*)	25.8	1.70 (3H, *s*)	25.9	1.71 (3H, *s*)
27	17.9	1.64 (3H, *s*)	17.9	1.64 (3H, *s*)	18.0	1.65 (3H, *s*)
28	31.4	1.35 (3H, *s*)	31.4	1.34 (3H, *s*)	28.4	1.09 (3H, *s*)
29	16.5	1.02 (3H, *s*)	16.5	1.00 (3H, *s*)	16.6	0.88 (3H, *s*)
30	17.1	0.97 (3H, *s*)	17.1	0.97 (3H, *s*)	17.4	0.94 (3H, *s*)
1′	105.5	4.38 (1H, *d*, *J* = 7.5)	103.8	4.47 (1H, *d*, *J* = 7.0)	105.4	4.46 (1H, *d*, *J* = 8.0)
2′	75.5		79.3		81.2	
3′	77.7		78.2		78.3	
4′	71.8		71.3		71.5	
5′	79.1		80.1		77.9	
6′	62.9		62.9		62.9	

1″	98.3	4.63 (1H, *d*, *J* = 8.0)	103.8	4.90 (1H, *d*, *J* = 6.0)	104.5	4.70 (1H, *d*, *J* = 8.0)
2″	75.4		75.5		76.8	
3″	77.9		77.6		78.3	
4″	71.2		71.9		71.6	
5″	78.2		66.9		78.5	
6″	62.5		-		63.1	
1‴			98.3	4.63 (1H, *d*, *J* = 8.0)	98.1	4.61 (1H, *d*, *J* = 8.0)
2‴			75.4		75.1	
3‴			77.9		77.9	
4‴			71.2		71.6	
5‴			78.2		76.3	
6‴			62.5		70.3	
1‴′					105.0	4.38 (1H, *d*, *J* = 8.0)
2‴′					75.3	
3‴′					77.7	
4‴′					71.9	
5‴′					78.5	
6‴′					62.9	