Supporting Information

***Rec. Nat. Prod*. 18:1 (2023) 107-113**

Pterosterone 20,22-Acetonide, a New Ecdysteroid and Other Constituents from *Acrostichum aureum* L.

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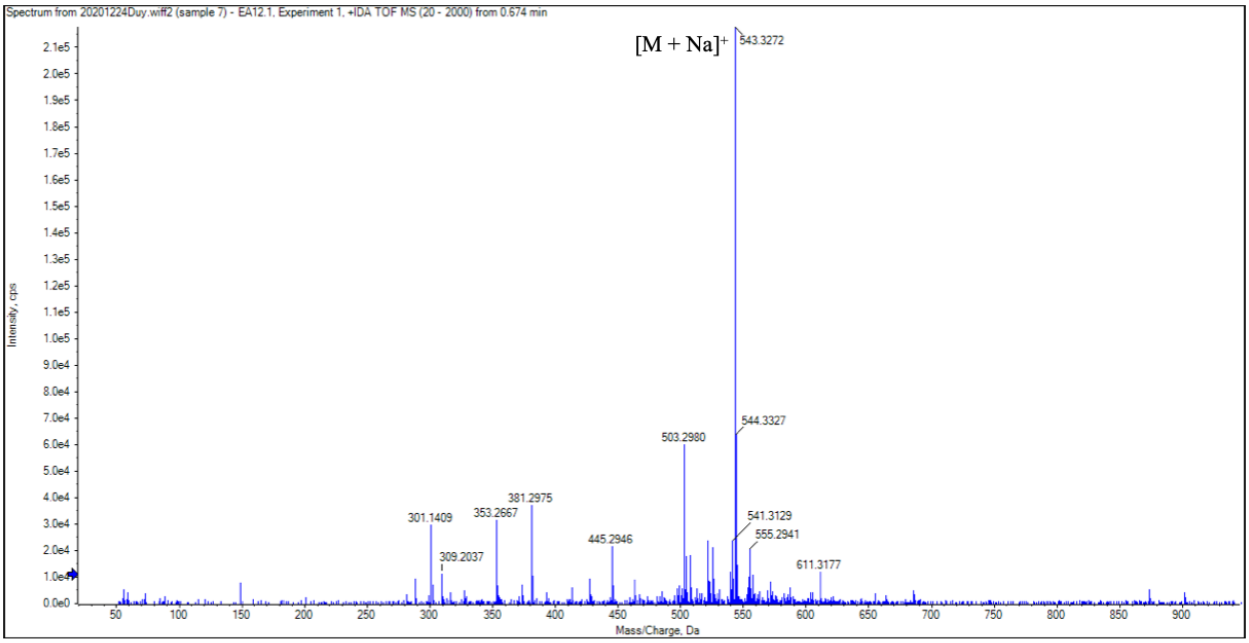


Hit	Formula	m/z	RDB	ppm	MS Rank	MSMS ppm	MSMS Rank	Found
1	C30H48O7	543.32922	7.0	-3.8	1			NA/NA

Figure S1: HR-ESI Mass Spectrum of Pterosterone 20,22-acetonide (**1**)

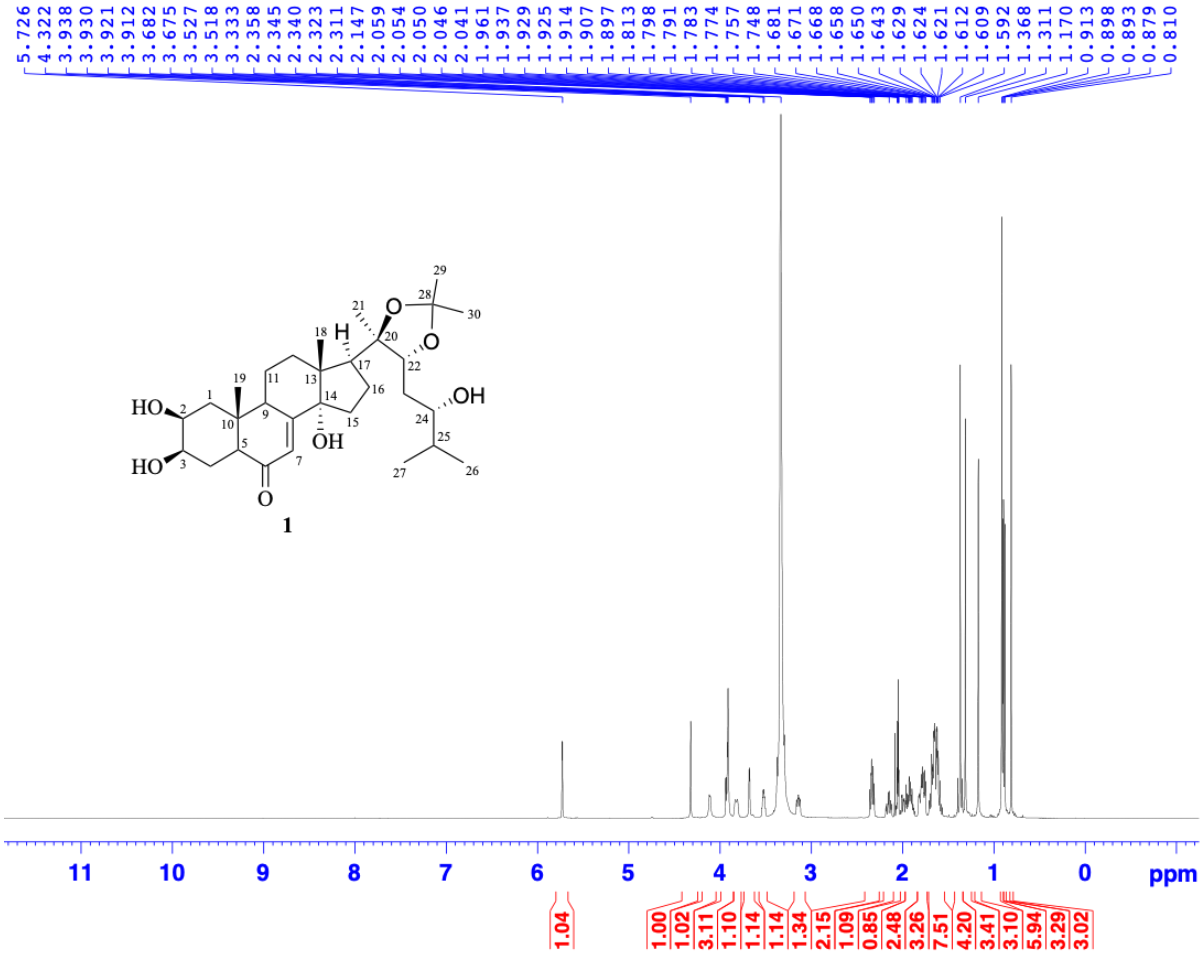


Figure S2: ^{1}H-NMR (500 MHz, acetone-d_6) Spectrum of Pterosterone 20,22-acetonide (**1**)

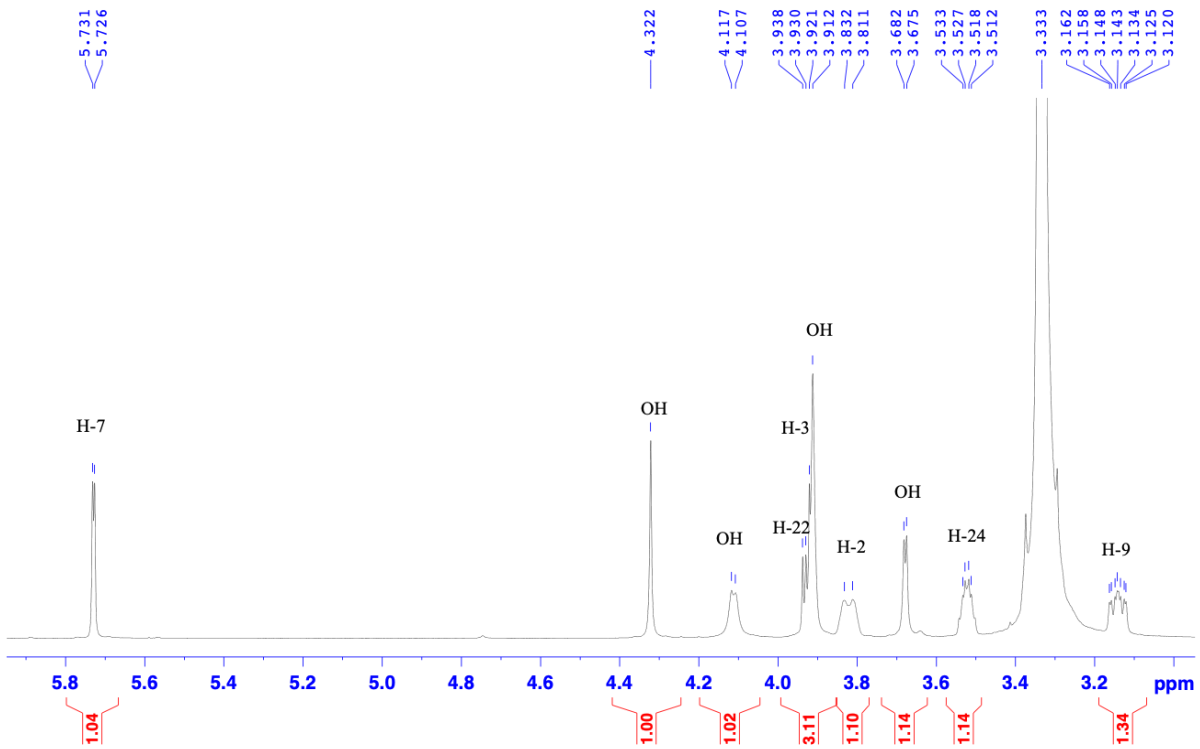


Figure S3: ^{1}H-NMR (500 MHz, acetone-d_6) Spectrum of **1** (from δ_H 3.0 ppm to 6.0 ppm)

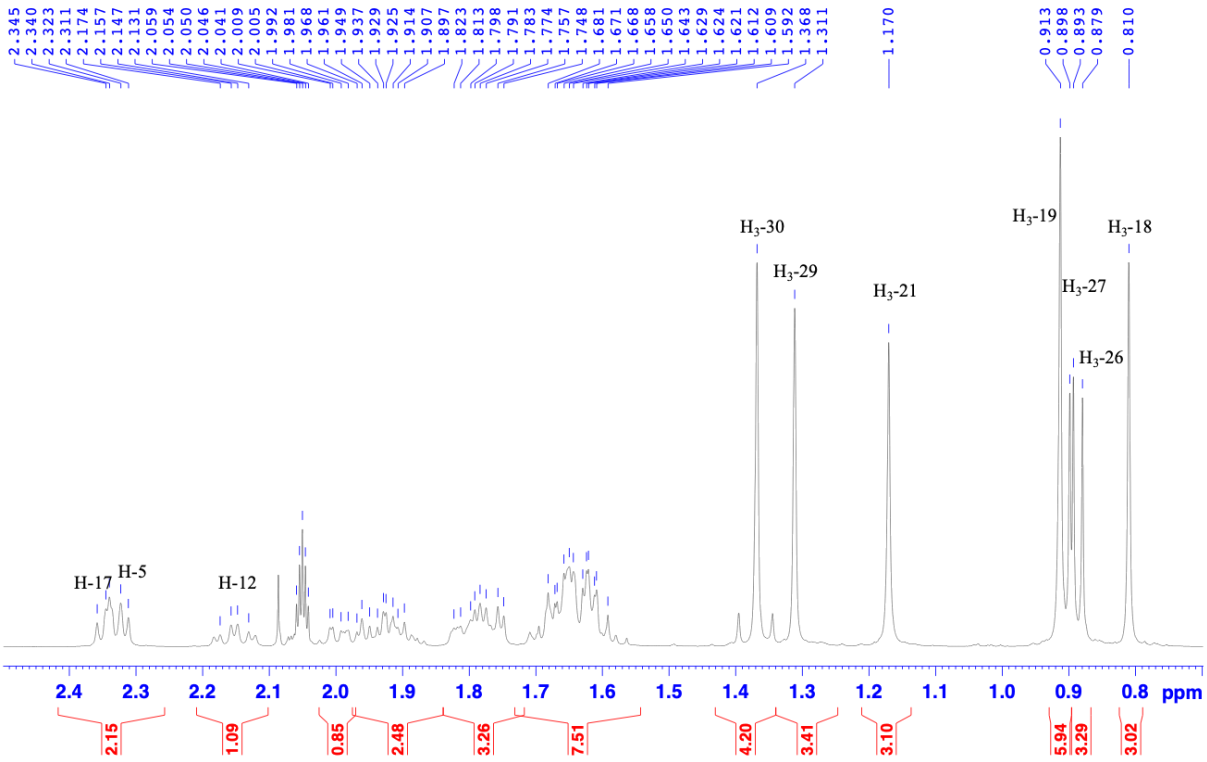


Figure S4: ^{1}H-NMR (500 MHz, acetone-d_6) Spectrum of **1** (from δ_H 0.5 ppm to 2.4 ppm)

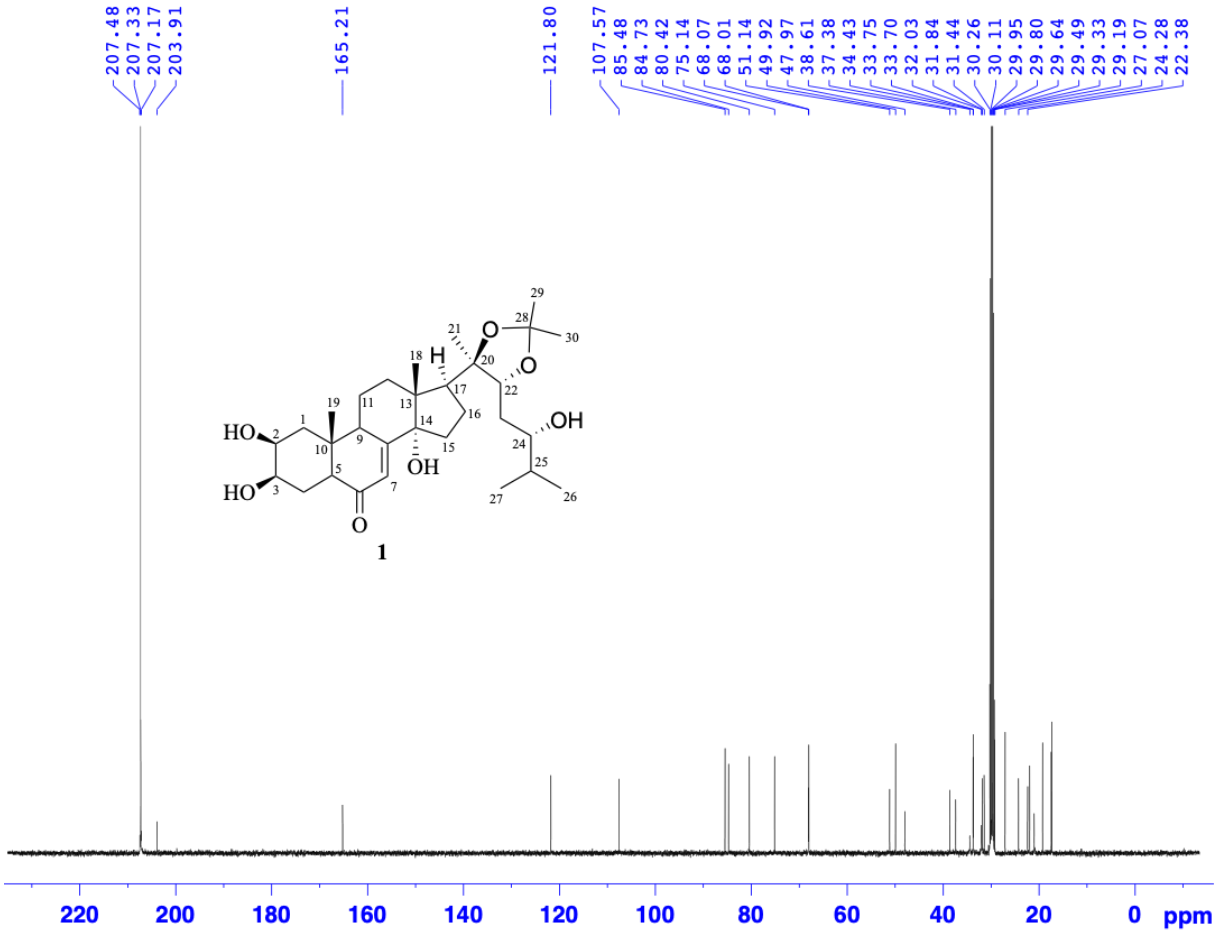


Figure S5: ^{13}C-NMR (125 MHz, acetone-d_6) Spectrum of Pterosterone 20,22-acetonide (**1**)

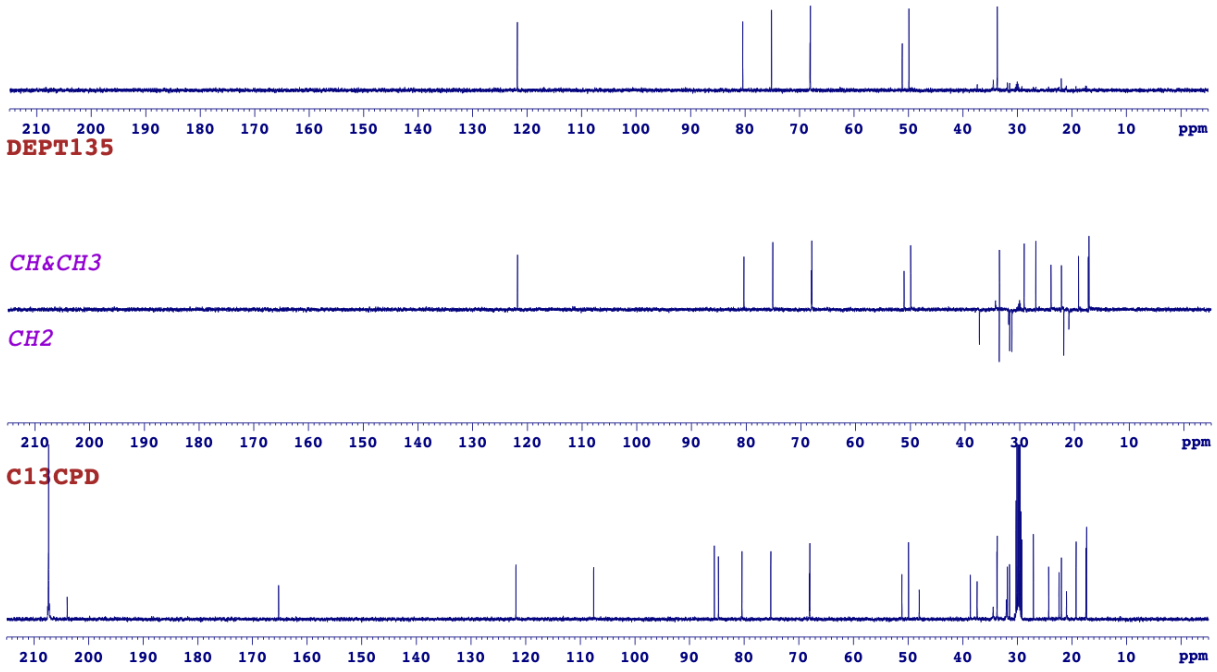


Figure S6: DEPT 90 and 135 (125 MHz, acetone-d_6) Spectrum of **1**

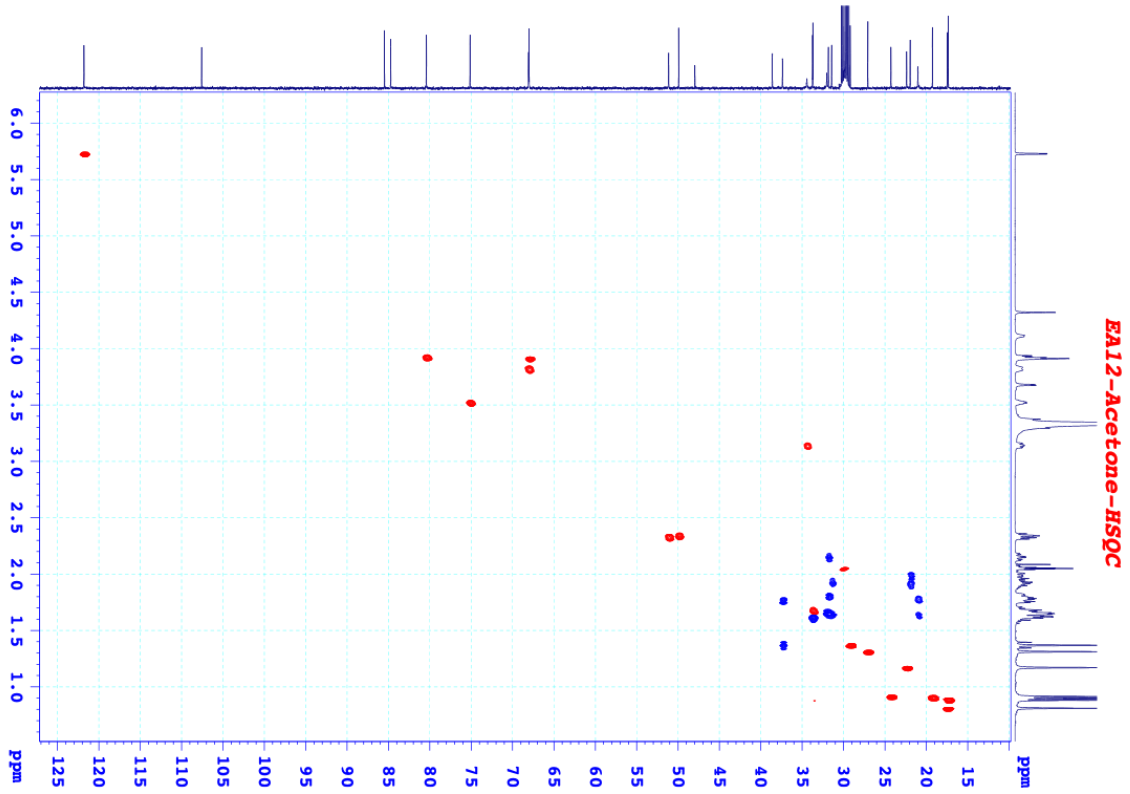


Figure S7: HSQC Spectrum of Pterosterone 20,22-acetonide (**1**)

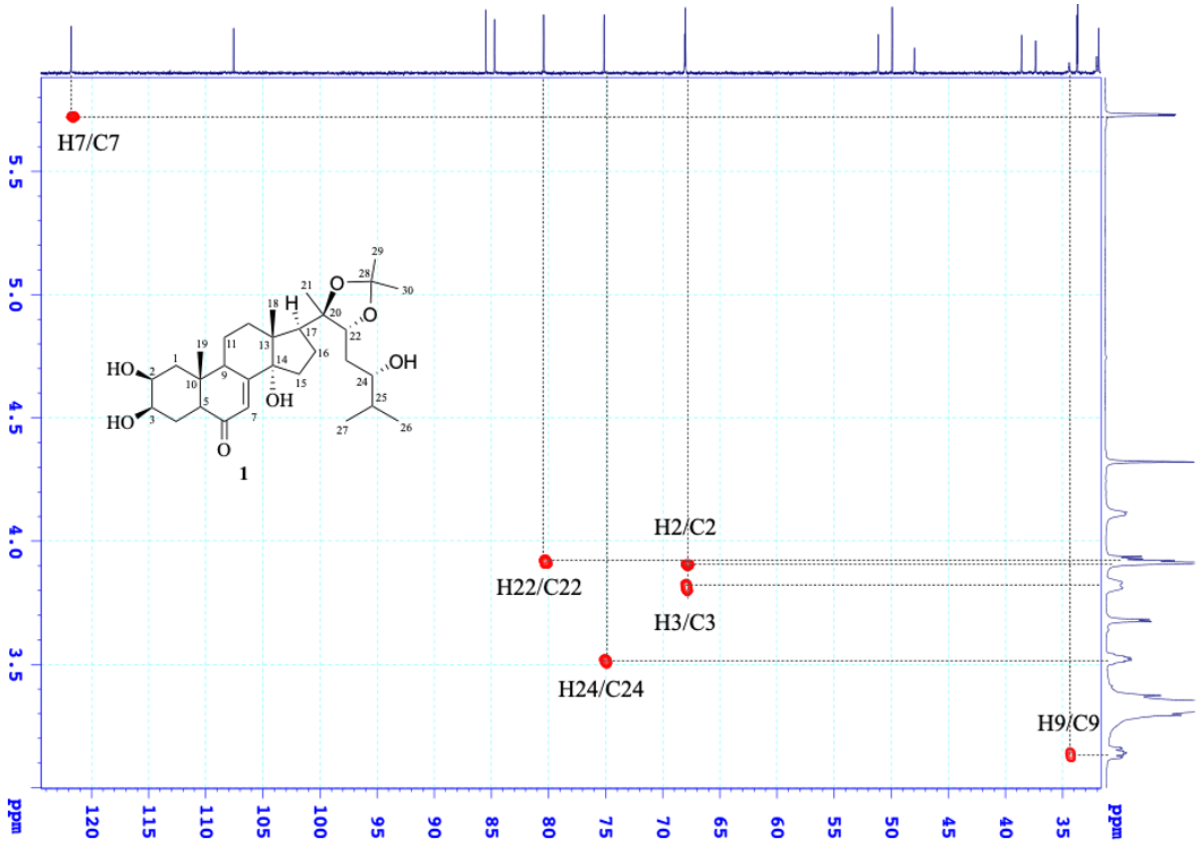


Figure S8: HSQC Spectrum of **1** (from δ_C 30 ppm to δ_C 125 ppm)

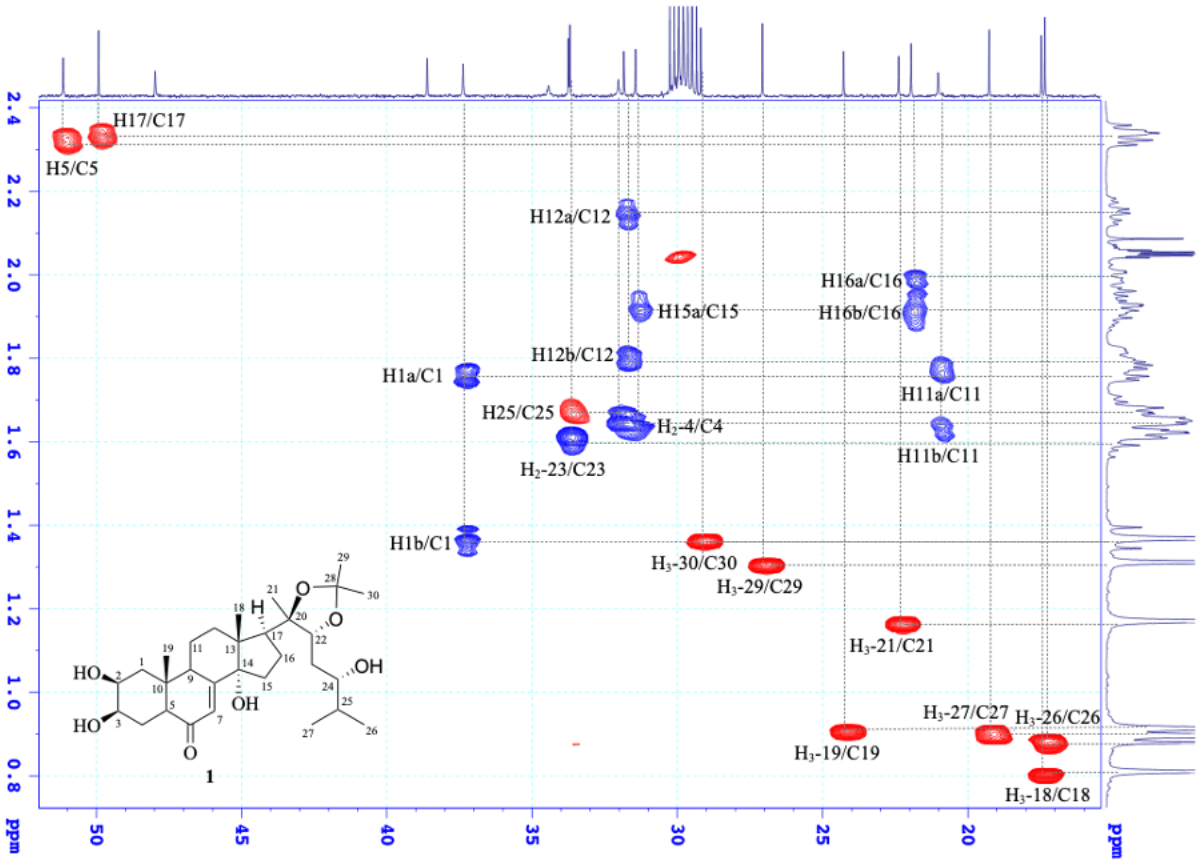


Figure S9: HSQC Spectrum of **1** (from δ_C 15 ppm to δ_C 55 ppm)

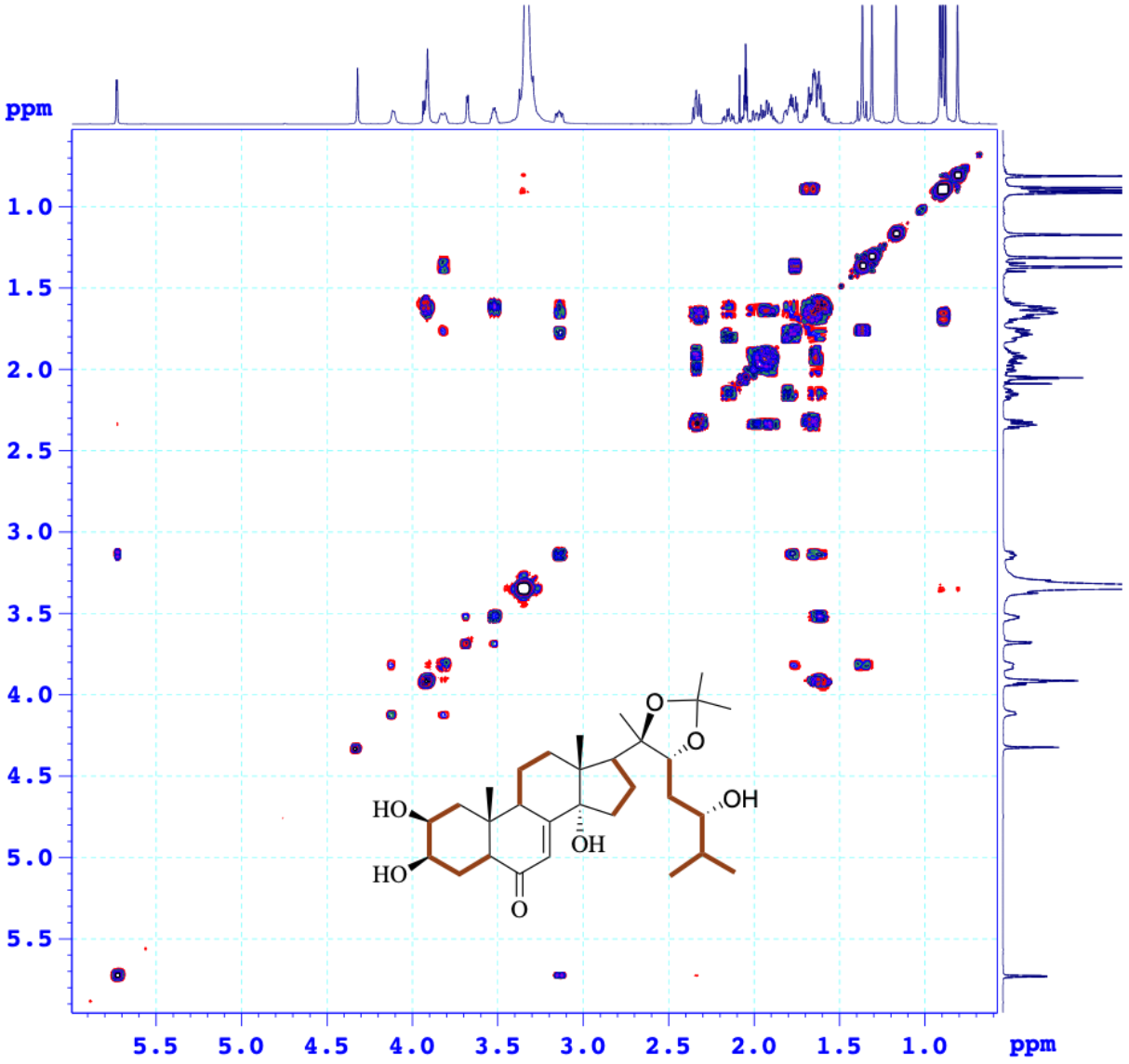


Figure S10: ^{1}H-^{1}H COSY Spectrum of Pterosterone 20,22-acetonide (**1**)

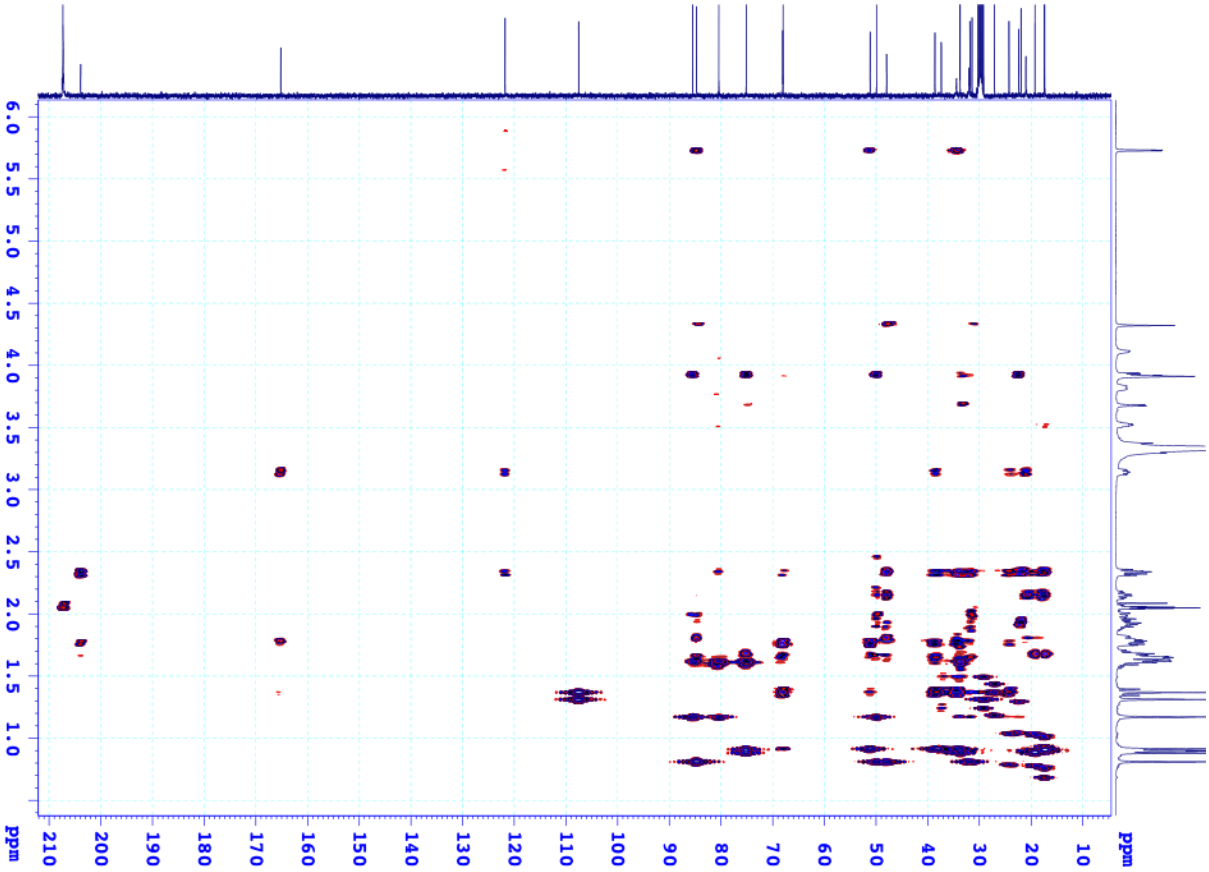


Figure S11: HMBC Spectrum of Pterosterone 20,22-acetonide (**1**)

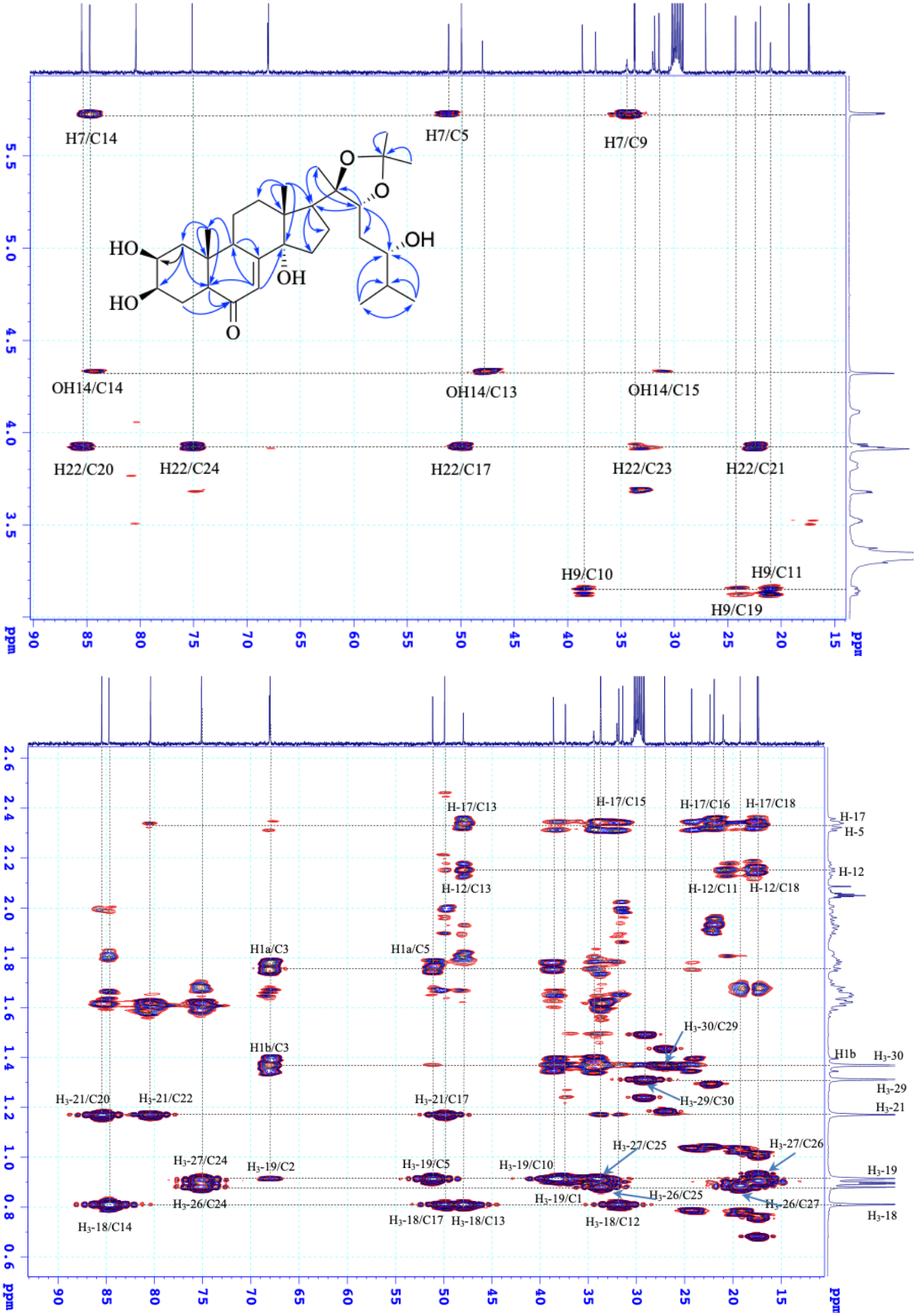


Figure S12: HMBC Spectrum of **1** (From δ_C 15 ppm to δ_C 90 ppm)

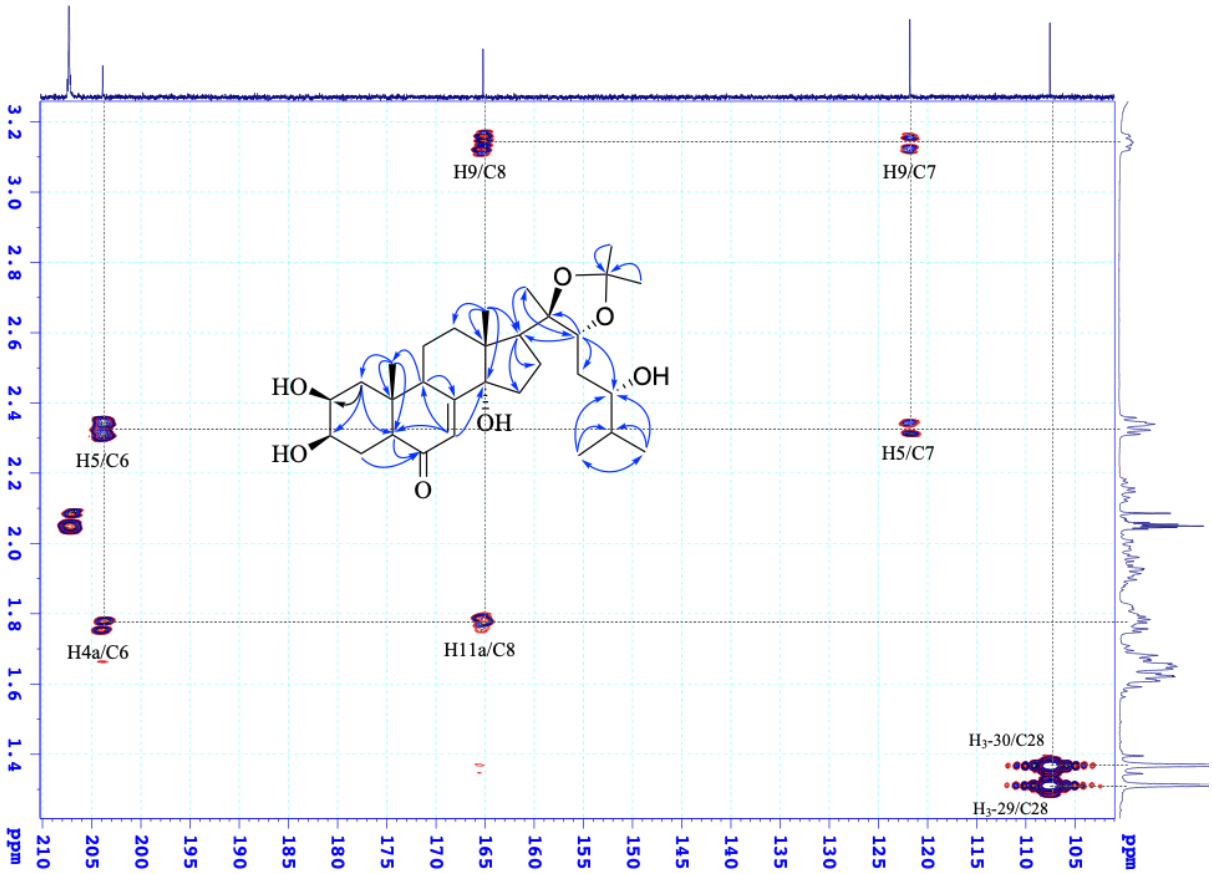


Figure S13: HMBC Spectrum of **1** (From δ_C 105 ppm to δ_C 210 ppm)

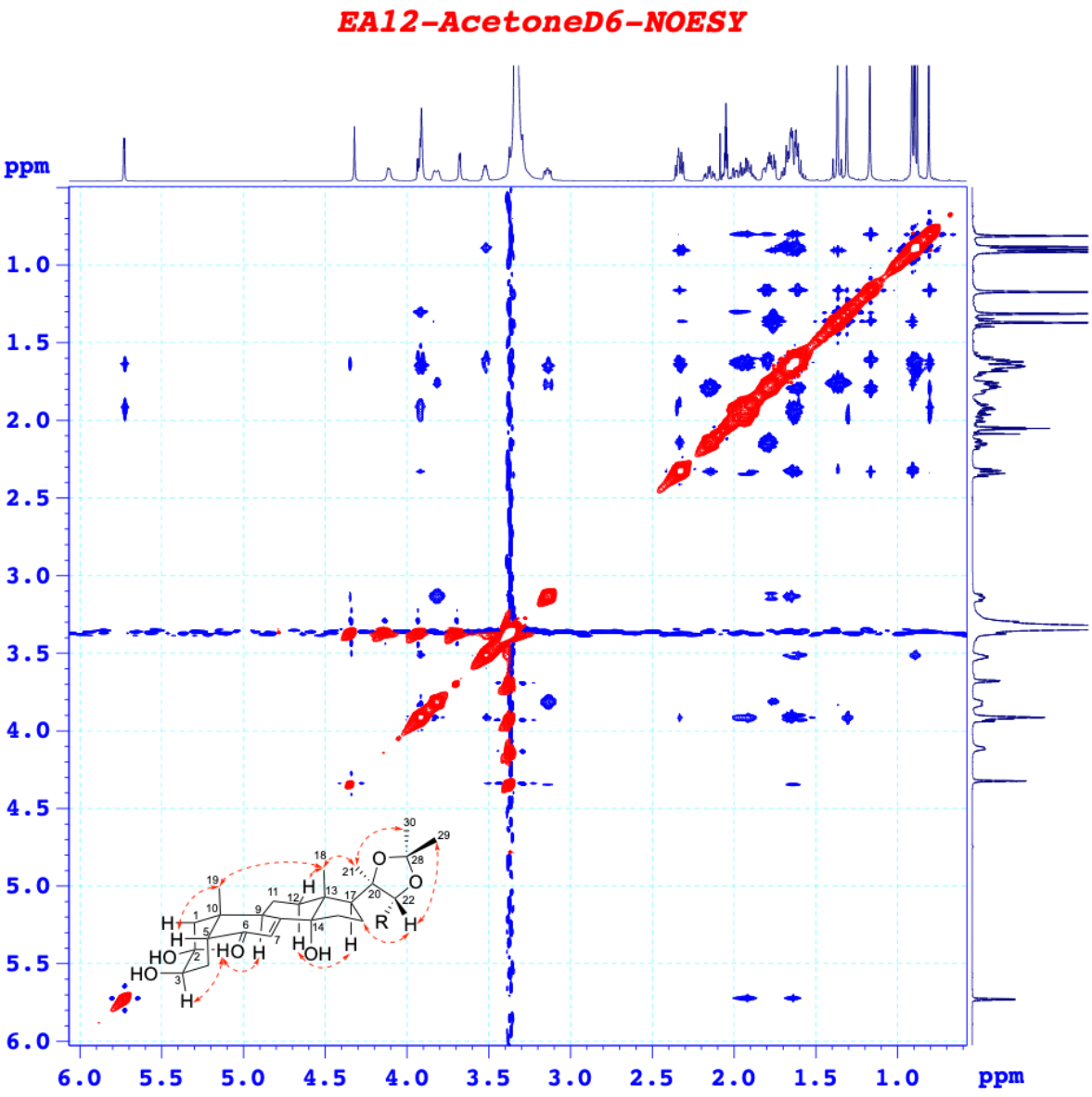


Figure S14: NOESY Spectrum of Pterosterone 20,22-acetonide (**1**)

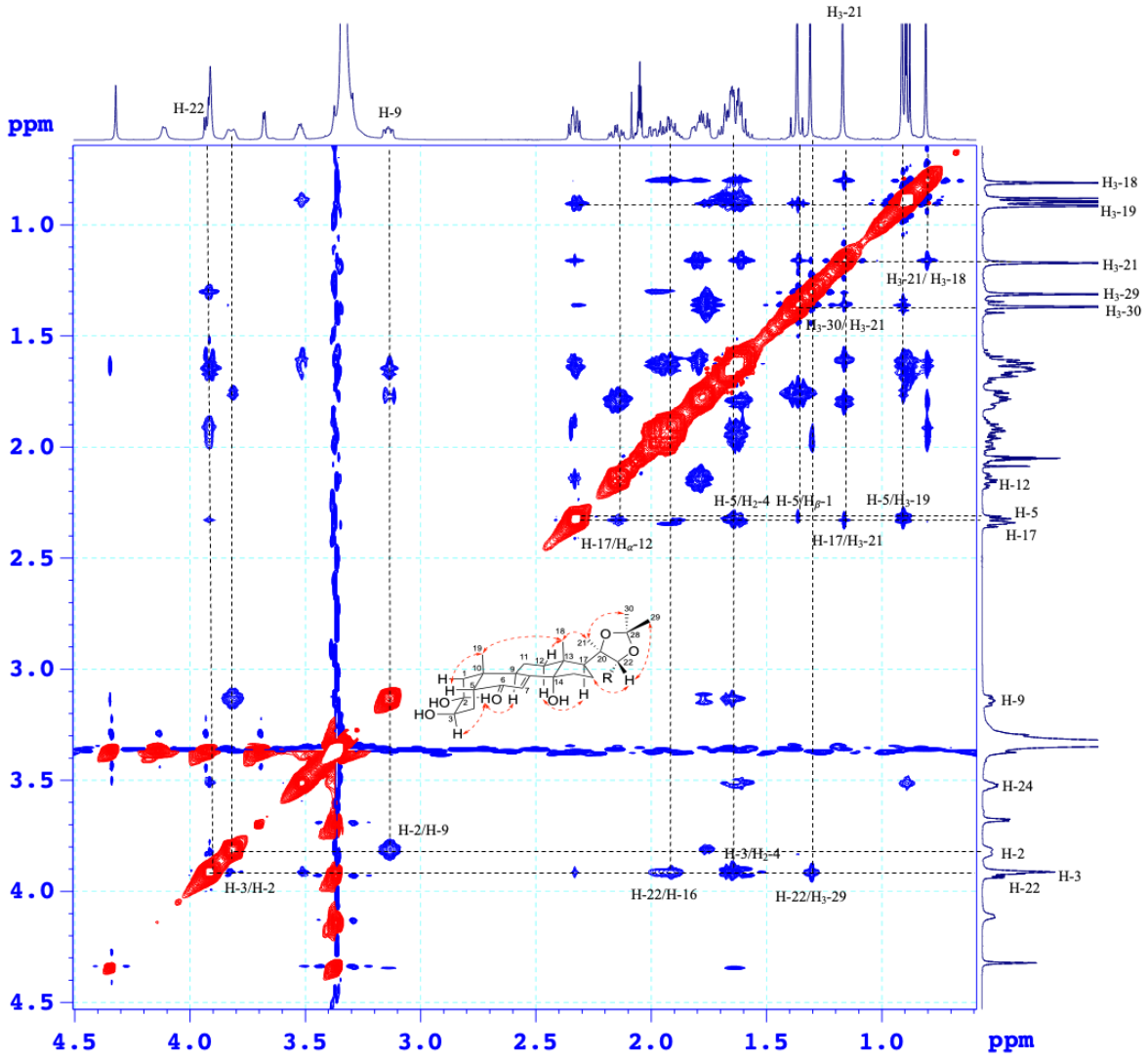


Figure S15: NOESY Spectrum of **1** (Expansion)

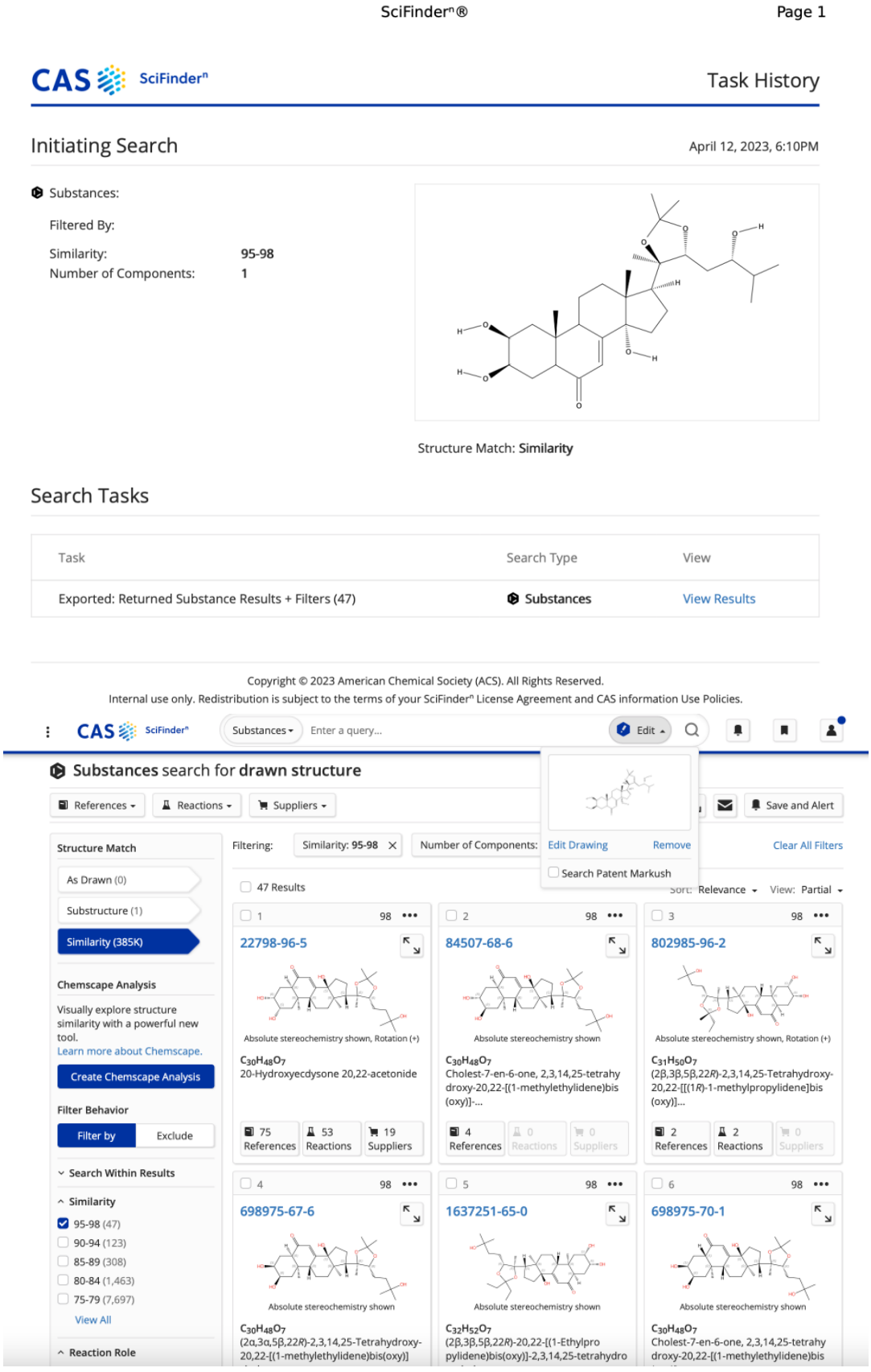


Figure S15: SciFinder Search Results of Compound **1**

Ponasterone A 20,22-acetonide (2): ^{1}H NMR (500 MHz, acetone-d_6) data (Table S1); ^{13}C NMR (125 MHz, acetone-d_6) data (Table S2).

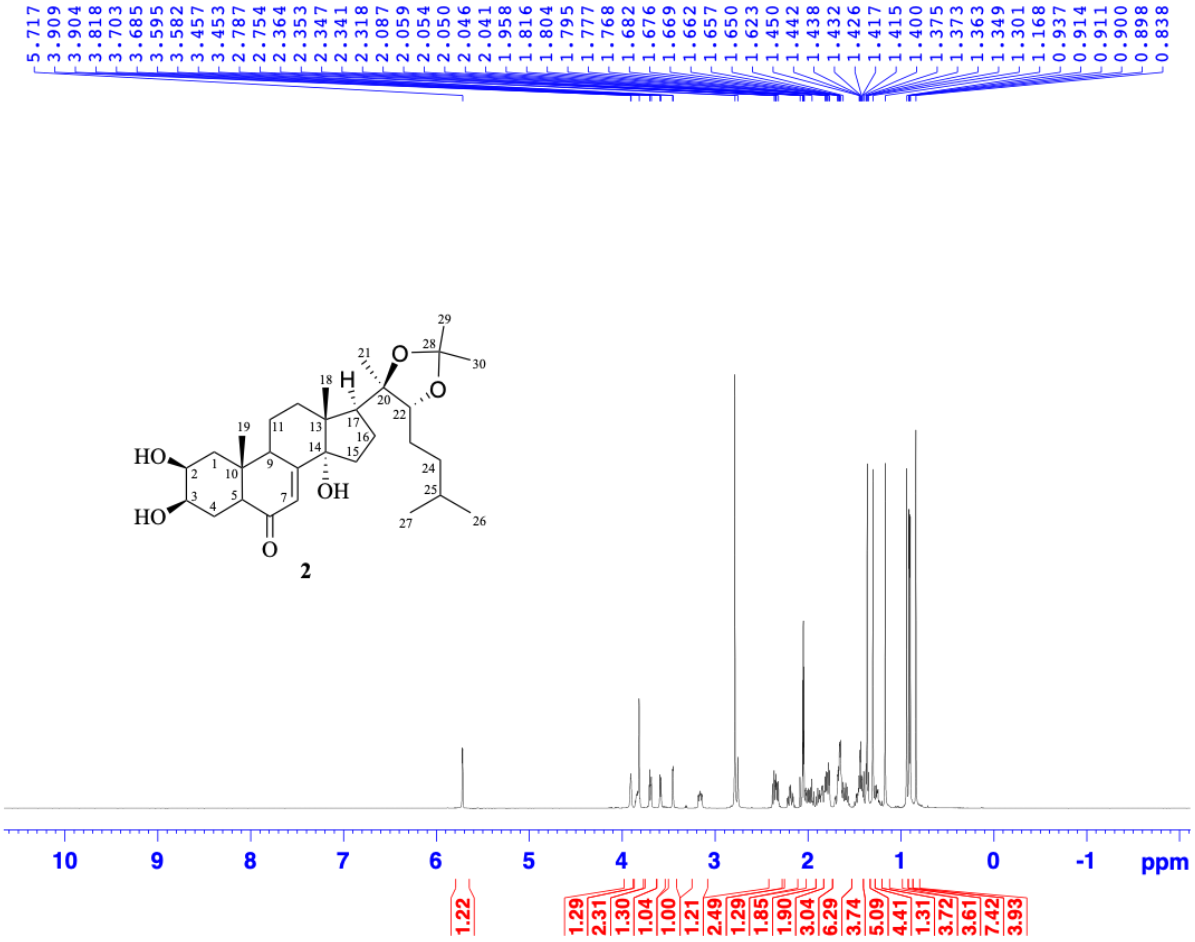


Figure S16: ^{1}H-NMR (500 MHz, acetone-d_6) Spectrum of Ponasterone A 20, 22-acetonide (**2**)

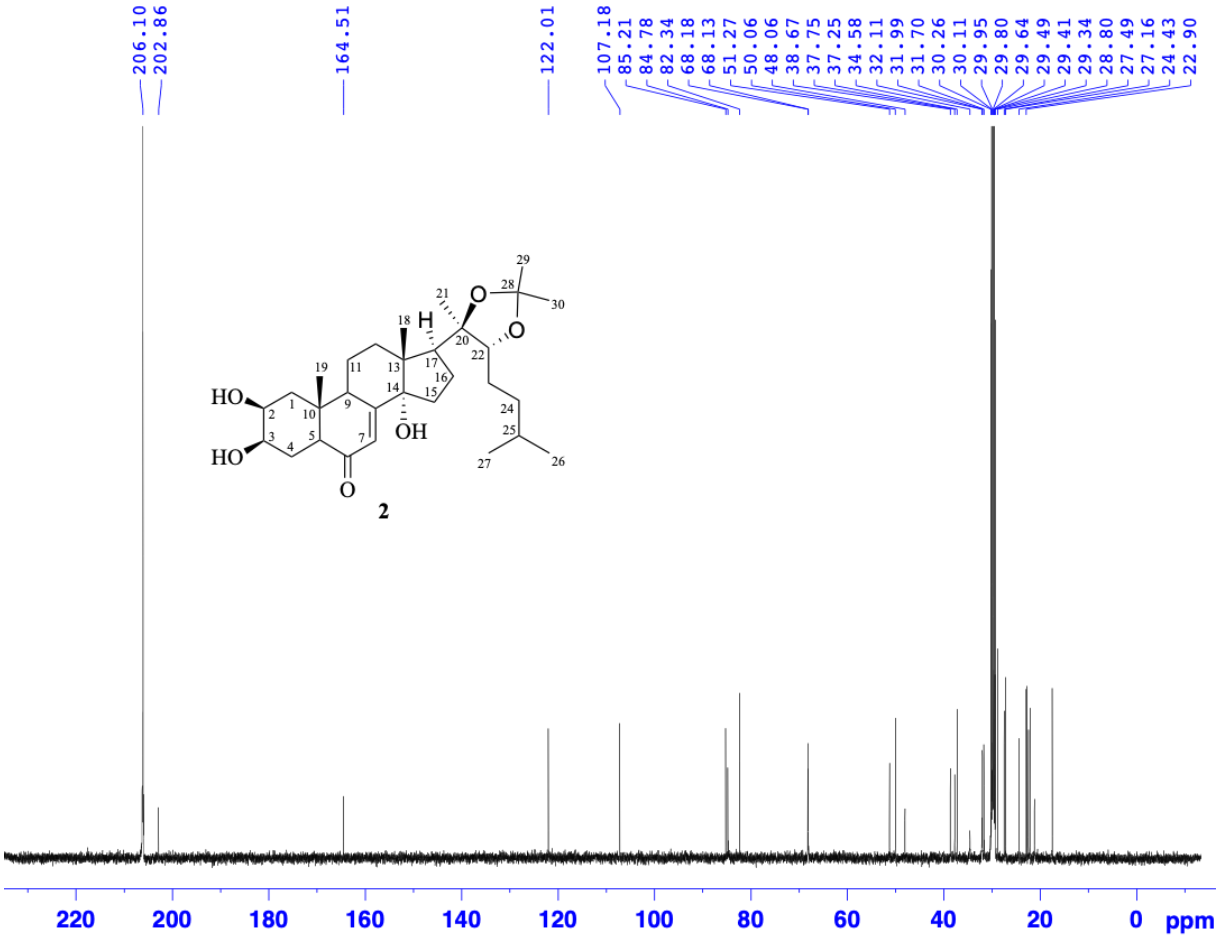


Figure S17: ^{13}C-NMR (125 MHz, acetone-d_6) Spectrum of Ponasterone A 20, 22-acetonide (**2**)

Pterosterone (3): ^{1}H NMR (500 MHz, CD_3OD) data (Table S1); ^{13}C NMR (125 MHz, CD_3OD) data (Table S2).

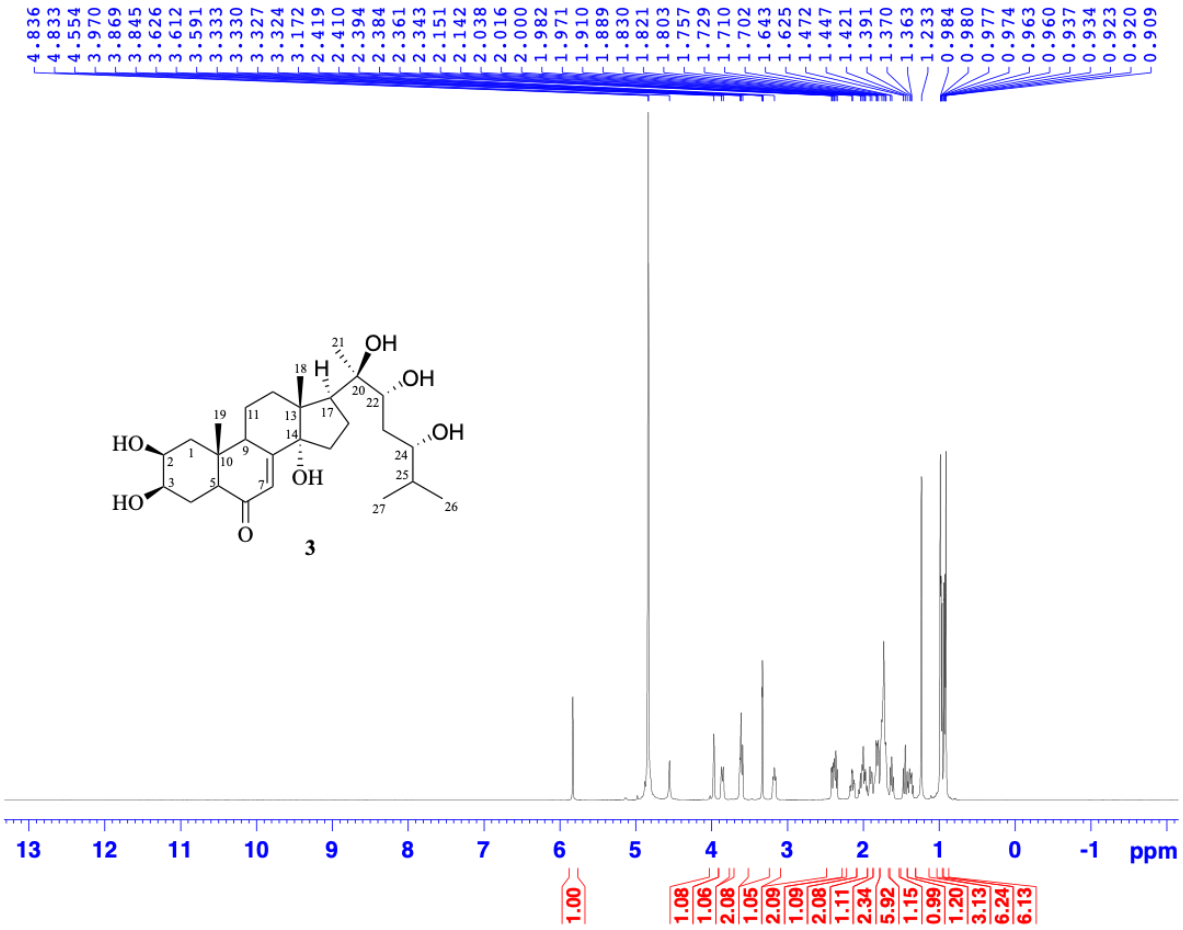


Figure S18: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Pterosterone (**3**)

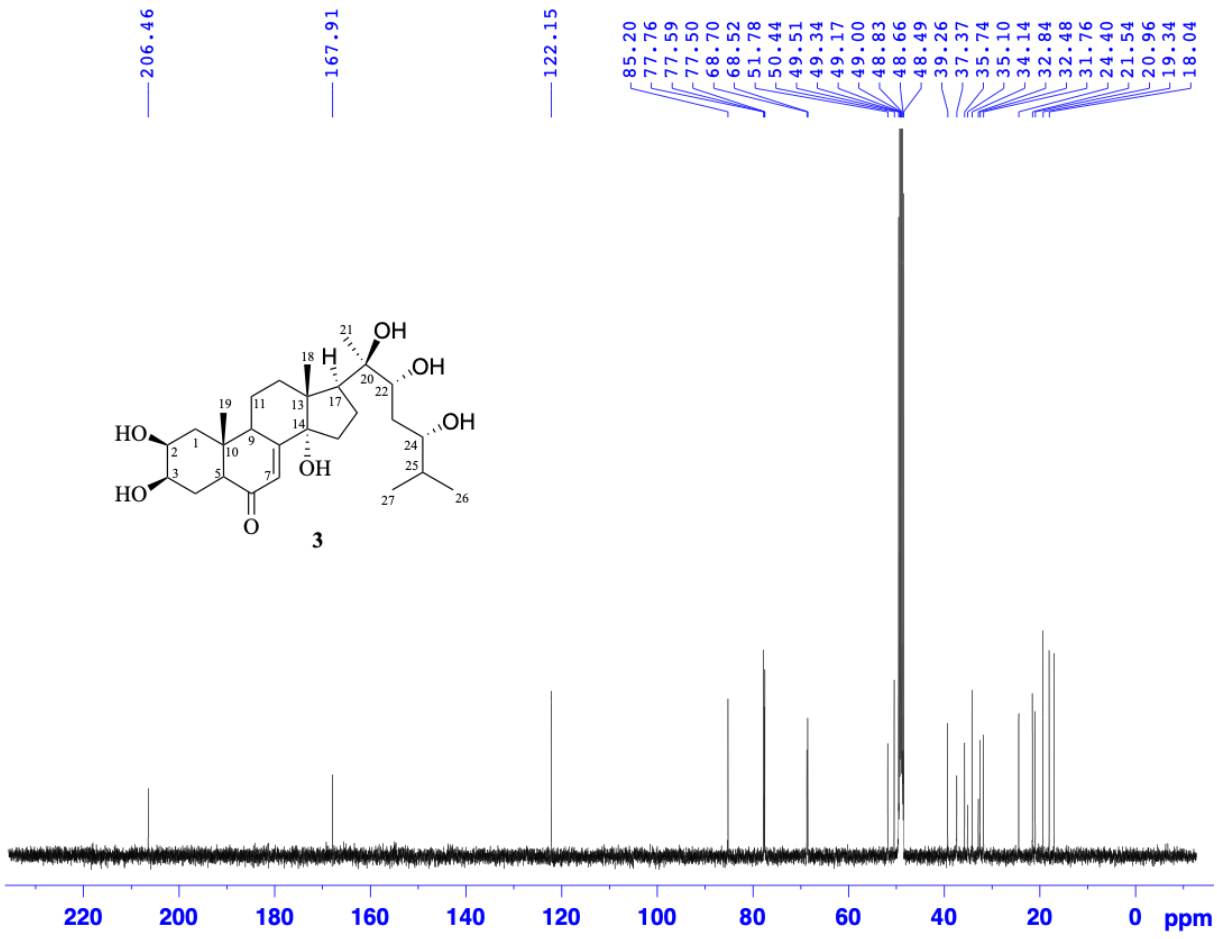


Figure S19: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Pterosterone (**3**)

Ponasterone A (4): ^{1}H NMR (500 MHz, CD_3OD) data (Table S1); ^{13}C NMR (125 MHz, CD_3OD) data (Table S2).

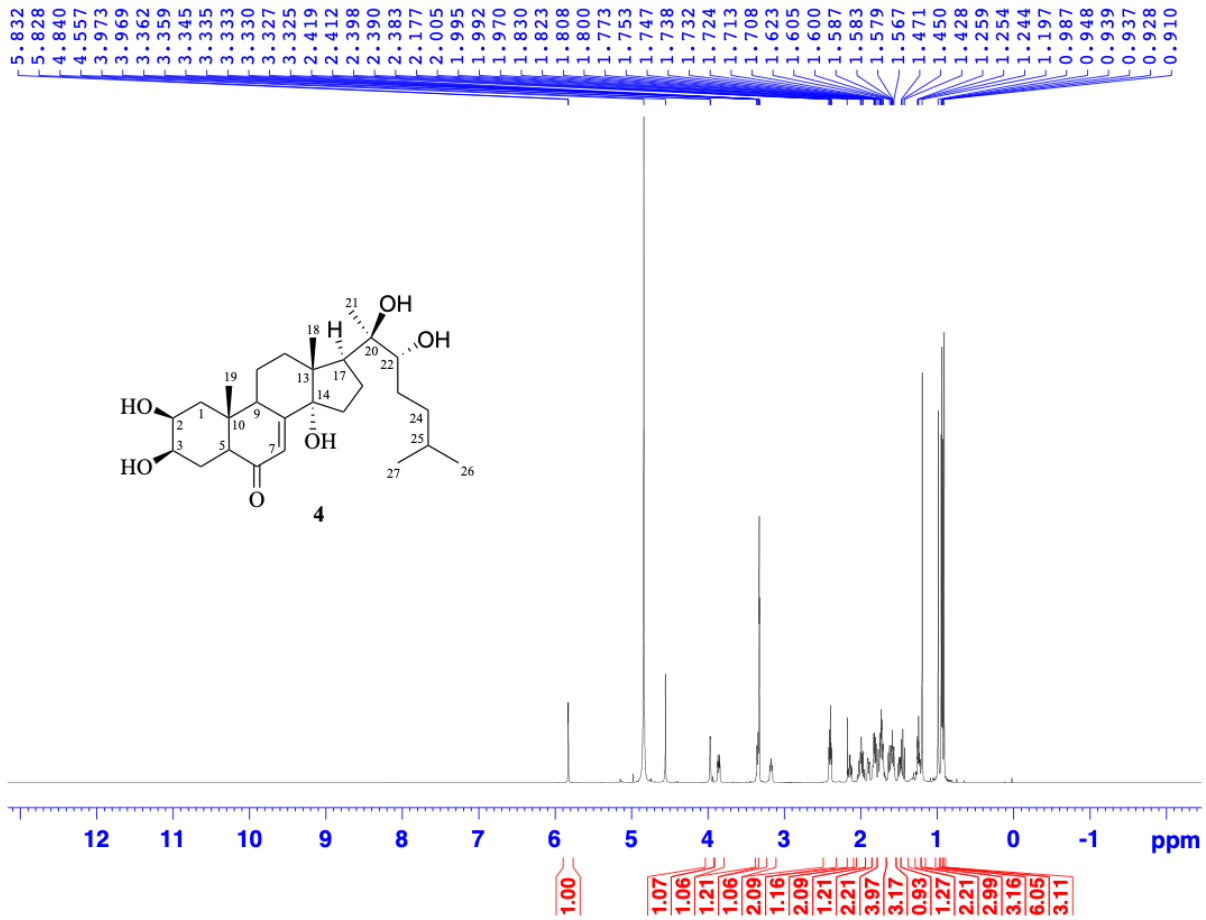


Figure S20: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Ponasterone A (**4**)

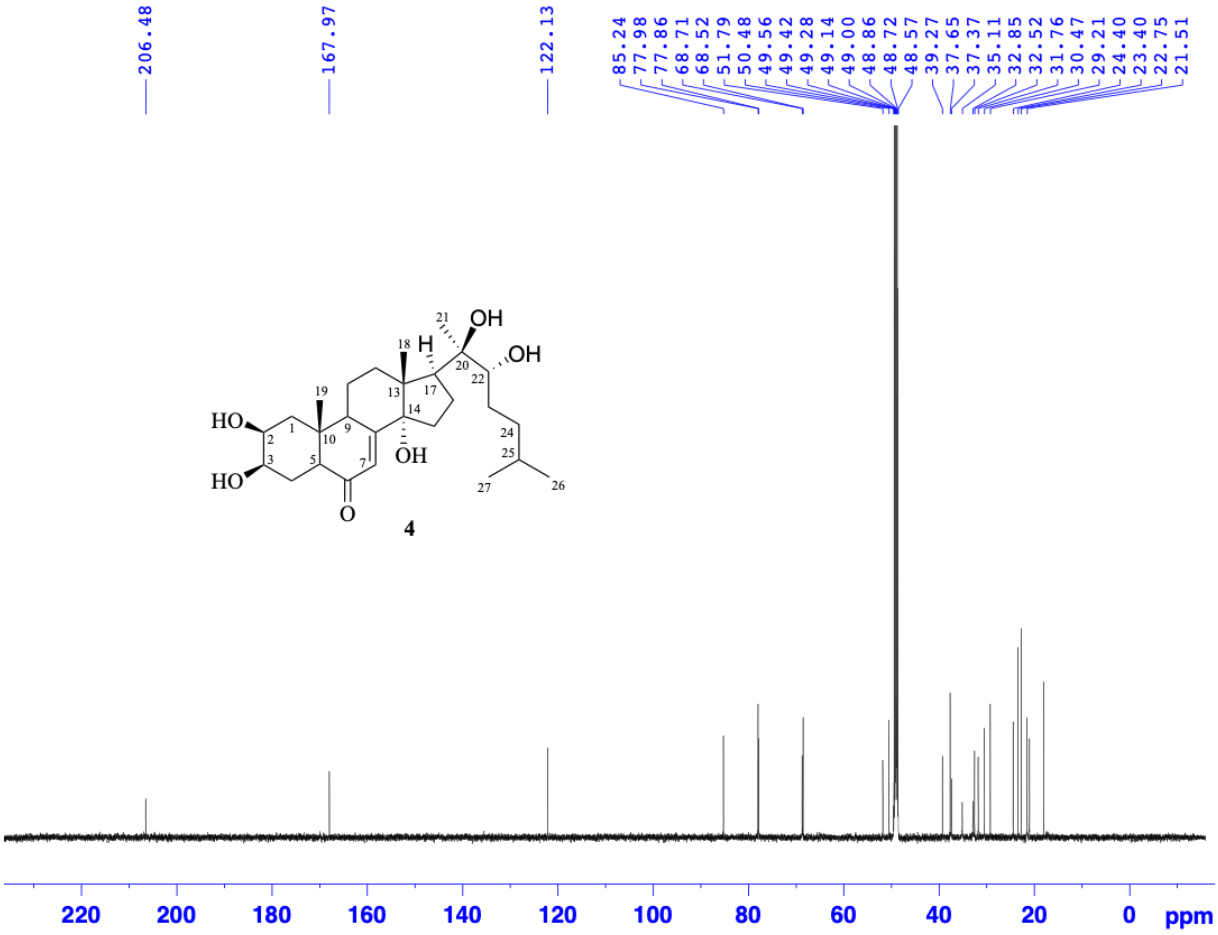


Figure S21: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Ponasterone A (**4**)

24-(2-Hydroxyethyl)-20-hydroxyecdysone (5): ^{1}H NMR (500 MHz, DMSO-d_6) data (Table S1); ^{13}C NMR (125 MHz, DMSO-d_6) data (Table S2).

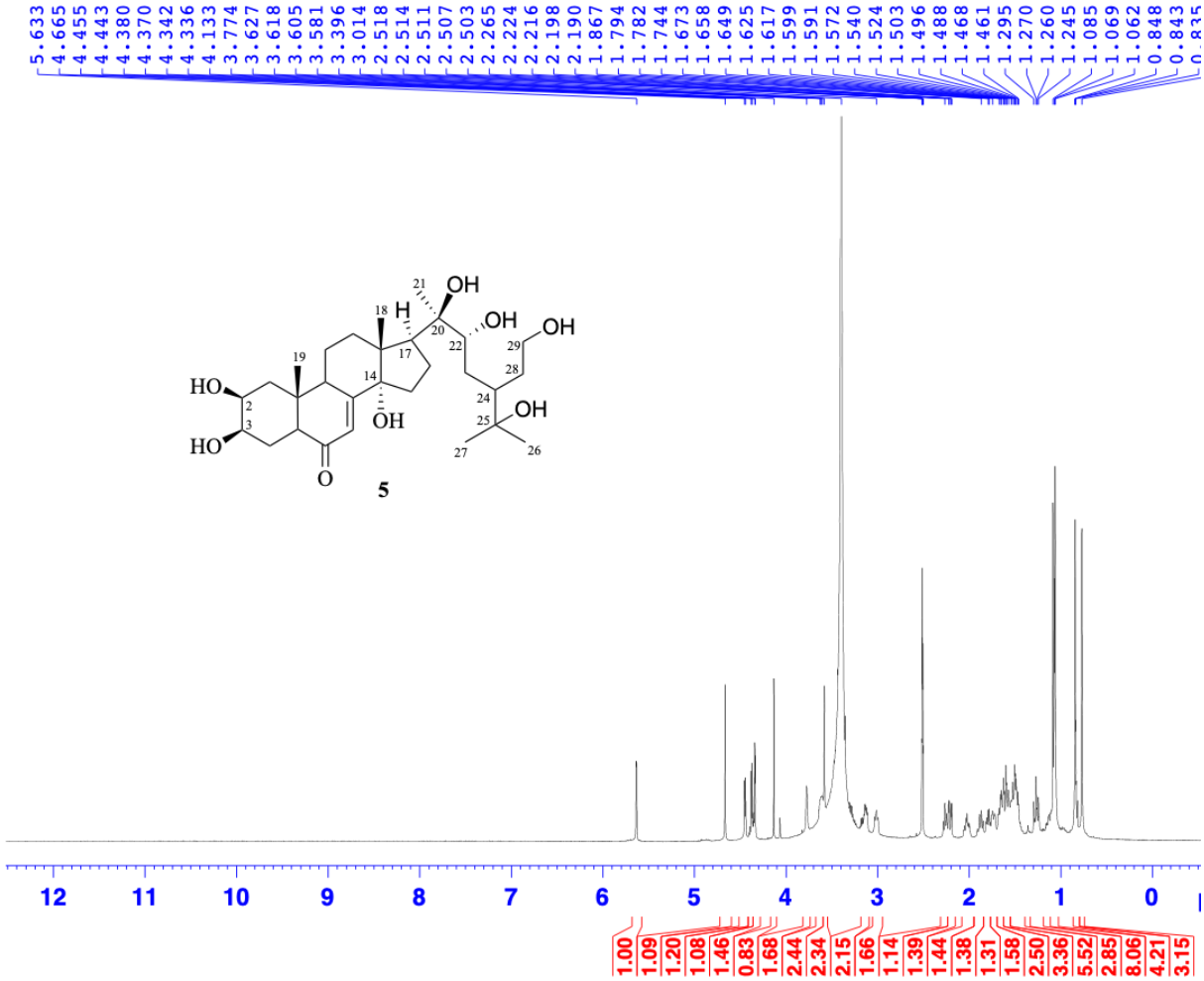


Figure S22: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of 24-(2-Hydroxyethyl)-20-hydroxyecdysone (**5**)

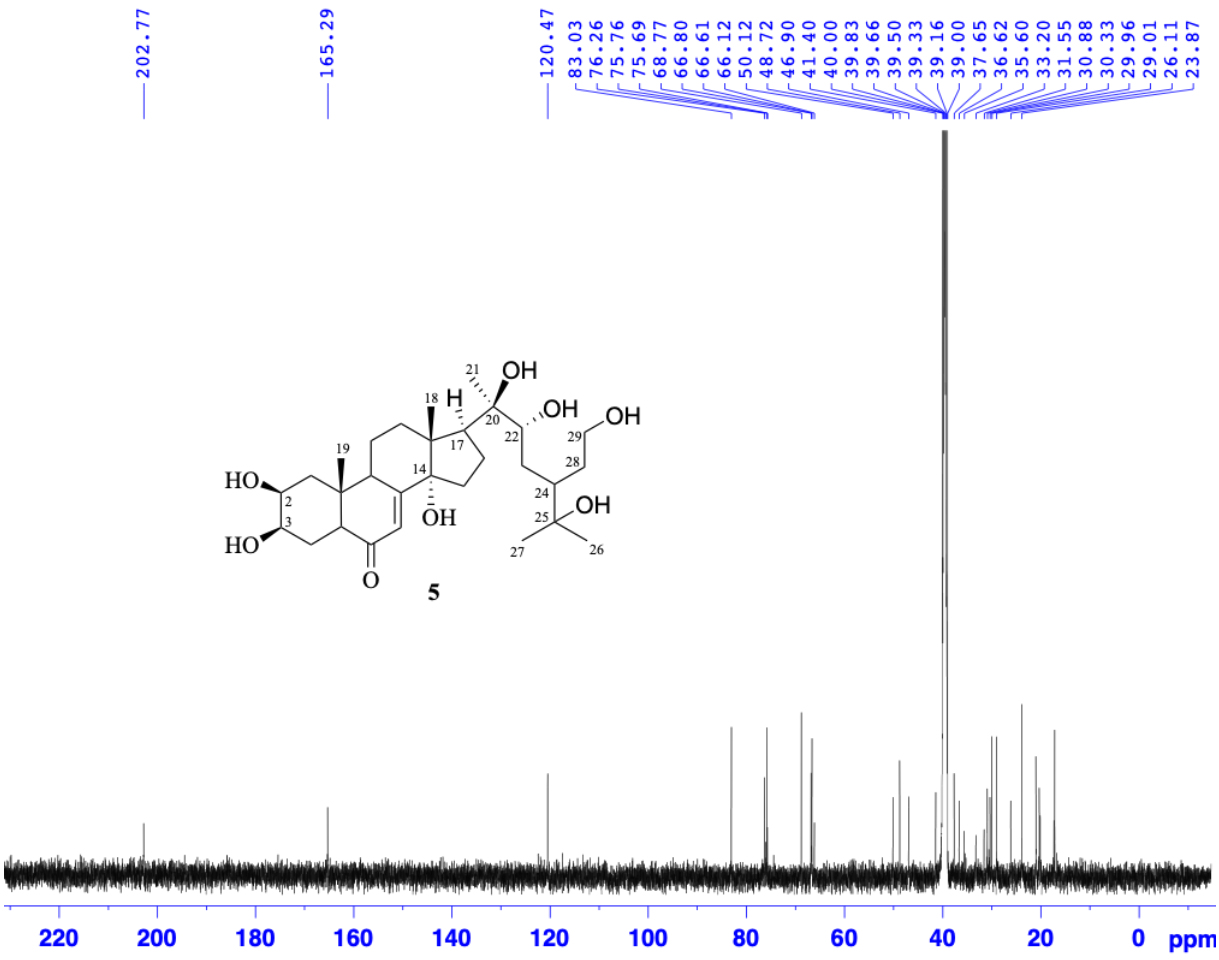


Figure S23: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of 24-(2-Hydroxyethyl)-20-hydroxyecdysone (**5**)

Quercetin (6): ^{1}H NMR (500 MHz, DMSO-d_6) data (Table S3); ^{13}C NMR (125 MHz, DMSO-d_6) data (Table S4).

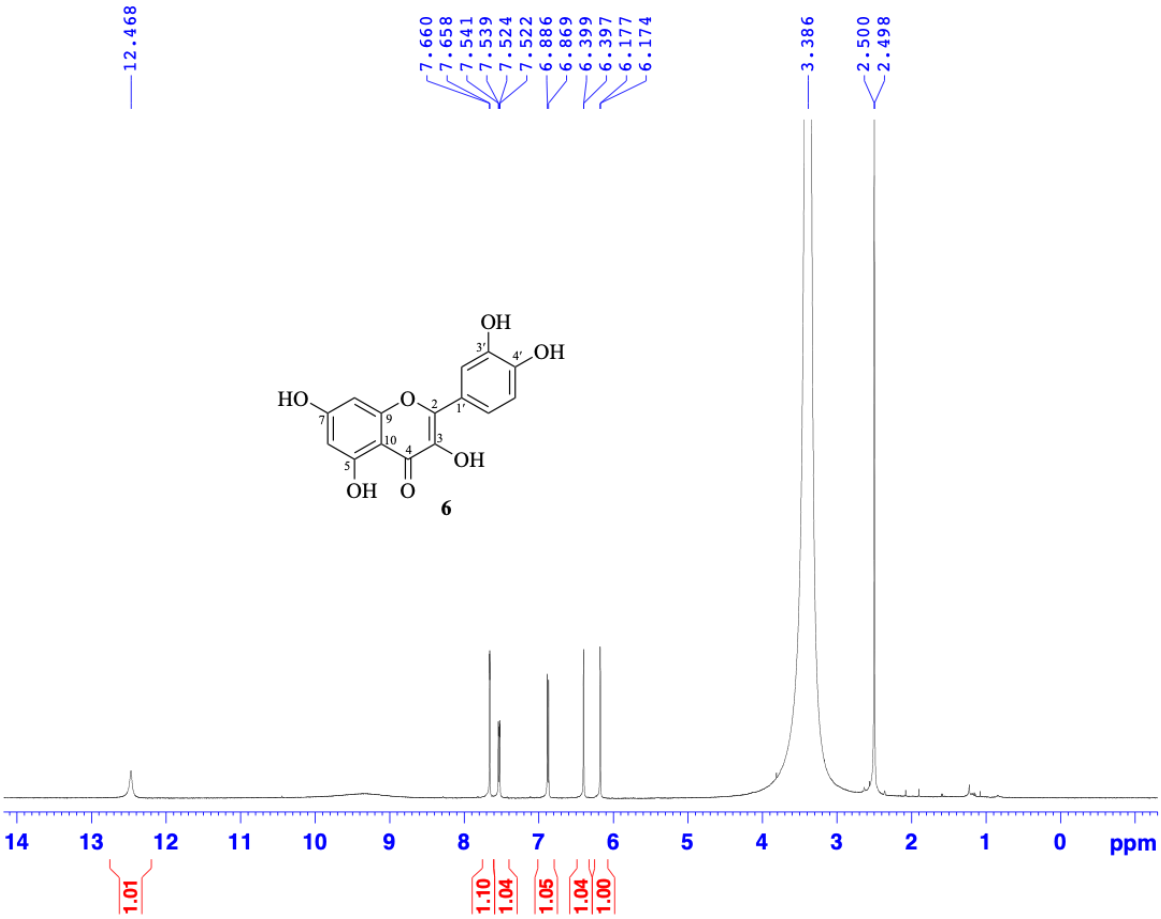


Figure S24: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of Quercetin (**6**)

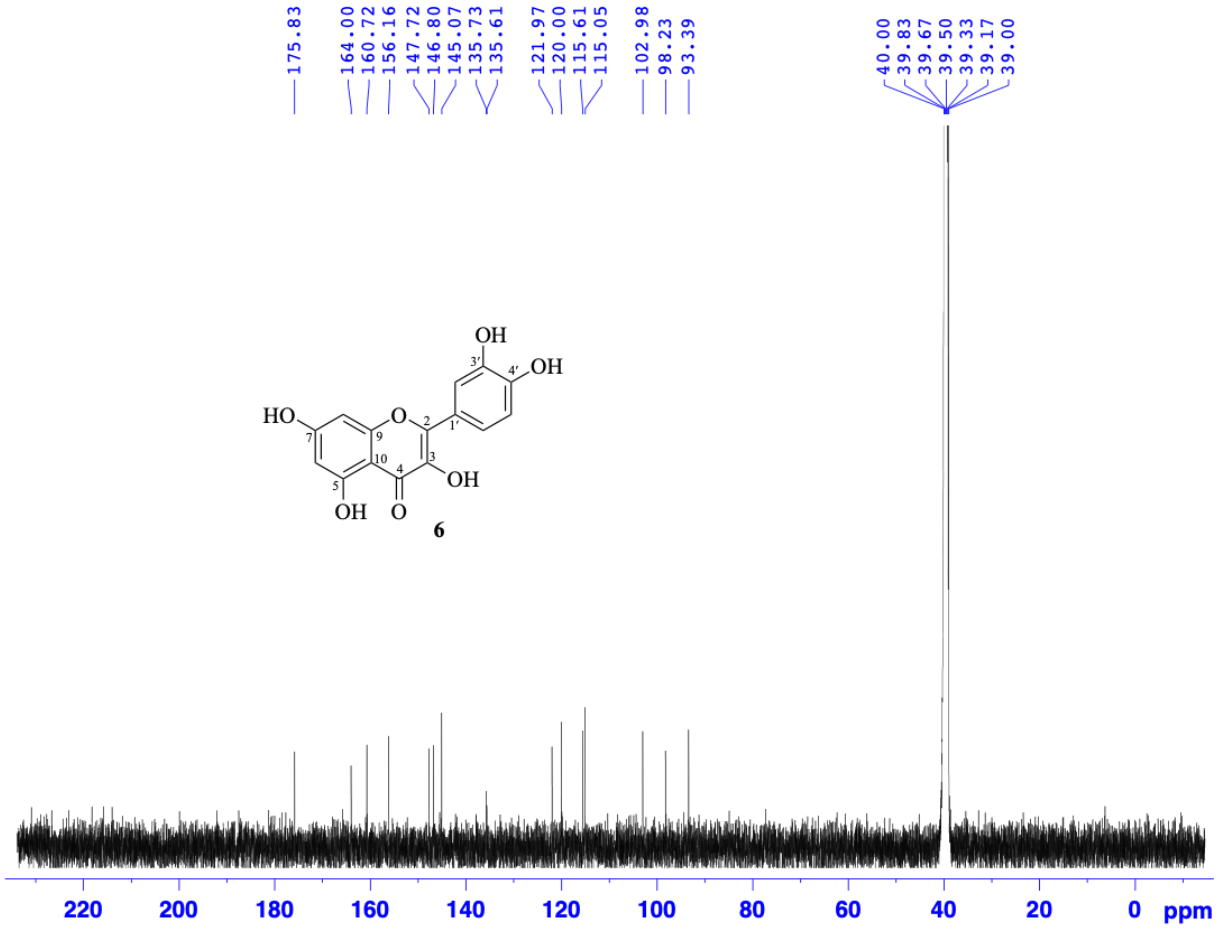


Figure S25: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of Quercetin (**6**)

Quercitrin (7): ESI-MS: *m/z* = 301 $[M-H-146]^-$ ($C_{21}H_{20}O_{11}$);
^{1}H NMR (500 MHz, DMSO-d_6) data (Table S3); ^{13}C NMR (125 MHz, DMSO-d_6) data (Table S4).

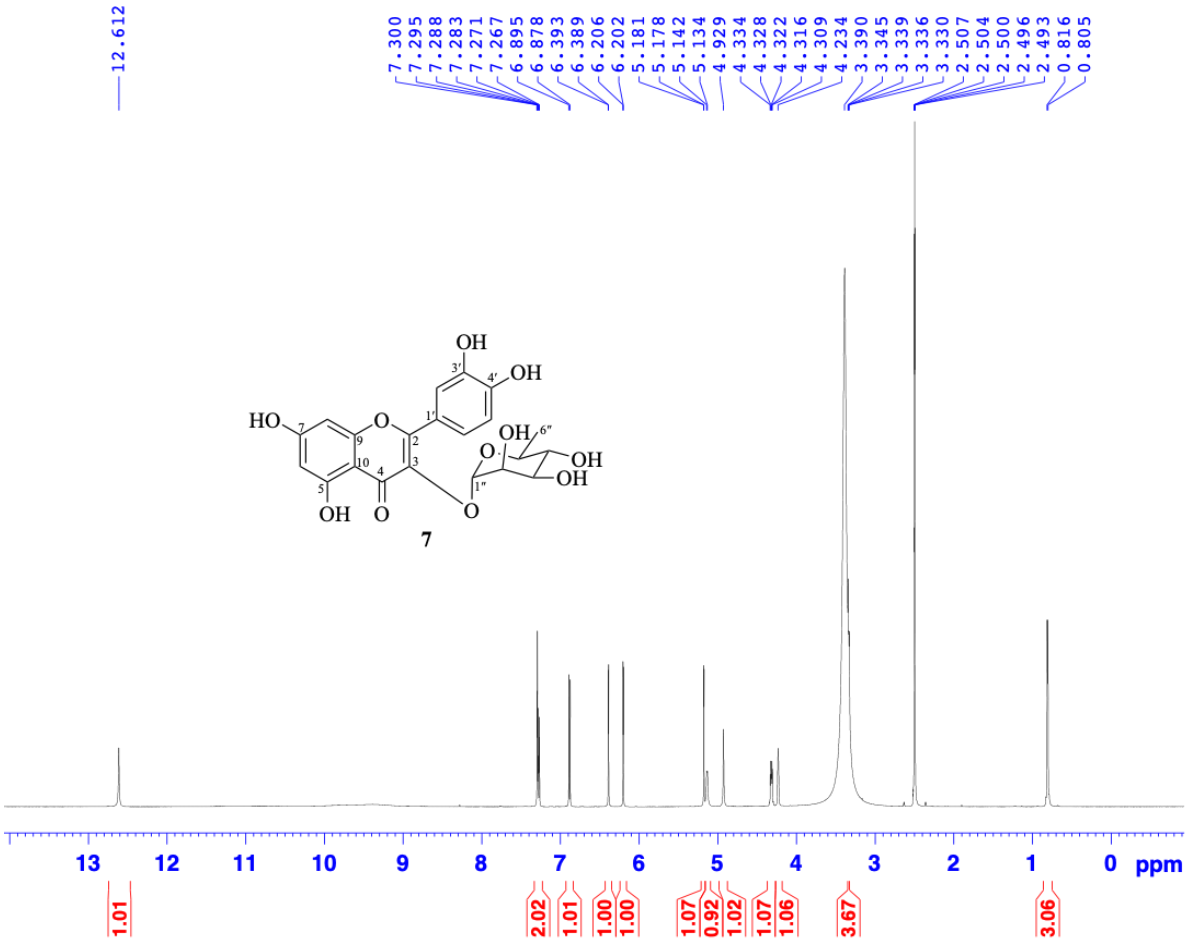


Figure S26: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of Quercitrin (**7**)

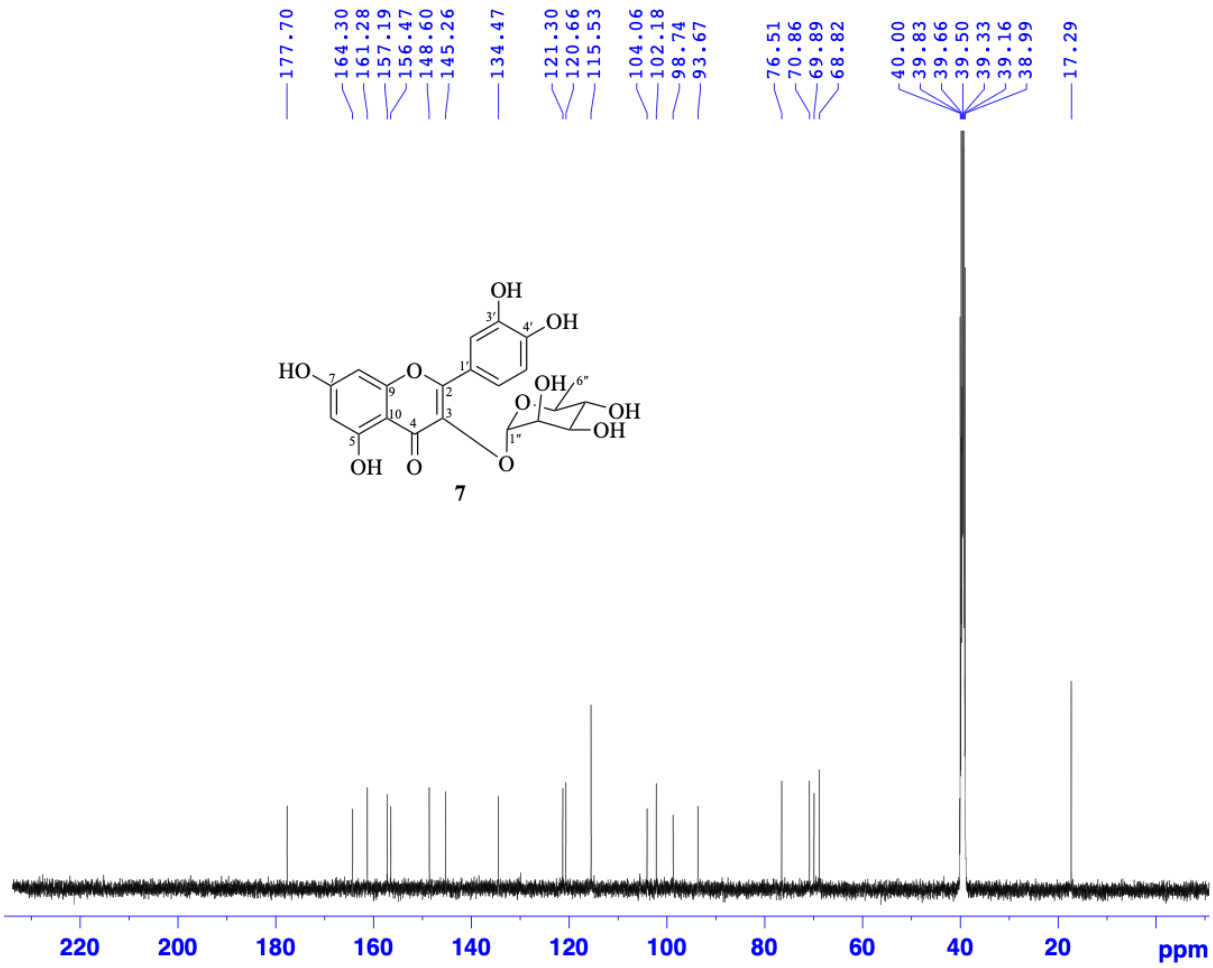


Figure S27: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of Quercitrin (**7**)

Isoquercitrin (8): ESI-MS (positive): *m/z* 465[M+H]$^+$ ($C_{21}H_{21}O_{12}$), 303[M+H-162]$^+$ ($C_{15}H_{11}O_7$); ^{1}H NMR (500 MHz, DMSO-d_6) data (Table S3); ^{13}C NMR (125 MHz, DMSO-d_6) data (Table S4).

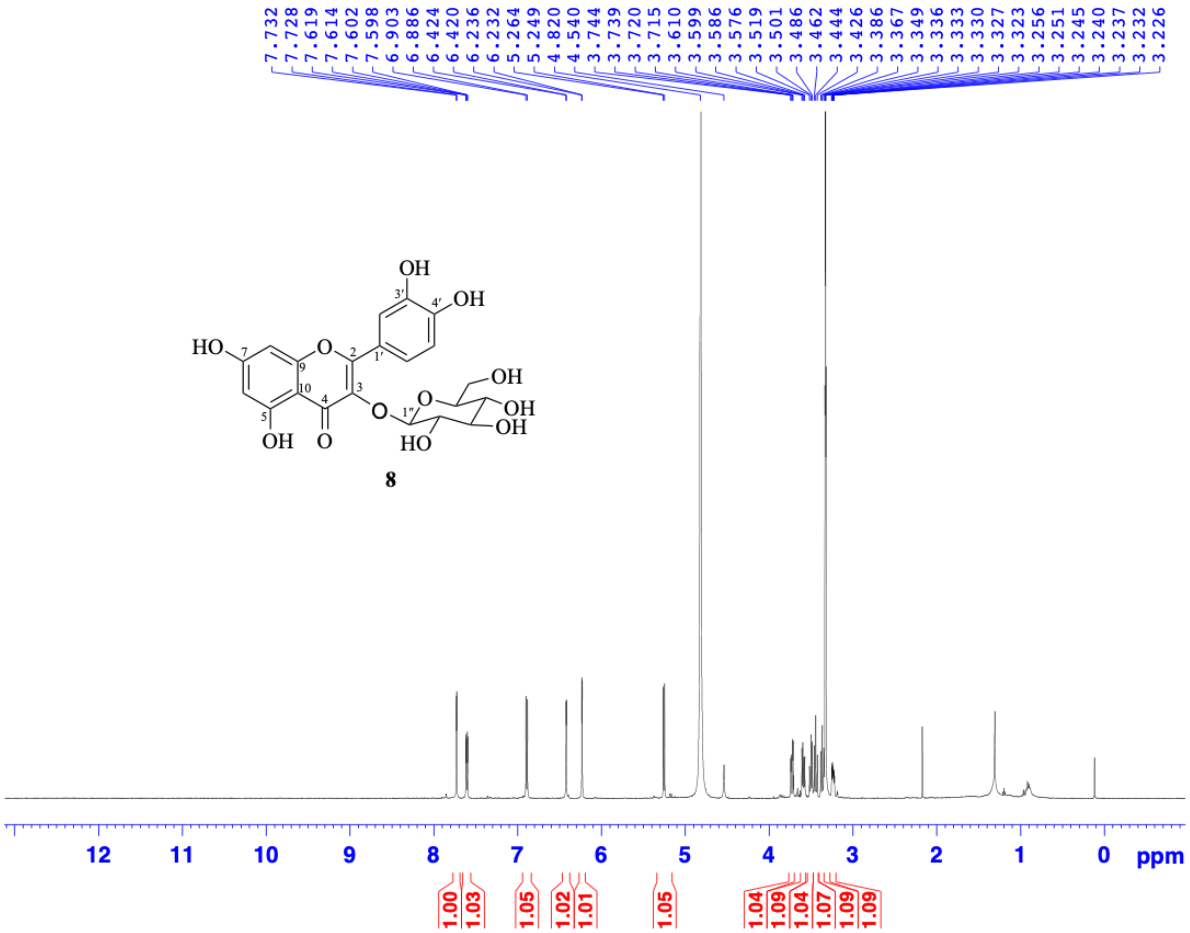


Figure S28: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Isoquercitrin (**8**)

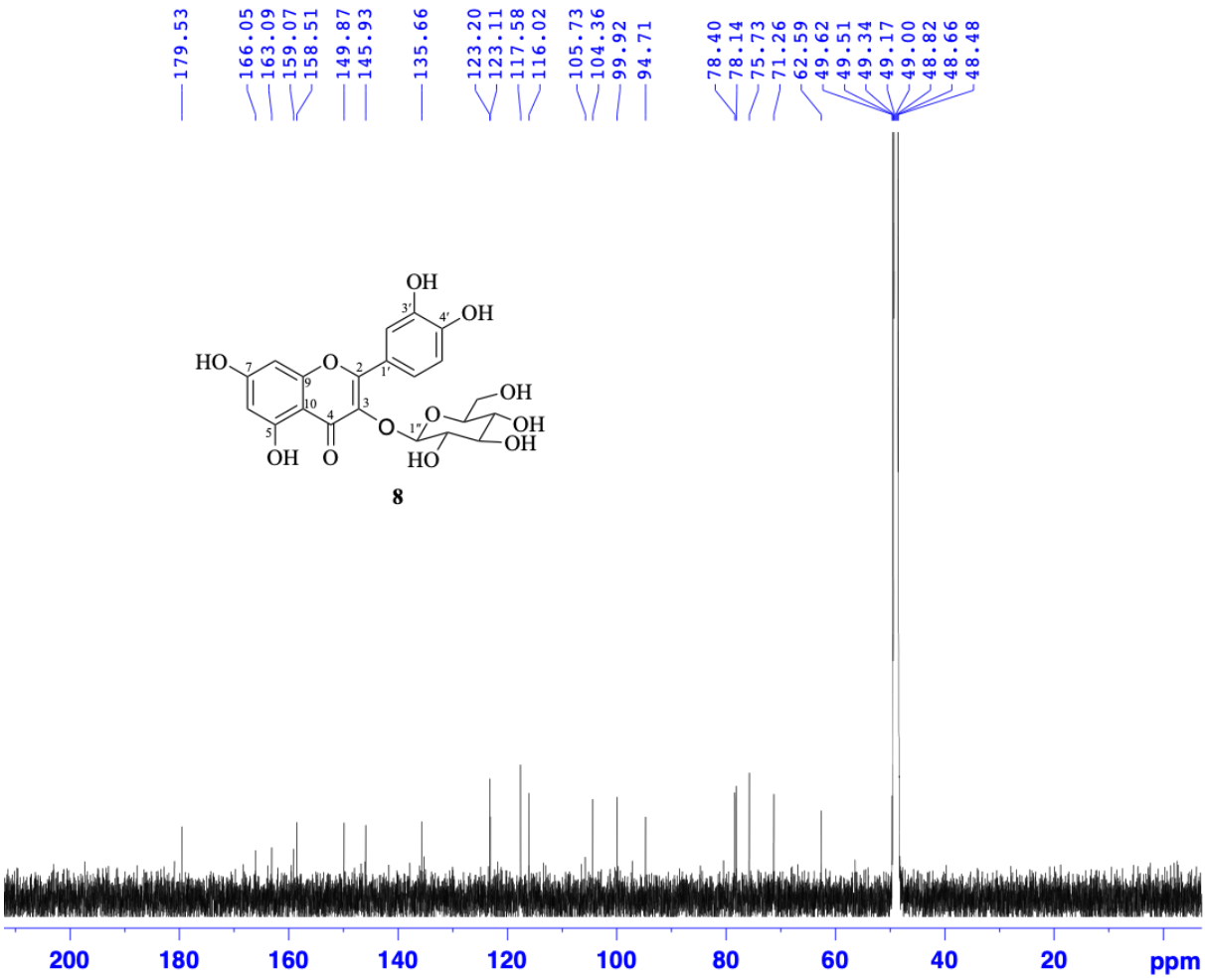


Figure S29: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Isoquercitrin (**8**)

Rutin (9): ^{1}H NMR (500 MHz, CD_3OD) data (Table S3); ^{13}C NMR (125 MHz, CD_3OD) data (Table S4).

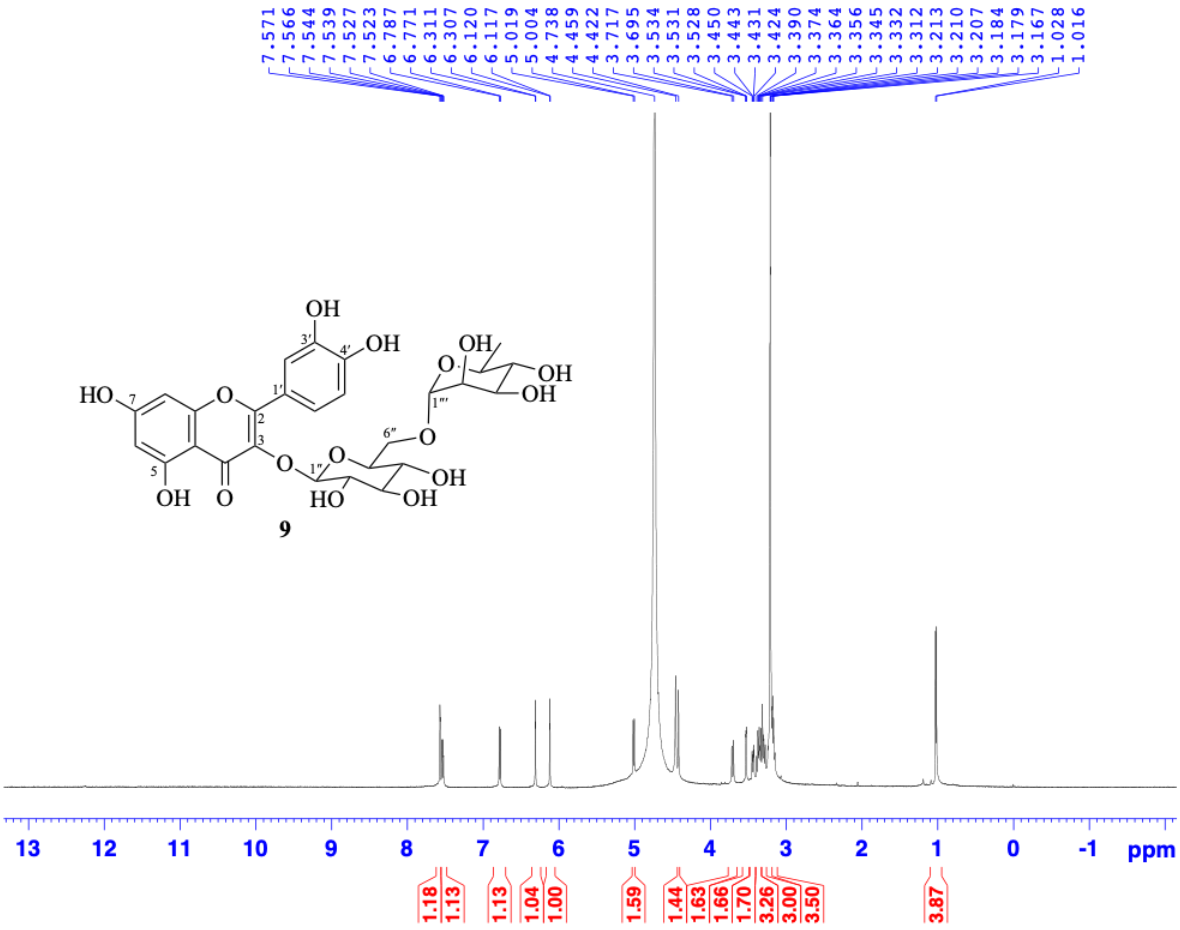


Figure S30: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Rutin (**9**)

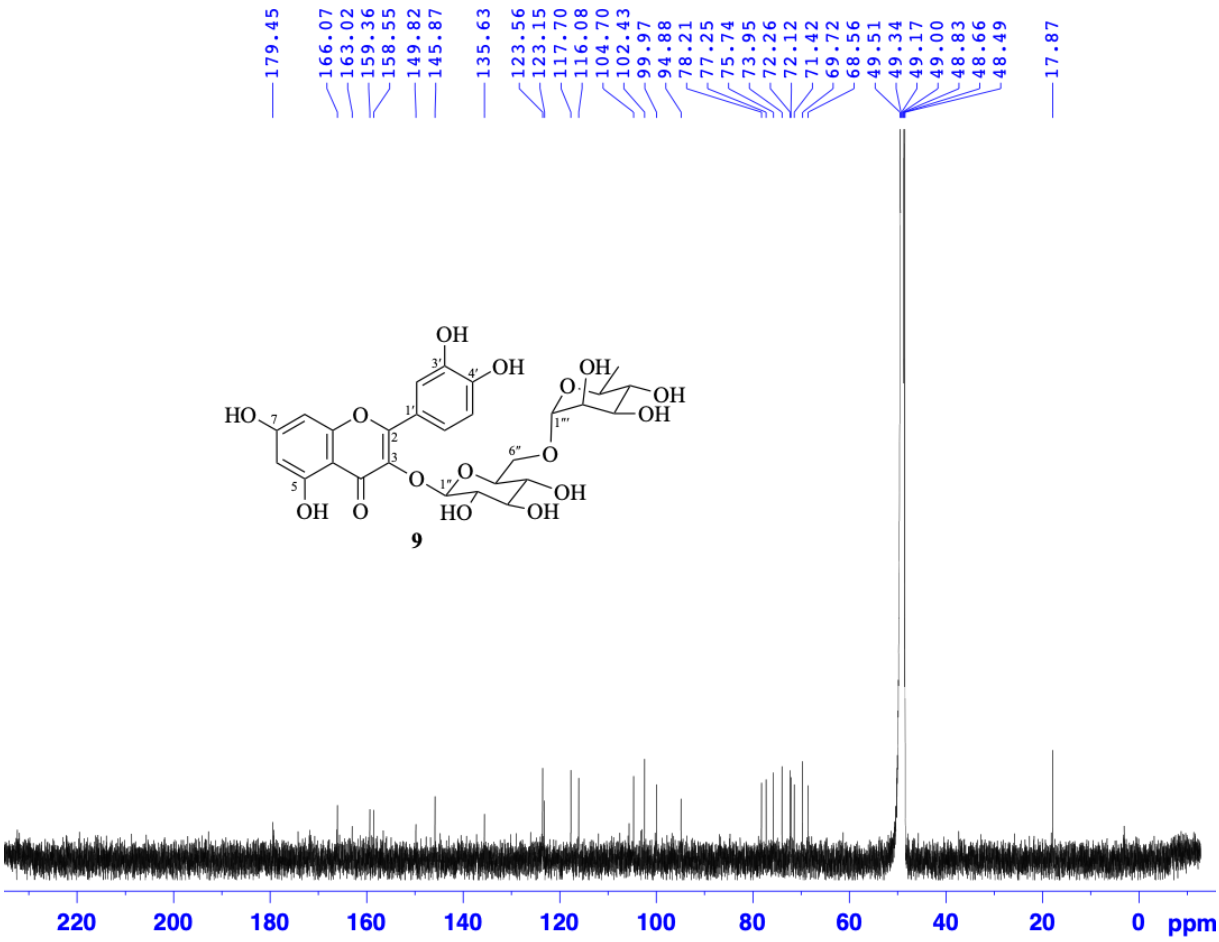


Figure S31: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Rutin (**9**)

Afzelin (10): ^{1}H NMR (500 MHz, DMSO-d_6) data (Table S3); ^{13}C NMR (125 MHz, DMSO-d_6) data (Table S4).

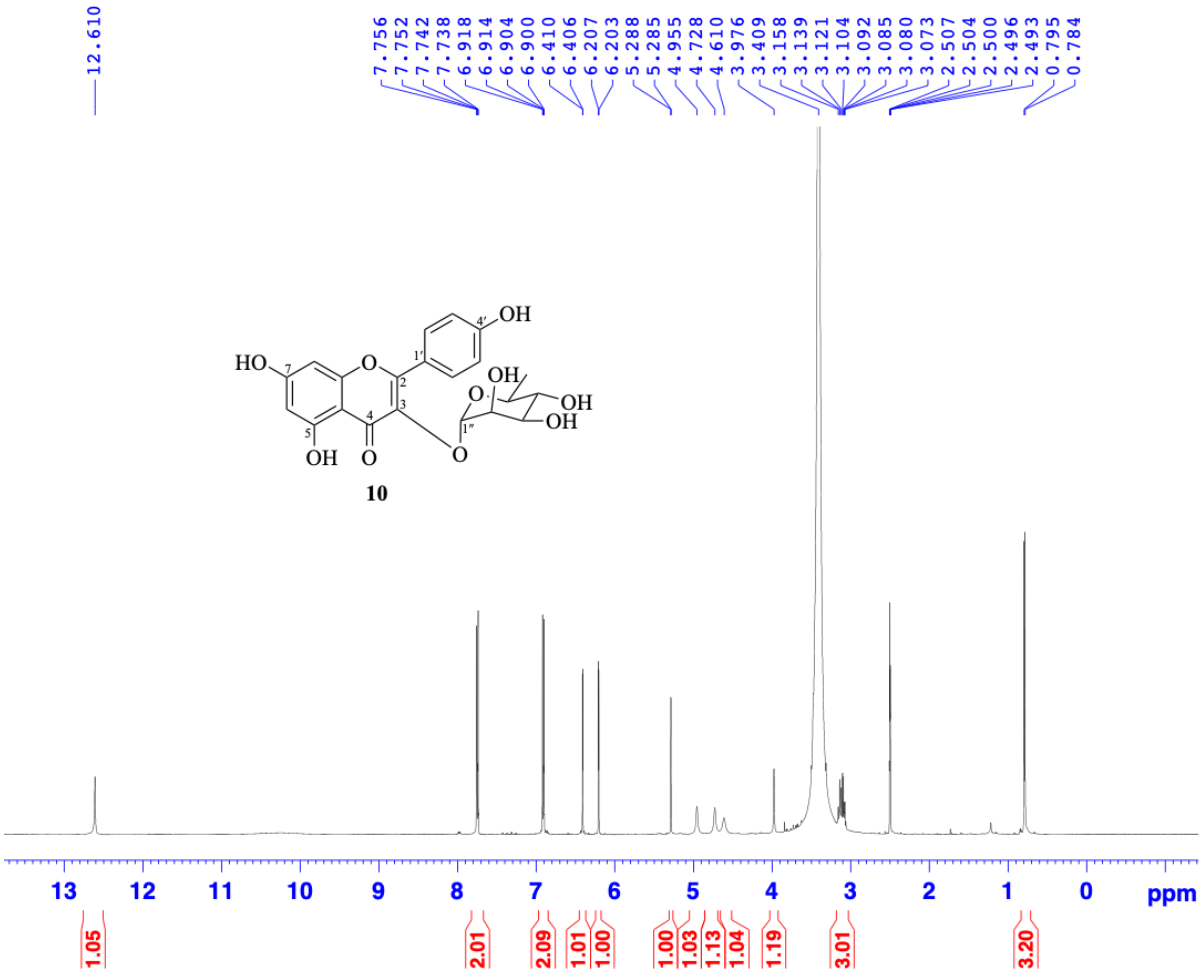


Figure S32: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of Afzelin (**10**)

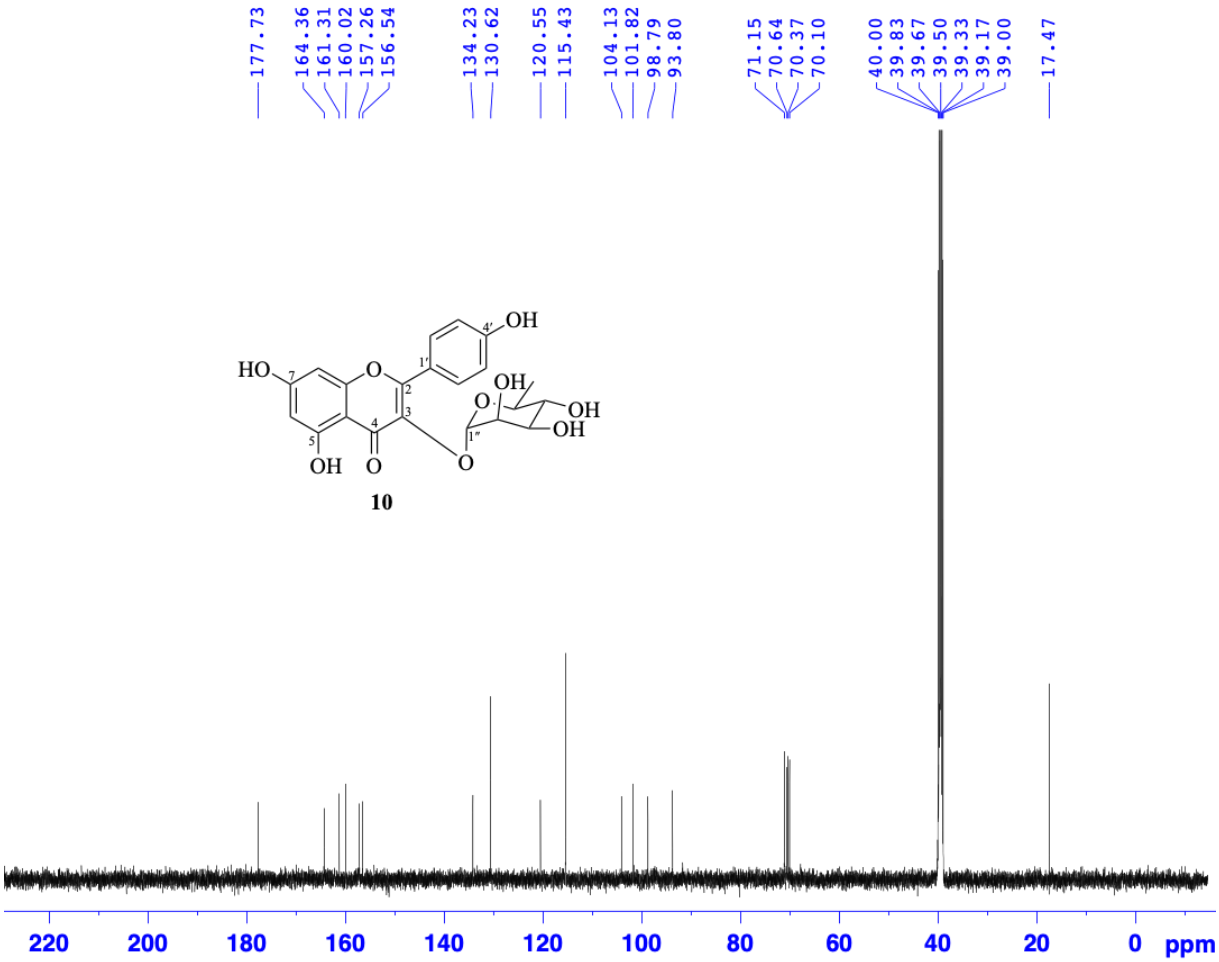


Figure S33: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of Afzelin (**10**)

Astragalin (11): ^{1}H NMR (500 MHz, DMSO-d_6) data (Table S3); ^{13}C NMR (125 MHz, DMSO-d_6) data (Table S4).

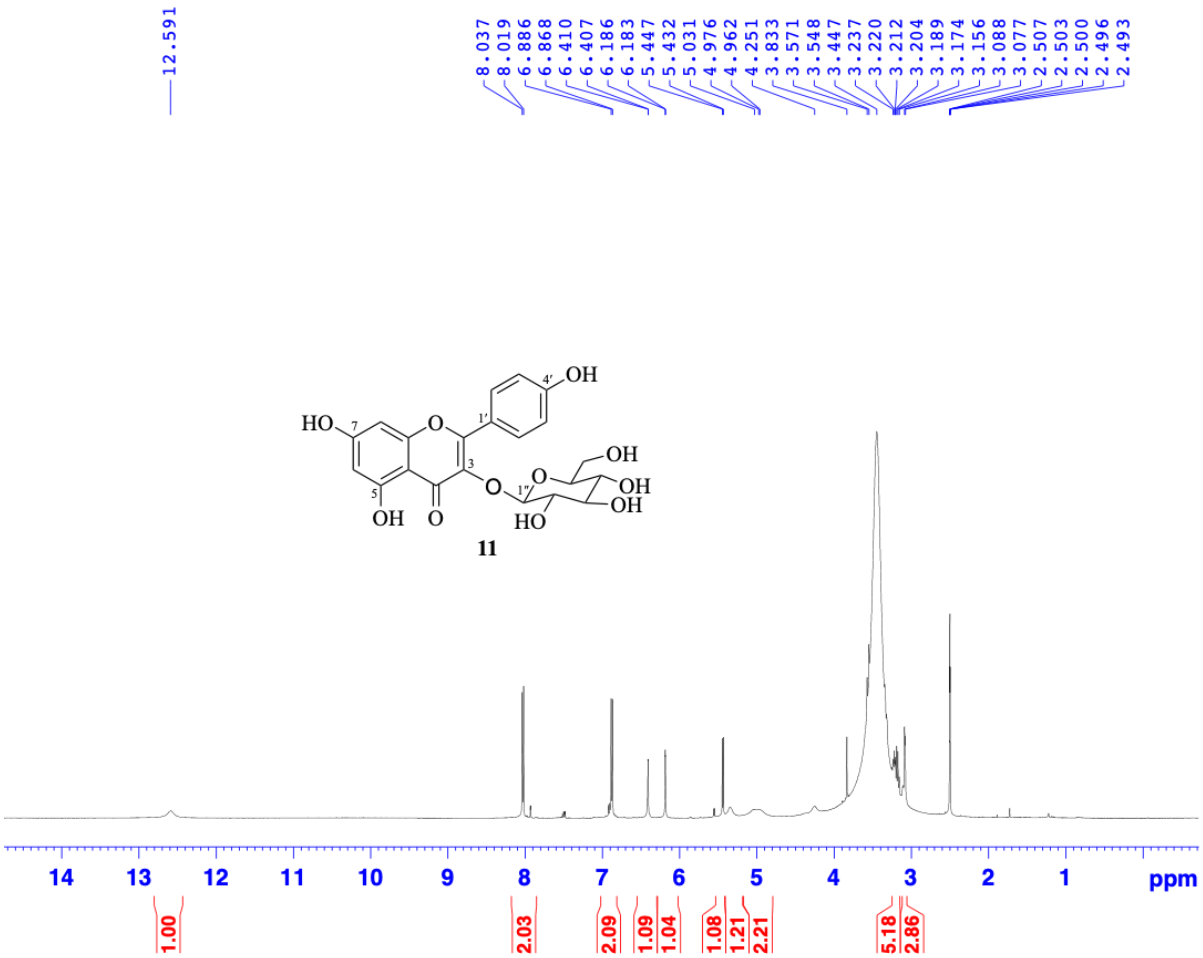


Figure S34: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of Astragalin (**11**)

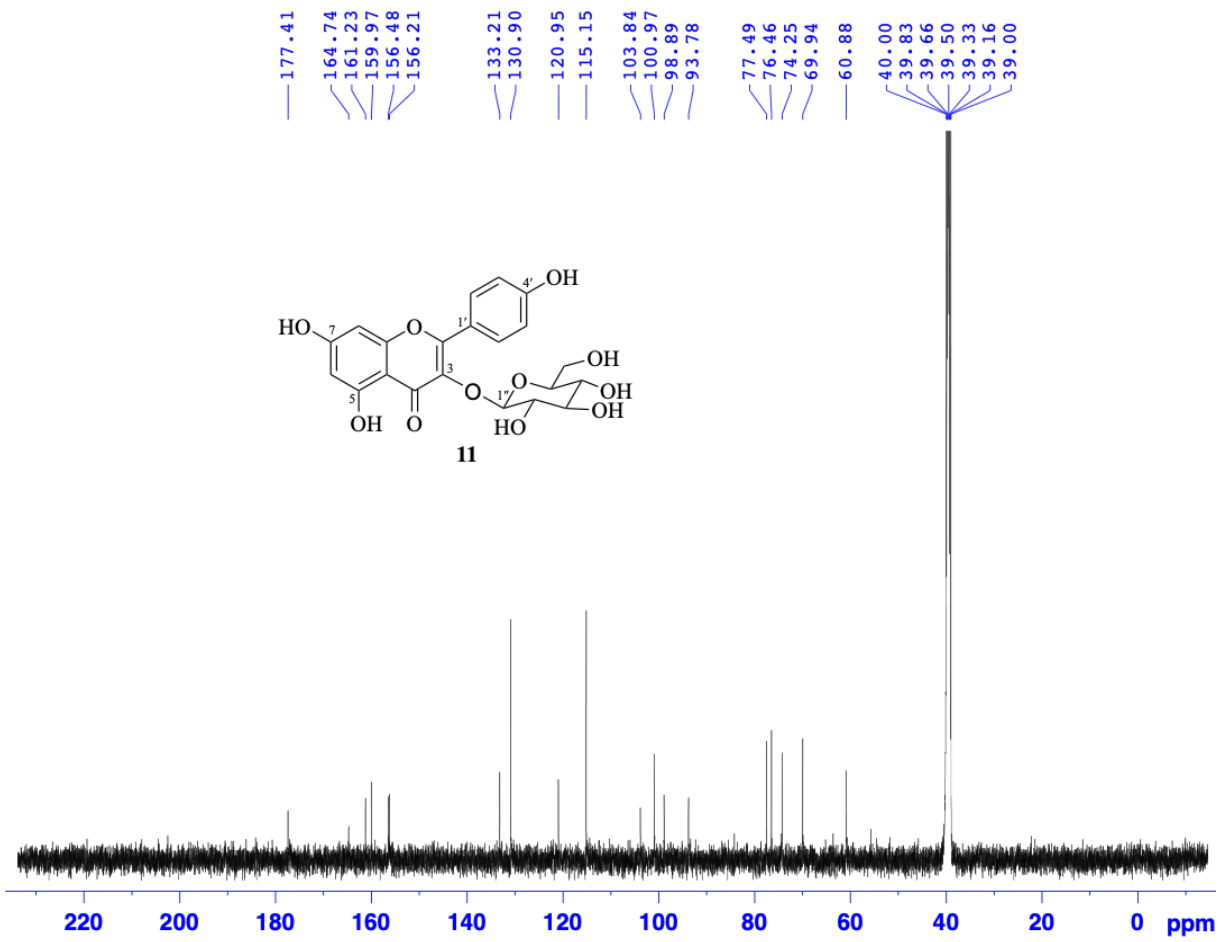


Figure S35: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of Astragalin (**11**)

Naringenin (12): ^{1}H NMR (500 MHz, CD_3OD) data (Table S3); ^{13}C NMR (125 MHz, CD_3OD) data (Table S4).

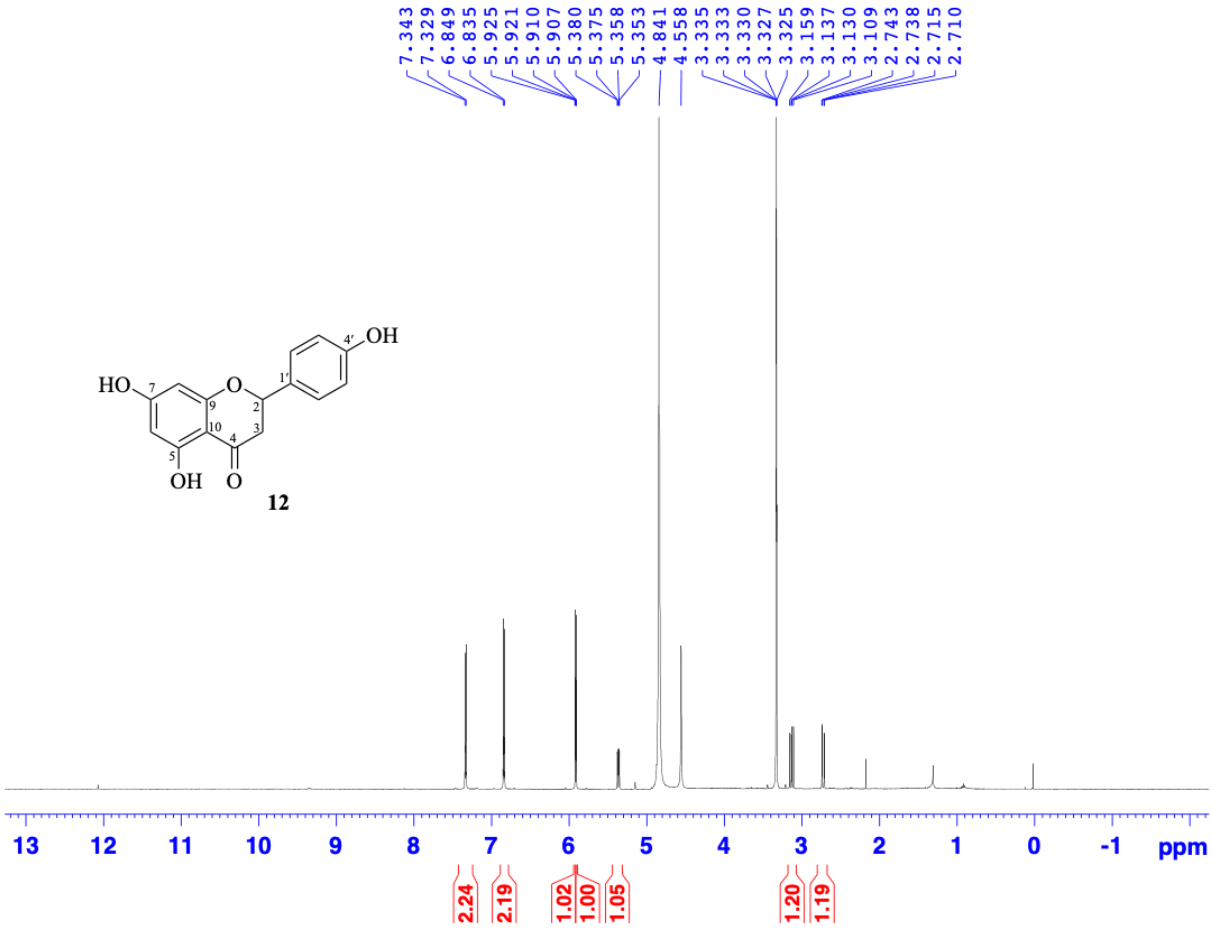


Figure S36: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Naringenin (**12**)

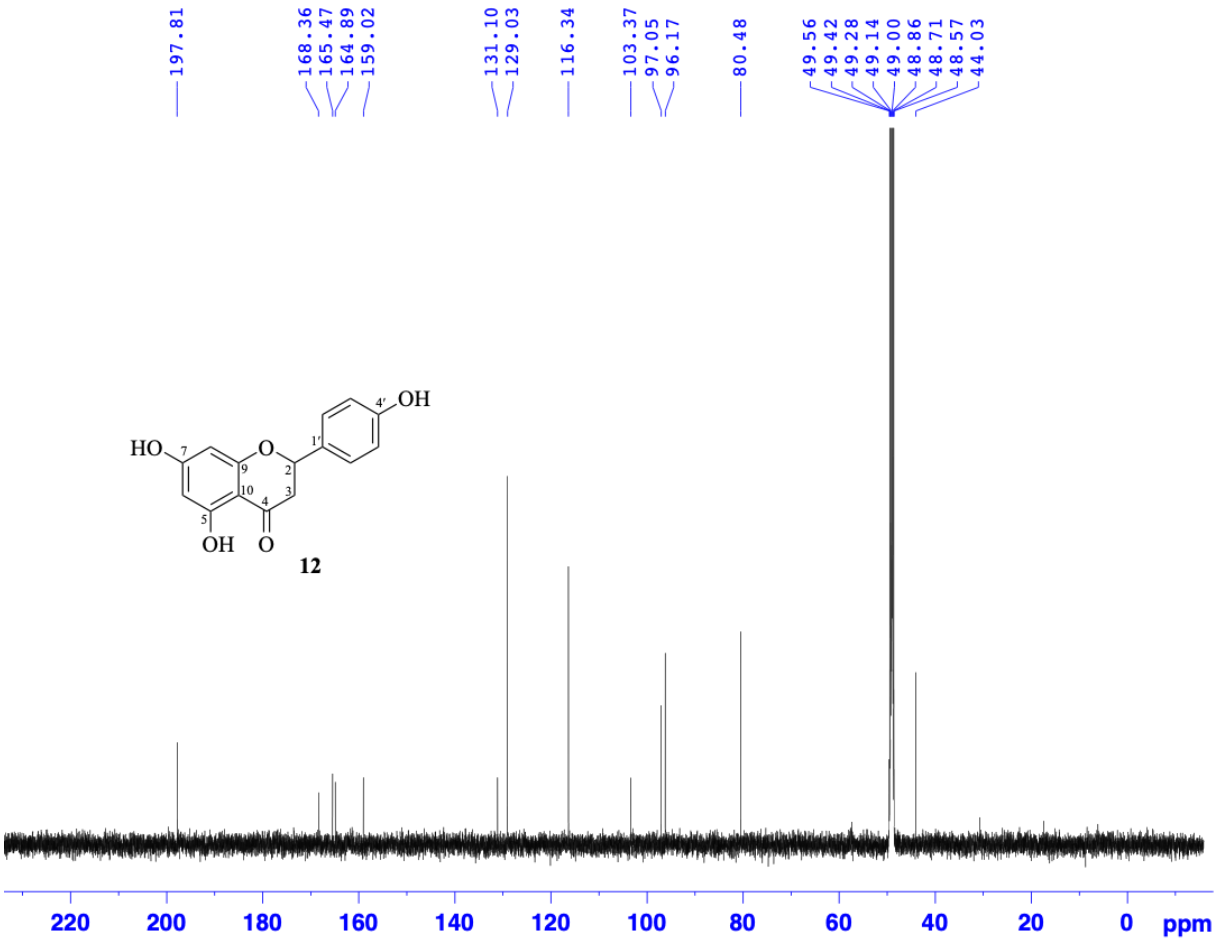


Figure S37: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Naringenin (**12**)

Myrciaphenone A (13): ^{1}H NMR (500 MHz, CD_3OD) δ: 6.21 (1H, *d*, *J* = 2.5 Hz, H-3), 5.97 (1H, *d*, *J* = 2.5 Hz, H-5), 5.05 (1H, *d*, *J* = 7.5 Hz, H-1'), 3.94 (1H, *dd*, *J* = 2.0, 12.0 Hz, H-6'a), 3.75 (1H, dd, *J* = 5.5, 12.0 Hz, H-6'b), 3.55 (1H, *t*, *J* = 9.0 Hz, H-2'), 3.48 (2H, *m*, H-3', H-5'), 3.44 (1H, *t*, *J* = 9.0 Hz, H-4'), 2.71 (3H, *s*, H_3-8); ^{13}C NMR (125 MHz, CD_3OD) δ: 204.8 (C-7), 166.2 (C-6), 165.7 (C-4), 162.4 (C-2), 105.5 (C-1), 102.0 (C-1'), 98.2 (C-5), 95.4 (C-3), 78.5 (C-3'), 78.3 (C-5'), 74.7 (C-2'), 71.1 (C-4'), 62.4 (C-6'), 33.4 (C-8).

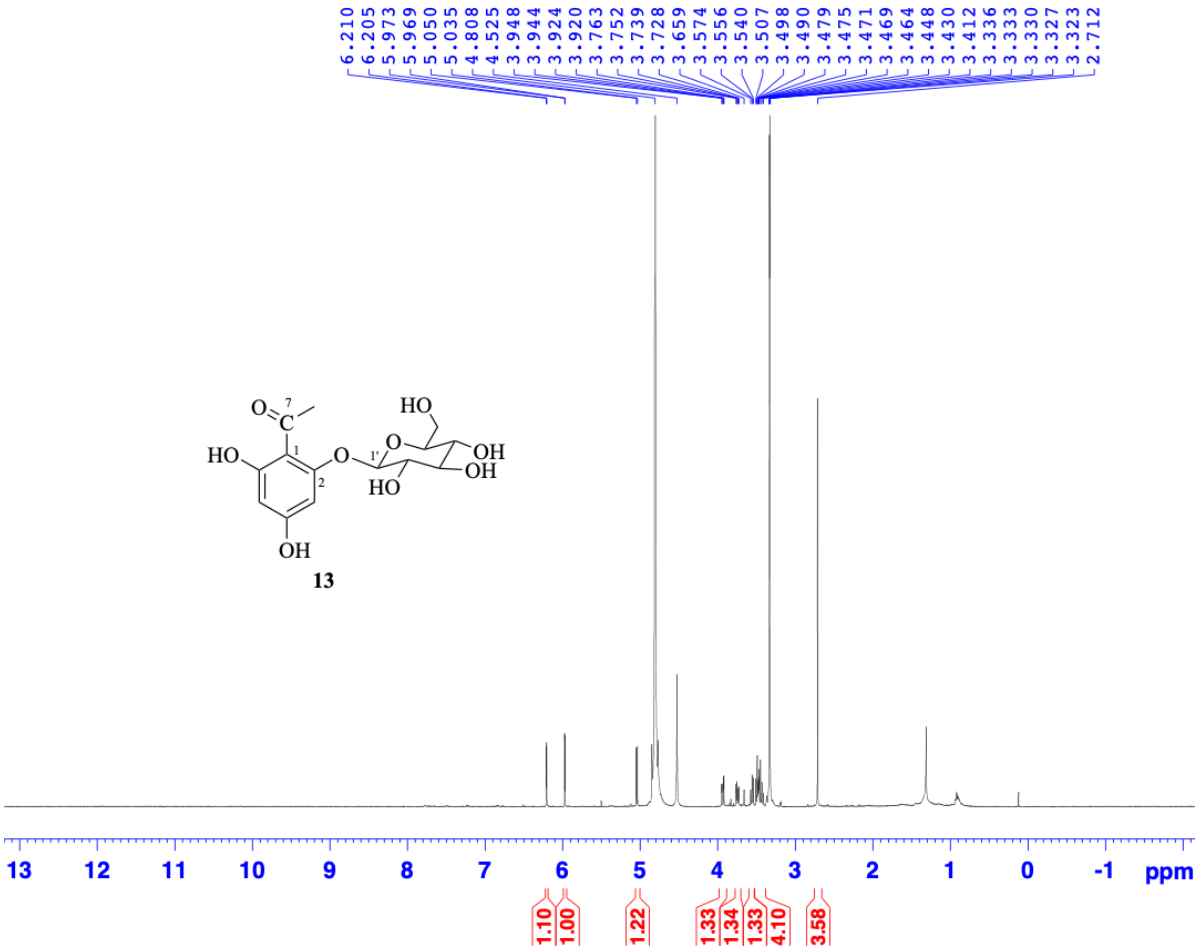


Figure S38: ^{1}H-NMR (500 MHz, CD_3OD) Spectrum of Myrciaphenone A (**13**)

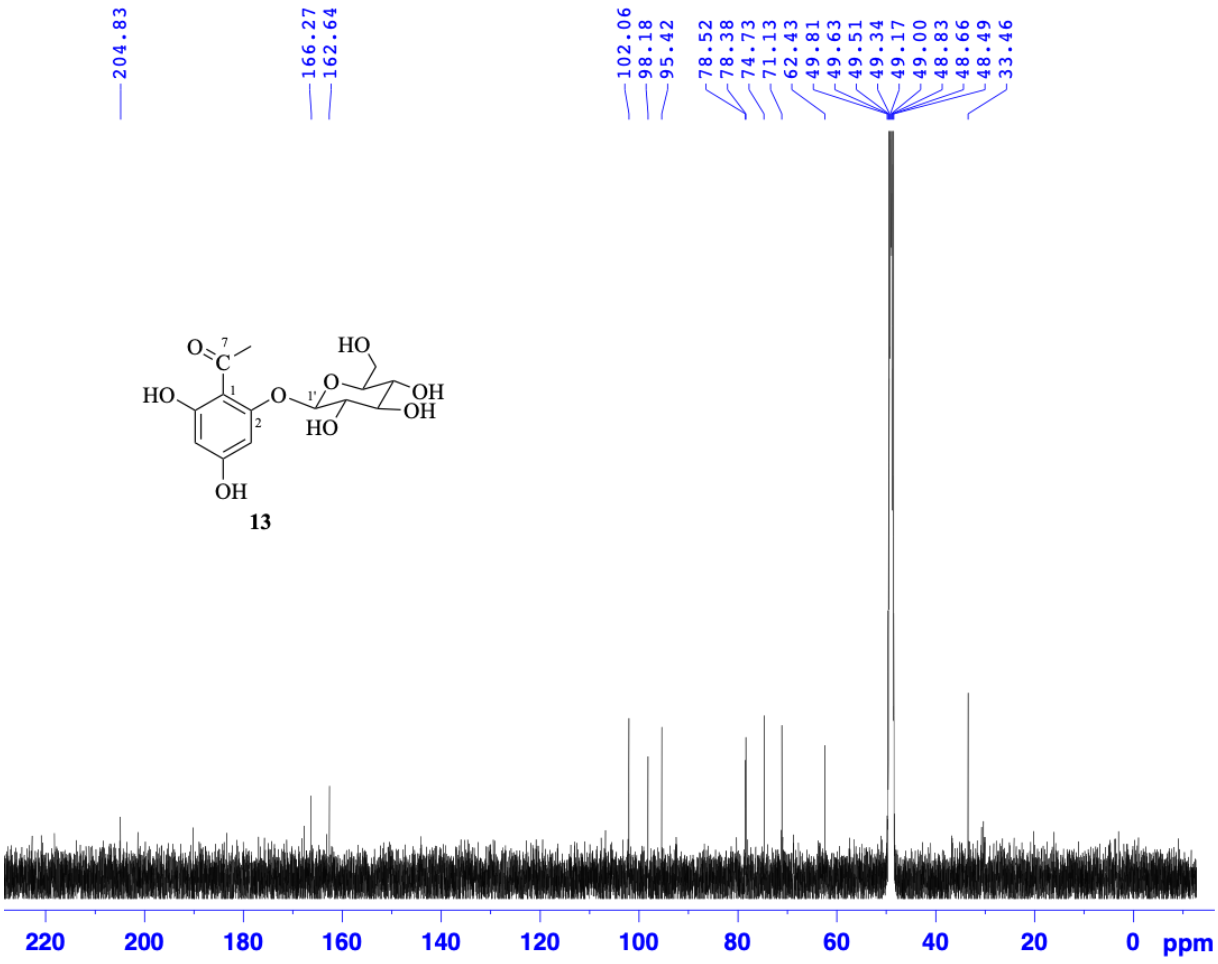
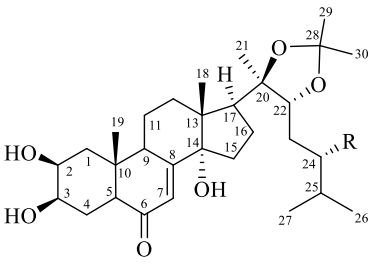
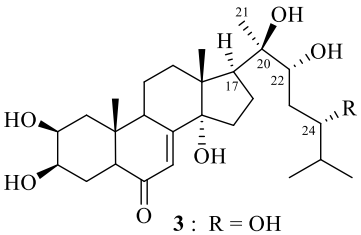


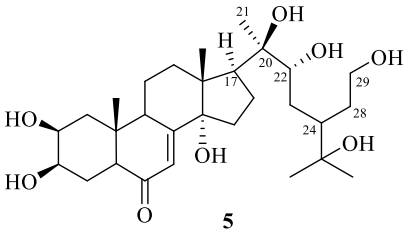
Figure S39: ^{13}C-NMR (125 MHz, CD_3OD) Spectrum of Myrciaphenone A (**13**)



1 : R = OH
2 : R = H



3 : R = OH
4 : R = H

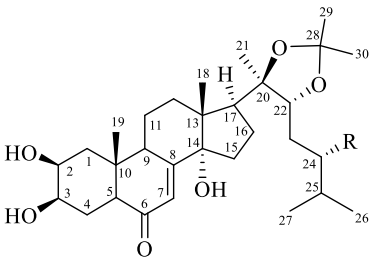


5

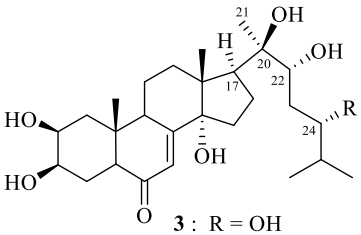
Table S1: ^{1}H NMR (500 MHz) data spectroscopic of compounds **1**-**5** (δ in ppm, *J* in Hz)

Position	**1**[a]	**2**[a]	**3**[b]	**4**[b]	**5**[c]
1	1.77 *m*, 1.39 *m*	1.77 *m*, 1.38 *m*	1.80 *m*, 1.44 *m*	1.83 *m*, 1.47 *m*	1.62 *m*, 1.26 *m*
2	3.83 *brd* (10.5)	3.82 *m*	3.86 *brd* (12.0)	3.86 *td* (4.2, 7.2)	3.77 *brs*
3	3.92 *m*	3.90 *m*	3.97 *brs*	3.97 *brd* (2.4)	3.62 *m*
4	1.65 *m*	1.66 *m*	1.72 *m*	1.73 *m*	1.62 *m*, 1.50 *m*
5	2.32 *m*	2.33 *m*	2.41 *dd* (4.5, 12.5)	2.41 *m*	2.21 *dd* (4.0,13.0)
6	-	-	-	-	-
7	5.73 *d* (2.5)	5.72 *d* (2.5)	5.83 *brs*	5.83 *d* (2.4)	5.63 *d* (1.5)
8	-	-	-	-	-
9	3.14 *m*	3.16 *m*	3.17 *m*	3.18 *m*	3.01 *m*
10	-	-	-	-	-
11	1.79 *m*, 1.65 *m*	1.76 *m*, 1.63 *m*	1.82 *m*, 1.69 *m*	1.82 *m*, 1.70 *m*	1.65 *m*, 1.53 *m*
12	2.14 *td* (6.0, 15.6)	2.19 *td* (5.0, 12.5)	2.14 *td* (4.5, 13.0)	2.14 *td* (4.8, 13.2)	1.80 *m*
	1.79 *m*	1.81 *m*	1.88 *m*	1.90 *m*	1.50 *m*
13	-	-	-	-	-
14	-	-	-	-	-
15	1.92 *m*, 1.67 *m*	1.95 *m*, 1.67 *m*	1.98 *m*, 1.62 *m*	2.00 *m*, 1.60 *m*	2.03 *m*, 1.74 *m*
16	2.04 *m*, 1.98 *m*	2.19 *m*, 1.87 *m*	2.01 *m*, 1.69 *m*	2.0 *m*, 1.73 *m*	1.87 *m*, 1.52 *m*
17	2.34 *m*	2.34 *m*	2.36 *m*	2.39 *m*	2.26 *m*
18	0.81 *s*	0.83 *s*	0.91 *s*	0.91 *s*	0.77 *s*
19	0.91 *s*	0.93 *s*	0.98 *s*	0.98 *s*	0.84 *s*
20	-	-	-	-	-
21	1.17 *s*	1.16 *s*	1.23 *s*	1.19 *s*	1.07 *s*
22	3.93 *m*	3.70 *dd* (3.0, 10.0)	3.61 *m*	3.34 *m*	3.13 *m*
23	1.61 *m*	1.44 *m*	1.73 *m*, 1.36 *m*	1.47 *m*, 1.25 *m*	1.47 *m*, 1.15 *m*
24	3.52 *m*	1.45 *m*, 1.26 *m*	3.61 *m*	1.53 *m*, 1.24 *m*	1.45 *m*
25	1.67 *m*	1.58 *m*	1.70 *m*	1.60 *m*	-
26	0.89 *d* (7.0)	0.91 *d* (6.5)	0.93 *d* (7.0)	0.93 *d* (6.6)	1.06 *s*
27	0.90 *d* (7.0)	0.91*d* (6.5)	0.97 *d* (7.0)	0.94 *d* (6.6)	1.09 *s*
28	-	-			1.26 *m*, 1.63 *m*
29	1.31 *s*	1.30 *s*			3.17 *m*, 3.29 *m*
30	1.36 *s*	1.36 *s*			-
C2-O<u>H</u>	4.11 *d* (5.0)	3.59 *d* (6.5)			4.45 *d* (6.0)
C3-O<u>H</u>	3.91 *m*	3.45 *d* (2.0)			4.34 *d* (3.0)
C14-O<u>H</u>	4.32 *s*	3.81 *s*			4.67 *s*
C20-O<u>H</u>	-	-			3.58 *s*
C22-O<u>H</u>	-	-			4.38 *d* (5.0)
C24-OH	3.68 *d* (3.5)	-			-
C25-OH	-	-			4.13 *s*

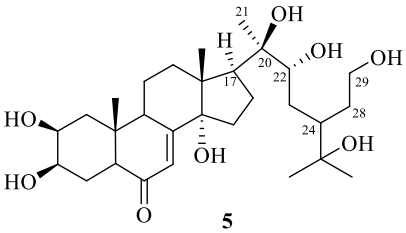
[a] Recorded in CD_3COCD_3, [b] in CD_3OD, [c] in DMSO-d_6



1 : R = OH
2 : R = H



3 : R = OH
4 : R = H



5

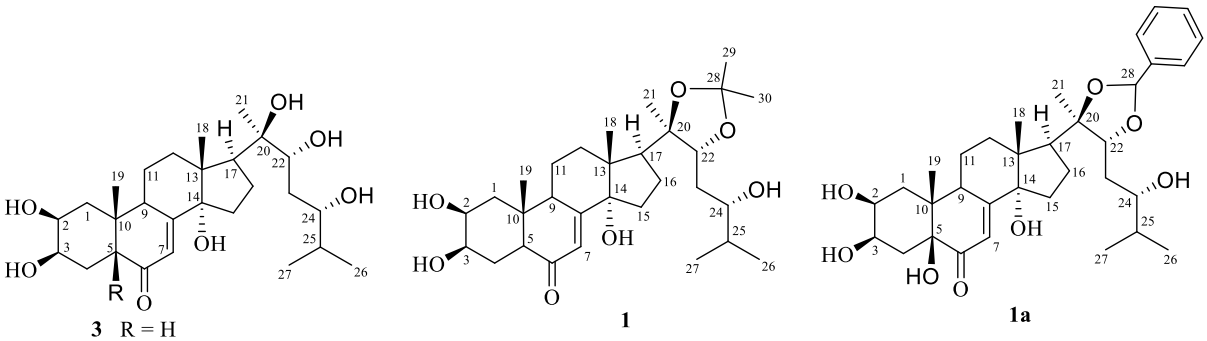
Table S2 : ^{13}C NMR (125 MHz) data spectroscopic of compounds **1**-**5**

Position	**1**[a]	**2**[a]	**3**[b]	**4**[b]	**5**[c]
1	37.4	37.8	37.4	37.4	36.6
2	68.1	68.2	68.7	68.7	66.8
3	68.0	68.1	68.5	68.5	66.6
4	32.0	32.1	32.8	32.9	31.6
5	51.1	51.3	51.8	51.8	50.1
6	203.9	202.9	206.4	206.5	202.8
7	121.8	122.0	122.2	122.1	120.5
8	165.2	164.5	167.9	168.0	165.3
9	34.4	34.6	35.1	35.1	33.2
10	38.6	38.7	39.3	39.3	37.7
11	21.0	21.2	21.5	21.5	20.1
12	31.8	32.0	32.5	32.5	30.3
13	48.0	48.1	*overlap	*overlap	46.9
14	84.7	84.8	85.2	85.2	83.0
15	31.4	31.7	31.8	31.8	30.9
16	22.0	22.1	21.5	21.5	20.3
17	49.9	50.1	50.4	50.5	48.7
18	17.5	17.5	18.0	18.0	17.2
19	24.3	24.4	24.4	24.4	23.8
20	85.5	85.2	77.8	77.9	76.3
21	22.4	22.4	21.0	21.0	21.0
22	80.4	82.3	77.6[d]	78.0	75.8
23	33.8	27.5	35.7	37.7	26.1
24	75.1	37.3	77.5[d]	30.5	35.6
25	33.7	28.8	34.1	29.2	68.8
26	17.4	22.9[d]	17.0	22.8[d]	29.0
27	19.3	22.8[d]	19.3	23.4[d]	30.0
28	107.6	107.2			41.4
29	27.1	27.2			66.6
30	29.2	29.3			

[a] Recorded in CD_3COCD_3, [b] in CD_3OD, [c] in DMSO-d_6

[d] Assignments may be interchanged in each column

*Overlapped with intensive solvent multiplet (CD_3OD: δ_C 49.0)



3 R = H
3a R = OH

1

1a

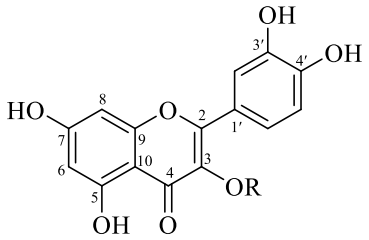
Table S3 : ^{13}C NMR data spectroscopic of compounds **1, 3** and **1a**

Position	**3**[b]	**1**[a]	**3a**[c]	**1a**[c]
1	37.4	37.4	34.6	34.8
2	68.7	68.1	67.8	67.9
3	68.5	68.0	69.7	69.7
4	32.8	32.0	35.9	35.9
5	51.8	51.1	79.7	79.8
6	206.4	203.9	200.8	200.5
7	122.2	121.8	119.8	119.9
8	167.9	165.2	166.8	166.2
9	35.1	34.4	38.2	38.2
10	39.3	38.6	44.6	44.6
11	21.5	21.0	21.3	21.9
12	32.5	31.8	31.5	31.6
13	*overlap	48.0	48.0	47.8
14	85.2	84.7	83.9	83.9
15	31.8	31.4	32.0	31.6
16	21.5	22.0	22.0	22.4
17	50.4	49.9	49.8	50.7
18	18.0	17.5	17.8	17.4
19	24.4	24.3	17.7	17.1
20	77.8	85.5	76.8	85.3
21	21.0	22.4	21.5	23.3
22	77.6[d]	80.4	76.7[d]	82.6
23	35.7	33.8	35.6	33.5
24	77.5[d]	75.1	77.5[d]	74.3
25	34.1	33.7	34.0	34.2
26	17.0	17.4	17.0	17.2
27	19.3	19.3	19.5	19.6
C-acetal	-	107.6	-	104.0
		Dimethyl: 27.1, 29.2		Phenyl: 139.9, 129.3, 128.6, 127.4

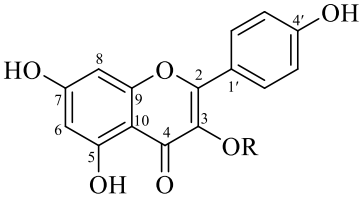
[a] Recorded in acetone-d_6, [b] in CD_3OD, [c] in pyridine-d_5

[d] Assignments may be interchanged in each column

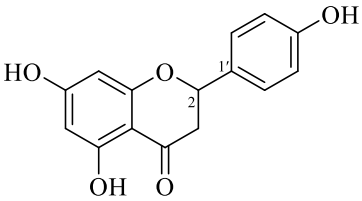
3a: ponasterone C; **1a**: ponasterone C-20,22-benzylidene acetal [11]



6 : R = H
7 : R = O-α-L-Rha
8 : R = O-β-D-Glc
9 : R = O-β-D-Glc^{6}-α-L-Rha



10 : R = O-α-L-Rha
11 : R = O-β-D-Glc

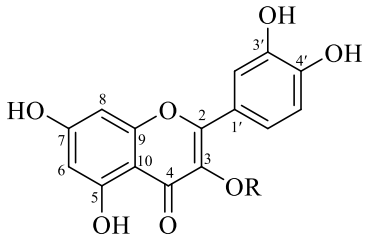


12

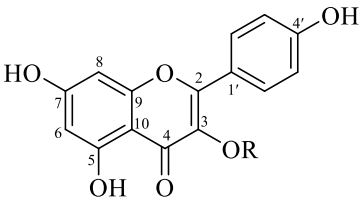
Table S4 : ^{1}H NMR (500 MHz) data spectroscopic of compounds **6-12** (δ in ppm, *J* in Hz)

Position	**6**[a]	**7**[a]	**8**[b]	**9**[b]	**10**[a]	**11**[a]	**12**[b]
2	-	-	-	-	-	-	5.37 *dd* (13. 3)
3	-	-	-	-	-	-	3.13 *dd* (13.0, 17.0) 2.71 *dd* (3.0, 17.0)
4	-	-	-	-	-	-	-
5	-	-	-	-	-	-	-
6	6.17 *d* (1.5)	6.20 *d* (2.0)	6.23 *d* (2.0)	6.12 *d* (2.0)	6.20 *d* (2.0)	6.18 *d* (1.5)	5.92 *d* (2.0)
7	-	-	-	-	-	-	-
8	6.39 *d* (1.5)	6.39 *d* (2.0)	6.42 *d* (2.0)	6.31 *d* (2.0)	6.41 *d* (2.0)	6.41 *d* (1.5)	5.91 *d* (2.0)
9	-	-	-	-	-	-	-
10	-	-	-	-	-	-	-
1′	-	-	-	-	-	-	-
2′	7.66 *d* (1.0)	7.30 *d* (2.5)	7.73 *d* (2.0)	7.57 *d* (2.5)	7.75 *d* (9.0)	8.03 *d* (9.0)	7.34 *d* (8.4)
3′	-	-	-	-	6.91 *d* (9.0)	6.88 *d* (9.0)	6.84 *d* (8.4)
4′	-	-	-	-	-	-	-
5′	6.88 *d* (8.5)	6.89 *d* (8.5)	6.90 *d* (8.5)	6.78 *d* (8.5)	6.91 *d* (9.0)	6.88 *d* (9.0)	6.84 *d* (8.4)
6′	7.53 *dd* (1.0, 8.5)	7.28 *dd* (2.5, 8.5)	7.61 *dd* (2.0, 8.5)	7.53 *dd* (2.5, 8.5)	7.75 *d* (9.0)	8.03 *d* (9.0)	7.34 *d* (8.4)
5-OH	12.46 s	12.61 s	-	-	12.61 *s*	12.59 *brs*	-
1″	-	5.18 *d* (1.5)	5.26 *d* (7.5)	5.01 *d* (7.5)	5.28 *d* (1.5)	5.44 *d* (7.5)	-
2″	-	3.33 *m*	3.50 *t* (9.0)	3.16-3.39	3.10	3.08-3.54	-
3″	-	4.23 *m*	3.44 *t* (9.0)	(6H, *m*)	(3H, *m*)	(6H, *m*)	-
4″	-	4.32 *m*	3.36 *t* (9.0)				-
5″	-	3.33 *m*	3.23 *m*		3.97 *brs*		-
6″	-	0.81 *d* (5.5)	3.73 *dd* (2.5, 12.0) 3.59 *dd* (5.5, 12.0)		0.79 *d* (5.5)		-
1‴	-	-	-	4.45 *brs*	-	-	-
2‴-5‴	-	-	-	3.16-3.39 (4H, *m*)	-	-	-
6‴	-	-	-	1.02 *d* (6.0)	-	-	-

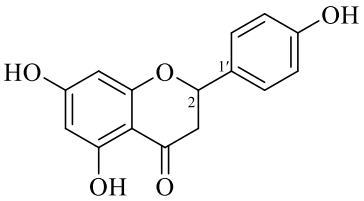
[a] Recorded in DMSO-d_6, [b] in CD_3OD



6 : R = H
7 : R = O-α-L-Rha
8 : R = O-β-D-Glc
9 : R = O-β-D-Glc^{6}-α-L-Rha



10 : R = O-α-L-Rha
11 : R = O-β-D-Glc



12

Table S5 : ^{13}C NMR (125 MHz) data spectroscopic of compounds **6-12**

Position	**6**[a]	**7**[a]	**8**[b]	**9**[b]	**10**[a]	**11**[a]	**12**[b]
2	146.8	156.5	158.5	158.6	157.3	156.2	80.5
3	135.6	134.5	135.7	135.6	134.2	133.2	44.0
4	175.8	177.7	179.5	179.5	177.7	177.4	197.8
5	160.7	161.3	163.1	163.0	161.3	161.2	165.5
6	98.2	98.7	99.9	100.0	98.8	98.9	97.1
7	164.0	164.3	166.1	166.1	164.4	164.7	168.4
8	93.4	93.7	94.7	94.9	93.8	93.8	96.2
9	156.2	157.2	159.1	159.4	156.6	156.5	164.9
10	103.0	104.1	105.7	105.5	104.1	103.8	103.4
1′	122.0	120.7	123.1	123.2	120.6	121.0	131.1
2′	115.1	115.5	117.6	117.7	130.6	130.9	129.0
3′	145.1	145.3	145.9	145.9	115.4	115.2	116.3
4′	147.7	148.6	149.9	149.8	160.0	160.0	159.0
5′	115.6	115.5	116.0	116.1	115.4	115.2	116.3
6′	120.0	121.3	123.2	123.6	130.6	130.9	129.0
1″		102.2	104.4	104.7	101.9	101.0	
2″		70.9	75.7	75.7	70.4	74.3	
3″		68.8	78.1	77.3	70.6	76.5	
4″		76.5	71.3	71.4	71.2	69.9	
5″		69.9	78.4	78.2	70.1	77.5	
6″		17.3	62.6	68.4	17.5	60.9	
1‴				102.4			
2‴				72.3			
3‴				72.1			
4‴				74.0			
5‴				69.7			
6‴				17.9			

[a] Recorded in DMSO-d_6, [b] in CD_3OD