

Supplemental File S3: NMR and mass spectrometry of dihydrostilbenes and a related substance

Table C1: NMR assignments of lunularin-4'-O-glucoside (16) and dihydioresveratrol-3-O-glucoside (17)

	lunularin-4'-O-glucoside (16)			dihydioresveratrol-3-O-glucoside (17)		
No	δ_{H} (Multiplicity, J, nH)	δ_{C}	HMBC	δ_{H} (Multiplicity, J, nH)	δ_{C}	HMBC
1	-	142.9	-	-	143.7	-
2	6.60 (s, 1H)	115.3	37.3(7)	6.34 (s, 1H)	107.1	37.6(7), 101.1(4), 109.1(6)
3	-	157.4	-	-	158.5	-
4	6.55 (d, 8.0 Hz, 1H)	112.8	118.9(6)	6.26 (s, 1H)	101.1	-
5	7.04 (t, 8.0, 7.4 Hz, 1H)	129.1	142.9(1), 157.4(3)	-	158.1	-
6	6.61 (d, 7.6 Hz, 1H)	118.9	37.3(7), 115.3(2)	6.26 (s, 1H)	109.1	-
7	2.74 (m, 2H)	37.3	36.1(8)	2.7 (m, 2H)	37.6	131.6(1'), 143.7(1)
8	2.79 (m, 2H)	36.1	37.3(7)	2.7 (m, 2H)	35.9	129.1(6'), 129.1(2'), 131.6(1')
1'	-	134.8	-	-	131.6	-
2'	7.11 (m, 1H)	129.1	36.1(8), 155.7(4')	7.00 (m, 1H)	129.1	129.1(6'), 155.4(4')
3'	6.92 (m, 1H)	116.0	116.0(5'), 134.8(1'), 155.7(4')	6.64 (m, 1H)	115.0	115.0(5'), 131.6(1'), 155.4(4')
4'	-	155.7	-	-	155.4	-
5'	6.92 (m, 1H)	116	116.0(3'), 134.8(1'), 155.7(4')	6.64 (m, 1H)	115	115.0(3'), 131.6(1'), 155.4(4')
6'	7.11 (m, 1H)	129.1	36.1(8), 155.7(4')	7.00 (m, 1H)	129.1	35.9(8), 129.1(2'), 155.4(4')
A1	4.81 (d, 7.7 Hz, 1H)	100.6	155.7(4')	4.73 (d, 7.7 Hz, 1H)	100.5	158.5(3)
A2	3.21 (m, 1H)	73.3	100.6(A1)	3.18 (m, 1H)	73.2	100.5(A1)
A3	3.26 (m 1H)	76.7	69.7(A4), 73.3(A2)	3.24 (m, 1H)	76.7	69.7(A4), 73.2(A2)
A4	3.15 (m, 1H)	69.7	-	3.16 (m, 1H)	69.7	-
A5	3.3 (m, 1H)	77.0	-	3.26 (m, 1H)	77	-
A6a	3.68 (m, 1H)	60.7	-	3.68 (m, 1H)	60.6	-
A6b	3.46 (m, 1H)	60.7	-	3.48 (m, 1H)	60.6	-

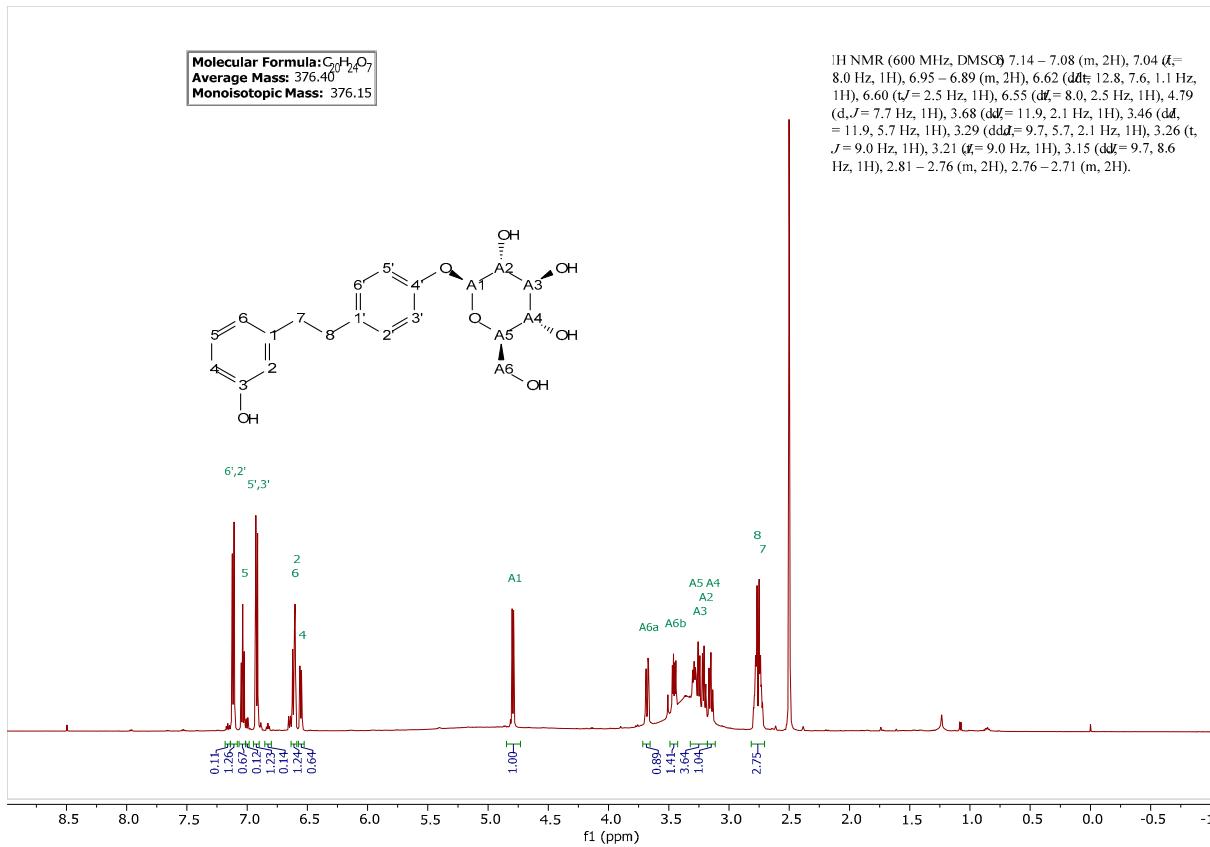


Figure C1: 1H NMR spectrum (600 MHz, DMSO) of lunularin-4'-O-glucoside (16)

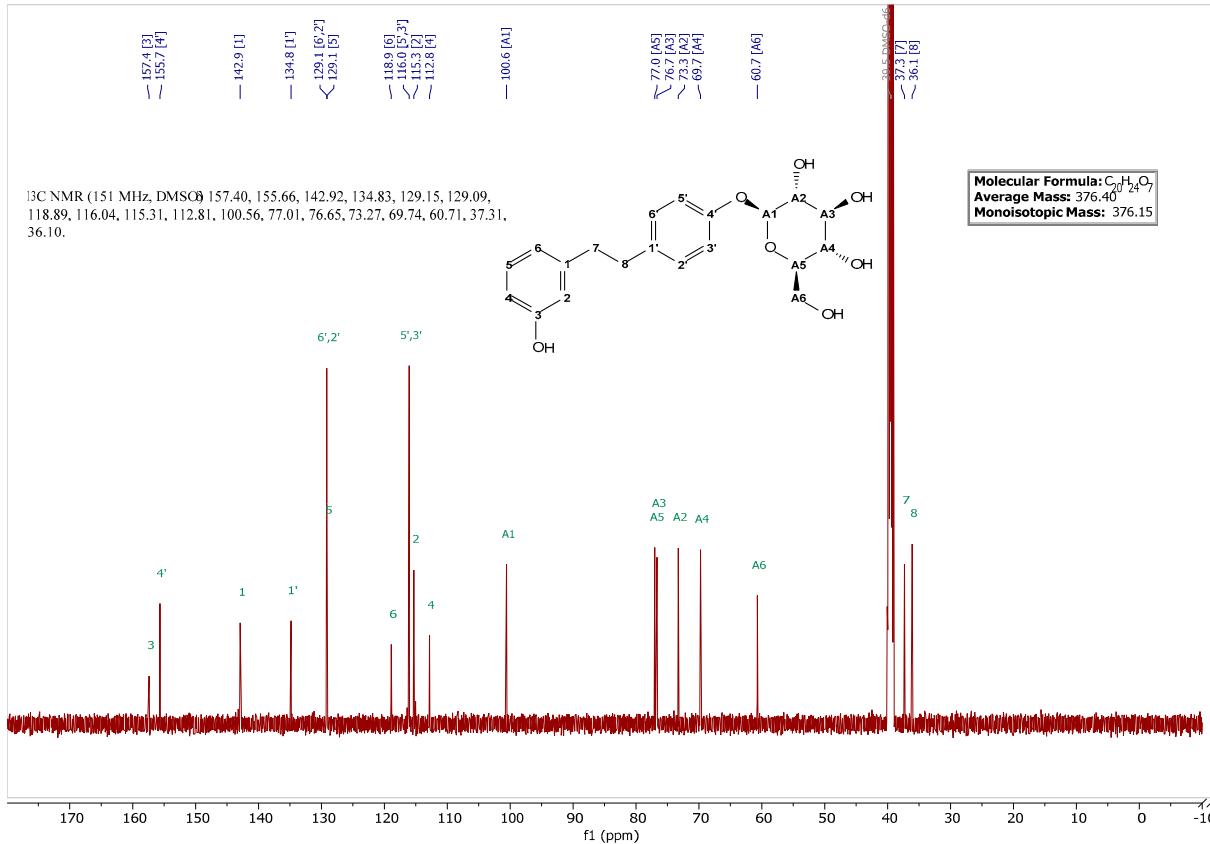


Figure C2: ^{13}C NMR spectrum (151 MHz, DMSO) of lunularin-4'-O-glucoside (16)

¹H NMR (600 MHz, DMSO) δ 7.02 – 6.97 (m, 2H), 6.67 – 6.61 (m, 2H), 6.36 – 6.32 (m, 1H), 6.29 – 6.22 (m, 2H), 4.73 (δ = 7.7 Hz, 1H), 3.68 (δ = 11.8, 2.1 Hz, 1H), 3.47 (δ = 11.8, 5.5 Hz, 1H), 3.26 (ddd, J = 9.8, 5.5, 2.1 Hz, 1H), 3.27 – 3.22 (m, 1H), 3.17 (δ = 8.9 Hz, 1H), 3.15 (δ = 9.8 Hz, 1H), 2.77 – 2.62 (m, 4H).

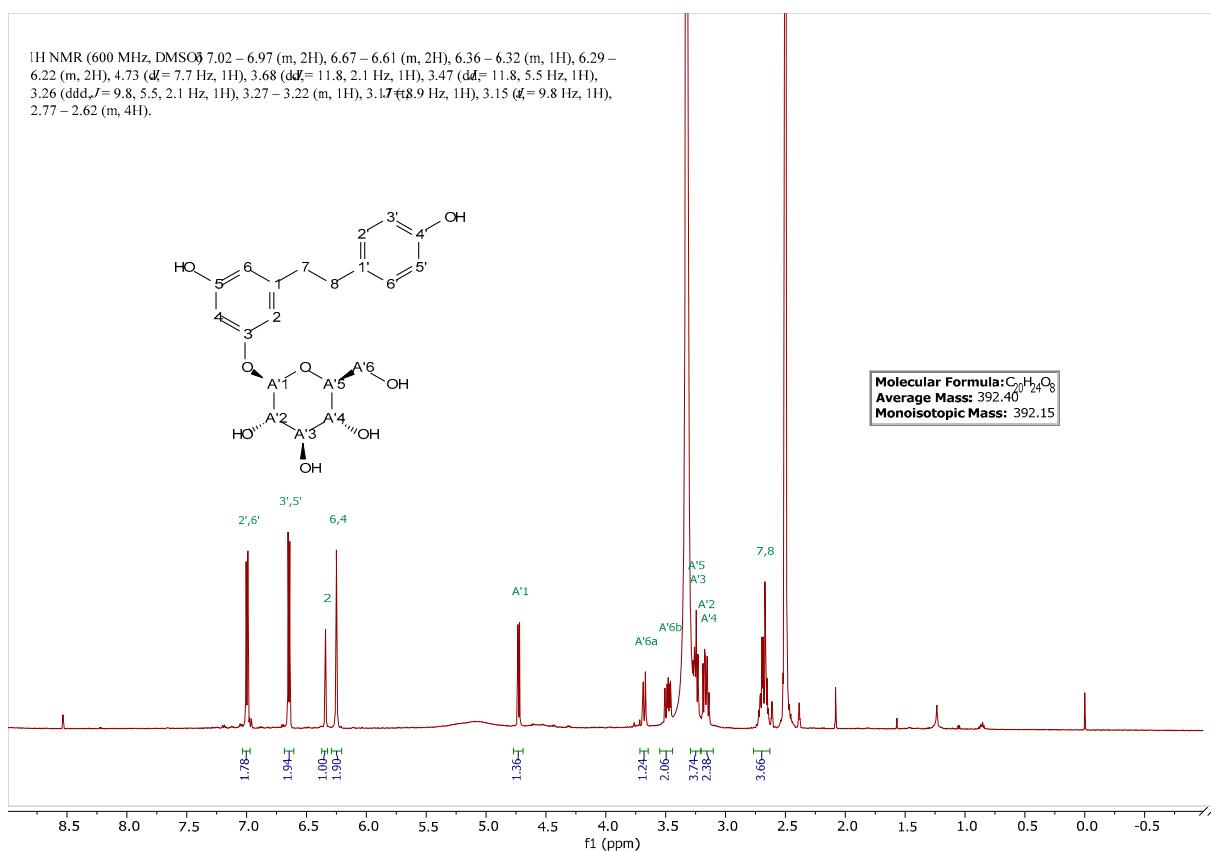


Figure C3: ¹H NMR spectrum (600 MHz, DMSO) of dihydroresveratrol-3-O-glucoside (17)

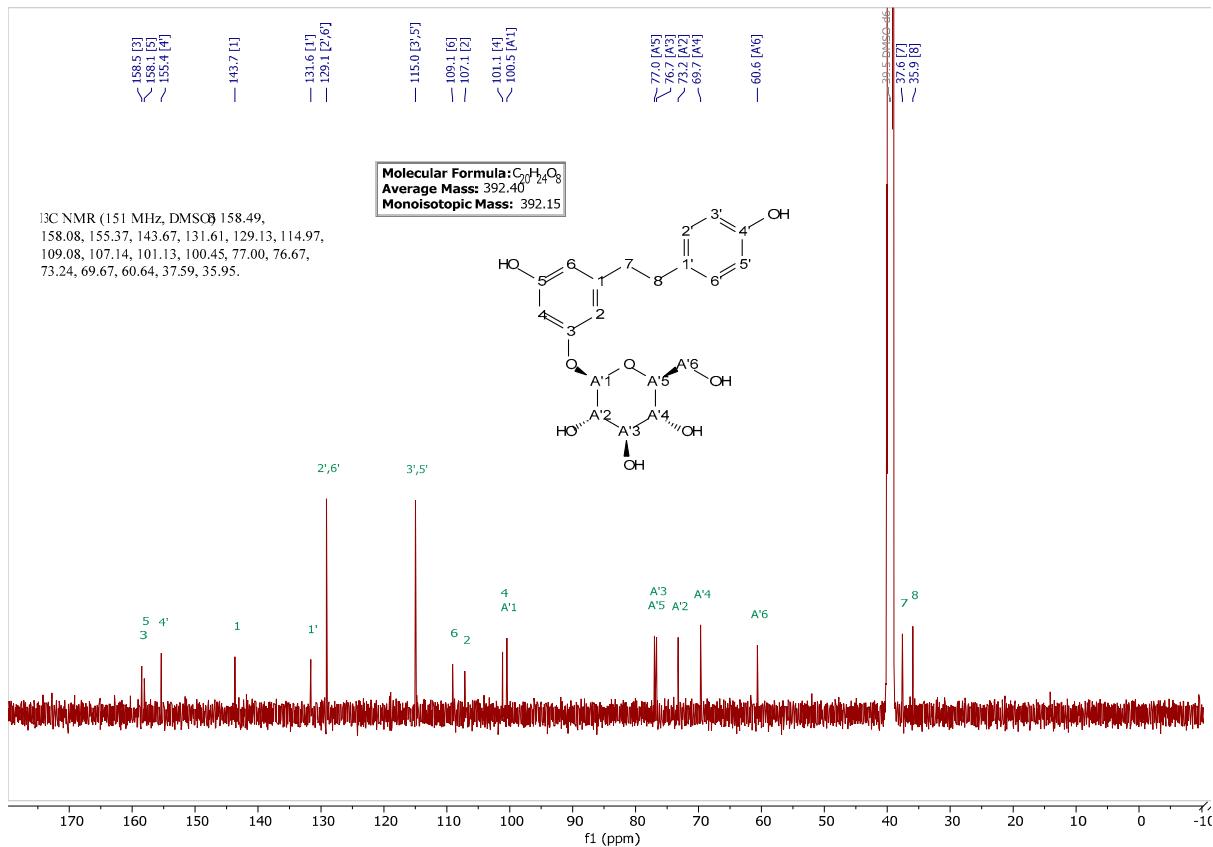
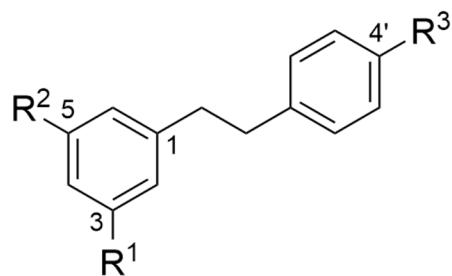


Figure C4: ¹³C NMR spectrum (151 MHz, DMSO) of dihydroresveratrol-3-O-glucoside (17)



Lunularin 4'-O-glc (**16**) R1: OH, R2: H, R3: O- β -Glc
dihydroresveratrol 3-O-glc (**17**) R1: OH, R2: O- β -Glc, R3: OH

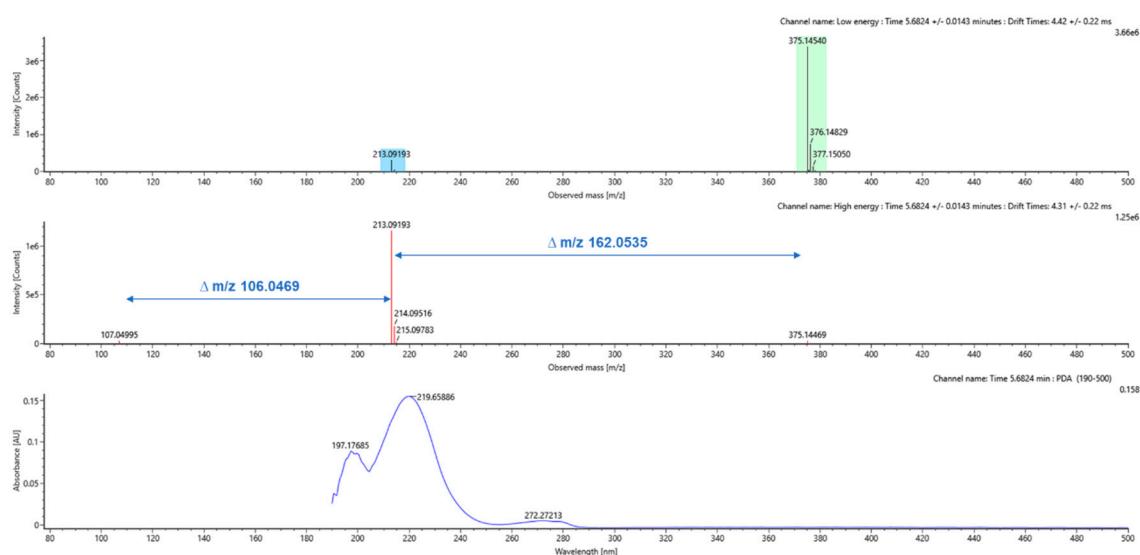


Figure C5: mass and UV-spectra of lunularin-4'-O-glucoside (16)

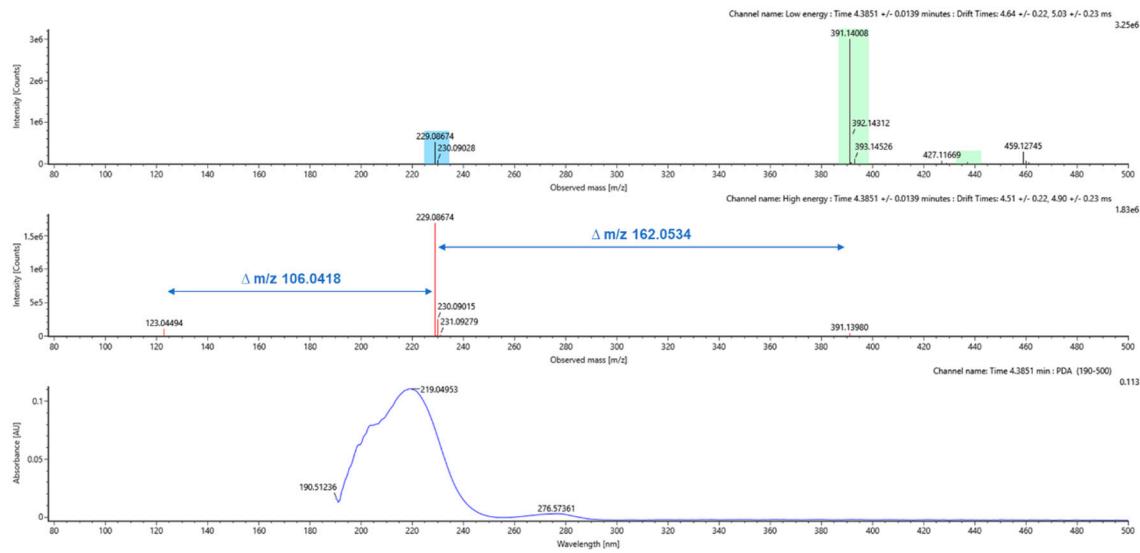


Figure C6: mass and UV spectra of dihydroresveratrol-3-O-glucoside (17)

Table C2: NMR assignments of 4-hydroxy-8-[4-glucopyranosyl]hydroxyphenyl]octane-2,6-dione (18)

No	δ H (Multiplicity, J, nH)	δ c	HMBC
1	2.08 (s, 3H)	30.5	50.7(3), 207.4(2)
2	-	207.4	-
3	2.47 (m, 2H)	50.7	49.9(5), 63.5(4), 207.4(2)
4	4.29 (tt, 7.7,5.5 Hz, 1H)	63.5	49.9(5), 50.7(3), 207.4(2), 208.5(6)
5	2.47 (m, 2H)	49.9	50.7(3), 63.5(4), 208.5(6)
6	-	208.5	-
7	2.72 (m, 2H)	44.4	134.4(1'), 208.5(6)
8	2.72 (m, 2H)	28	44.4(7), 129.0(2'), 129.0(6'), 134.4(1'), 208.5(6)
1'	-	134.4	-
2'	7.12 (m, 1H)	129	28.0(8), 155.7(4')
3'	6.94 (m, 1H)	116.2	134.4(1'), 155.7(4')
4'	-	155.7	-
5'	6.94 (m, 1H)	116.2	135.4(1'), zz155.7(4')
6'	7.12 (m, 1H)	129	28.0(8), 155.7(4')
A1	4.77 (d, 7.6 Hz, 1H)	100.6	155.7(4')
A2	3.20 (m, 1H)	73.3	76.6(A3), 100.6(A1)
A3	3.25 (m, 1H)	76.6	69.8(A4), 73.3(A2)
A4	3.14 (m, 1H)	69.8	60.7(A6), 76.6(A3)
A5	3.29 (m, 1H)	77	-
A6a	3.66 (m, 1H)	60.7	69.8(A4)
A6b	3.45 (m, 1H)	60.7	77.0(A5)

¹H NMR (600 MHz, DMSO) 7.19 – 7.06 (m, 2H), 7.01 – 6.87 (m, 2H), 4.79 (d, 7.6 Hz, 1H), 4.32 (tt, *J*= 7.5, 5.5 Hz, 1H), 3.68 (dd= 11.8, 2.1 Hz, 1H), 3.45 (dd= 11.8, 5.8 Hz, 1H), 3.29 (dd= 9.5, 5.8, 2.1 Hz, 1H), 3.25 (*q*= 9.1 Hz, 1H), 3.20 (*q*= 9.1 Hz, 1H), 3.14 (*q*= 9.5 Hz, 1H), 2.72 (ddt, *J*= 12.3, 9.1, 7.3 Hz, 4H), 2.49 – 2.44 (m, 4H), 2.08 (s, 3H).

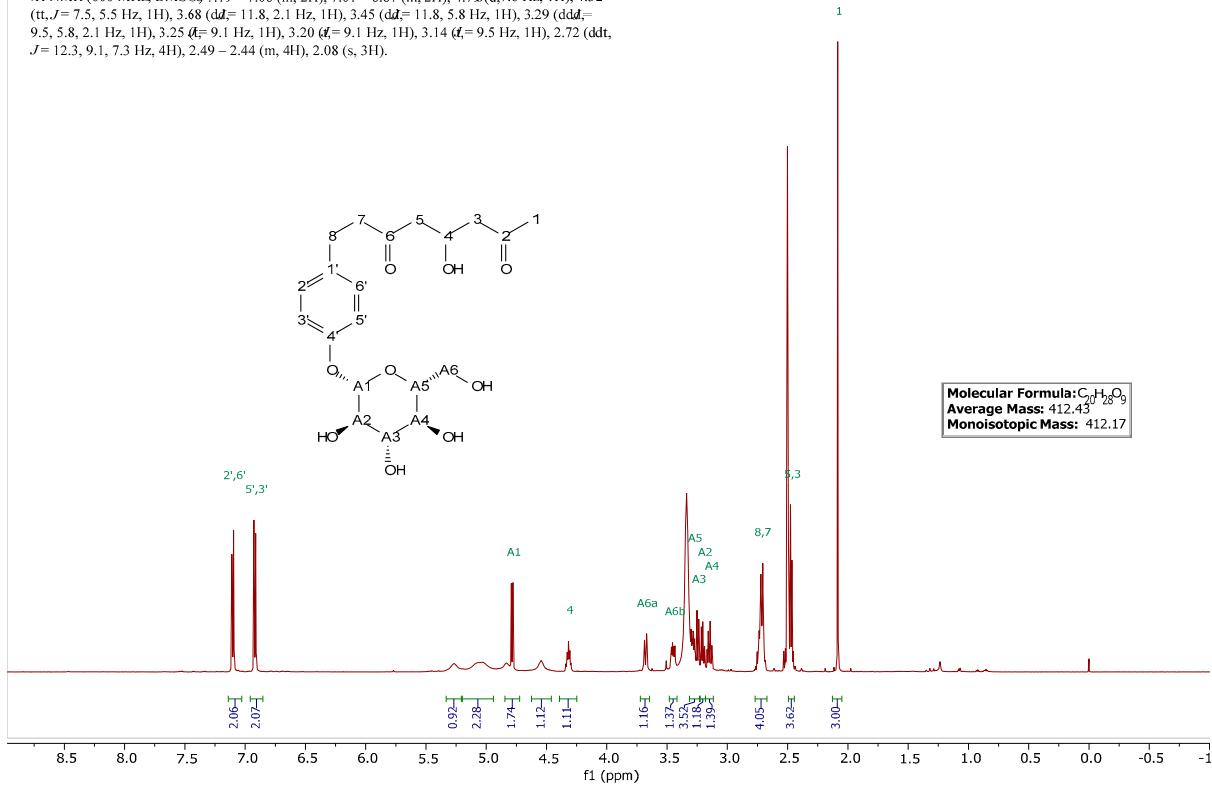


Figure C7: ¹H NMR spectrum (600 MHz, DMSO) of 4-hydroxy-8-[4-glucopyranosyl]hydroxyphenyl]octane-2,6-dione (18)

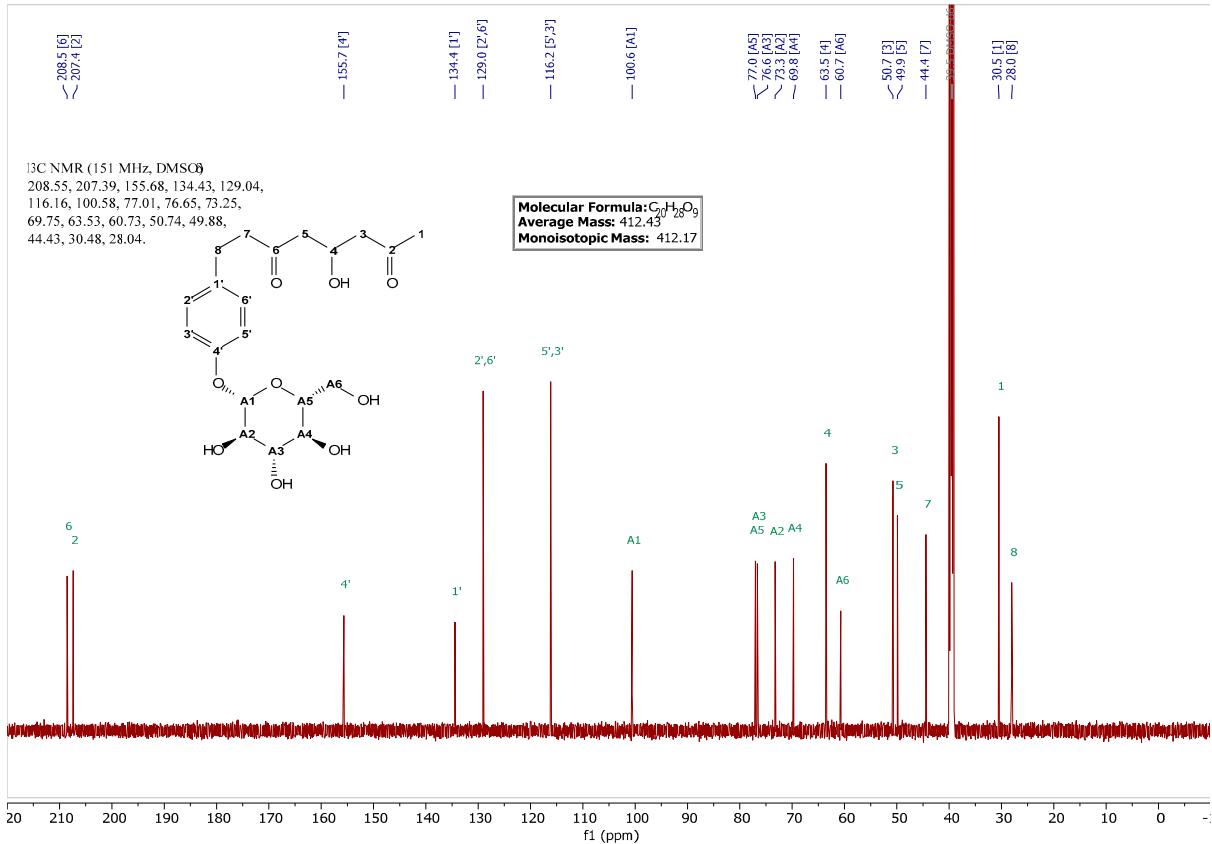
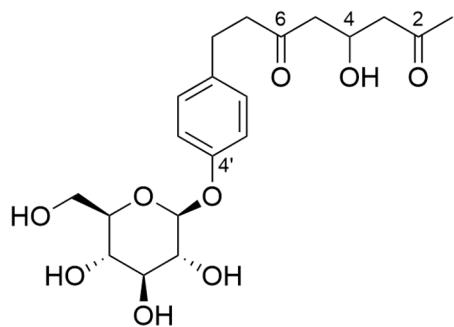


Figure C8: ¹³C NMR spectrum (151 MHz, DMSO) of 4-hydroxy-8-[4-glucopyranosyl]hydroxyphenyl]octane-2,6-dione (18)



4-hydroxy-8-[4-glucopyranosyl]hydroxyphenyl]octane-2,6-dione (**18**)

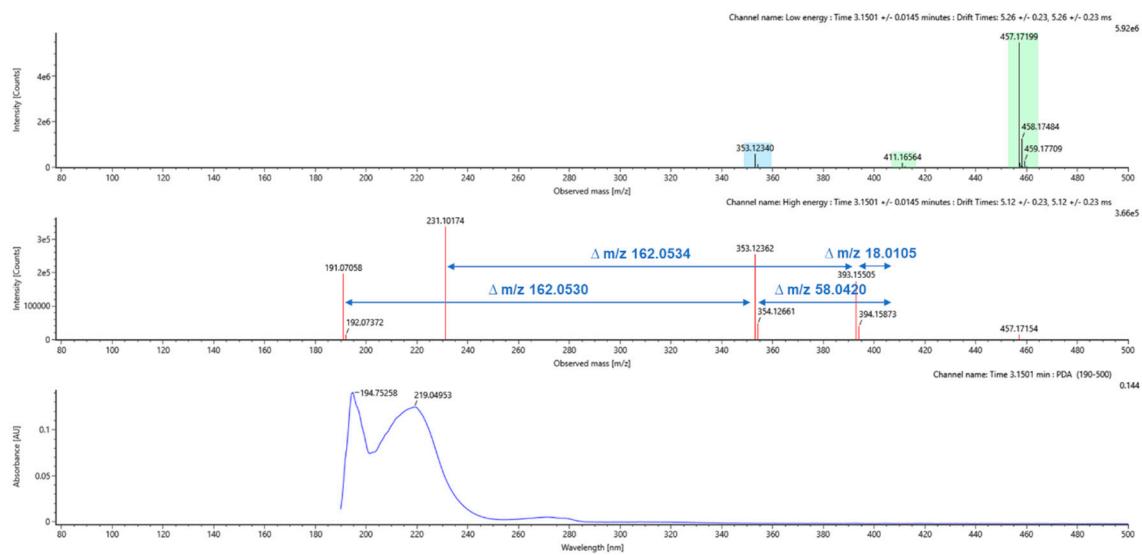


Figure C9: mass and UV-spectra of 4-hydroxy-8-[4-glucopyranosyl]hydroxyphenyl]octane-2,6-dione (**18**)