

Deciphering the phytochemical profile of an Alpine rose (*Rhododendron ferrugineum* L.)
leave extract for a better understanding of its senolytic and skin-rejuvenation effects

Supplementary data

NMR data (experimental data)

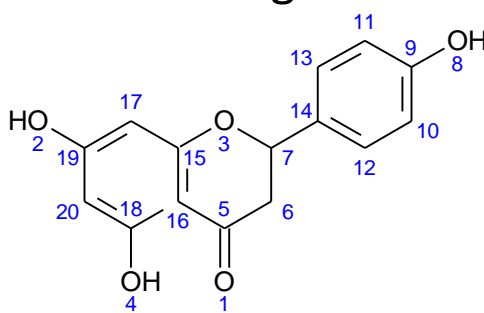
NMR data validated after interpretation of 1D and 2D NMR spectra (^1H , ^{13}C , HSQC, HMBC and COSY)

Spectrometer: Bruker Avance 600 MHz – cryoprobe

Solvent: DMSO- d_6

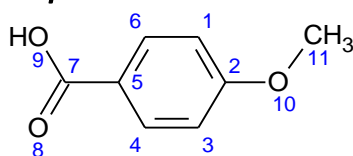
Note: Molecular structure numbering is different from the IUPAC numbering

Naringenin



$\text{C}_{15}\text{H}_{12}\text{O}_5$	272.2 g/mol	CAS 480-41-1
Atom number	^{13}C (ppm)	^1H (ppm)
5	196.8	-
6	42.2	2.68/3.27
7	78.9	5.43
9	158.2	-
10/11	115.5	6.80
12/13	128.8	7.33
14	129.4	-
15	163.2	-
16	102.2	-
17	95.4	5.88
18	163.9	-
19	167.1	-
20	96.2	5.88

p-anisic acid



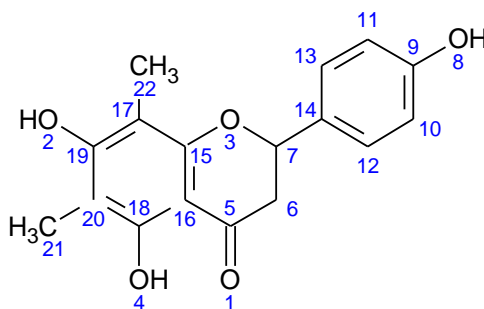
C₈H₈O₃

152.1 g/mol

CAS 100-09-4

Atom number	¹³ C (ppm)	¹ H (ppm)
1/3	114.3	7.03
2	163.3	-
4/6	131.8	7.89
5	123.5	-
7	167.5	-
11	55.9	3.82

Farrerol



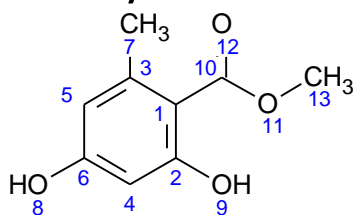
C₁₇H₁₆O₅

300.3 g/mol

CAS 24211-30-1

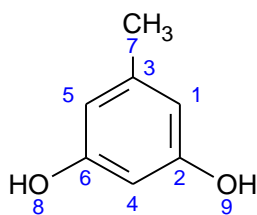
Atom number	¹³ C (ppm)	¹ H (ppm)
5	197.2	-
6	42.4	2.74/3.20
7	78.2	5.42
9	158.0	-
10/11	115.6	6.80
12/13	128.4	7.32
14	129.7	-
15	157.9	-
16	102.1	-
17	103.0	-
18	158.8	-
19	162.9	-
20	103.6	-
21	7.9	1.95
22	8.5	1.93

Methyl-orcellinate



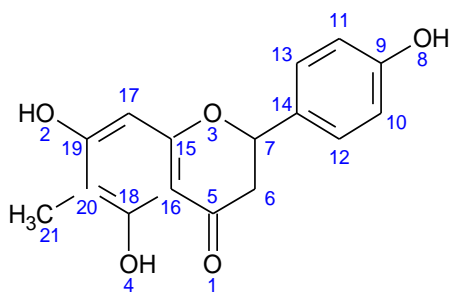
C ₉ H ₁₀ O ₄ 182.2 g/mol CAS 3187-58-4		
Atom number	¹³ C (ppm)	¹ H (ppm)
1	107.7	-
2	161.3	-
3	141.2	-
4	100.7	6.15
5	110.4	6.17
6	161.3	-
7	22.3	2.28
10	170.2	-
13	52.0	3.78

Orcinol



C ₇ H ₈ O ₂ 124.2 g/mol CAS 504-15-4		
Atom number	¹³ C (ppm)	¹ H (ppm)
1/5	107.3	6.00
2/6	158.5	-
3	139.1	-
4	99.7	5.99
7	21.5	2.10

Poriol



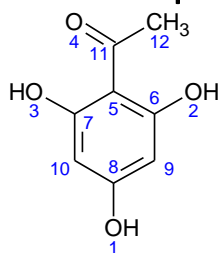
C₁₆H₁₄O₅

286.3 g/mol

CAS 14348-16-4

Atom number	¹³ C (ppm)	¹ H (ppm)
5	196.6	-
6	42.2	2.75/3.27
7	78.6	5.40
9	158.1	-
10/11	115.3	6.80
12/13	128.3	7.32
14	128.9	-
15	161.0	-
16	101.8	-
17	94.5	5.98
18	160.8	-
19	164.6	-
20	163.2	-
21	7.2	1.88

Phloroacetophenone



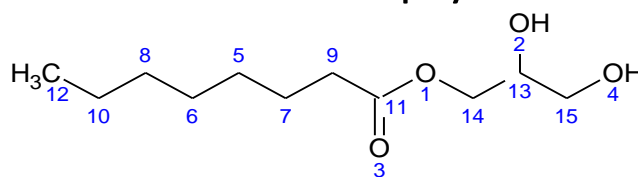
C₈H₈O₄

168.1 g/mol

CAS 480-66-0

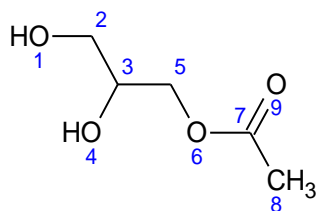
Atom number	¹³ C (ppm)	¹ H (ppm)
5	104.5	-
6/7	157.7	-
8	165.3	-
9/10	94.9	5.80
11	202.9	-
12	32.7	2.54

α-monocaprylin



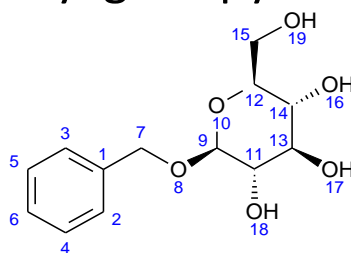
C ₁₁ H ₂₂ O ₄			218.3 g/mol	CAS 502-54-5
Atom number	¹³ C (ppm)	¹ H (ppm)		
5	28.8	1.25		
6	29.0	1.26		
7	24.6	1.50		
8	31.7	1.23		
9	33.5	2.28		
10	22.2	1.26		
11	173.3	-		
12	14.2	0.86		
13	69.5	3.63		
14	65.8	3.90/4.03		
15	63.0	3.33		

Monoacetin



C ₅ H ₁₀ O ₄			134.1 g/mol	CAS 106-61-6
Atom number	¹³ C (ppm)	¹ H (ppm)		
2	63.1	3.33		
3	69.7	3.63		
5	66.0	3.89/4.03		
7	170.7	-		
8	21.1	2.01		

Benzyl glucopyranoside



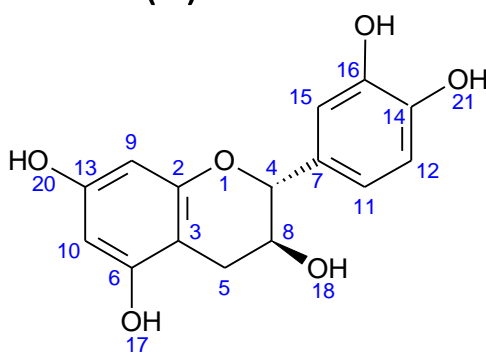
C₁₃H₁₈O₆

270.3 g/mol

CAS 4304-12-5

Atom number	¹³ C (ppm)	¹ H (ppm)
1	138.6	-
2/3	128.1	7.39
4/5	128.6	7.34
6	127.9	7.28
7	69.9	4.85/4.82
9	102.5	4.22
11	73.9	3.04
12	77.1	3.10
13	77.3	3.14
14	70.6	3.06
15	62.7	3.35/3.43

(+)-catechin



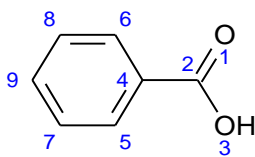
C₁₅H₁₄O₆

290.3 g/mol

CAS 154-23-4

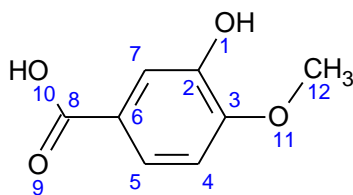
Atom number	¹³ C (ppm)	¹ H (ppm)
2	155.7	-
3	99.6	-
4	81.4	4.48
5	28.3	2.66/2.35
6	156.6	-
7	131.0	-
8	66.6	3.81
9	95.6	5.89
10	94.1	5.68
11	118.8	6.59
12	115.3	6.68
13	156.8	-
14	145.3	-
15	114.9	6.72
16	145.2	-

Benzoic acid



C ₇ H ₆ O ₂		122.1 g/mol	CAS 65-85-0
Atom number	¹³ C (ppm)	¹ H (ppm)	
2	168.1	-	
4	131.0	-	
5	129.5	7.96	
6	129.5	7.96	
7	128.8	7.51	
8	128.8	7.51	
9	132.8	7.63	

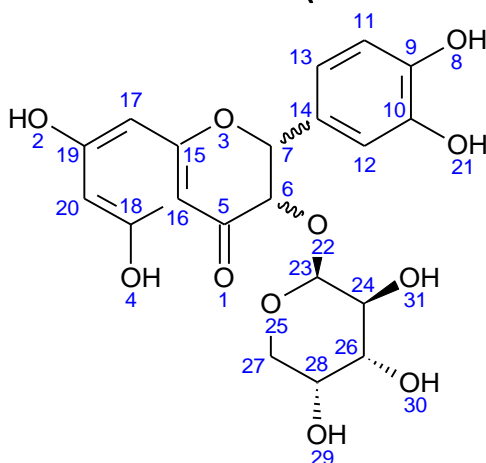
Isovanillic acid



C ₈ H ₈ O ₄		168.1 g/mol	CAS 645-08-9
Atom number	¹³ C (ppm)	¹ H (ppm)	
2	148.9	-	
3	152.9	-	
4	111.4	7.04	
5	123.5	7.56	
6	Nd*	-	
7	112.4	7.44	
8	167.7	-	
12	56.0	3.82	

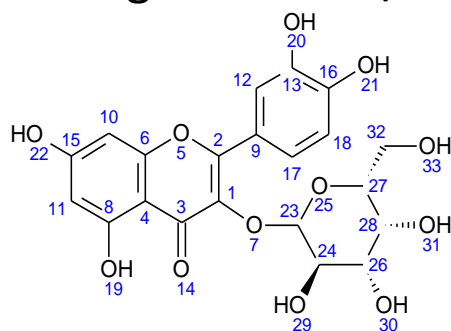
Nd* not well detected

Taxifolin 3-*O*-arabinoside (isomer 1 / isomer 2)



C ₂₀ H ₂₀ O ₁₁		436.4 g/mol	CAS ?? (two isomers)
Atom number	¹³ C (ppm)	¹ H (ppm)	
5	193.7 (193.7)	-	
6	75.3 (75.7)	4.68 (4.62)	
7	81.5 (81.7)	5.34 (5.35)	
9	146.2 (146.2)	-	
10	145.5 (145.7)	-	
11	115.8 (115.8)	6.70 (6.72)	
12	115.1 (115.1)	6.85 (6.79)	
13	119.1 (119.1)	6.71 (6.64)	
14	127.1 (127.3)	-	
15	162.2 (162.4)	-	
16	100.9 (101.1)	-	
17	95.6 (95.6)	5.87 (5.87)	
18	164.0 (164.0)	-	
19	168.5 (168.5)	-	
20	96.4 (96.4)	5.86 (5.86)	
23	100.8 (102.9)	3.95 (4.63)	
24	70.2 (70.7)	3.36 (3.49)	
26	71.8 (72.0)	3.39 (3.40)	
27	62.4 (63.2)	3.24/3.74 (3.15/3.28)	
28	65.3 (66.1)	3.65 (3.60)	

Quercetin-3-*O*-galactoside / Hyperoside



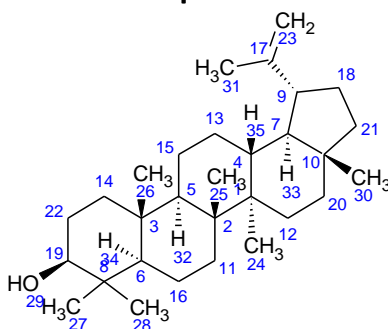
C₂₁H₂₀O₁₂

464.4 g/mol

CAS: 482-36-0

Atom number	¹³ C (ppm)	¹ H (ppm)
1	133.8	-
2	156.6	-
3	177.9	-
4	104.3	-
6	156.7	-
8	161.6	-
9	121.5	-
10	93.9	6.41
11	99.1	6.21
12	116.4	7.54
13	145.2	-
15	164.6	-
16	148.9	-
17	122.4	7.67
18	115.6	6.82
23	102.2	5.39
24	71.6	3.57
26	73.6	3.38
27	76.2	3.33
28	68.4	3.65
32	60.6	3.30/3.46

Lupeol



C₃₀H₅₀O

426.7 g/mol

CAS 545-47-1

Atom number	¹³ C (ppm)	¹ H (ppm)
1	42.8	-
2	40.6	-
3	37.1	-
4	38.0	1.62
5	50.3	1.24
6	55.2	0.63
7	48.2	1.33
8	38.8	-
9	47.9	2.37
10	43.0	-
11	34.3	1.33
12	27.4	0.96/1.62
13	25.0	1.02/1.62
14	38.7	0.83/1.56
15	20.9	1.18/1.35
16	18.4	1.34/1.45
17	150.7	-
18	29.6	1.24
19	77.2	2.97
20	35.5	1.44/1.36
21	40.0	1.19/1.34
22	27.6	1.44
23	110.2	4.54/4.68
24	14.8	0.91
25	16.2	0.99
26	16.4	0.77
27	28.5	0.87
28	16.3	0.66
30	18.2	0.76
31	19.4	1.65