Supplementary Data

This supplementary data is a part of a paper entitled “Isolation and Evaluation of the Antioxidant Capacity of Compounds from *Ehretia asperula* Zoll. & Moritzi”.

1. Supplementary Spectroscopic Data of Compound 1

**Kaempferol (1):** ¹H-NMR (600 MHz, DMSO-*d*₆), δ_H (ppm): 6.19 (1H, d, J = 2.0 Hz, H-6), 6.44 (1H, d, J = 2.0 Hz, H-8), 6.93 (2H, d, J = 8.0 Hz, H-3’, H-5’), 8.04 (2H, d, J = 8.0 Hz, H-2’, H-6’), 12.50 (1H, s, 5-OH); ¹³C-NMR (150 MHz, DMSO-*d*₆), δ_C (ppm): 146.8 (C-2), 136.0 (C-3), 176.0 (C-4), 160.7 (C-5), 98.2 (C-6), 164.0 (C-7), 93.5 (C-8), 156.2 (C-9), 103.0 (C-10), 121.7 (C-1’), 129.5 (C-2’), 115.4 (C-3’), 159.2 (C-4’), 115.4 (C-5’), 129.5 (C-6’).

![Fig S1. FTIR spectrum of compound 1](image1.png)

![Fig S2. ¹H-NMR spectrum of compound 1](image2.png)
Fig S3. Expanded $^1$H-NMR spectrum of compound 1

Fig S4. $^{13}$C-NMR spectrum of compound 1
2. Supplementary Spectroscopic Data of Compound 2

*Kaempferol-3-O-β-D-glucopyranoside (astragalin) (2):* $^1$H-NMR (600 MHz, DMSO-$d_6$), $\delta_H$ (ppm): 3.09 (2H, $m$, H-3", H-4"), 3.18 (1H, $m$, H-2"), 3.22 (1H, $m$, H-5"), 3.32 (1H, $s$, H-6"a), 3.57 (1H, $d$, $J = 12.0$ Hz, H-6"b), 5.46 (1H, $d$, $J = 7.2$ Hz, H-1"), 6.20 (1H, $d$, $J = 2.0$ Hz, H-6), 6.42 (1H, $d$, $J = 2.0$ Hz, H-8), 6.88 (2H, $d$, $J = 9.0$ Hz, H-3", H-5"), 8.04 (2H, $d$, $J = 9.0$ Hz, H-2", H-6"), 12.60 (1H, $s$, 5-OH); $^{13}$C-NMR (150 MHz, DMSO-$d_6$), $\delta_C$ (ppm): 156.2 (C-2), 133.2 (C-3), 177.4 (C-4), 161.2 (C-5), 98.7 (C-6), 164.4 (C-7), 93.6 (C-8), 156.4 (C-9), 103.9 (C-10), 120.9 (C-1"), 130.8 (C-2"), 115.1 (C-3"), 159.9(C-4"), 115.1 (C-5"), 130.8 (C-6"), 100.9 (C-1"'), 74.2 (C-2"'), 77.4 (C-3"'), 69.9 (C-4"'), 76.4 (C-5"'), 60.8 (C-6"'); ESI-MS $m/z$ 449.1072 [M+H]$,^+$, calculated C$_{21}$H$_{20}$O$_{11}$, $m/z$ 448.1006.

![Fig S5. Expanded $^{13}$C-NMR spectrum of compound 1](image1)

![Fig S6. FTIR spectrum of compound 2](image2)
Fig S7. (+)ESI-MS spectrum of compound 2

Fig S8. $^{1}$H-NMR spectrum of compound 2

Fig S9. Expanded $^{1}$H-NMR spectrum of compound 2
Fig S10. $^{13}$C-NMR spectrum of compound 2

Fig S11. Expanded $^{13}$C-NMR spectrum of compound 2
Fig S12. HSQC spectrum of compound 2

Fig S13. Expanded HSQC spectrum of compound 2
**Fig S14.** Expanded HSQC spectrum of compound 2

**Fig S15.** HMBC spectrum of compound 2
3. Supplementary Spectroscopic Data of Compound 3

**Kaempferol-3-O-β-D-rutinoside (nicotiflorin) (3):** $^1$H-NMR (600 MHz, DMSO- $d_6$), $\delta$H (ppm): 0.98 (3H, d, $J = 6.0$ Hz, H-6”), 3.04 (1H, m, H-4”), 3.09 (1H, d, $J = 9.6$ Hz, H-4”), 3.16 (1H, m, H-2”), 3.22 (1H, m, H-3”), 3.27 (4H, m, H-5”, H-6”a, H-3”, H-5”), 3.35 (1H, m, H-2”), 3.69 (1H, d, $J = 10.2$ Hz, H-6”b), 4.38 (1H, d, $J = 1.2$ Hz, H-1”), 5.30 (1H, d, $J = 7.8$ Hz, H-1”), 6.20 (1H, d, $J = 2.0$ Hz, H-6), 6.41 (1H, d, $J = 2.0$ Hz, H-8), 6.88 (2H, dt, $J = 9.0$ Hz, 4.8 Hz, H-3’, H-5’), 8.00 (2H, dt, $J = 9.0$ Hz, 4.8 Hz, H-2’, H-6’), 12.55 (1H, s, 5-OH); $^{13}$C-NMR (150 MHz, DMSO- $d_6$), $\delta$C (ppm): 156.5 (C-2), 133.2 (C-3), 177.4 (C-4), 161.2 (C-5), 98.7 (C-6), 164.2 (C-7), 93.7 (C-8), 156.8 (C-9), 104.0 (C-10), 120.9 (C-1’), 130.8 (C-2’), 115.1 (C-3’), 159.9 (C-4’), 115.1 (C-5’), 130.8 (C-6’), 101.3 (C-1’’), 74.2 (C-2’’), 76.4 (C-3’’), 69.9 (C-4’’), 75.7 (C-5’’), 66.9 (C-6’’), 100.7 (C-1’’’), 70.3 (C-2’’’), 70.6 (C-3’’’), 71.8 (C-4’’’), 68.2 (C-5’’’), 17.7 (C-6’’’); ESI-MS m/z 595.1667 [M+H]$^+$, calculated C$_{27}$H$_{30}$O$_{15}$, m/z 594.1585.
Fig S18. FTIR spectrum of compound 3

Fig S19. (+)ESI-MS spectrum of compound 3

Fig S20. $^1$H-NMR spectrum of compound 3
Fig S21. Expanded $^1$H-NMR spectrum of compound 3

Fig S22. Expanded $^1$H-NMR spectrum of compound 3
Fig S23. $^{13}$C-NMR spectrum of compound 3

Fig S24. Expanded $^{13}$C-NMR spectrum of compound 3
**Figure S25.** Expanded $^{13}$C-NMR spectrum of compound 3

**Figure S26.** HSQC spectrum of compound 3

**Figure S27.** Expanded HSQC spectrum of compound 3
**Fig S28.** Expanded HSQC spectrum of compound 3

**Fig S29.** HMBC spectrum of compound 3
Fig S30. Expanded HMBC spectrum of compound 3

Fig S31. Expanded HMBC spectrum of compound 3
4. Supplementary Spectroscopic Data of Compound 4

**Quercetin-3-O-β-D-rutinoside (rutin) (4):**

$^1$H-NMR (600 MHz, DMSO-$d_6$), $\delta_H$ (ppm): 0.99 (3H, $d$, $J = 6.0$ Hz, H-6$''$), 3.71, (1H, $d$, $J = 10.8$ Hz, H-6$'$b), 4.38 (1H, $s$, H-1$'''$), 5.34 (1H, $d$, $J = 7.2$ Hz, H-1$''$), 6.19 (1H, $d$, $J = 2.4$ Hz, H-6), 6.38 (1H, $d$, $J = 1.8$ Hz, H-8), 6.84 (2H, $d$, $J = 8.4$ Hz, H-5), 7.53 (1H, $d$, $J = 2.4$ Hz, H-2$'$), 7.55 (1H, dd, $J = 8.4$, 2.4 Hz, H-6$'$), 12.60 (1H, s, 5-OH); $^1$C-NMR (150 MHz, DMSO-$d_6$), $\delta_C$ (ppm): 156.4 (C-2), 133.3 (C-3), 177.3 (C-4), 161.2 (C-5), 98.6 (C-6), 164.1 (C-7), 93.5 (C-8), 156.5 (C-9), 103.9 (C-10), 121.1 (C-1$'$), 115.2 (C-2$'$), 144.7 (C-3$'$), 148.4 (C-4$'$), 116.2 (C-5$'$), 121.5 (C-6$'$), 101.2 (C-1$''$), 74.0 (C-2$''$), 76.4 (C-3$''$), 70.0 (C-4$''$), 75.9 (C-5$''$), 66.9 (C-6$''$), 100.7 (C-1$'''$), 70.5 (C-2$'''$), 70.3 (C-3$'''$), 71.8 (C-4$'''$), 68.2 (C-5$'''$), 17.7 (C-6$'''$).
Fig S35. $^1$H-NMR spectrum of compound 4

Fig S36. Expanded $^1$H-NMR spectrum of compound 4
Fig S37. Expanded $^1$H-NMR spectrum of compound 4

Fig S38. $^{13}$C-NMR spectrum of compound 4
Fig S39. Expanded $^{13}C$-NMR spectrum of compound 4

Fig S40. Expanded $^{13}C$-NMR spectrum of compound 4
Fig S41. HSQC spectrum of compound 4

Fig S42. Expanded HSQC spectrum of compound 4
Fig S43. Expanded HSQC spectrum of compound 4

Fig S44. HMBC spectrum of compound 4
Fig S45. Expanded HMBC spectrum of compound 4

Fig S46. Expanded HMBC spectrum of compound 4
5. Supplementary Spectroscopic Data of Compound 5

3,4-Dihydroxycinnamic acid (caffeic acid) (5): $^1$H-NMR (600 MHz, MeOD), $\delta_H$ (ppm): 6.24 (1H, d, $J = 15.6$ Hz, H-8), 6.80 (1H, d, $J = 8.4$ Hz, H-5), 6.95 (1H, dd, $J = 8.4$ Hz, 2.4 Hz, H-6), 7.06 (1H, d, $J = 2.4$ Hz, H-2), 7.55 (1H, d, $J = 15.6$ Hz, H-7); $^{13}$C-NMR (150 MHz, MeOD), $\delta_C$ (ppm): 127.8 (C-1), 115.1 (C-2), 147.0 (C-3), 149.4 (C-4), 116.5 (C-5), 122.8 (C-6), 146.8 (C-7), 115.6 (C-8), 171.0 (C-9); ESI-MS m/z 181.0494 [M+H]$^+$, 163.0391 [M+H–H$_2$O]$^+$, calculated C$_9$H$_8$O$_4$, $m/z$ 180.0423.
Fig S49. (+)ESI-MS spectrum of compound 5

Fig S50. $^1$H-NMR spectrum of compound 5

Fig S51. Expanded $^1$H-NMR spectrum of compound 5
Fig S52. $^{13}$C-NMR spectrum of compound 5

Fig S52. Expanded $^{13}$C-NMR spectrum of compound 5
Fig S53. HSQC spectrum of compound 5

Fig S54. Expanded HSQC spectrum of compound 5
6. Supplementary Spectroscopic Data of Compound 6

\((6S,7aR)\)-6-hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydro-1-benzofuran-2(4H)-one((-)loliolide)\): $^1$H-NMR (600 MHz, CDCl$_3$), $\delta$H (ppm): 1.27 (3H, s, CH$_3$ at C-9), 1.47 (3H, s, CH$_3$ at C-8), 1.53 (1H, dd, $J = 14.4$, 3.6 Hz, H-5α), 1.77 (1H, d, $J = 3.6$ Hz, H-7α), 1.79 (3H, s, CH$_3$ at C-10), 1.99 (1H, dt, $J = 14.4$, 2.4 Hz, H-5β), 2.47 (1H, dt, $J = 14.4$, 2.4 Hz, H-7β), 4.33 (1H, s, H-6), 5.70 (1H, s, H-3); $^{13}$C-NMR (150 MHz, CDCl$_3$), $\delta$C (ppm): 172.0 (C-2), 112.8 (C-3), 183.0 (C-3a), 35.9 (C-4), 47.3 (C-5), 66.7 (C-6), 45.6 (C-7), 86.8 (C-7a), 26.5 (C-8), 30.7 (C-9), 27.0 (C-10); ESI-MS $m/z$ 197.1181 [M+H]$^+$, 179.1076 [M+H$_2$O]$^+$, calculated C$_{11}$H$_{16}$O$_3$, $m/z$ 196.1099.

![Fig S55. HMBC spectrum of compound 5](image1)

![Fig S56. Expanded HMBC spectrum of compound 5](image2)

![Fig S57. FTIR spectrum of compound 6](image3)
Fig S58. (+)ESI-MS spectrum of compound 6

Fig S59. $^1$H-NMR spectrum of compound 6

Fig S60. Expanded $^1$H-NMR spectrum of compound 6
Fig S61. Expanded $^1$H-NMR spectrum of compound 6

Fig S62. $^{13}$C-NMR spectrum of compound 6
Fig S63. Expanded $^{13}$C-NMR spectrum of compound 6

Fig S64. HSQC spectrum of compound 6

Fig S65. Expanded HSQC spectrum of compound 6
Fig S66. HMBC spectrum of compound 6

Fig S67. Expanded HMBC spectrum of compound 6
Fig S69. Expanded HMBC spectrum of compound 6

Fig S70. Complete assignment NOESY spectrum of compound 6

Fig S71. Expanded NOESY spectrum of compound 6

Fig S72. Expanded NOESY spectrum of compound 6
7. Supplementary Spectroscopic Data of Compound 7

\(\beta\)-Sitosterol-3-O-\(\beta\)-D-glucopyranoside (daucosterol) (7): \(^1\)H-NMR (600 MHz, DMSO-d\(_6\)), \(\delta_H\) (ppm): 0.65 (3H, s, CH\(_3\) at C-18), 1.00 (3H, s, CH\(_3\) at C-19); 2.90-3.64 (6H, m, H-2’ – H-6’), 4.22 (1H, d, \(J = 7.8\) Hz, H-1’), 5.32 (1H, t, H-6); \(^13\)C-NMR (150 MHz, DMSO-d\(_6\)), \(\delta_C\) (ppm): 36.8 (C-1), 29.2 (C-2), 76.8 (C-3), 39.3 (C-4), 140.4 (C-5), 121.2 (C-6), 31.4 (C-7), 31.3 (C-8), 49.6 (C-9), 36.2 (C-10), 20.6 (C-11), 38.3 (C-12), 41.8 (C-13), 56.1 (C-14), 23.8 (C-15), 27.8 (C-16), 55.4 (C-17), 11.6 (C-18), 19.1 (C-19), 35.4 (C-20), 18.9 (C-21), 33.3 (C-22), 25.4 (C-23), 45.1 (C-24), 28.7 (C-25), 18.6 (C-26), 19.7 (C-27), 22.6 (C-28), 11.8 (C-29), 100.8 (C-1’), 73.4 (C-2’), 76.9 (C-3’), 70.1 (C-4’), 76.7 (C-5’), 61.1 (C-6’).

Fig S73. FTIR spectrum of compound 7

Fig S74. \(^1\)H-NMR spectrum of compound 7
Fig S75. Expanded $^1$H-NMR spectrum of compound 7

Fig S76. Expanded $^1$H-NMR spectrum of compound 7
Fig S77. $^{13}$C-NMR spectrum of compound 7

Fig S78. Expanded $^{13}$C-NMR spectrum of compound 7
Fig S79. Expanded $^{13}$C-NMR spectrum of compound 7

Fig S80. Expanded $^{13}$C-NMR spectrum of compound 7