

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): $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$), 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); $^{13}\text{C-NMR}$ (150 MHz, $\text{DMSO-}d_6$), 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').

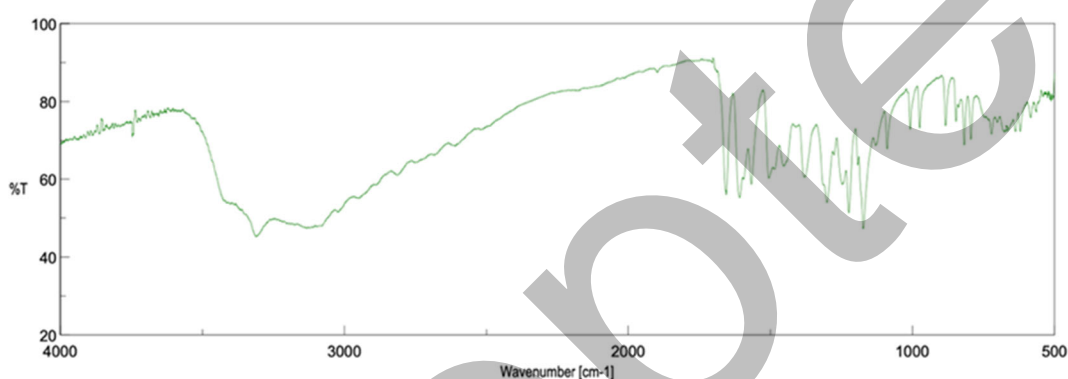


Fig S1. FTIR spectrum of compound 1

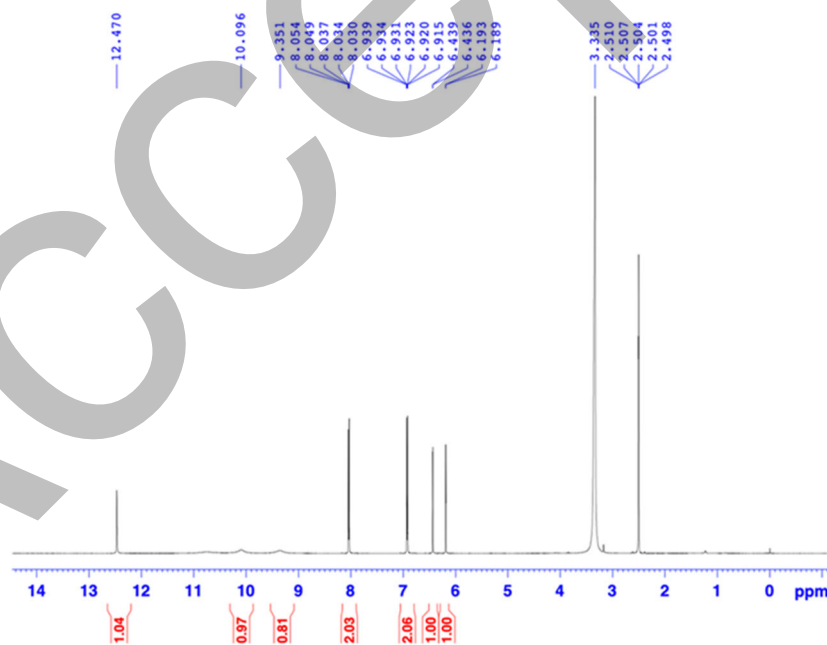
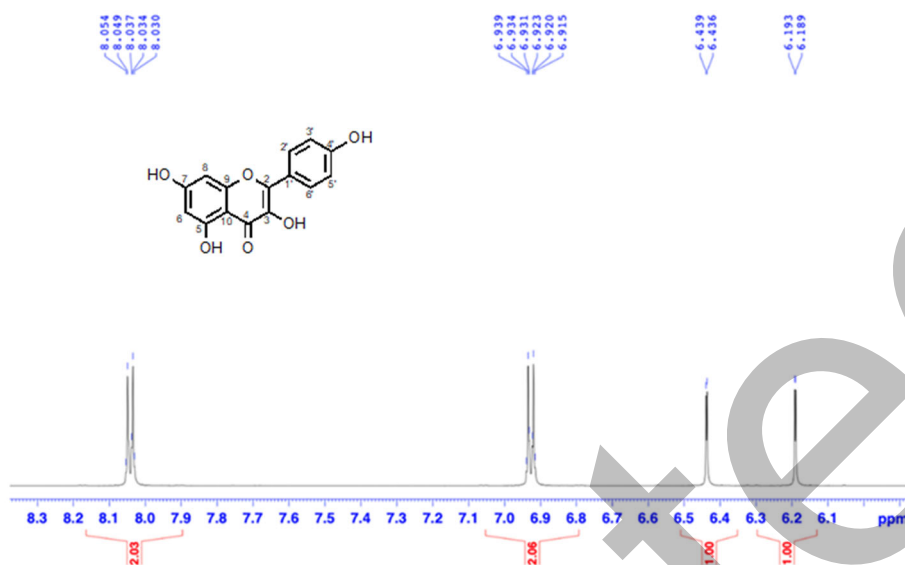
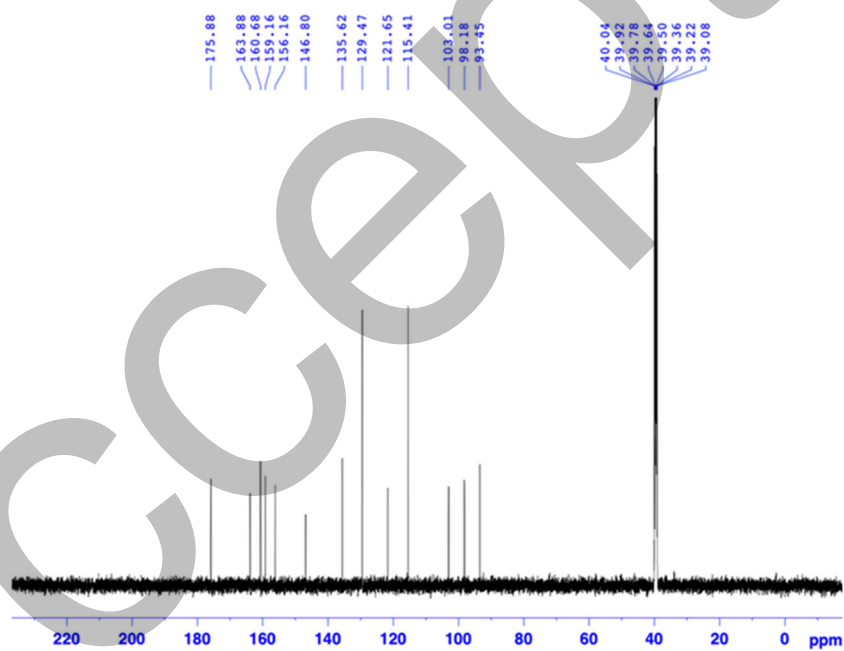
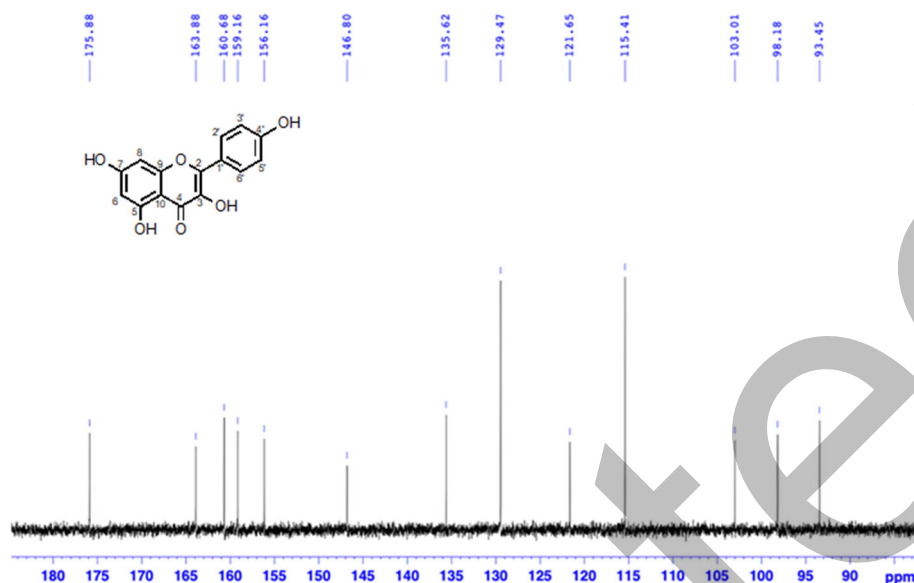


Fig S2. $^1\text{H-NMR}$ spectrum of compound 1

Fig S3. Expanded ¹H-NMR spectrum of compound 1Fig S4. ¹³C-NMR spectrum of compound 1

Fig S5. Expanded ^{13}C -NMR spectrum of compound 1

2. Supplementary Spectroscopic Data of Compound 2

Kaempferol-3-O- β -D-glucopyranoside (astragalin) (2): ^1H -NMR (600 MHz, $\text{DMSO-}d_6$), δ_{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, $\text{DMSO-}d_6$), δ_{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 $[\text{M}+\text{H}]^+$, calculated $\text{C}_{21}\text{H}_{20}\text{O}_{11}$, m/z 448.1006.

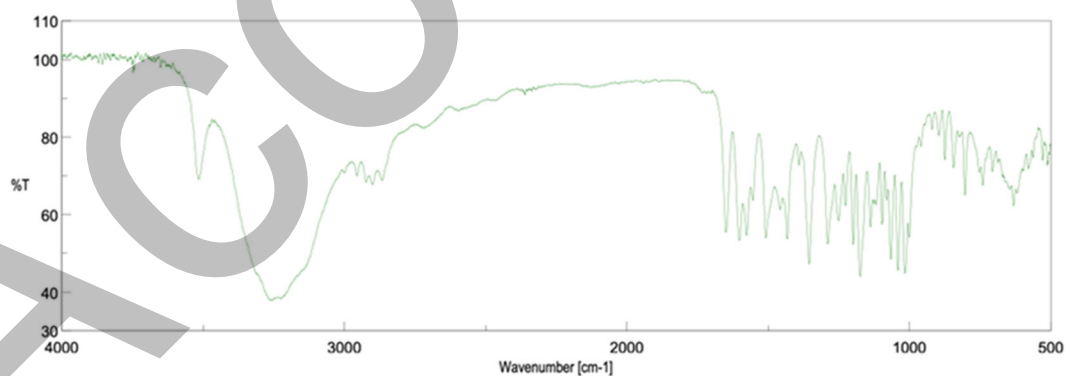


Fig S6. FTIR spectrum of compound 2

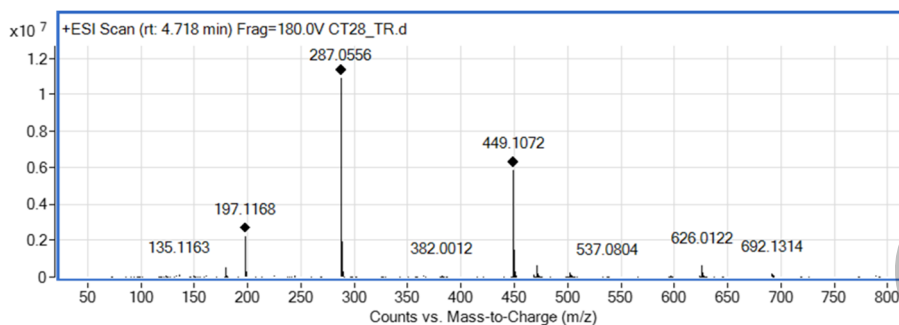
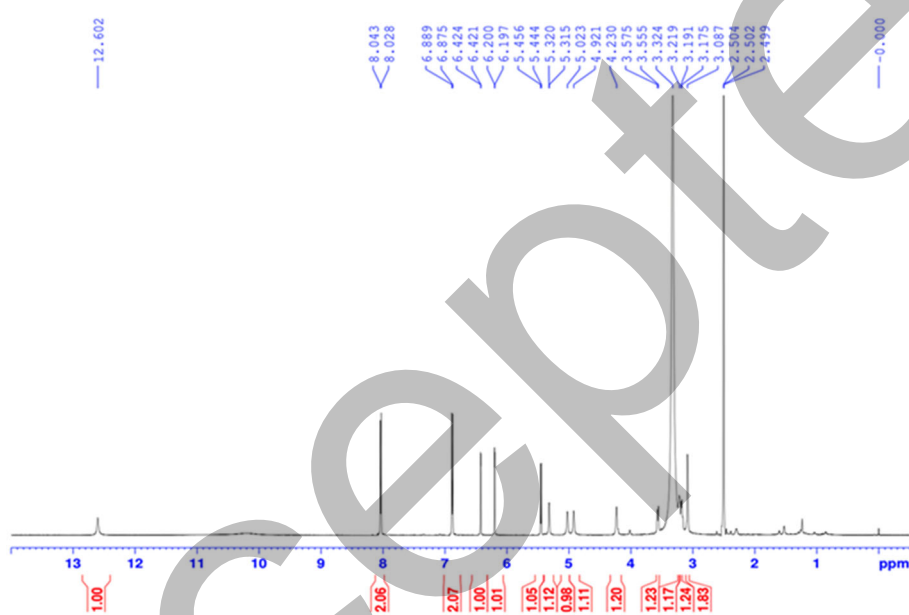
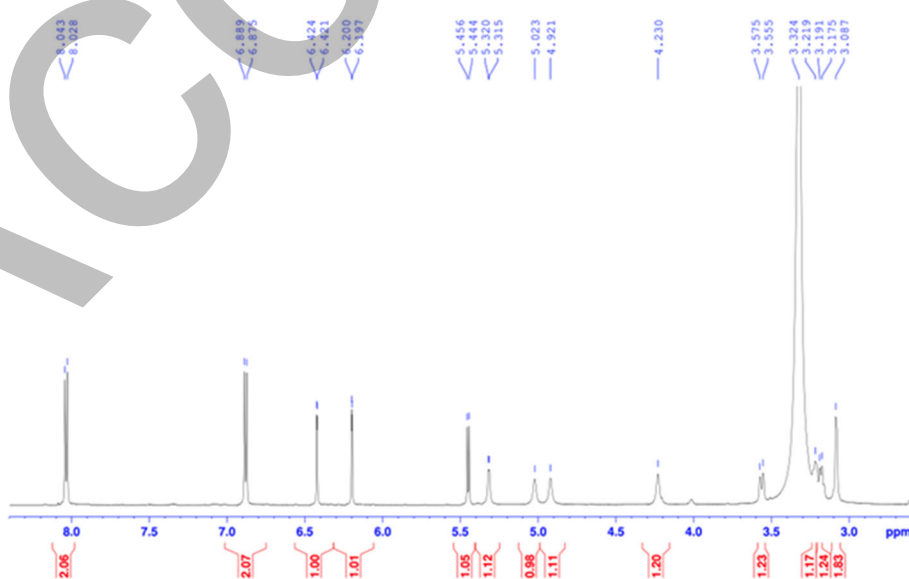
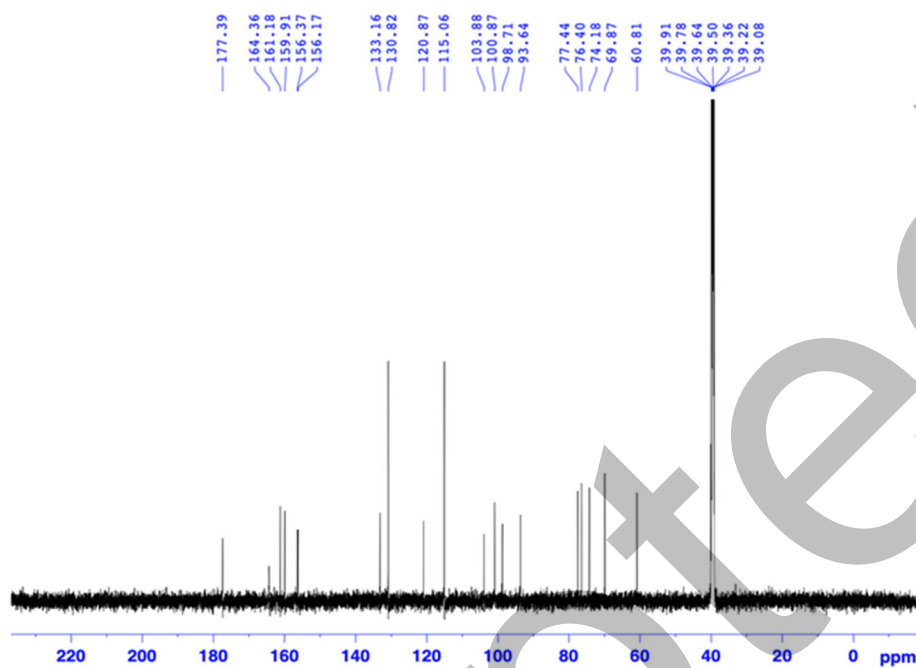
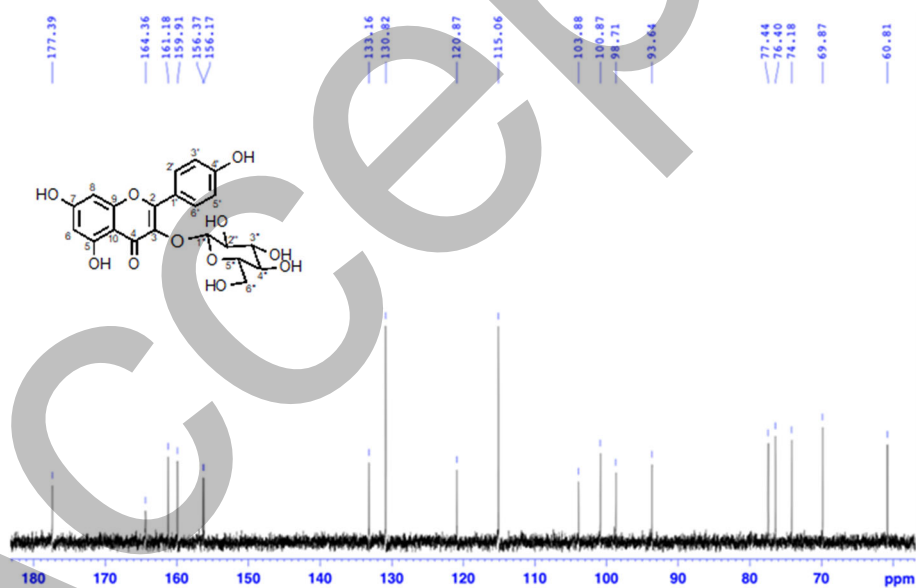


Fig S7. (+)ESI-MS spectrum of compound 2

Fig S8. ¹H-NMR spectrum of compound 2Fig S9. Expanded ¹H-NMR spectrum of compound 2

Fig S10. ^{13}C -NMR spectrum of compound 2Fig S11. Expanded ^{13}C -NMR spectrum of compound 2

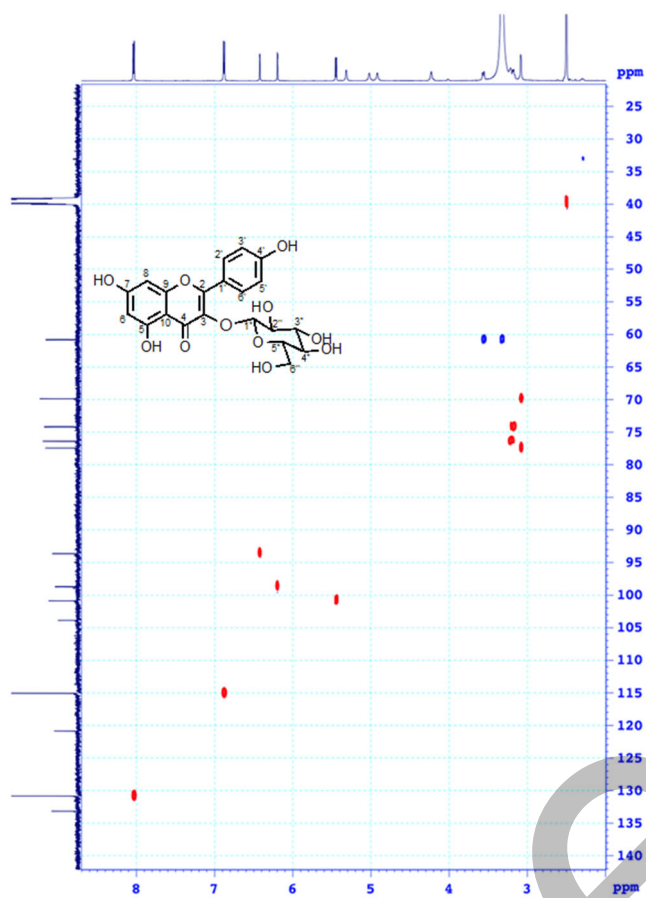


Fig S12. HSQC spectrum of compound 2

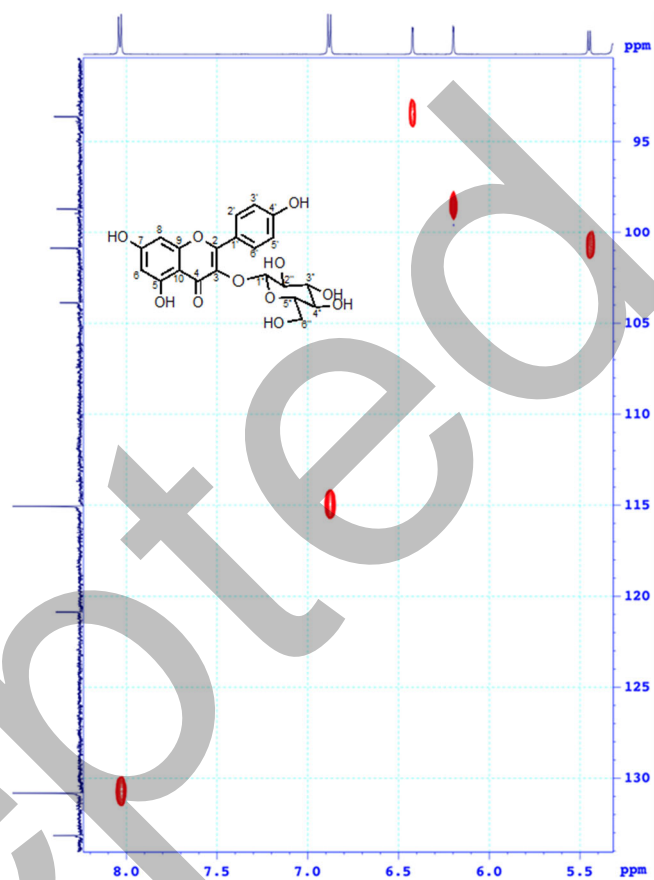
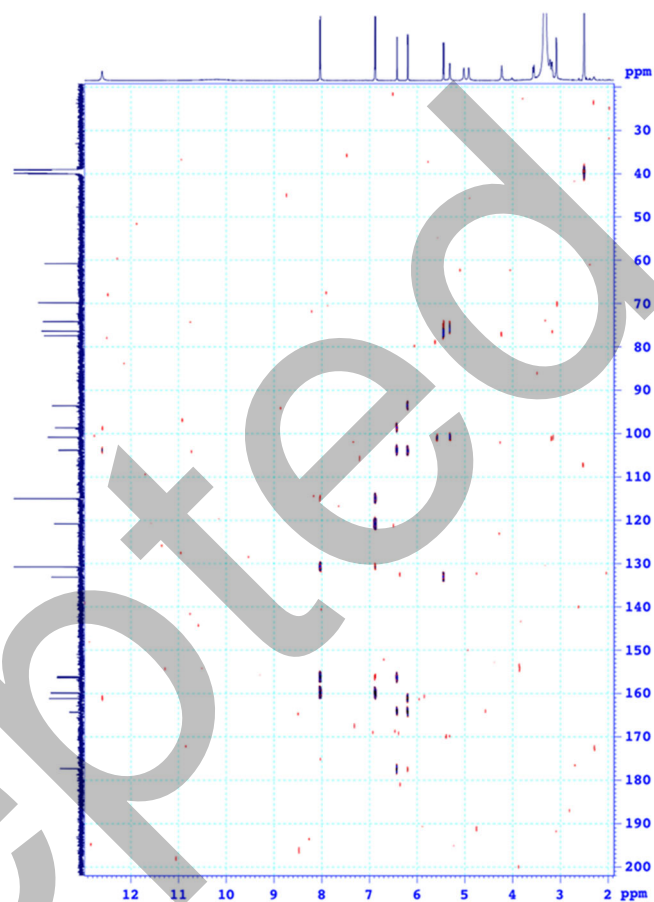
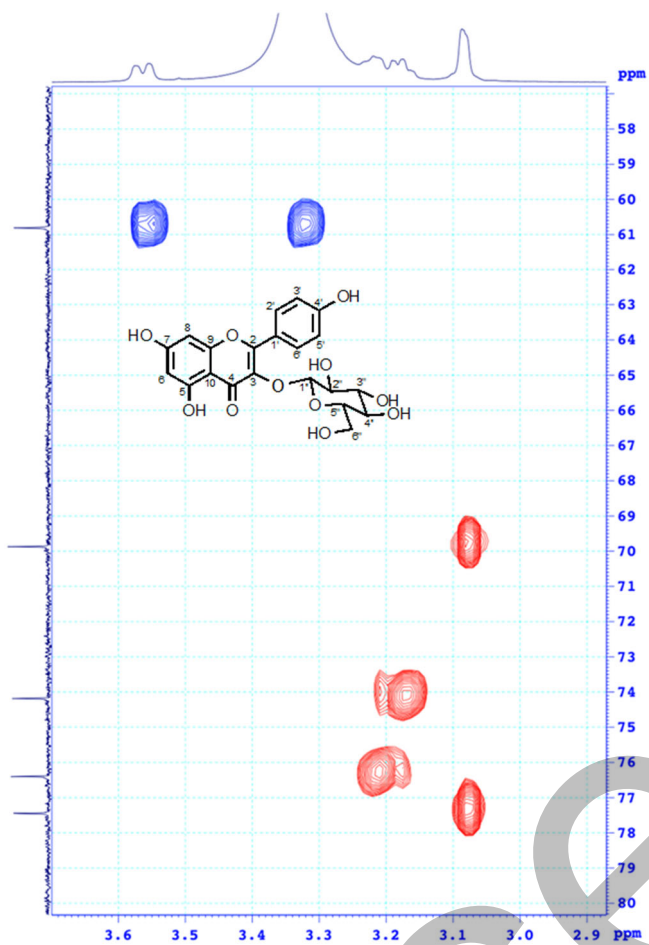


Fig S13. Expanded HSQC spectrum of compound 2



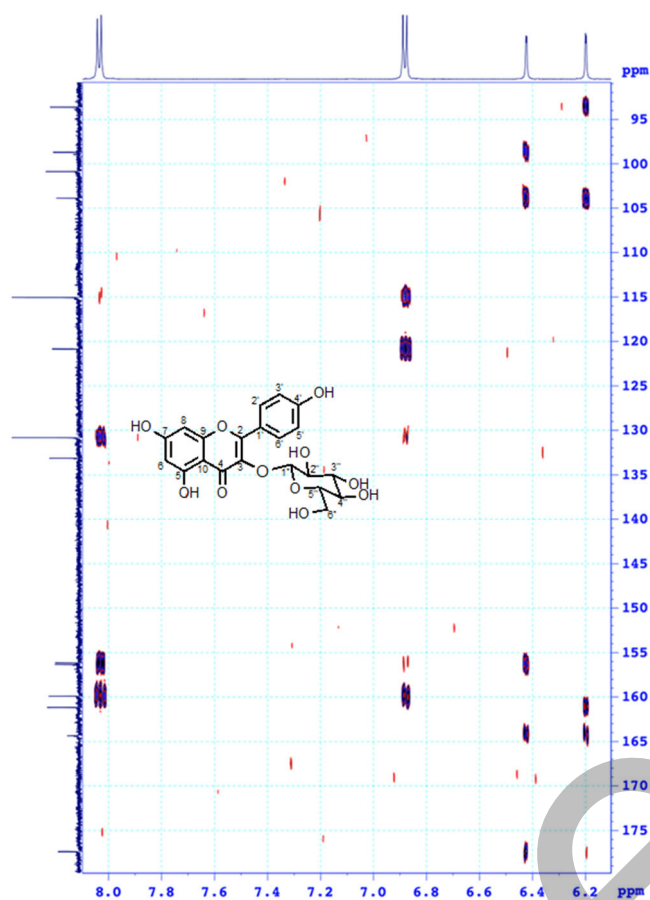


Fig S16. Expanded HMBC spectrum of compound 2

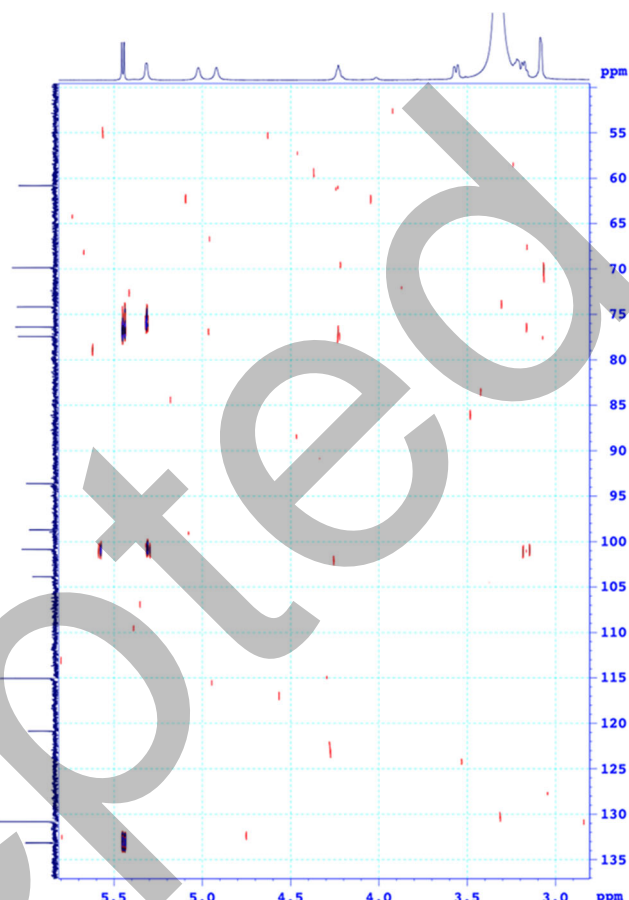


Fig S17. Expanded HMBC spectrum of compound 2

3. Supplementary Spectroscopic Data of Compound 3

Kaempferol-3-O- β -D-rutinoside (nicotiflorin) (3): $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$), δ_{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); $^{13}\text{C-NMR}$ (150 MHz, $\text{DMSO-}d_6$), δ_{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 $[\text{M}+\text{H}]^+$, calculated $\text{C}_{27}\text{H}_{30}\text{O}_{15}$, m/z 594.1585.

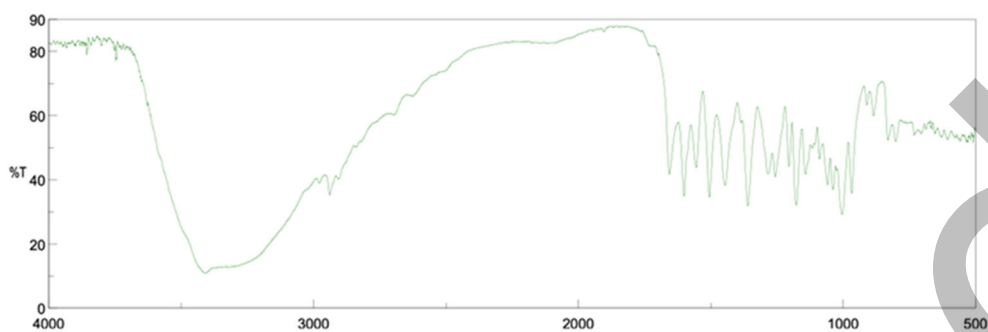


Fig S18. FTIR spectrum of compound 3

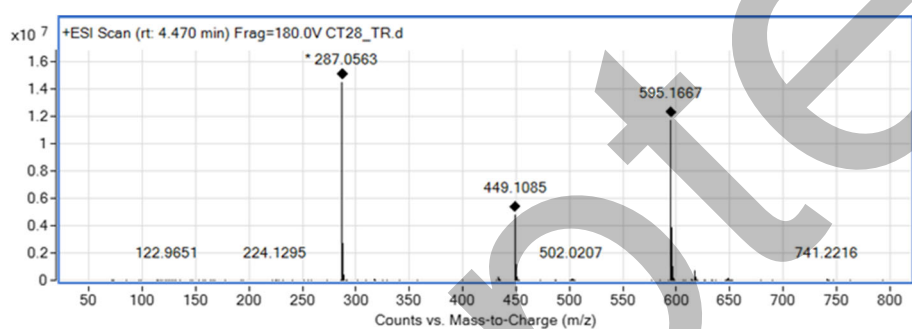
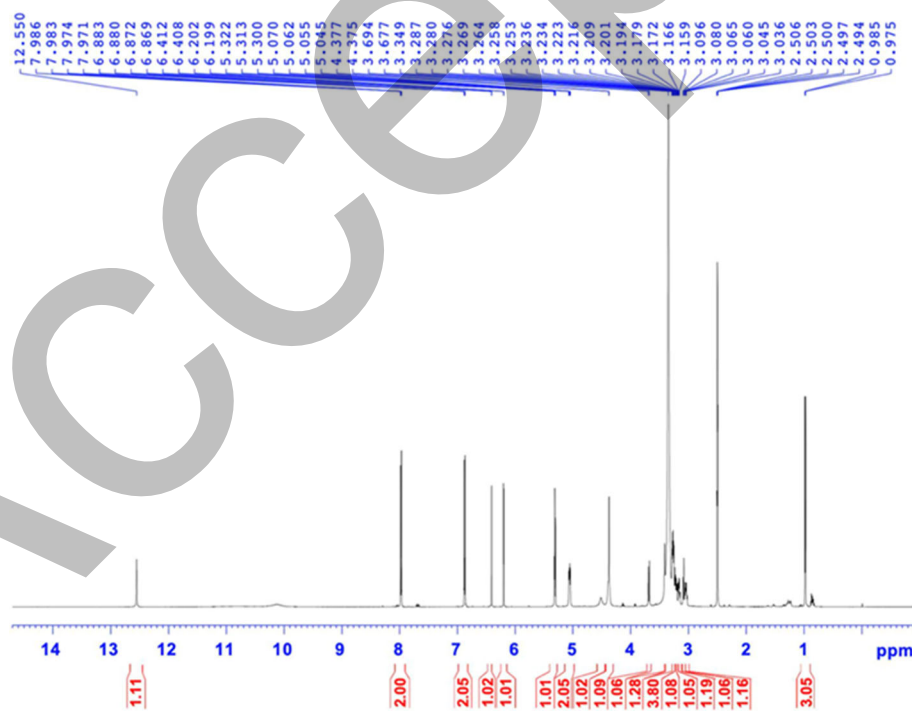
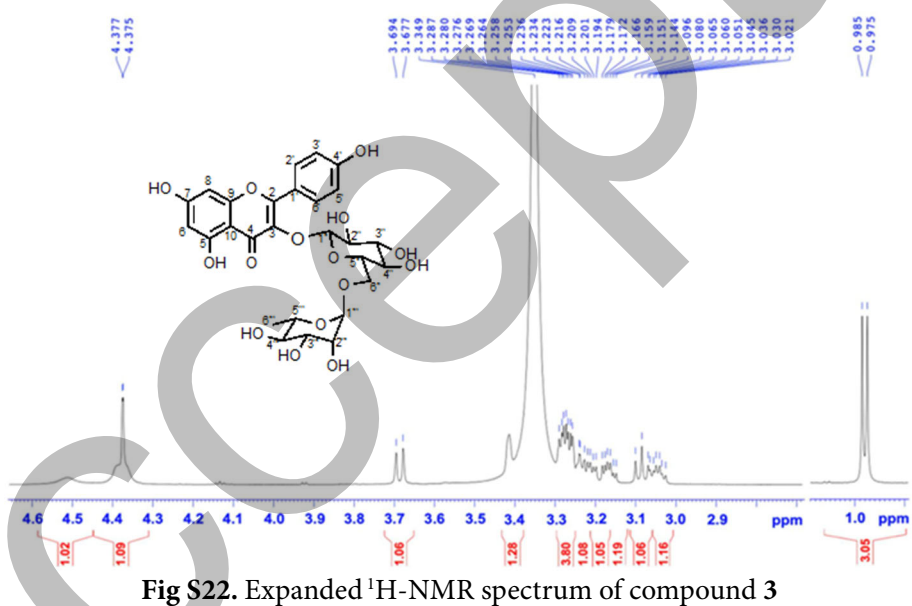
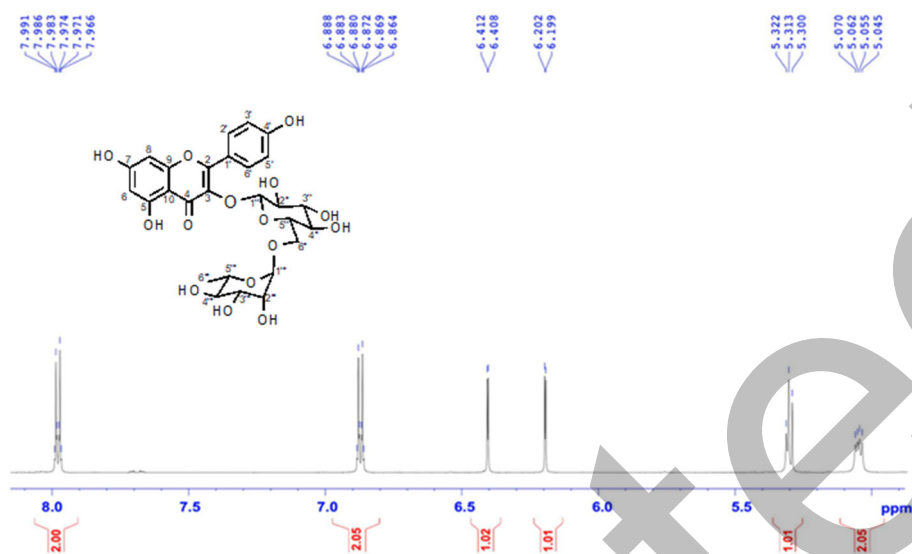
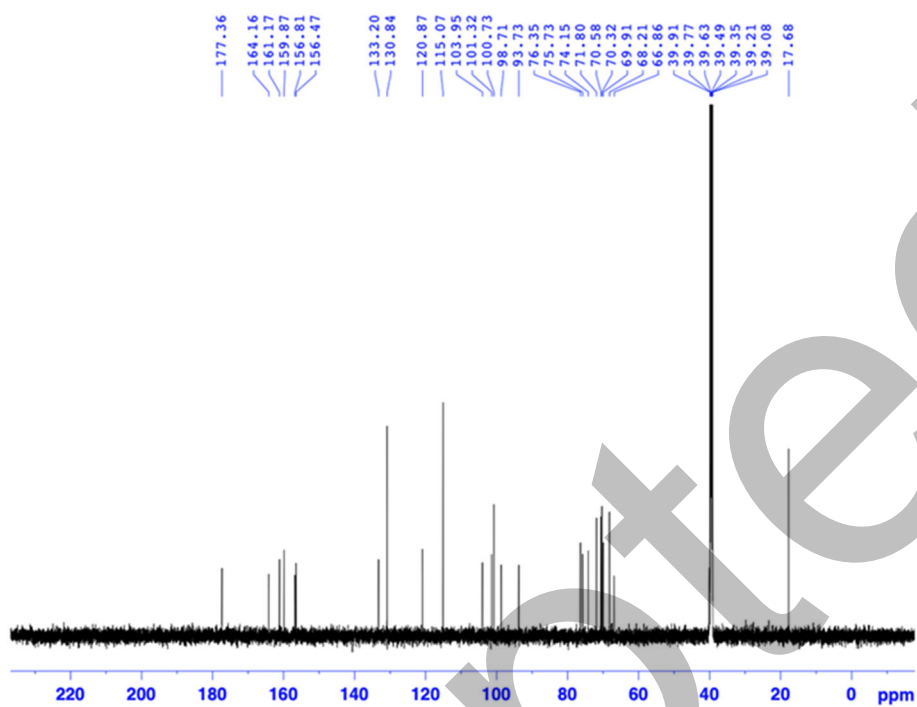
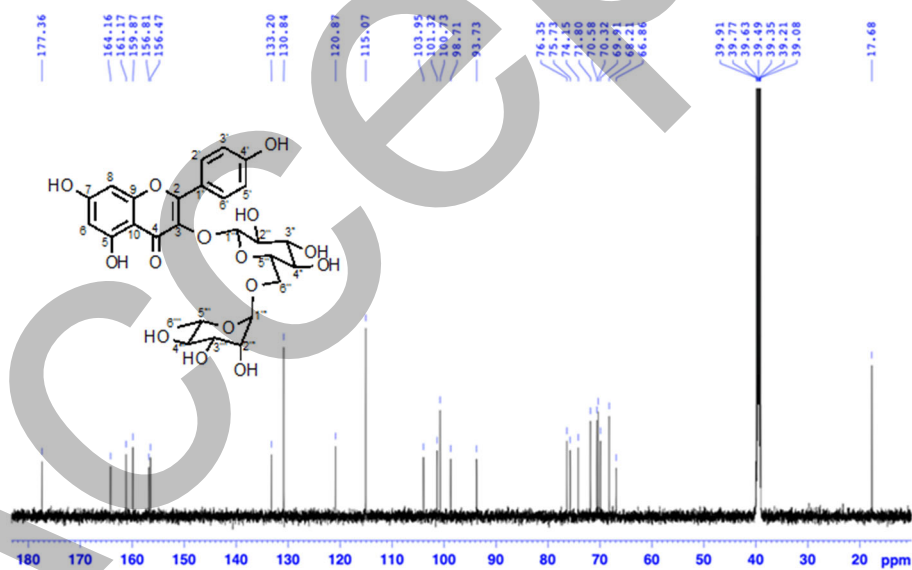


Fig S19. (+)ESI-MS spectrum of compound 3

Fig S20. ¹H-NMR spectrum of compound 3



Fig S23. ^{13}C -NMR spectrum of compound 3Fig S24. Expanded ^{13}C -NMR spectrum of compound 3

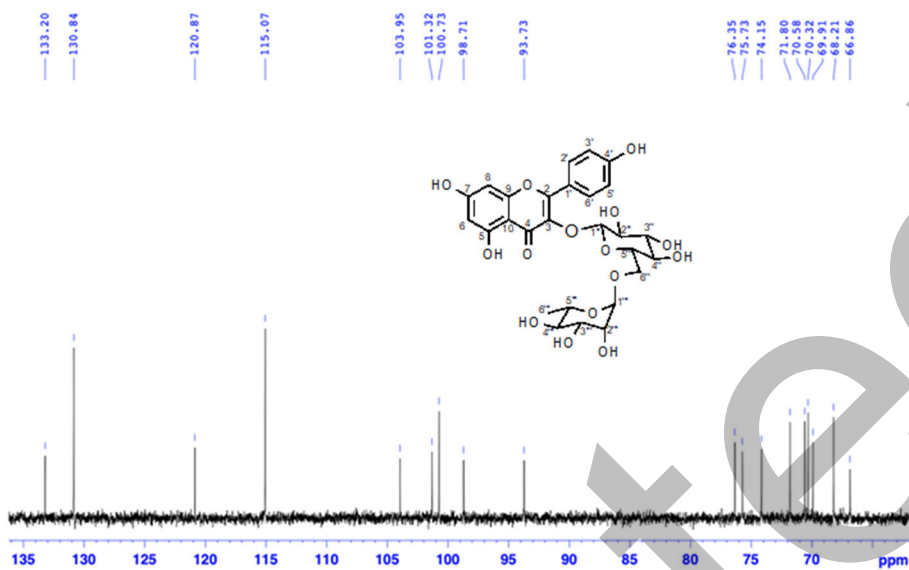
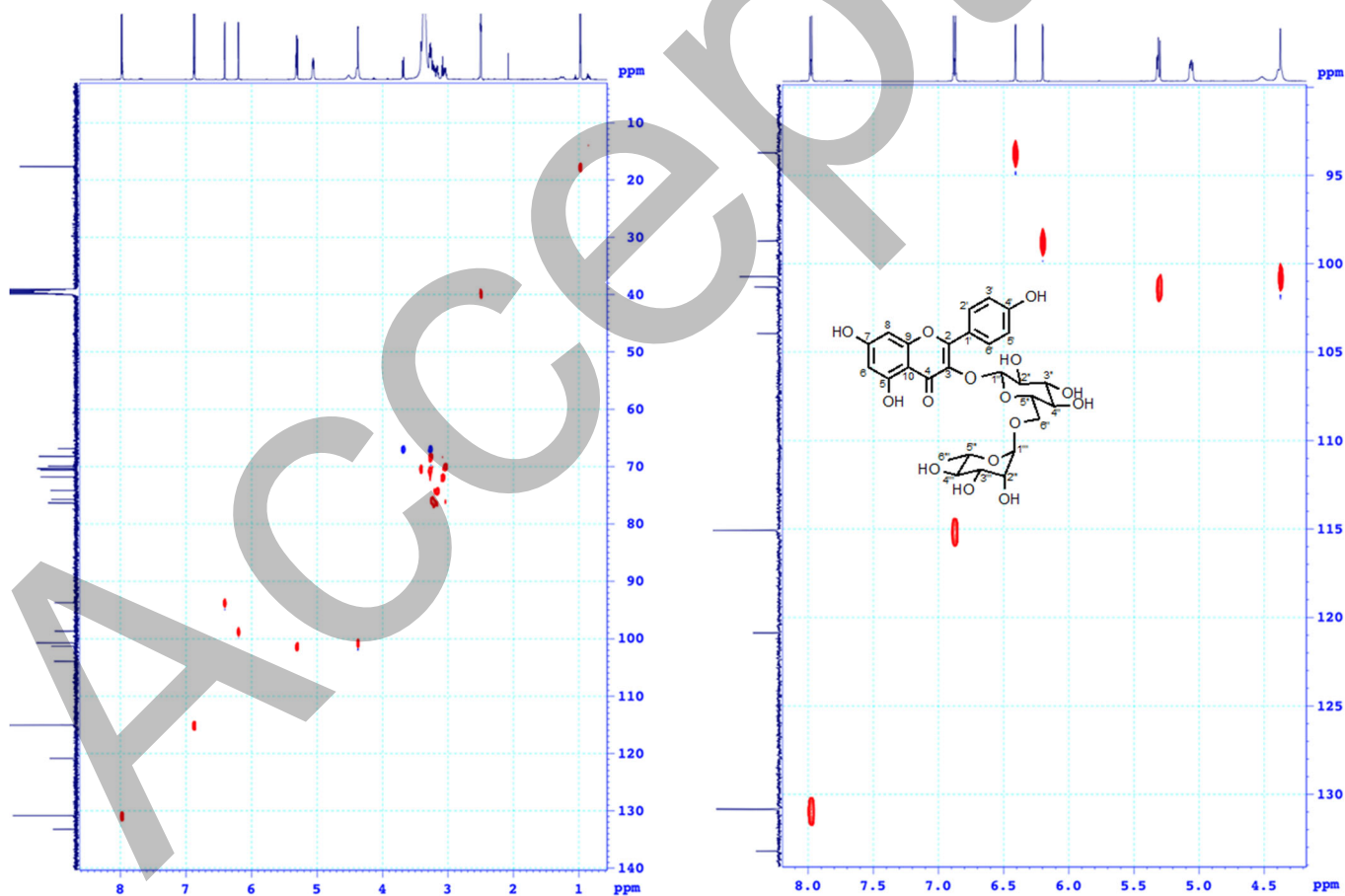
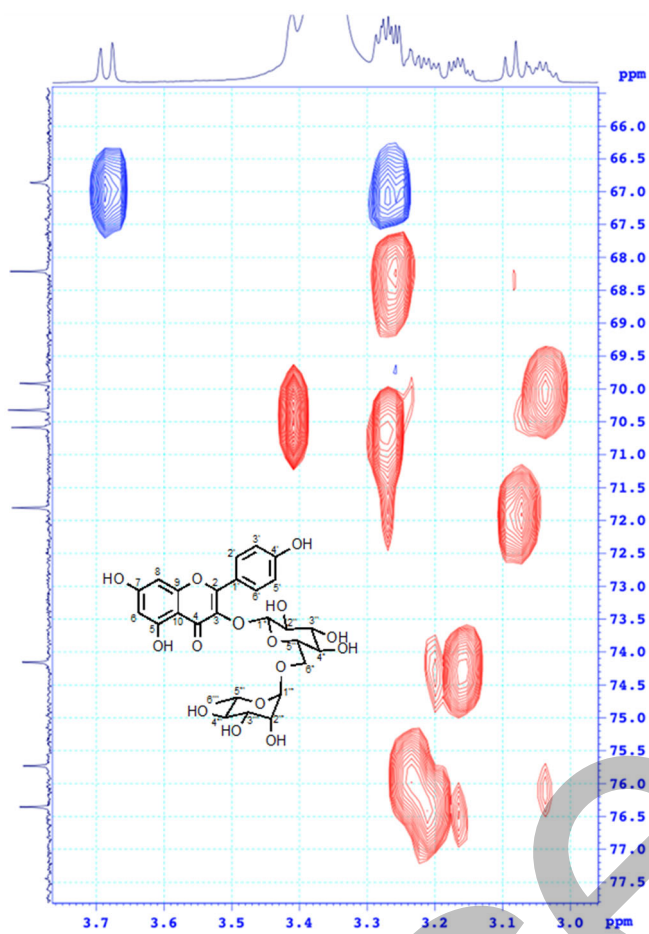
Figure S25. Expanded ^{13}C -NMR spectrum of compound 3

Figure S26. HSQC spectrum of compound 3

Figure S27. Expanded HSQC spectrum of compound 3



FigS28. Expanded HSQC spectrum of compound 3

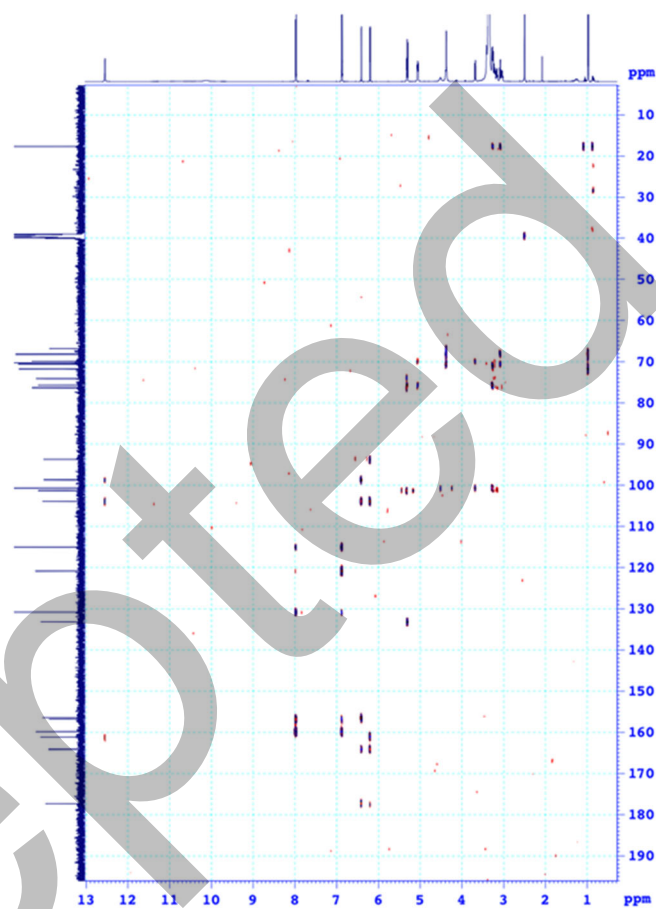


Fig S29. HMBC spectrum of compound 3

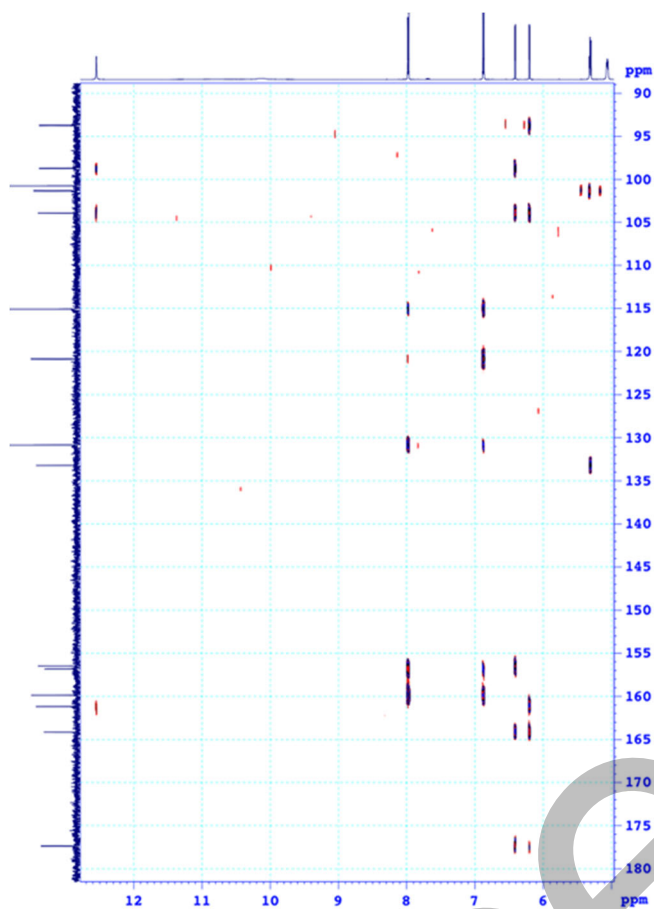


Fig S30. Expanded HMBC spectrum of compound 3

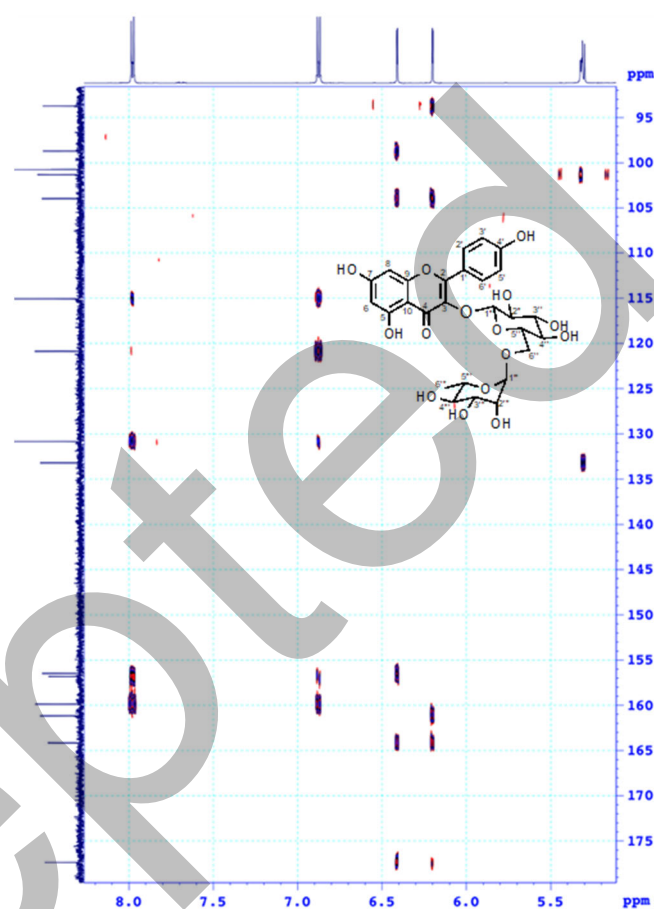


Fig S31. Expanded HMBC spectrum of compound 3

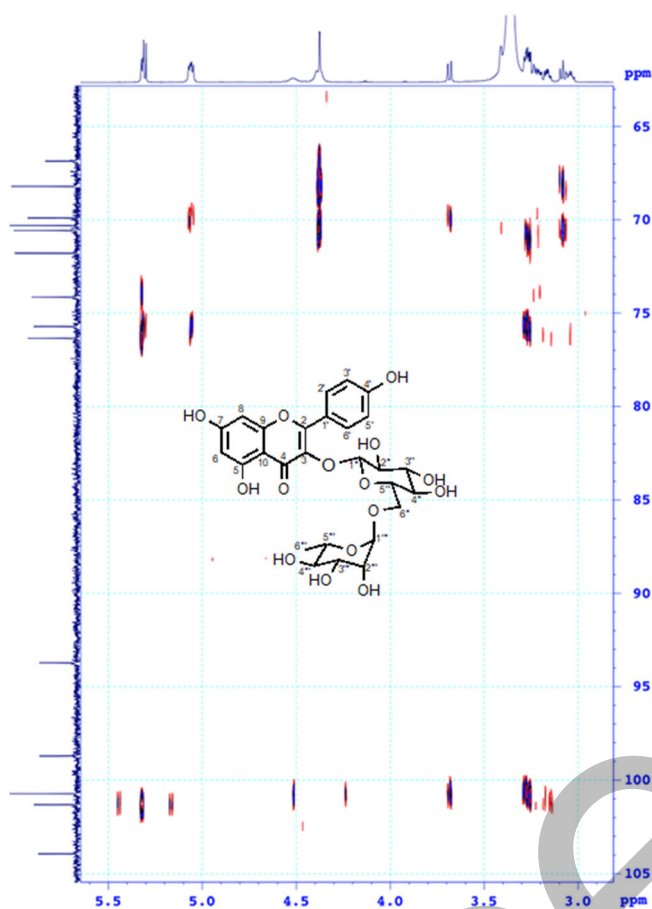


Fig S32. Expanded HMBC spectrum of compound 3

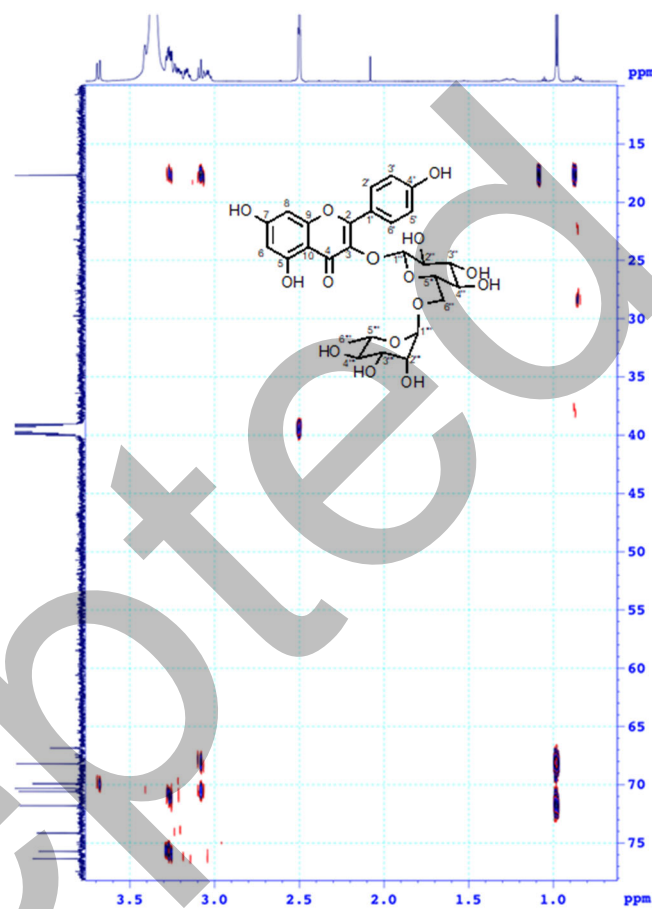


Fig S33. Expanded HMBC spectrum of compound 3

4. Supplementary Spectroscopic Data of Compound 4

Quercetin-3-O- β -D-rutinoside (rutin) (4): $^1\text{H-NMR}$ (600 MHz, $\text{DMSO-}d_6$), δ_{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); $^{13}\text{C-NMR}$ (150 MHz, $\text{DMSO-}d_6$), δ_{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''').

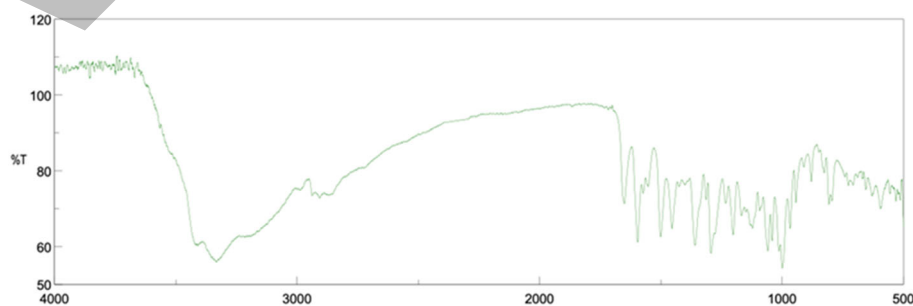
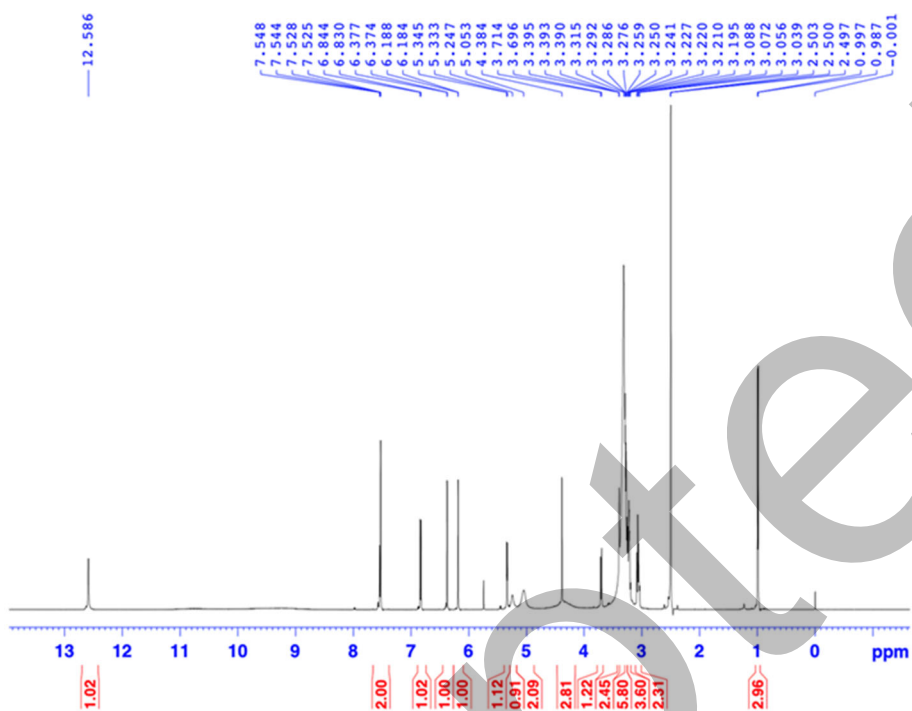
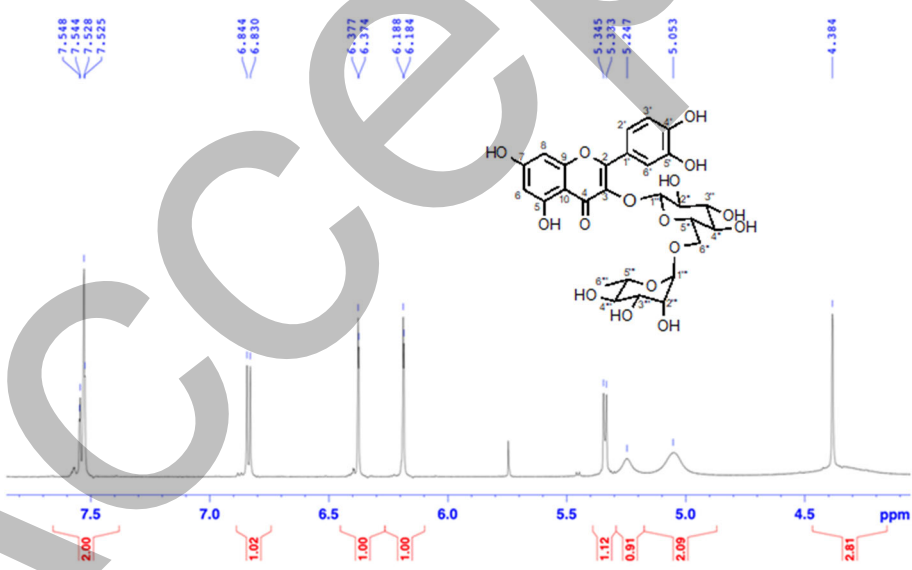
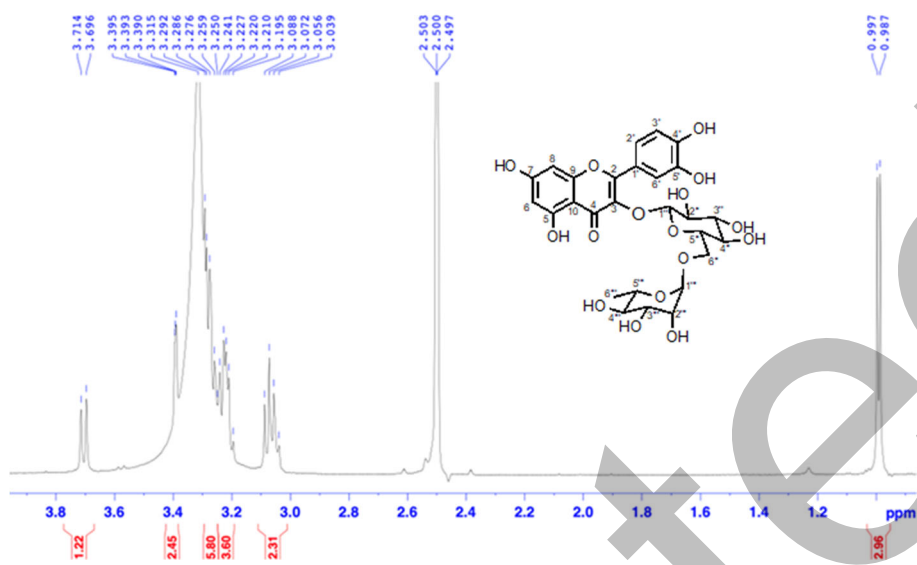
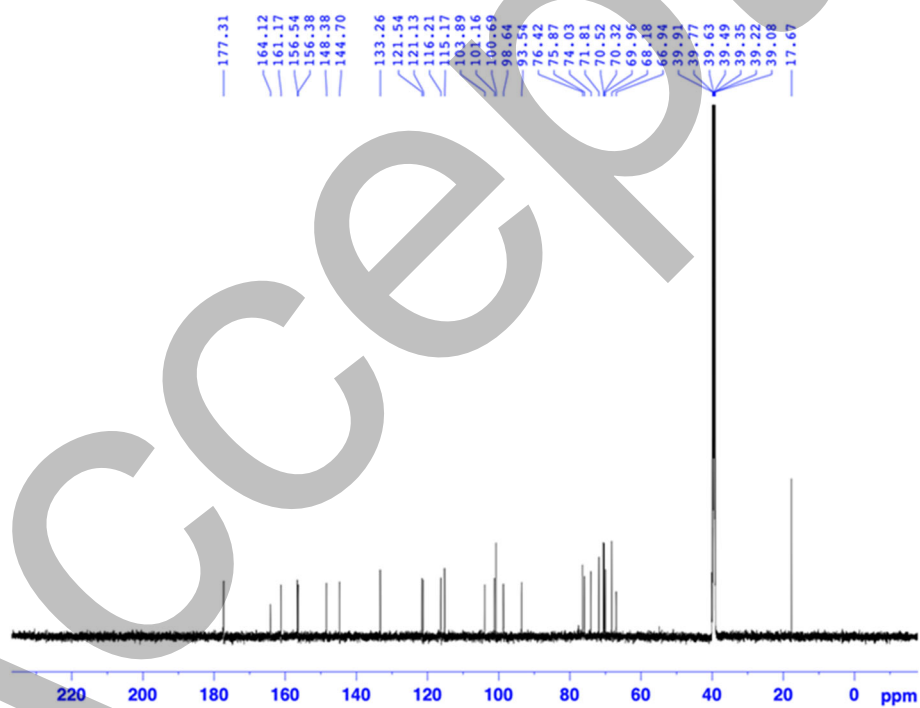
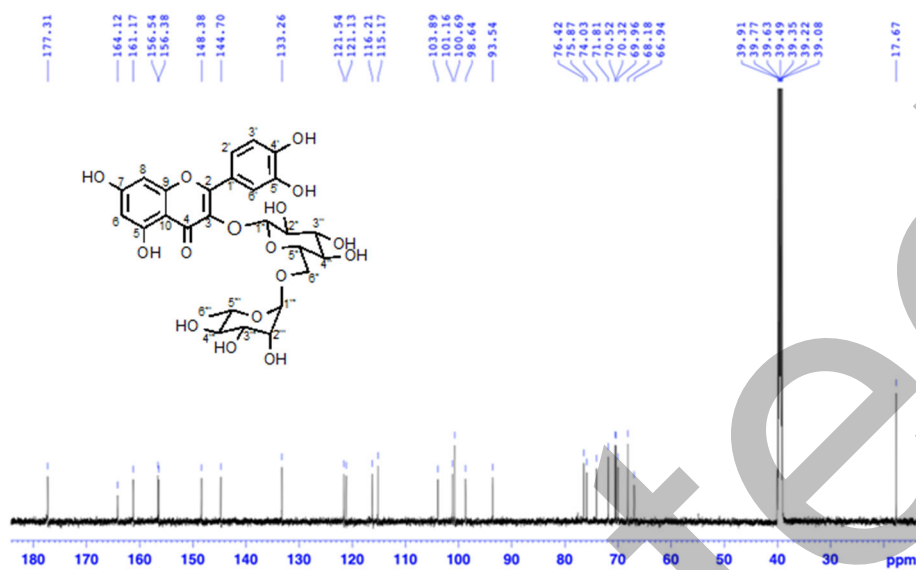
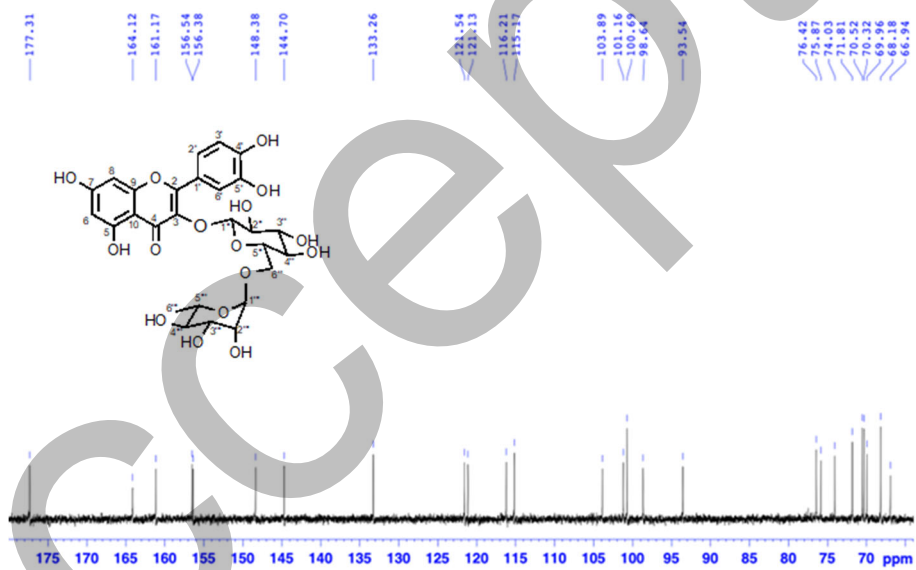


Fig S34. FTIR spectrum of compound 4

Fig S35. ¹H-NMR spectrum of compound 4Fig S36. Expanded ¹H-NMR spectrum of compound 4

Fig S37. Expanded ^1H -NMR spectrum of compound 4Fig S38. ^{13}C -NMR spectrum of compound 4

Fig S39. Expanded ^{13}C -NMR spectrum of compound 4Fig S40. Expanded ^{13}C -NMR spectrum of compound 4

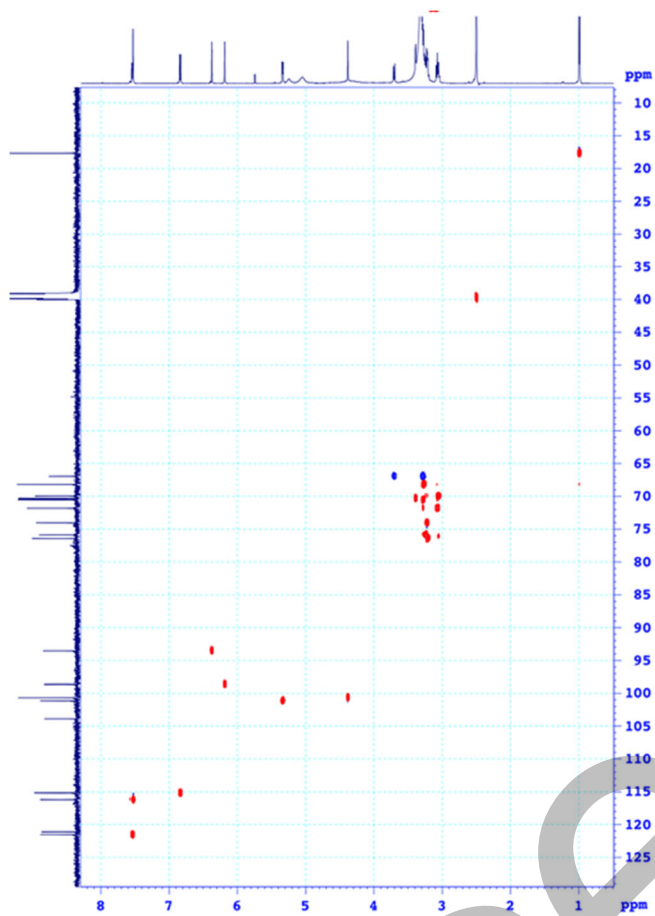


Fig S41. HSQC spectrum of compound 4

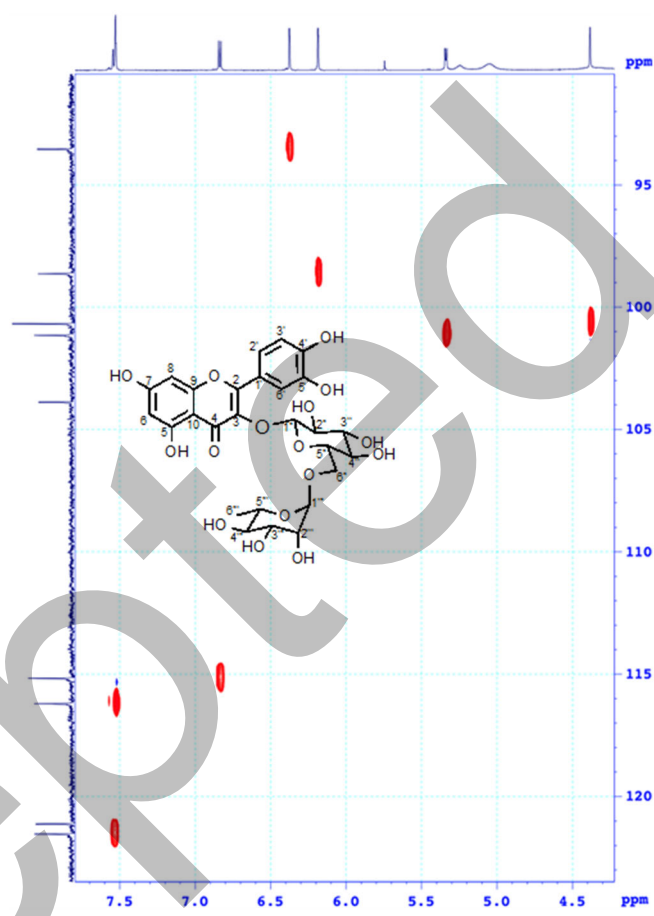


Fig S42. Expanded HSQC spectrum of compound 4

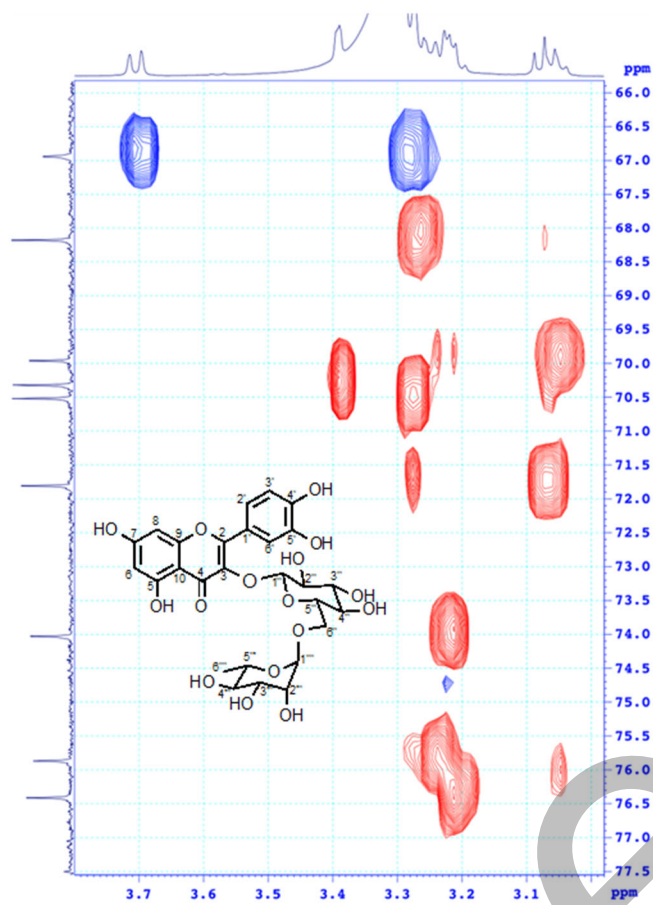


Fig S43. Expanded HSQC spectrum of compound 4

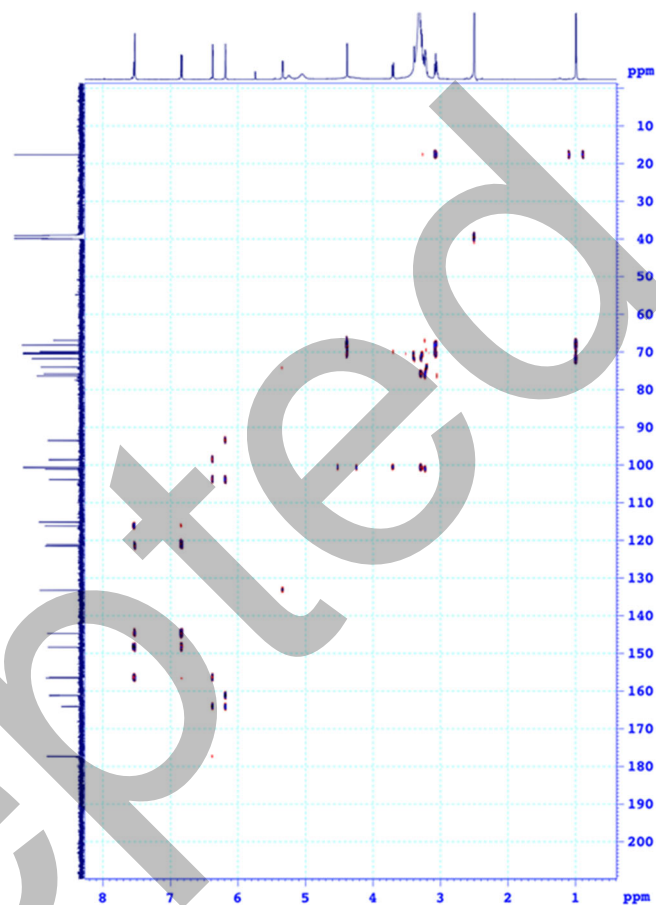
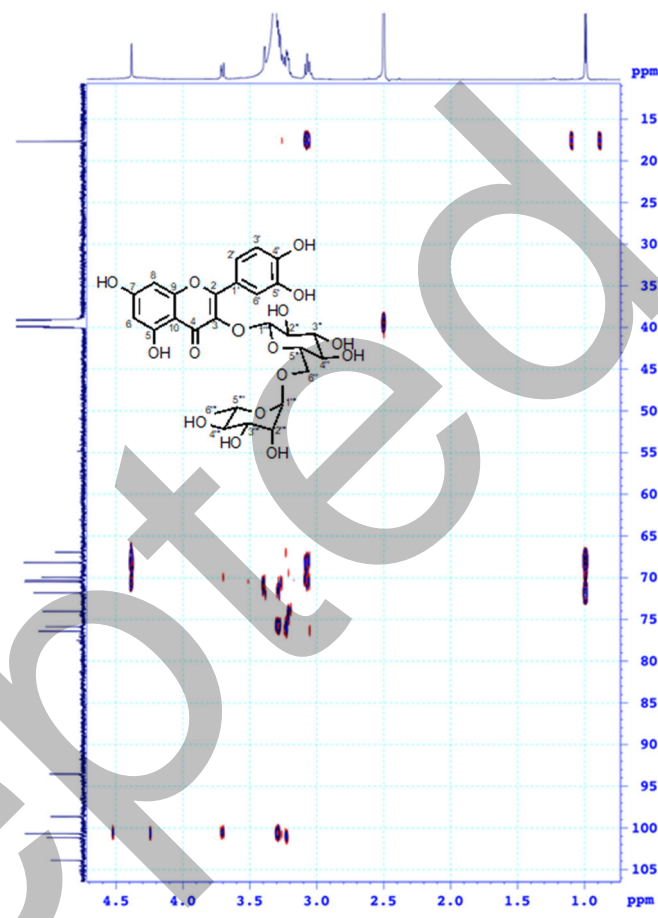
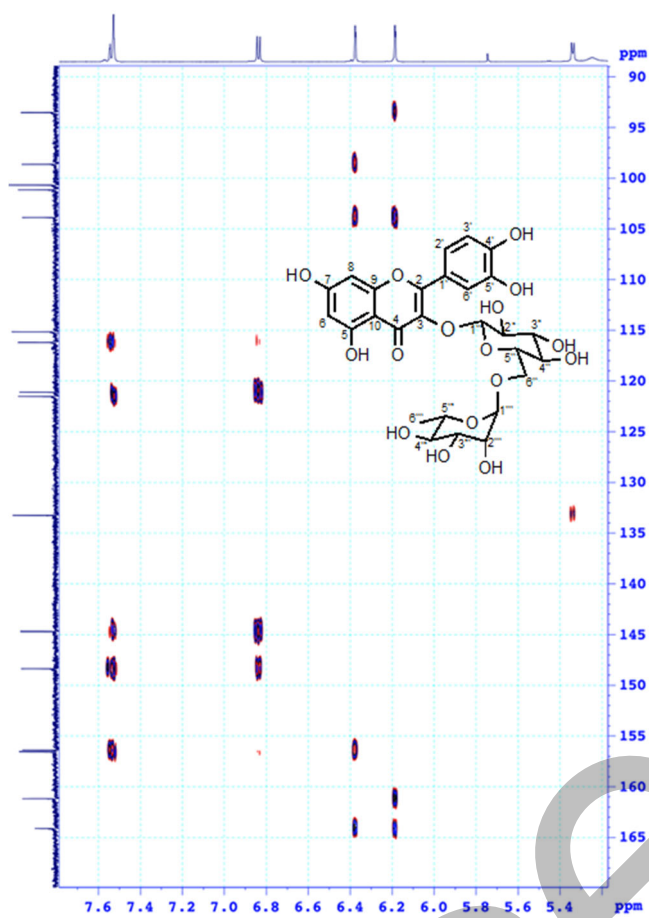


Fig S44. HMBC spectrum of compound 4



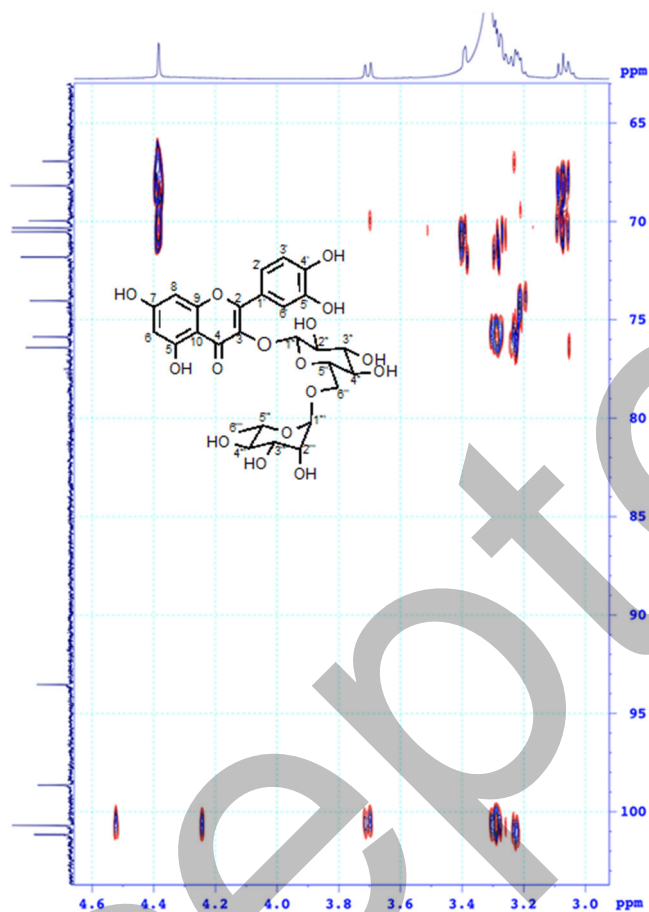


Fig S47. Expanded HMBC spectrum of compound 4

5. Supplementary Spectroscopic Data of Compound 5

3,4-Dihydroxycinnamic acid (caffeic acid) (5): $^1\text{H-NMR}$ (600 MHz, MeOD), δ_{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); $^{13}\text{C-NMR}$ (150 MHz, MeOD), δ_{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 $[\text{M}+\text{H}]^+$, 163.0391 $[\text{M}+\text{H}-\text{H}_2\text{O}]^+$, calculated $\text{C}_9\text{H}_8\text{O}_4$, m/z 180.0423.

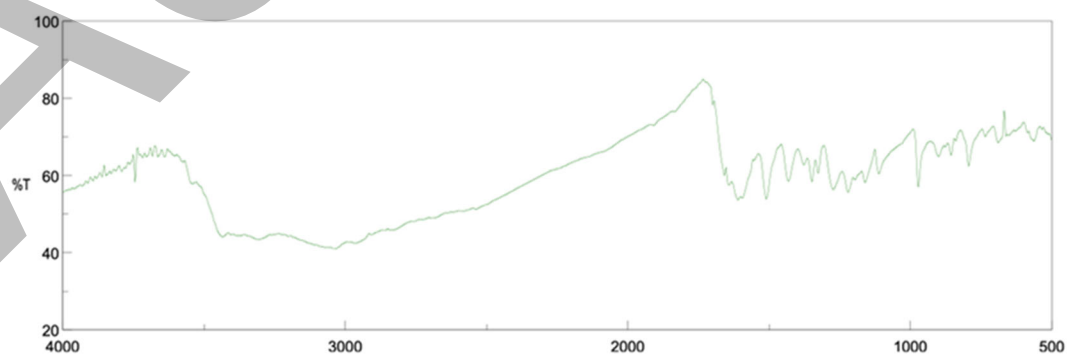


Fig S48. FTIR spectrum of compound 5

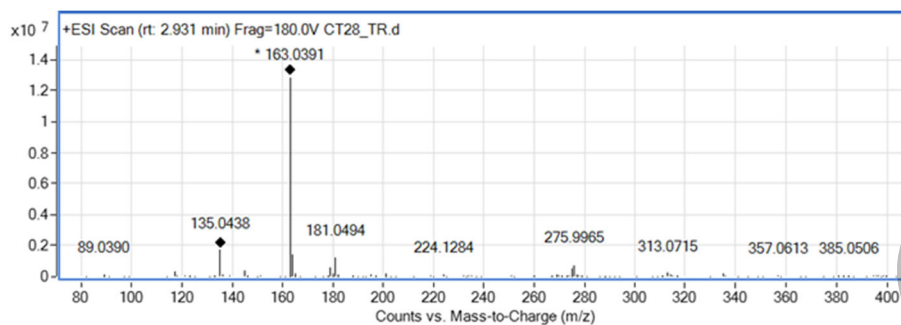


Fig S49. (+)ESI-MS spectrum of compound 5

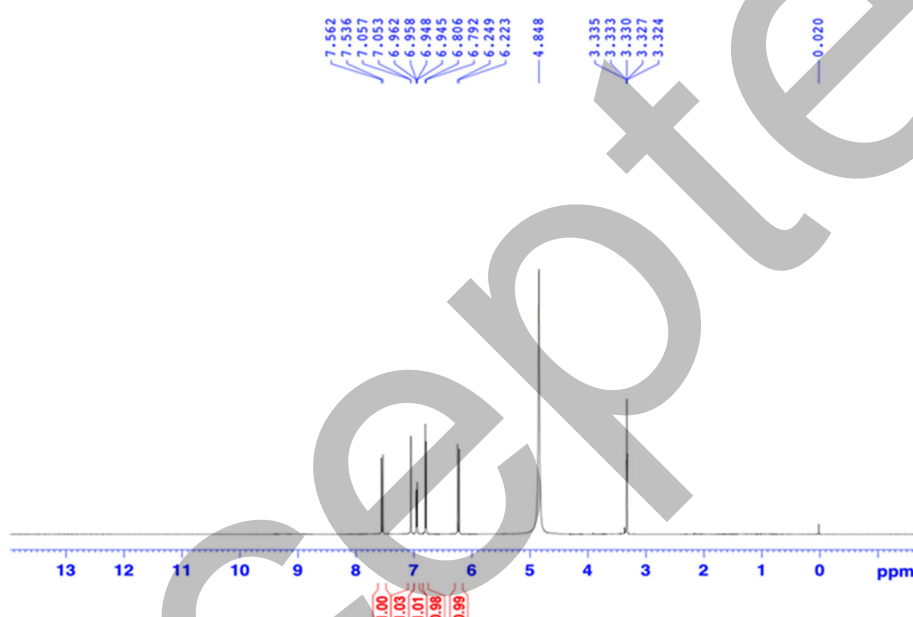


Fig S50. ¹H-NMR spectrum of compound 5

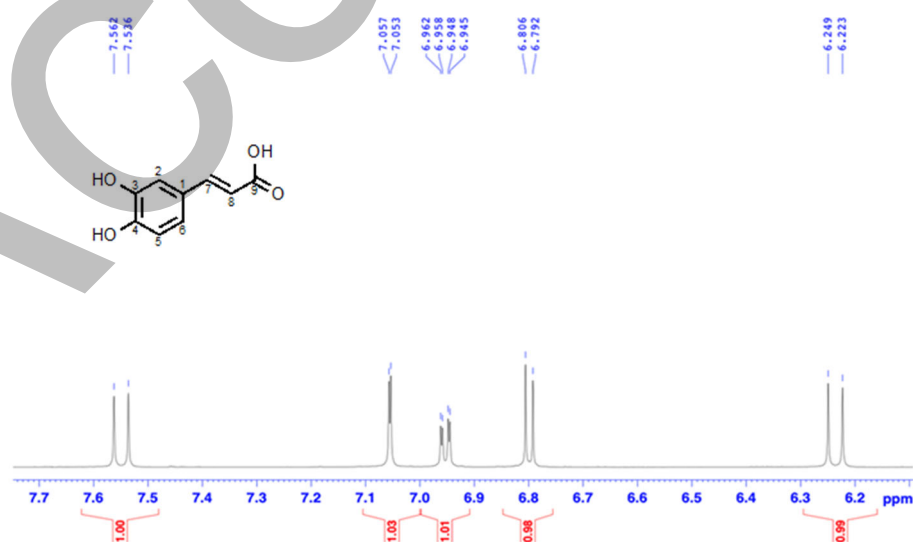
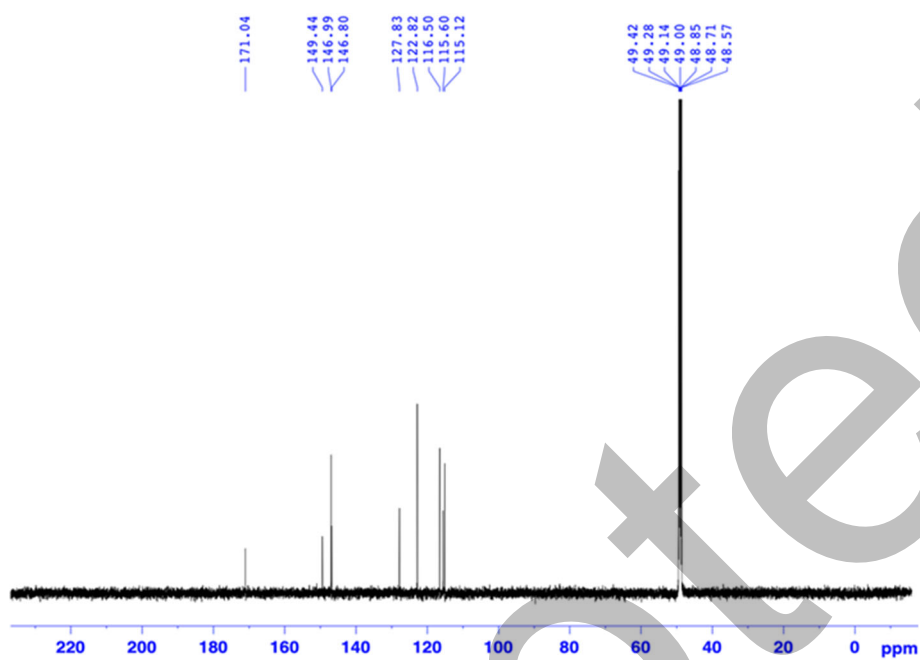
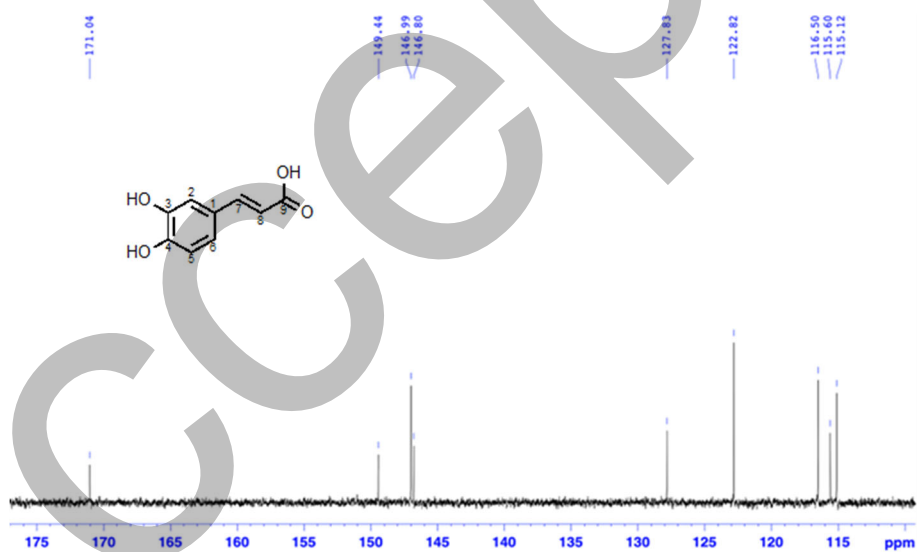


Fig S51. Expanded ¹H-NMR spectrum of compound 5

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

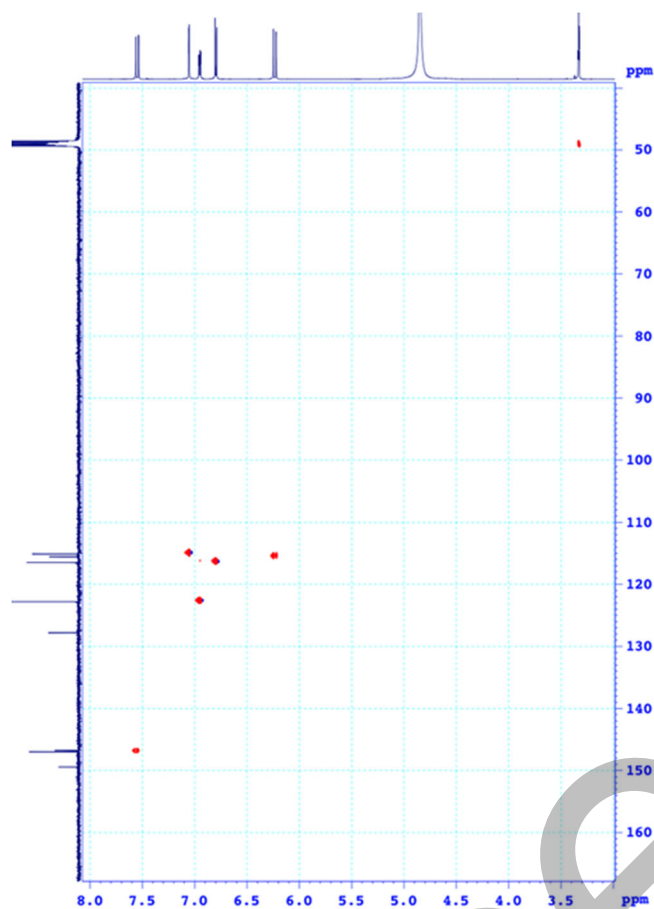


Fig S53. HSQC spectrum of compound 5

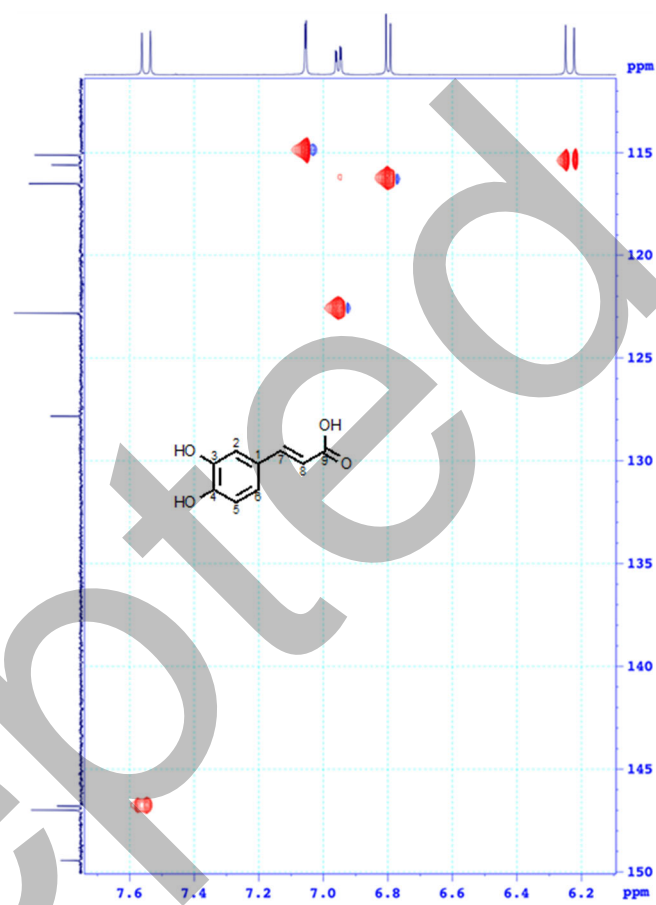


Fig S54. Expanded HSQC spectrum of compound 5

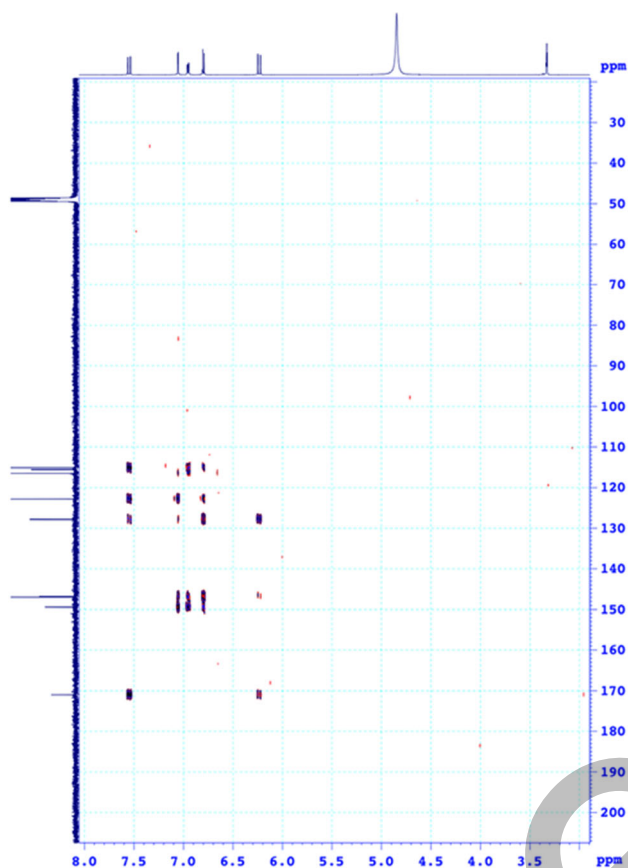


Fig S55. HMBC spectrum of compound 5

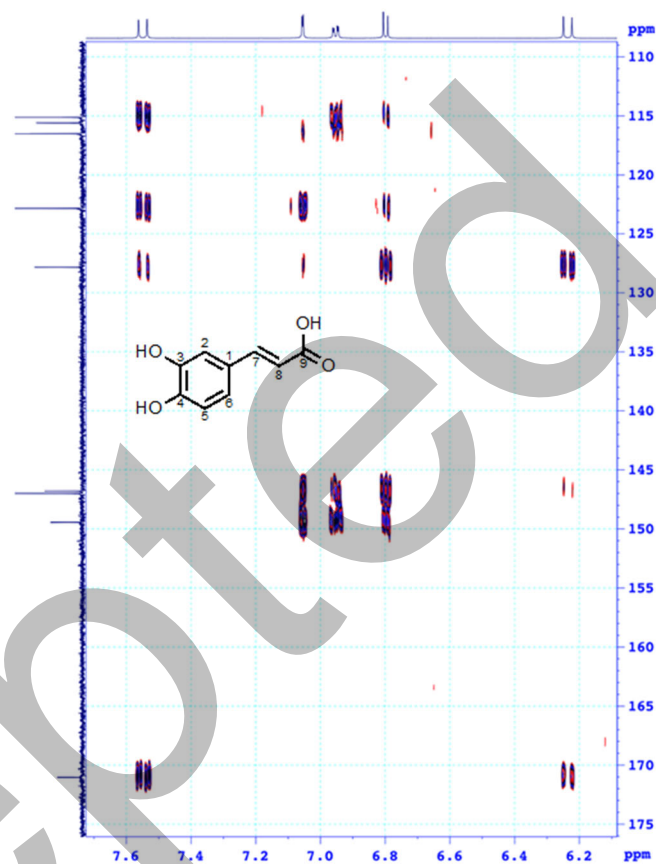


Fig S56. Expanded HMBC spectrum of compound 5

6. Supplementary Spectroscopic Data of Compound 6

(6*S*,7*a*R)-6-hydroxy-4,4,7*a*-trimethyl-5,6,7,7*a*-tetrahydro-1-benzofuran-2(4*H*)-one((-)-loliolide)(6): $^1\text{H-NMR}$ (600 MHz, CDCl_3), δ_{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-5 α), 1.77 (1H, *d*, $J = 3.6$ Hz, H-7 α), 1.79 (3H, s, CH_3 at C-10), 1.99 (1H, *dt*, $J = 14.4, 2.4$ Hz, H-5 β), 2.47 (1H, *dt*, $J = 14.4, 2.4$ Hz, H-7 β), 4.33 (1H, s, H-6), 5.70 (1H, s, H-3); $^{13}\text{C-NMR}$ (150 MHz, CDCl_3), δ_{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 $[\text{M}+\text{H}]^+$, 179.1076 $[\text{M}+\text{H}-\text{H}_2\text{O}]^+$, calculated $\text{C}_{11}\text{H}_{16}\text{O}_3$, m/z 196.1099.

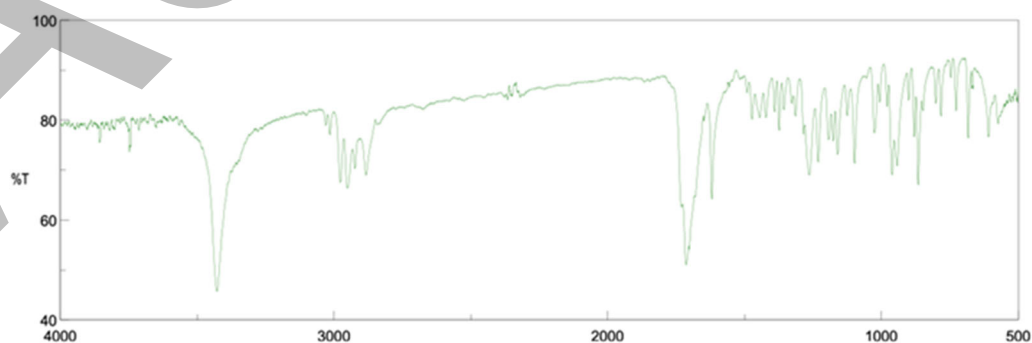


Fig S57. FTIR spectrum of compound 6

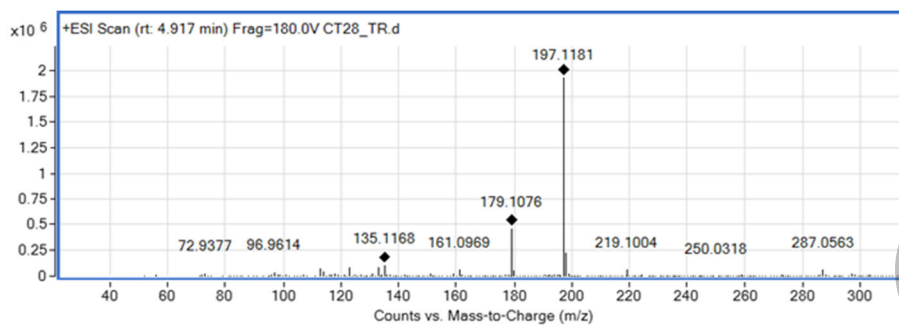
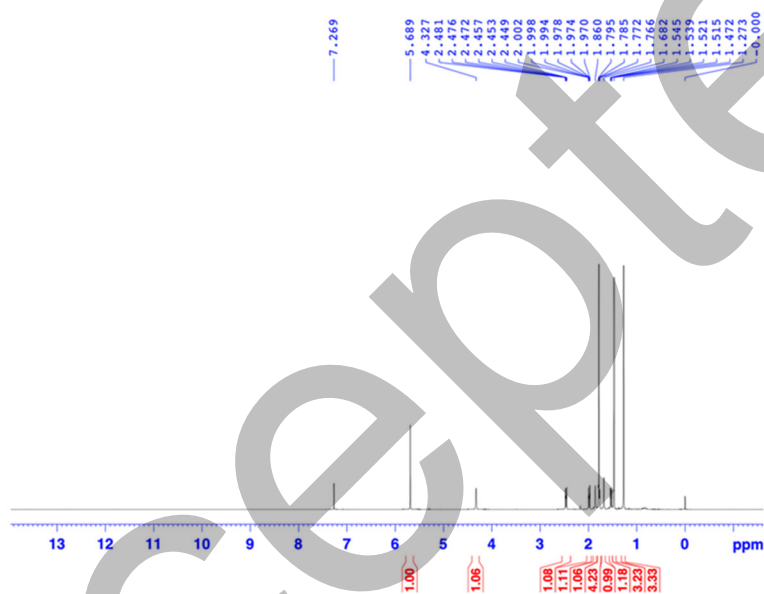
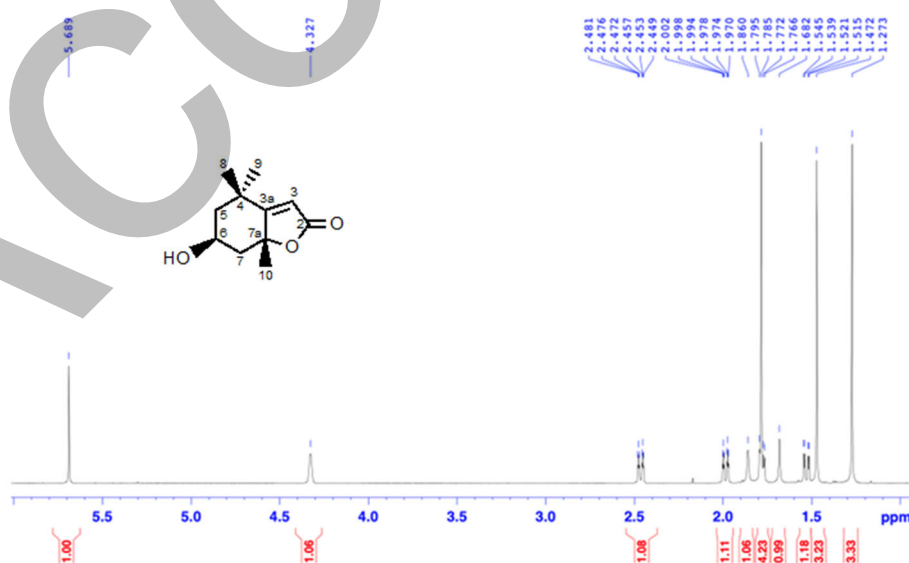
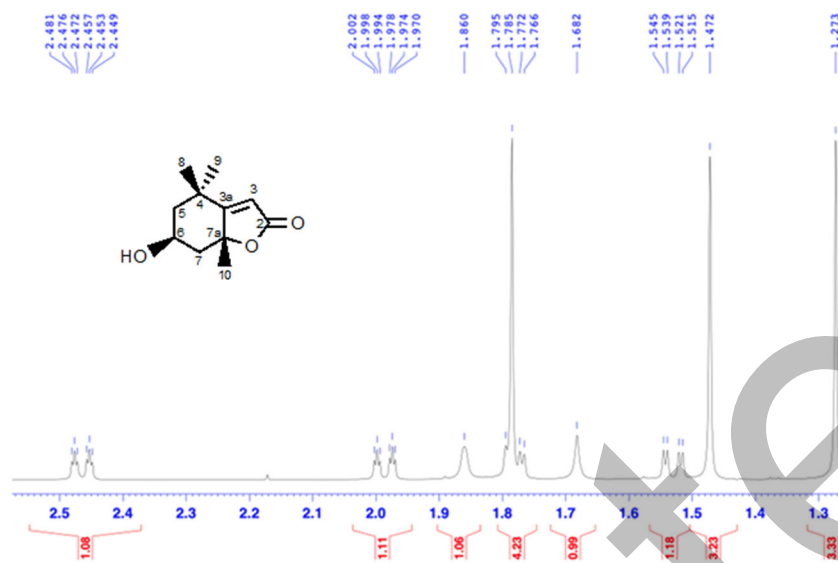
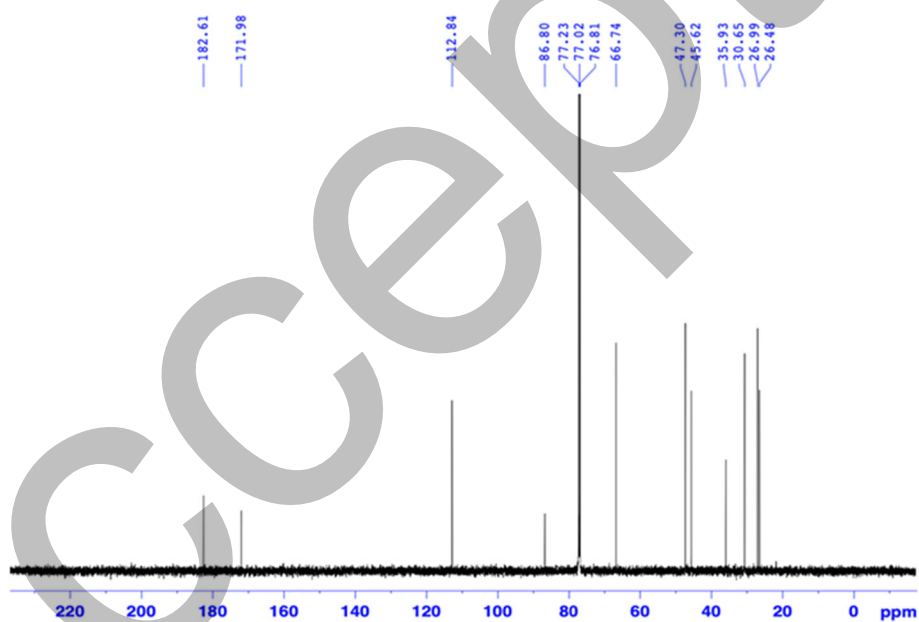


Fig S58. (+)ESI-MS spectrum of compound 6

Fig S59. ¹H-NMR spectrum of compound 6Fig S60. Expanded ¹H-NMR spectrum of compound 6

Fig S61. Expanded ¹H-NMR spectrum of compound 6Fig S62. ¹³C-NMR spectrum of compound 6

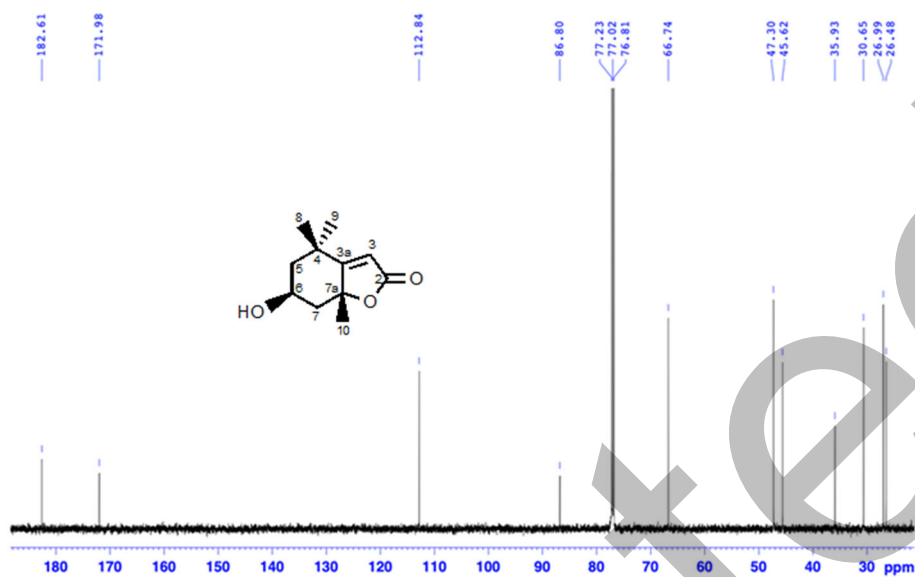
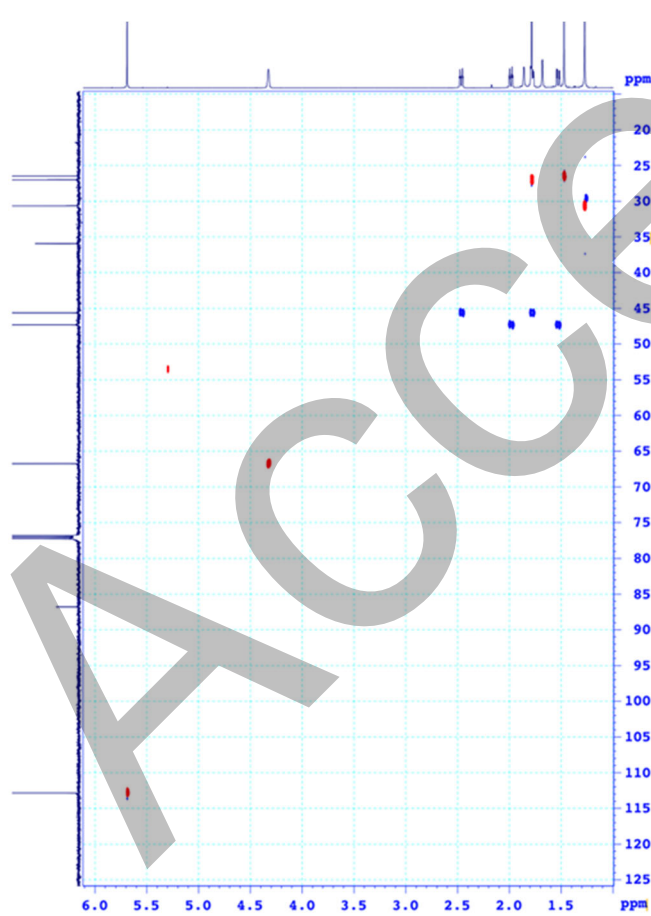
Fig S63. Expanded ^{13}C -NMR spectrum of compound 6

Fig S64. HSQC spectrum of compound 6

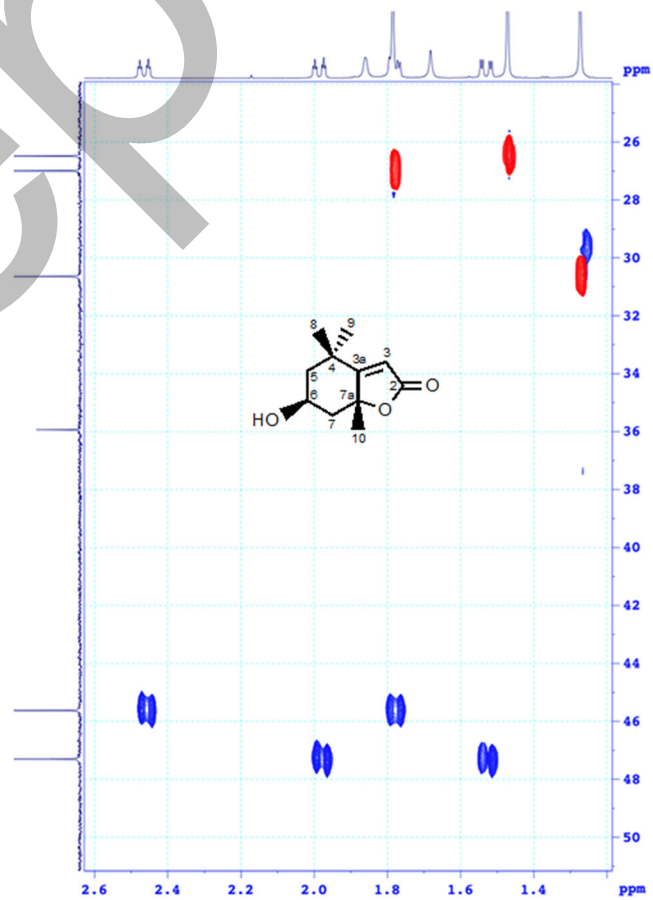


Fig S65. Expanded HSQC spectrum of compound 6

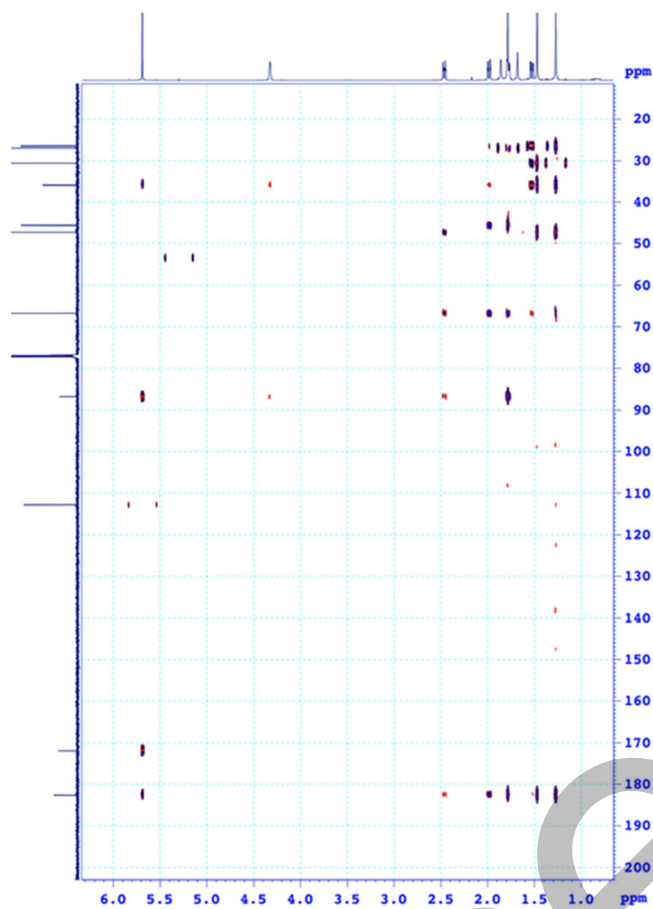


Fig S66. HMBC spectrum of compound 6

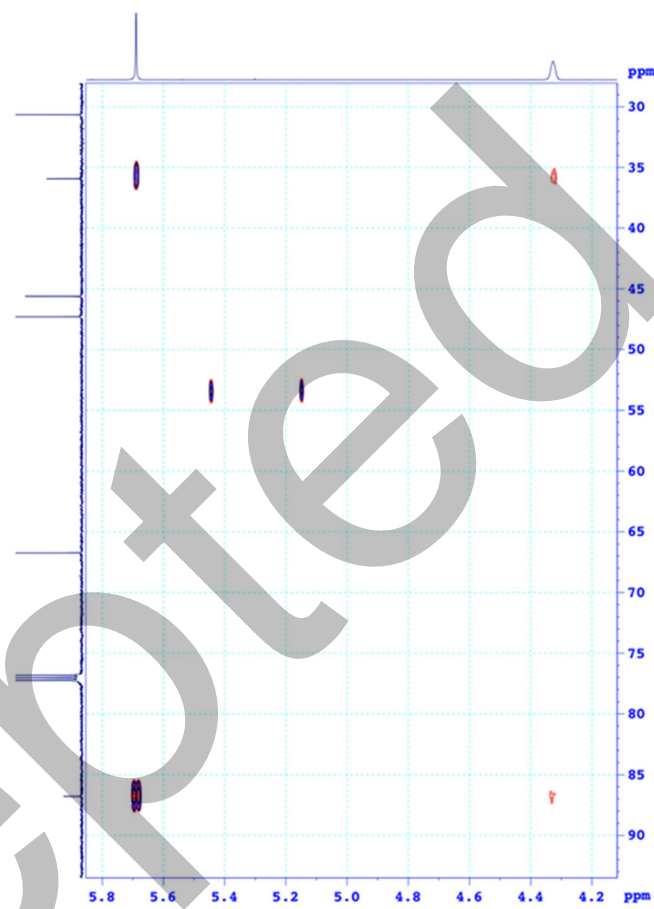


Fig S67. Expanded HMBC spectrum of compound 6

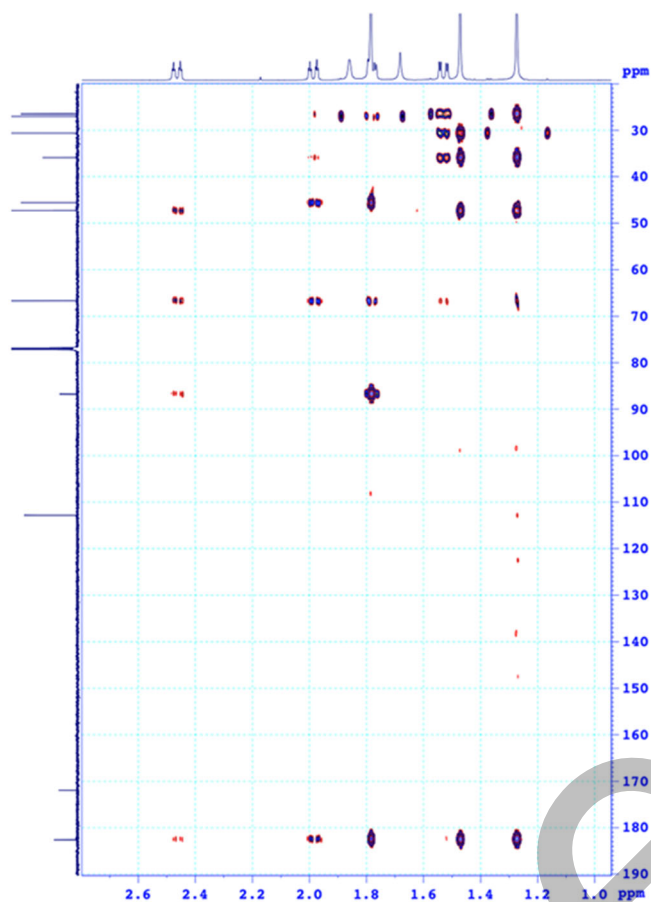


Fig S69. Expanded HMBC spectrum of compound 6

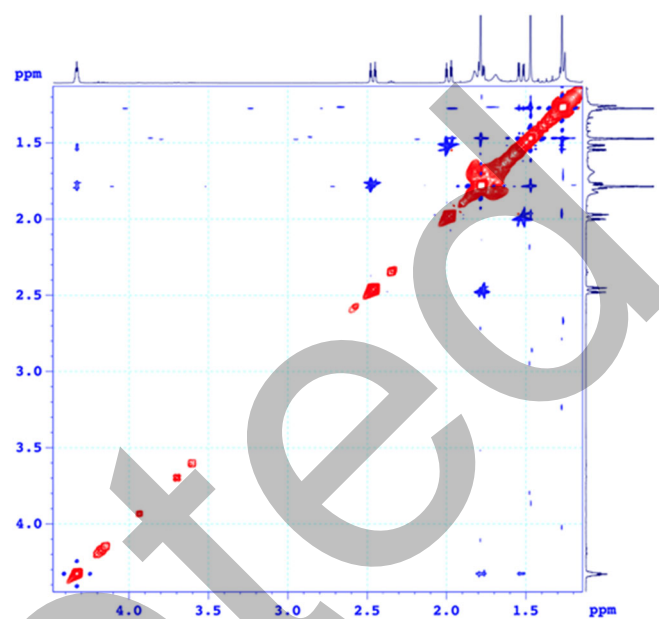


Fig S71. Expanded NOESY spectrum of compound 6

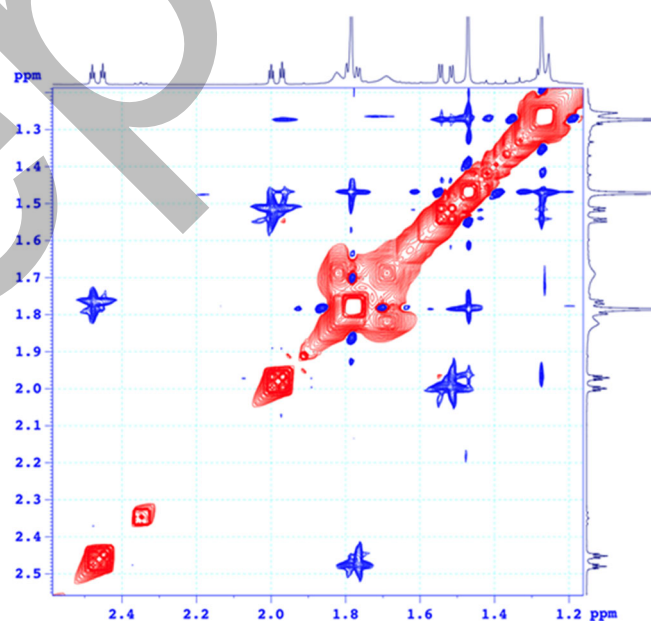


Fig S72. Expanded NOESY spectrum of compound 6

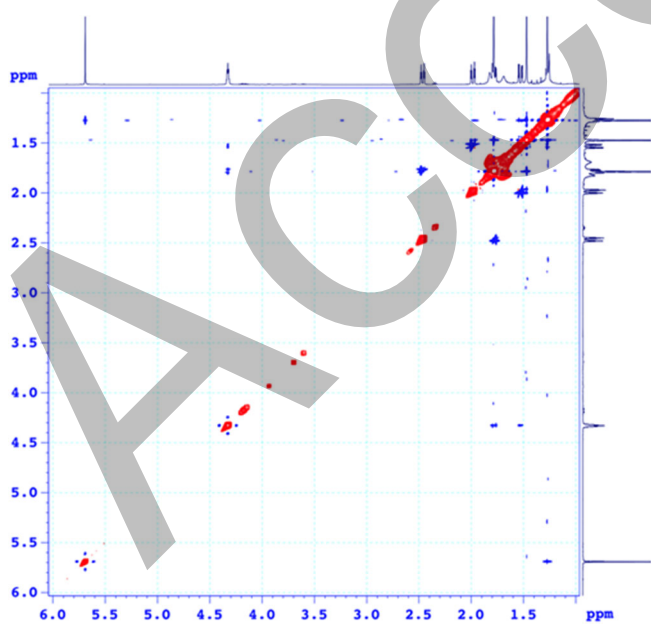


Fig S70. Complete assignment NOESY spectrum of compound 6

7. Supplementary Spectroscopic Data of Compound 7

***β*-Sitosterol-3-O-*β*-D-glucopyranoside (daucosterol) (7)**: ¹H-NMR (600 MHz, DMSO-*d*₆), δ_H (ppm): 0.65 (3H, s, CH₃ at C-18), 1.00 (3H, s, CH₃ 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); ¹³C-NMR (150 MHz, DMSO-*d*₆), δ_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').

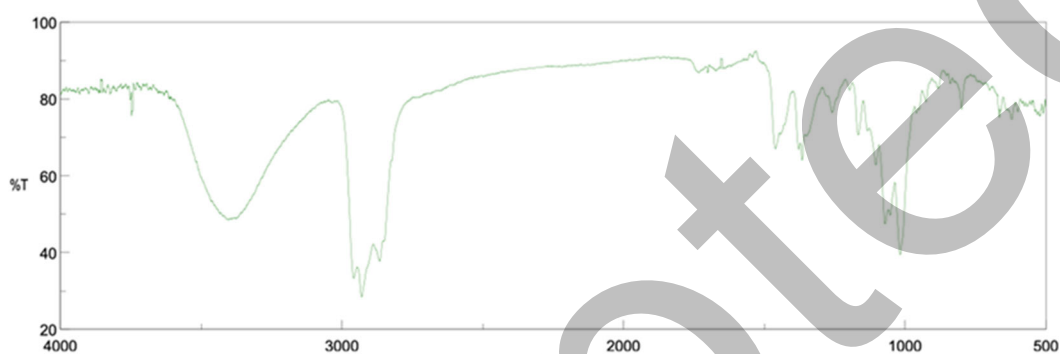


Fig S73. FTIR spectrum of compound 7

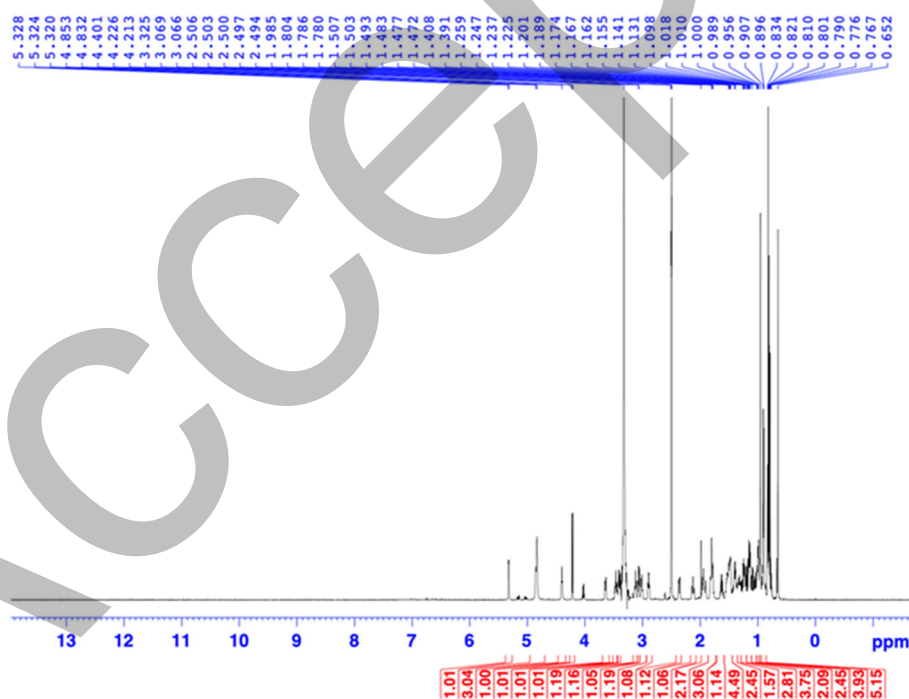
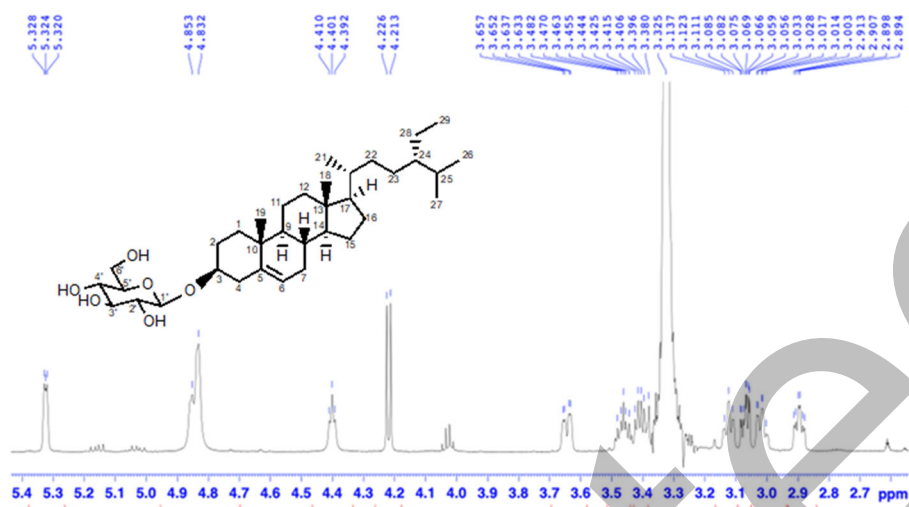
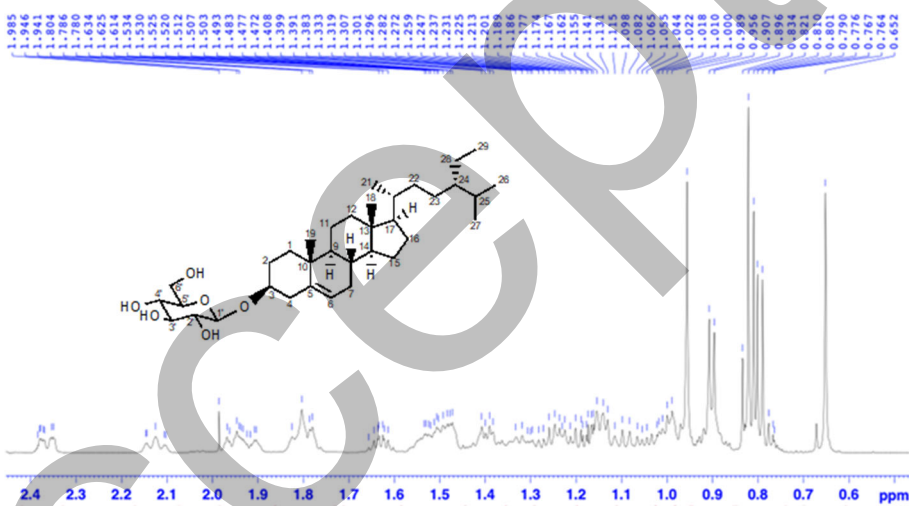
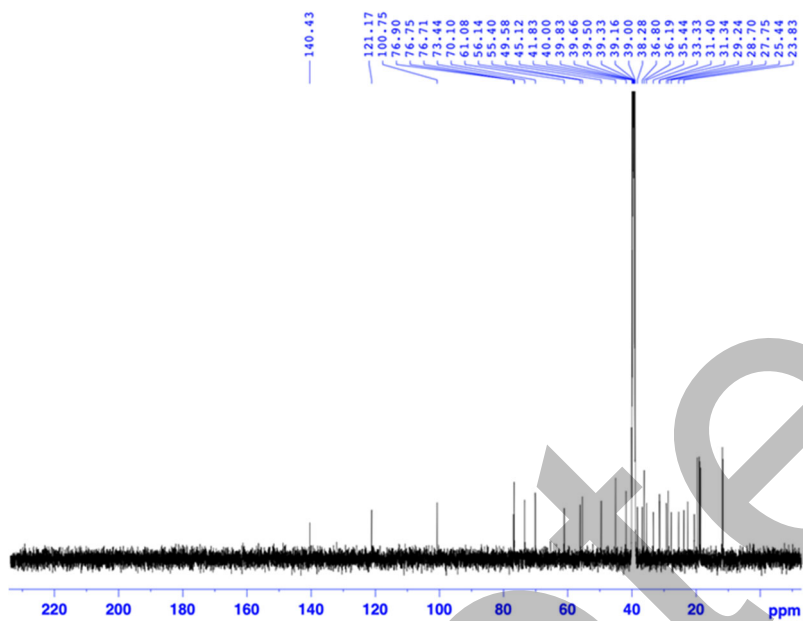
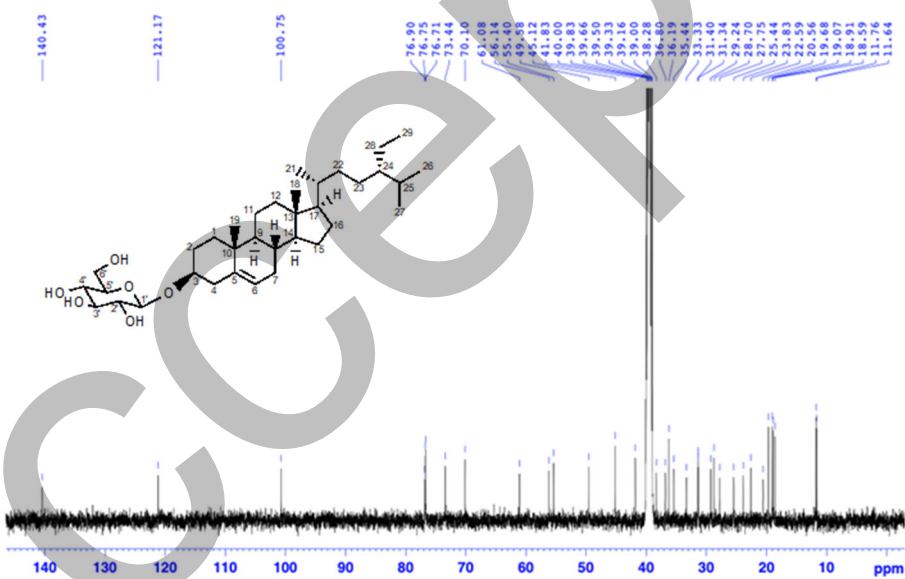


Fig S74. ¹H-NMR spectrum of compound 7

Fig S75. Expanded ^1H -NMR spectrum of compound 7Fig S76. Expanded ^1H -NMR spectrum of compound 7

Fig S77. $^{13}\text{C-NMR}$ spectrum of compound 7Fig S78. Expanded $^{13}\text{C-NMR}$ spectrum of compound 7

