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}H-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); ^{13}C-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').

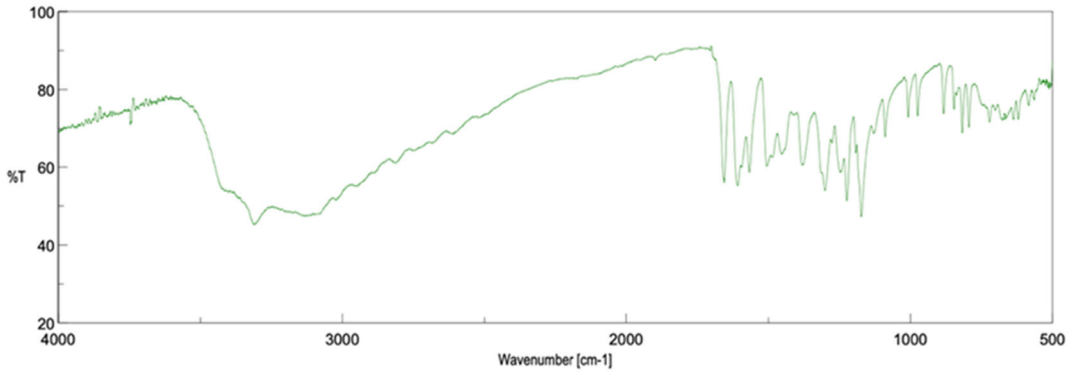


Fig S1. FTIR spectrum of compound **1**

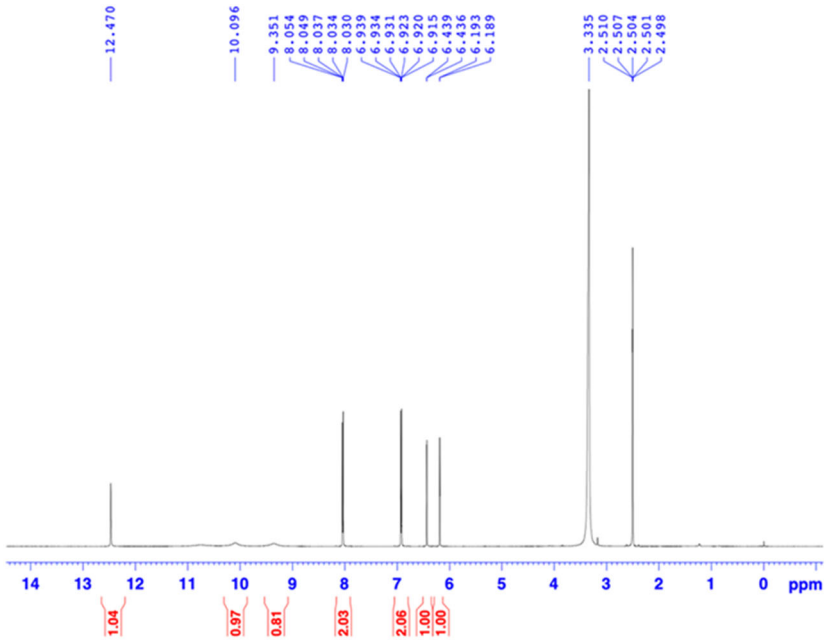


Fig S2. ^{1}H-NMR spectrum of compound **1**

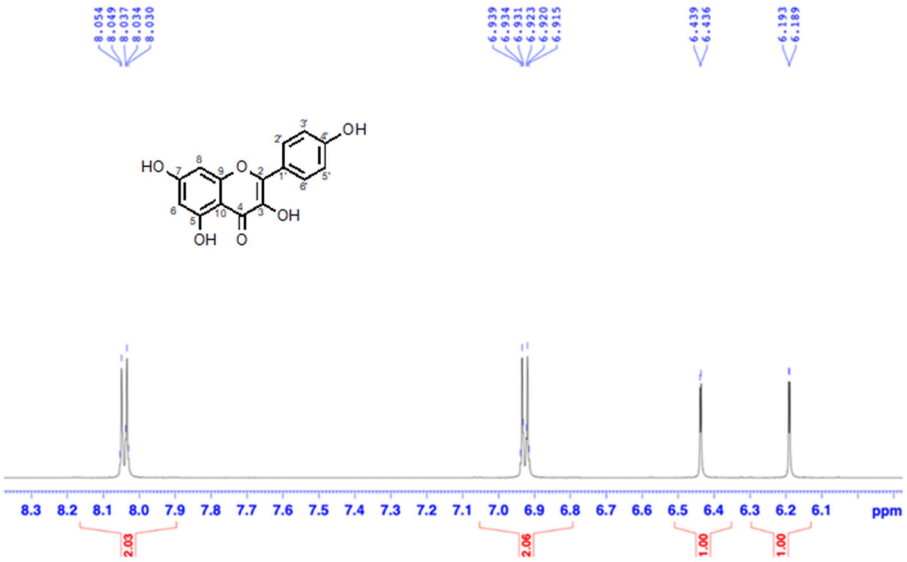


Fig S3. Expanded ^{1}H-NMR spectrum of compound **1**

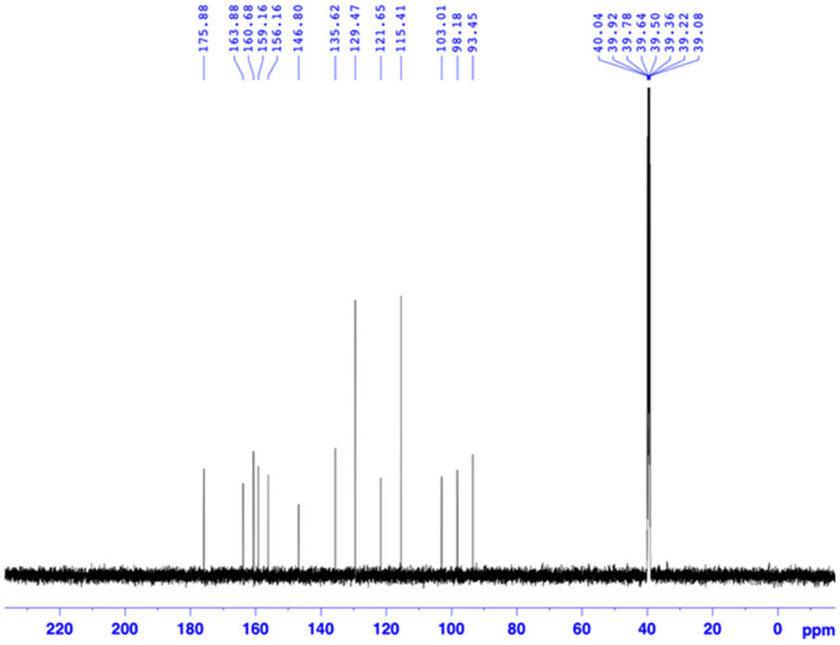


Fig S4. ^{13}C-NMR spectrum of compound **1**

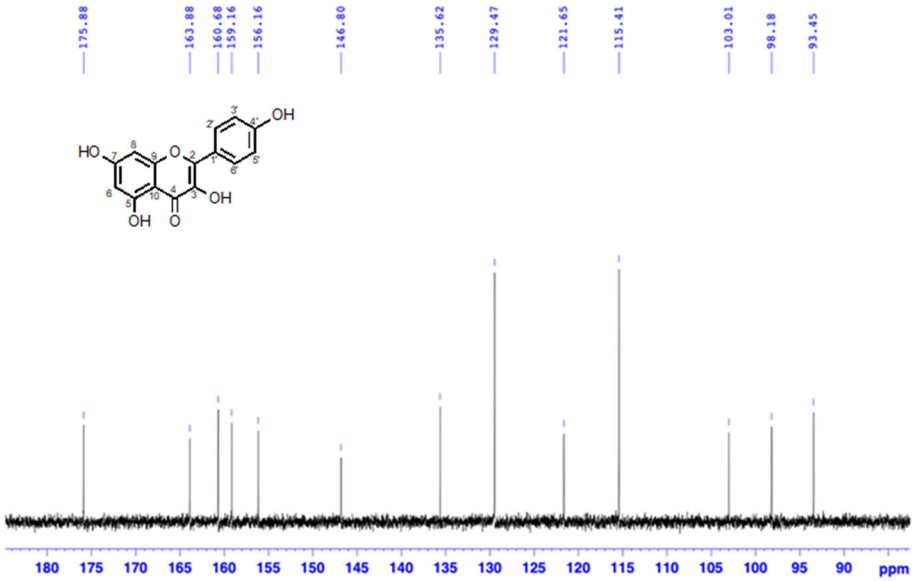


Fig S5. Expanded ^{13}C-NMR spectrum of compound **1**

2. Supplementary Spectroscopic Data of Compound 2

Kaempferol-3-O-β-D-glucopyranoside (astragalin) (2): ^{1}H-NMR (600 MHz, 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, 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 $[M+H]^+$, calculated $C_{21}H_{20}O_{11}$, *m/z* 448.1006.

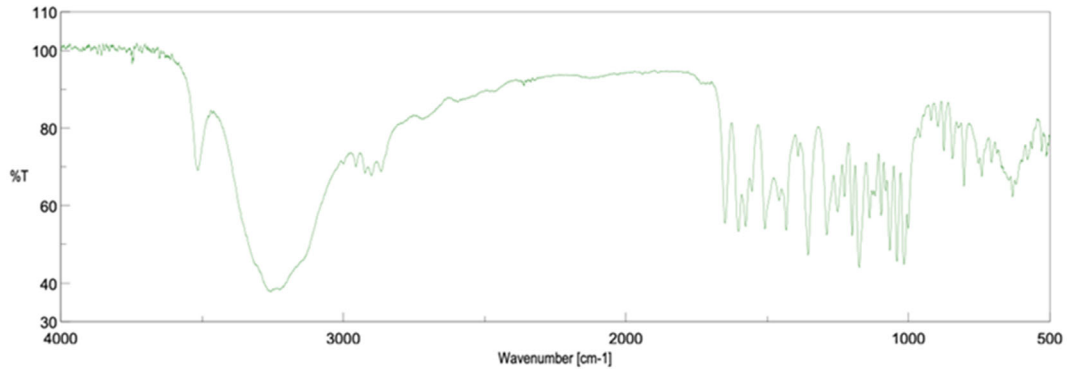


Fig S6. FTIR spectrum of compound **2**

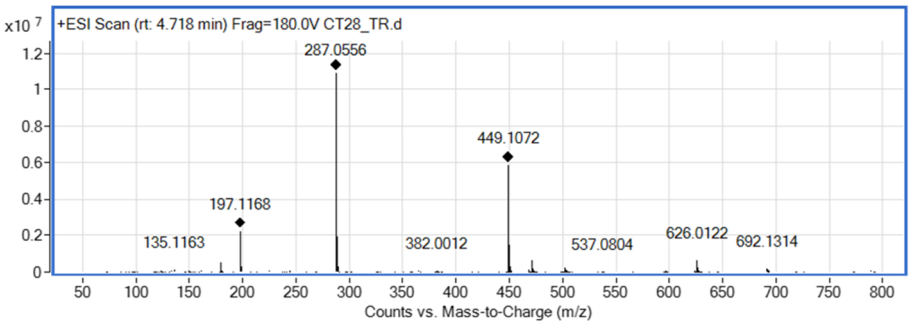


Fig S7. (+)ESI-MS spectrum of compound **2**

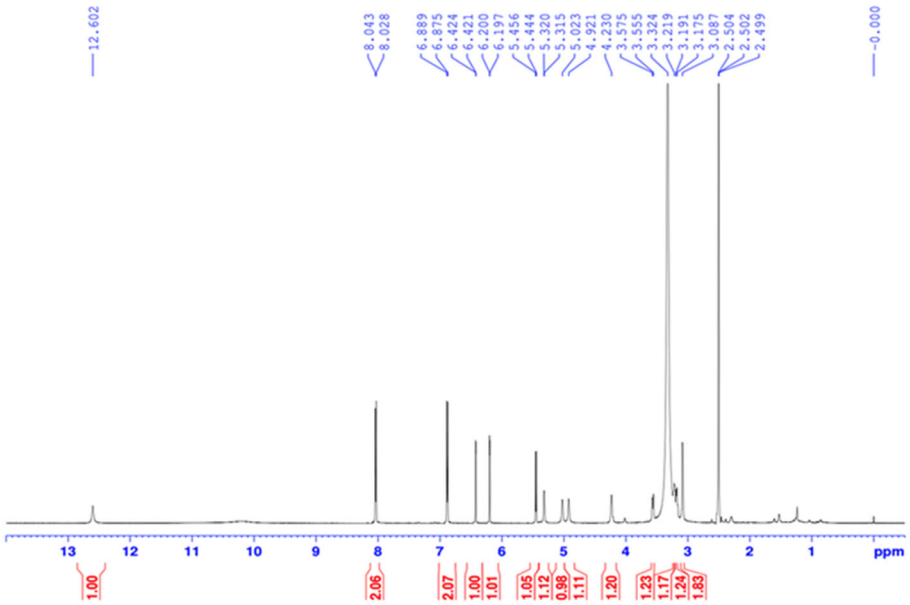


Fig S8. ^{1}H-NMR spectrum of compound **2**

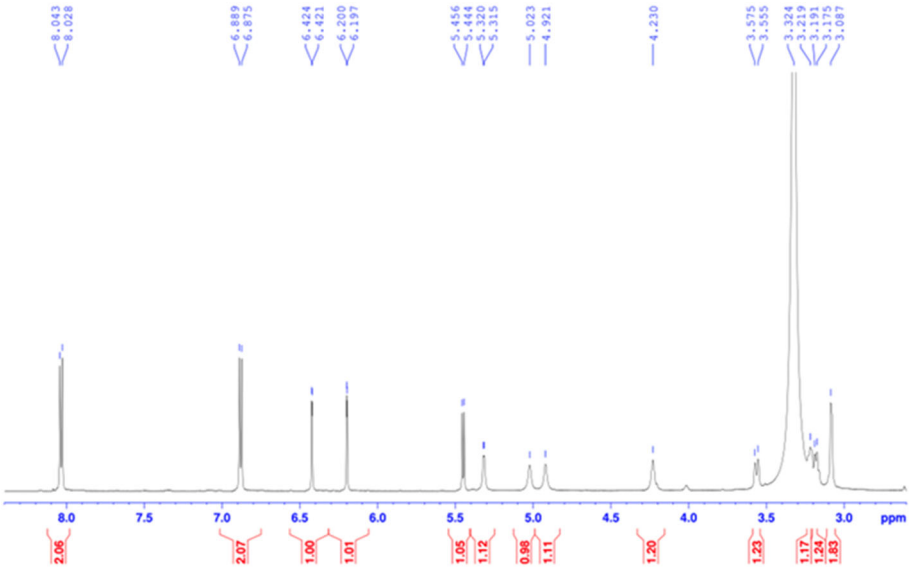


Fig S9. Expanded ^{1}H-NMR spectrum of compound **2**

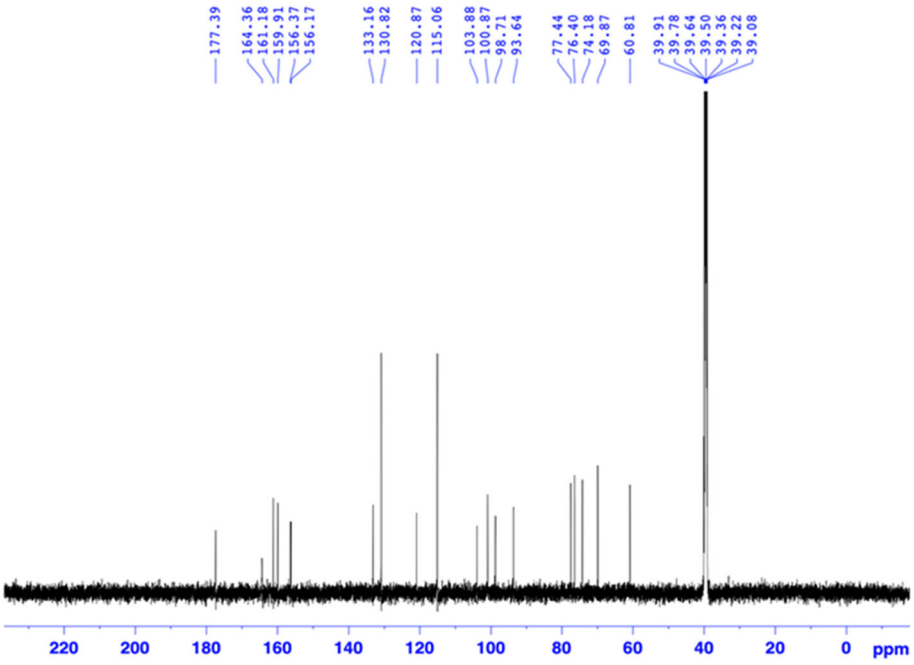


Fig S10. ^{13}C-NMR spectrum of compound **2**

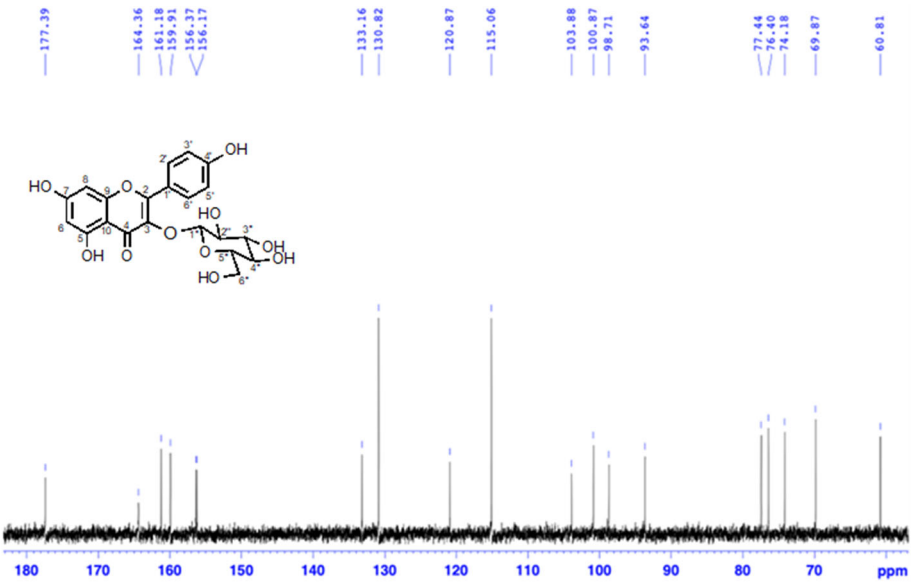


Fig S11. Expanded ^{13}C-NMR spectrum of compound **2**

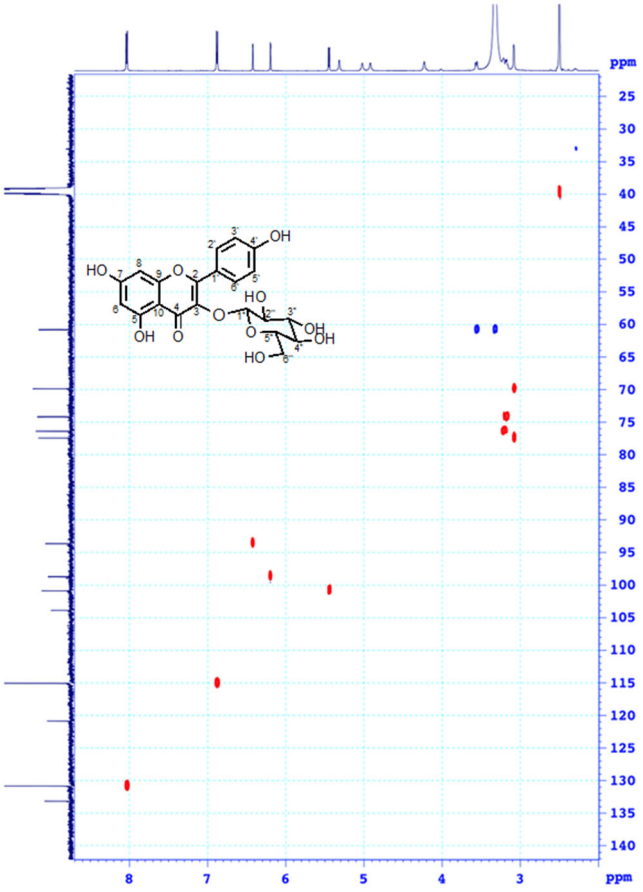


Fig S12. HSQC spectrum of compound **2**

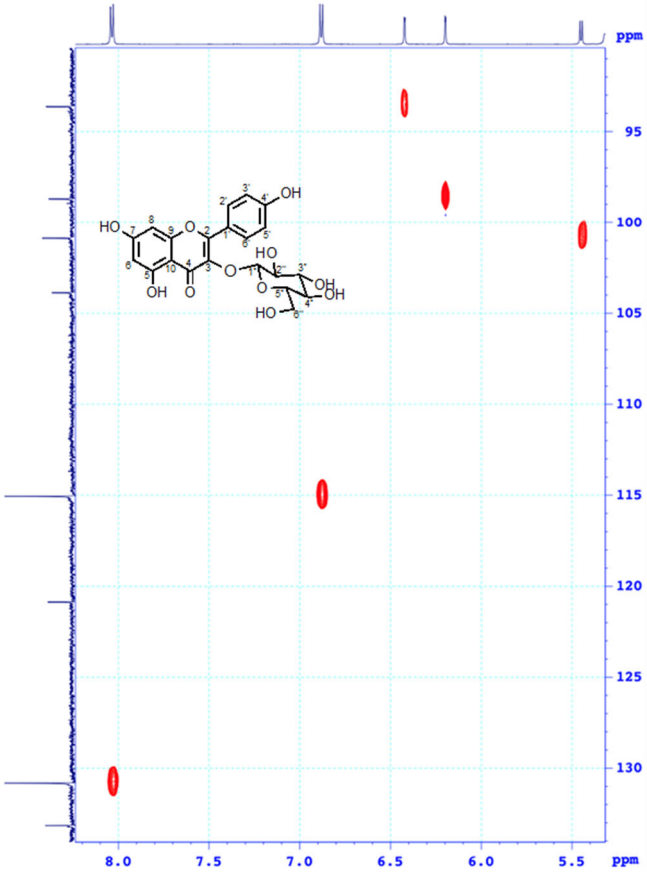


Fig S13. Expanded HSQC spectrum of compound **2**

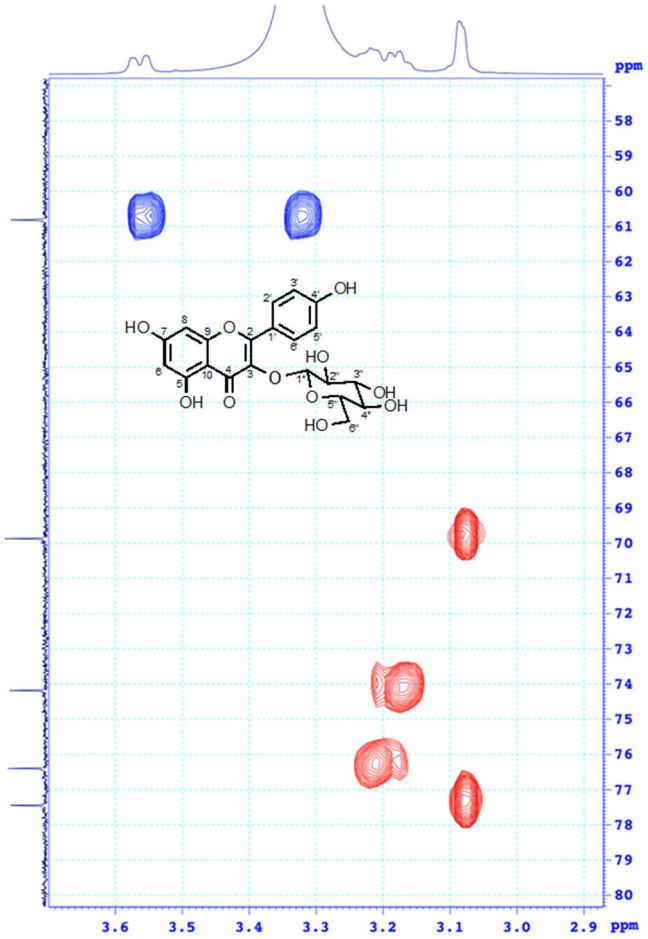


Fig S14. Expanded HSQC spectrum of compound **2**

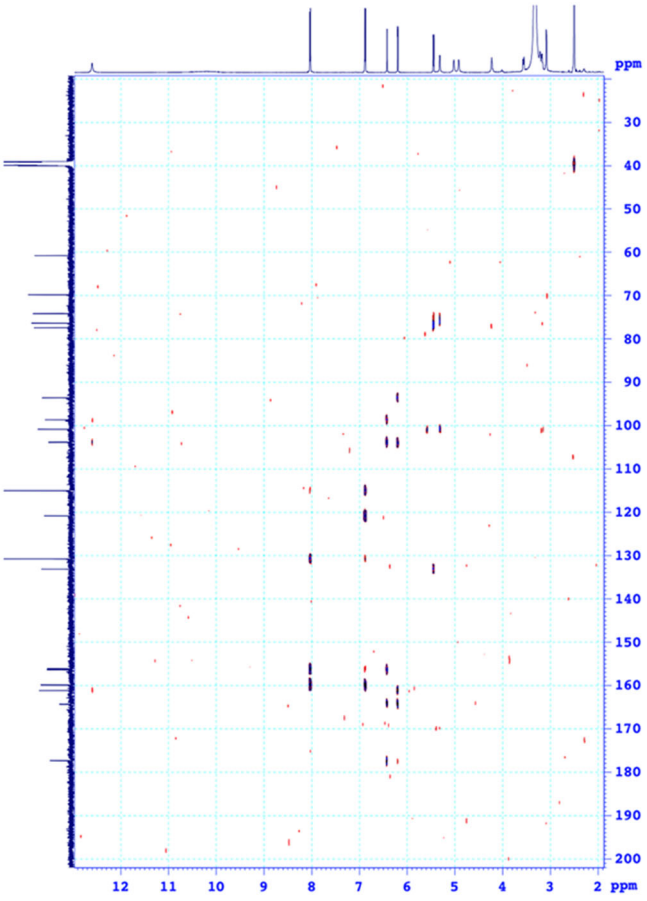


Fig S15. HMBC spectrum of compound **2**

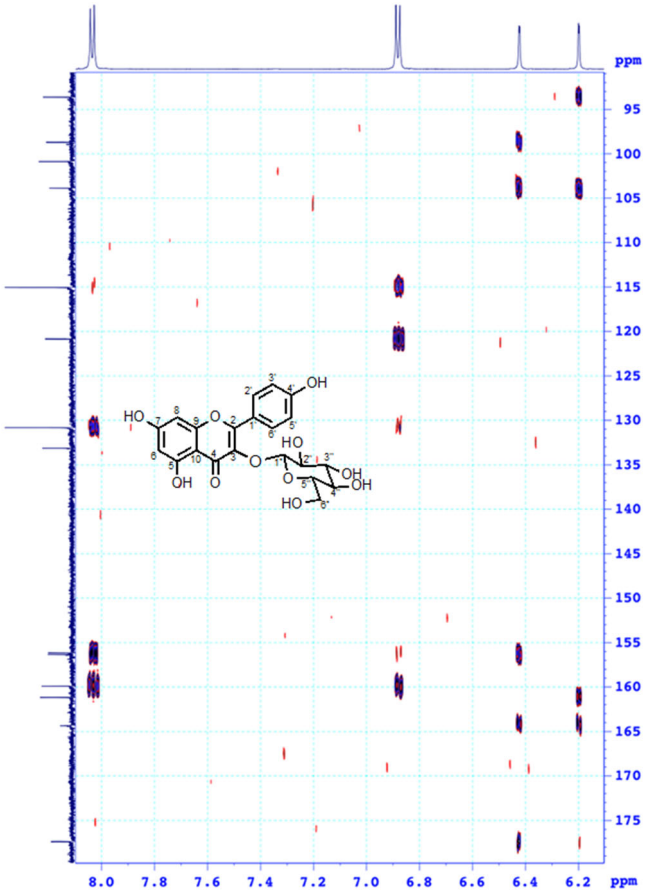


Fig S16. Expanded HMBC spectrum of compound **2**

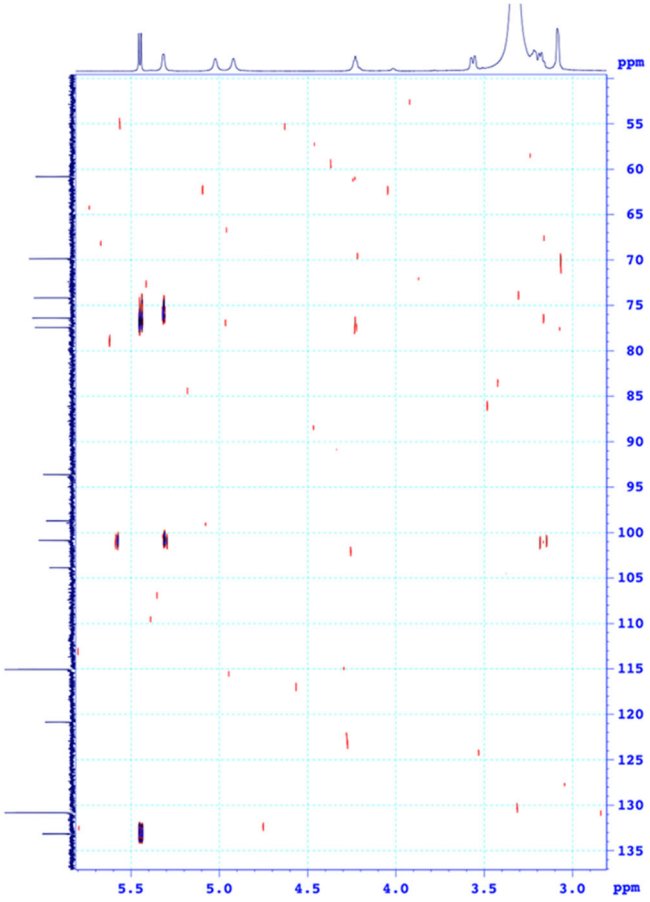


Fig S17. Expanded HMBC spectrum of compound **2**

3. Supplementary Spectroscopic Data of Compound 3

Kaempferol-3-O-β-D-rutinoside (nicotiflorin) (**3**): ^{1}H-NMR (600 MHz, 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}C-NMR (150 MHz, 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 $[M+H]^+$, calculated $C_{27}H_{30}O_{15}$, *m/z* 594.1585.

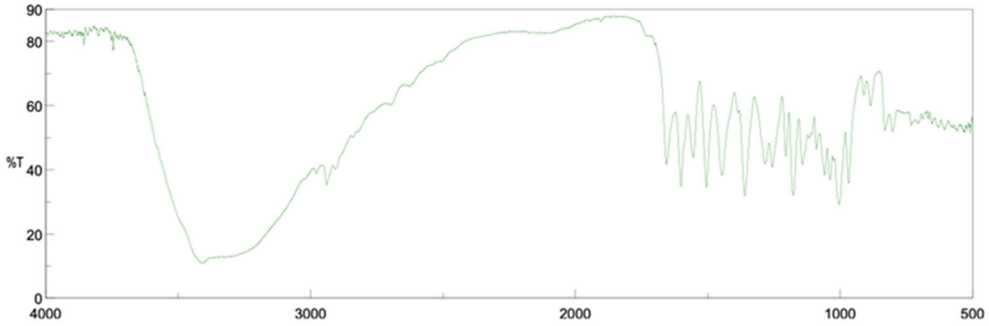


Fig S18. FTIR spectrum of compound **3**

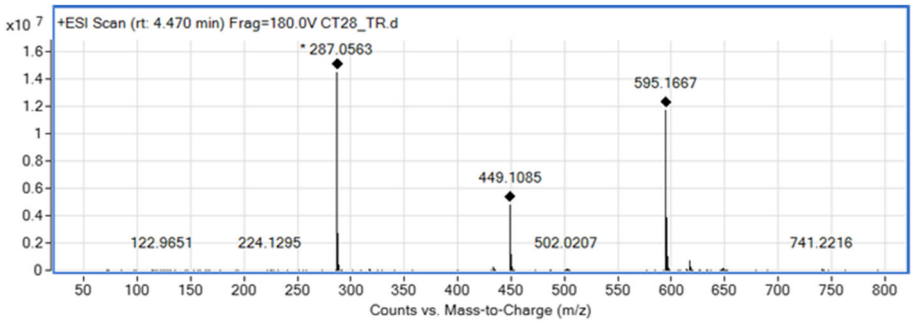


Fig S19. (+)ESI-MS spectrum of compound **3**

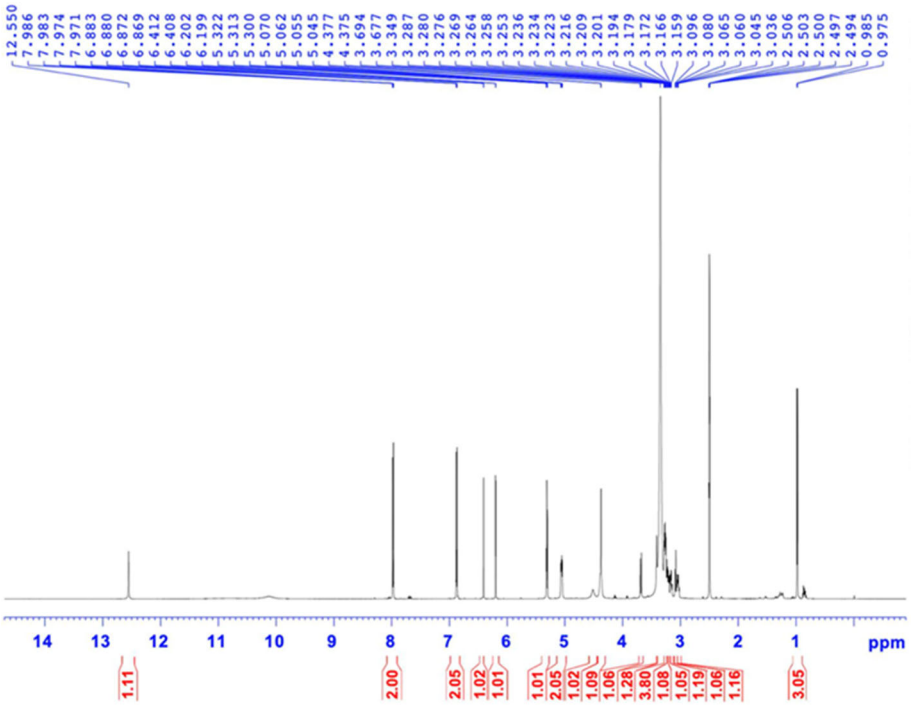


Fig S20. ^{1}H-NMR spectrum of compound **3**

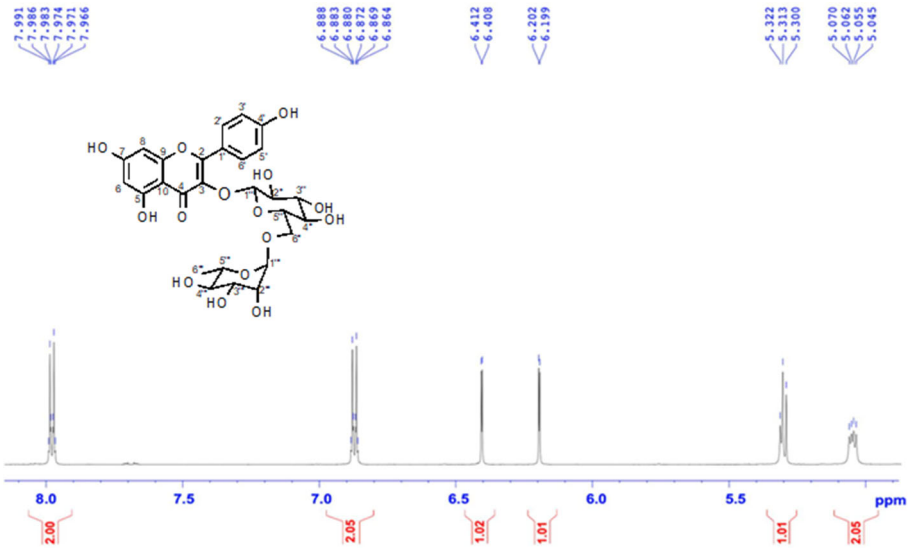


Fig S21. Expanded [1]H-NMR spectrum of compound **3**

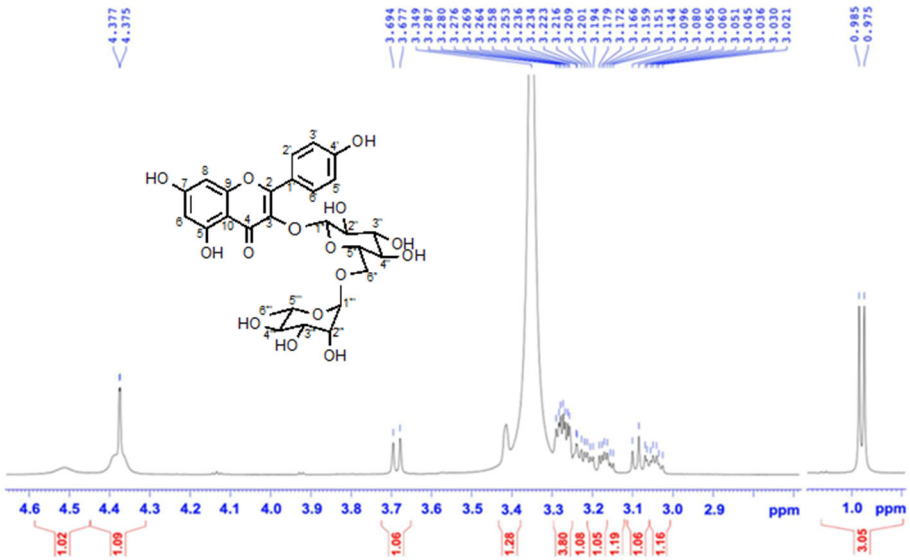


Fig S22. Expanded [1]H-NMR spectrum of compound **3**

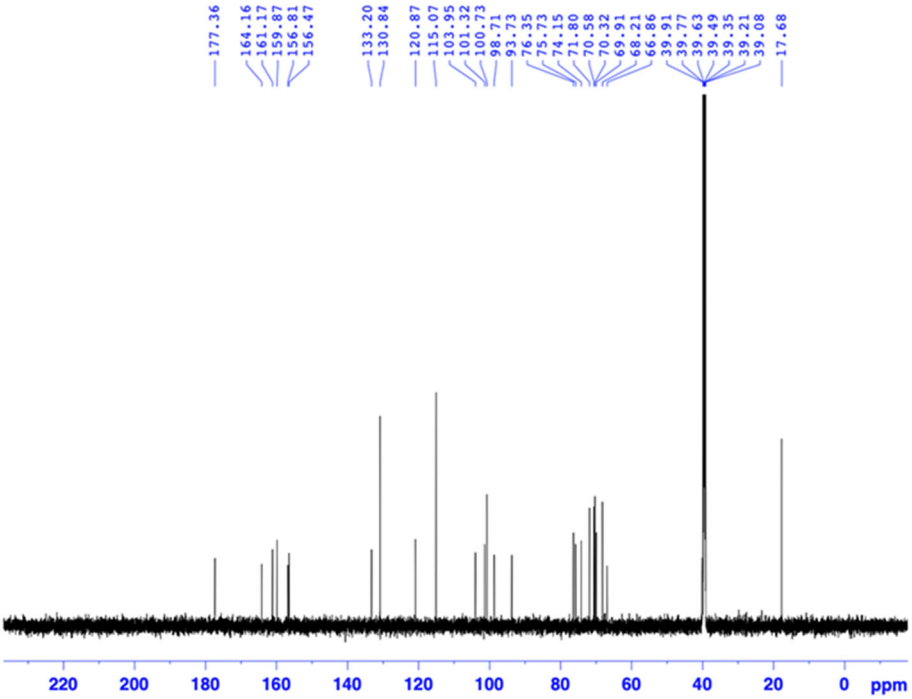


Fig S23. ^{13}C-NMR spectrum of compound **3**

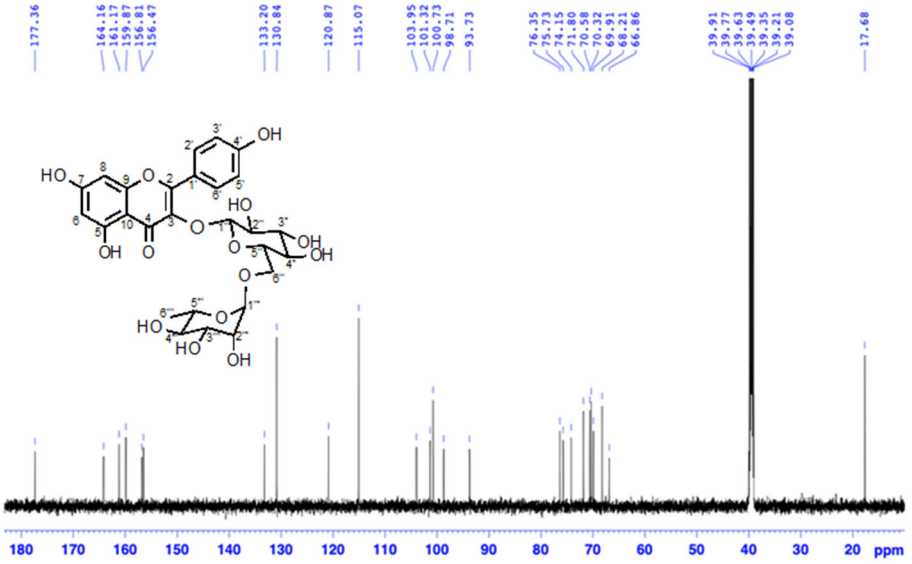


Fig S24. Expanded ^{13}C-NMR spectrum of compound **3**

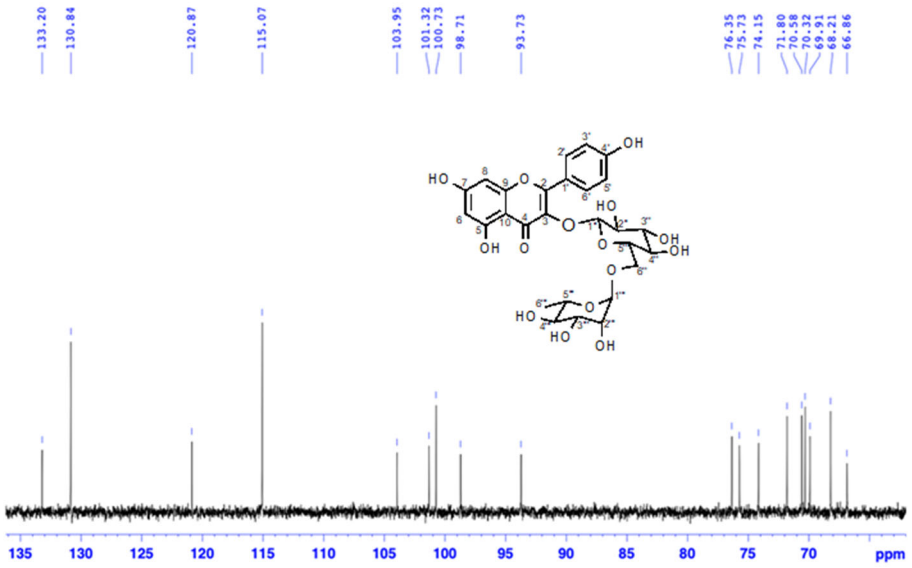
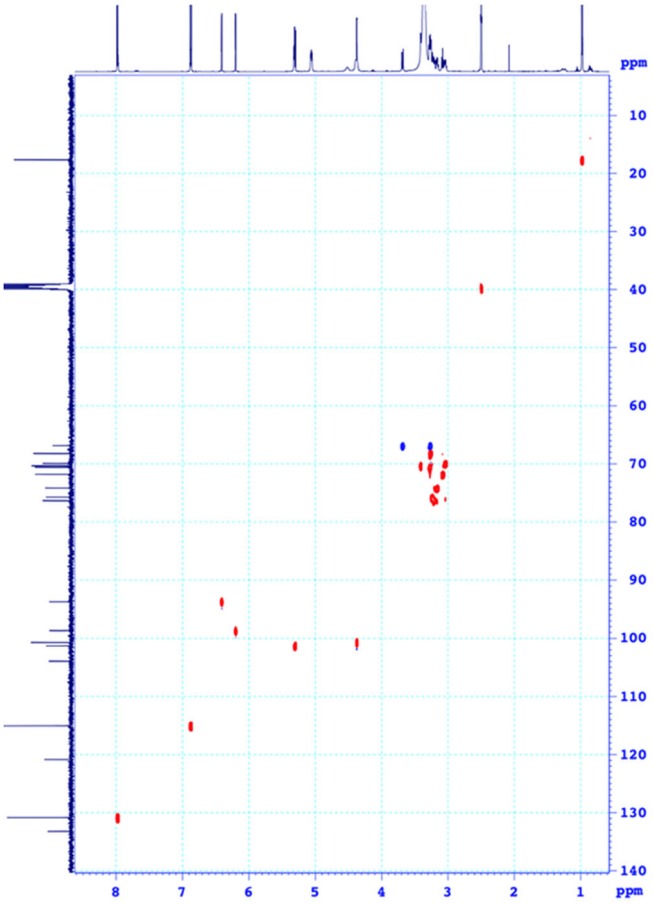


Figure S25. Expanded ^{13}C-NMR spectrum of compound **3**



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

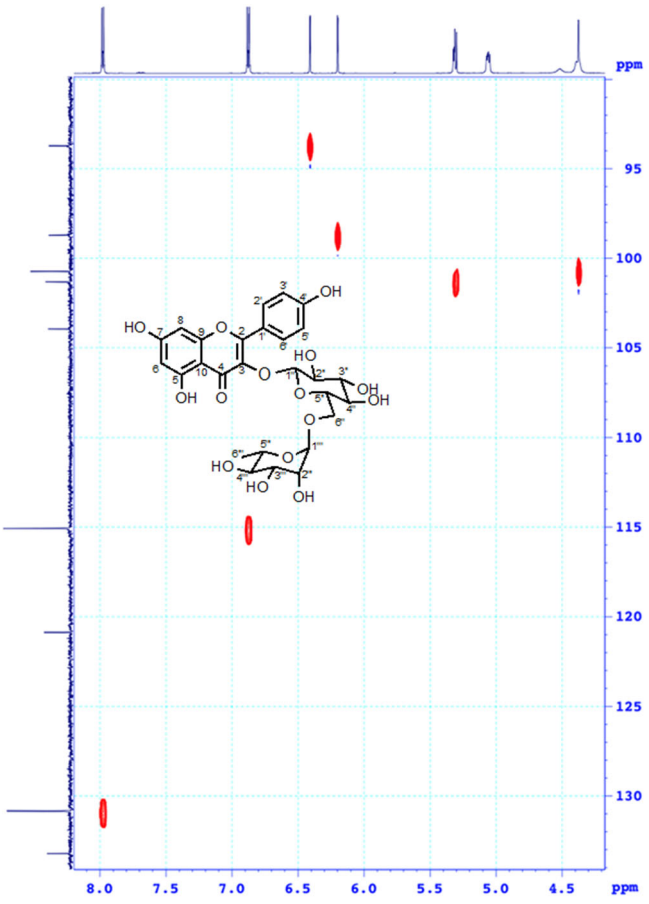
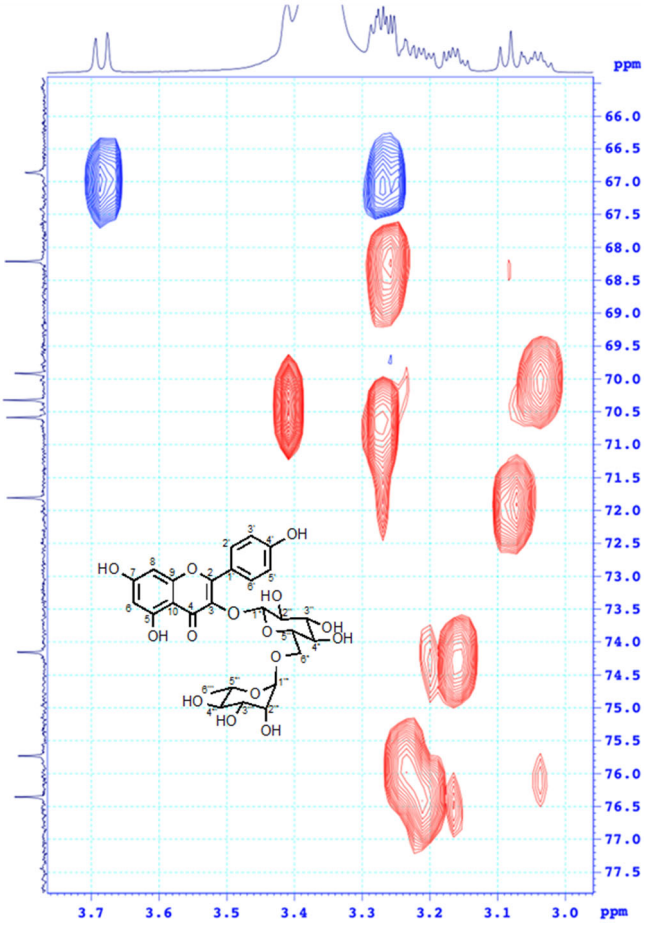


Fig S27. Expanded HSQC spectrum of compound **3**



FigS28. Expanded HSQC spectrum of compound **3**

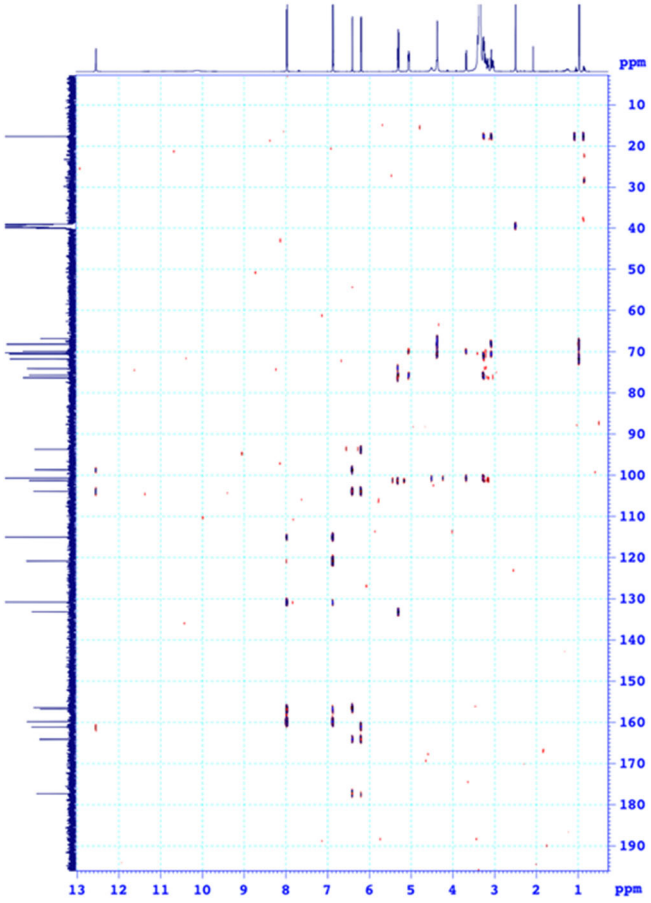


Fig S29. HMBC spectrum of compound **3**

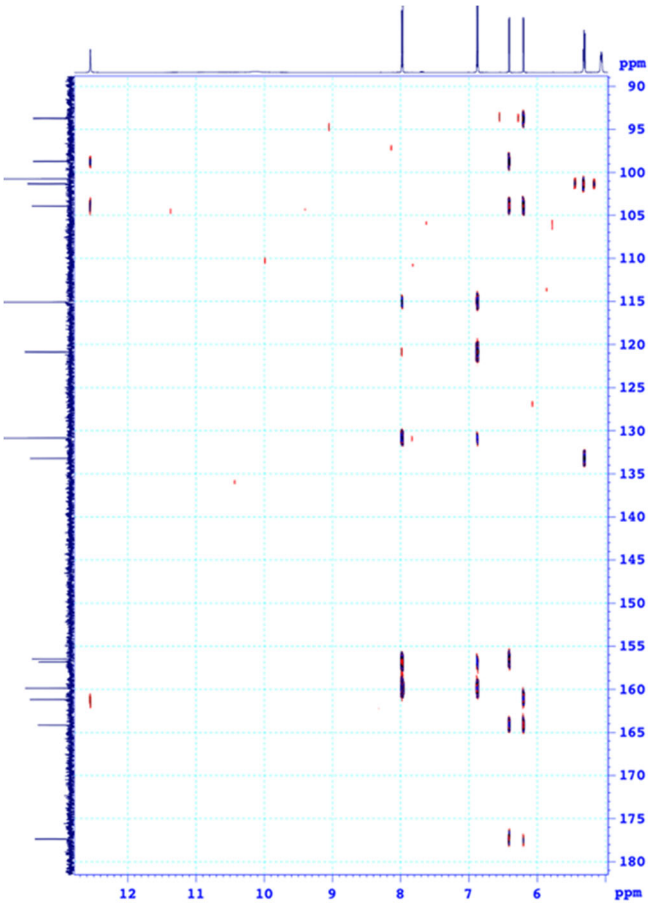


Fig S30. Expanded HMBC spectrum of compound **3**

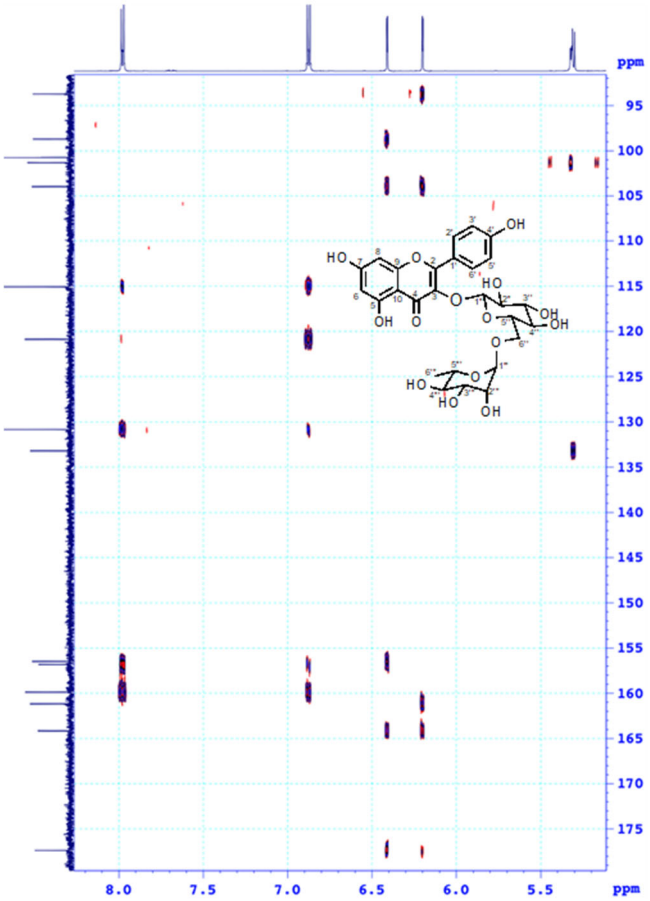


Fig S31. Expanded HMBC spectrum of compound **3**

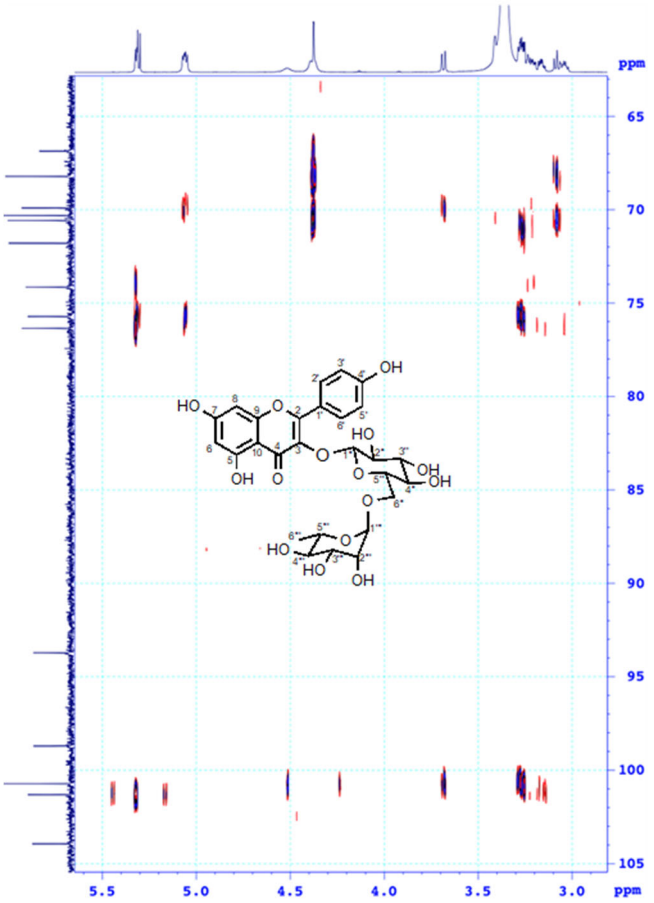


Fig S32. Expanded HMBC spectrum of compound **3**

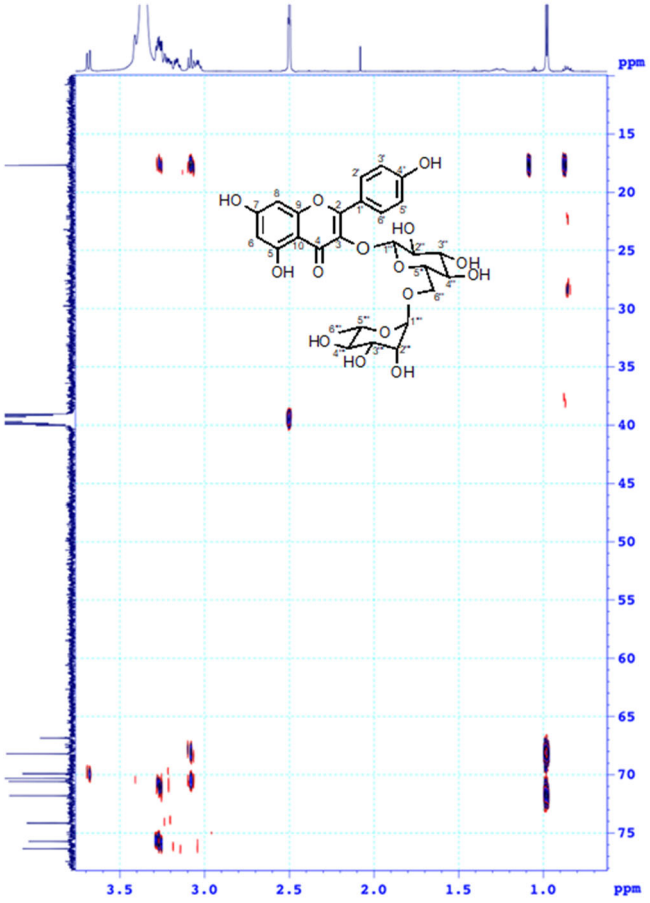


Fig S33. Expanded HMBC spectrum of compound **3**

4. Supplementary Spectroscopic Data of Compound 4

Quercetin-3-O-β-D-rutinoside (rutin) (**4**): ^{1}H-NMR (600 MHz, 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}C-NMR (150 MHz, 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''').

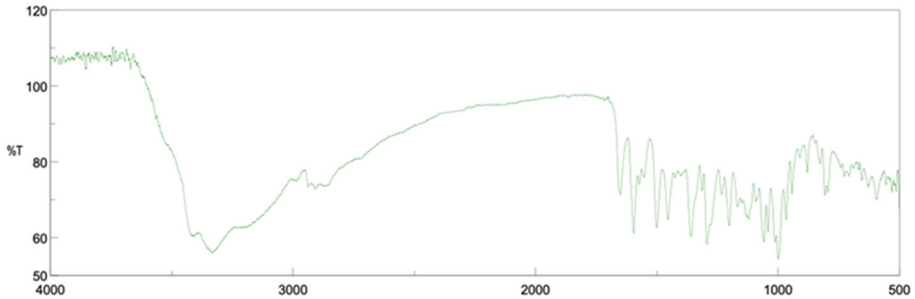


Fig S34. FTIR spectrum of compound **4**

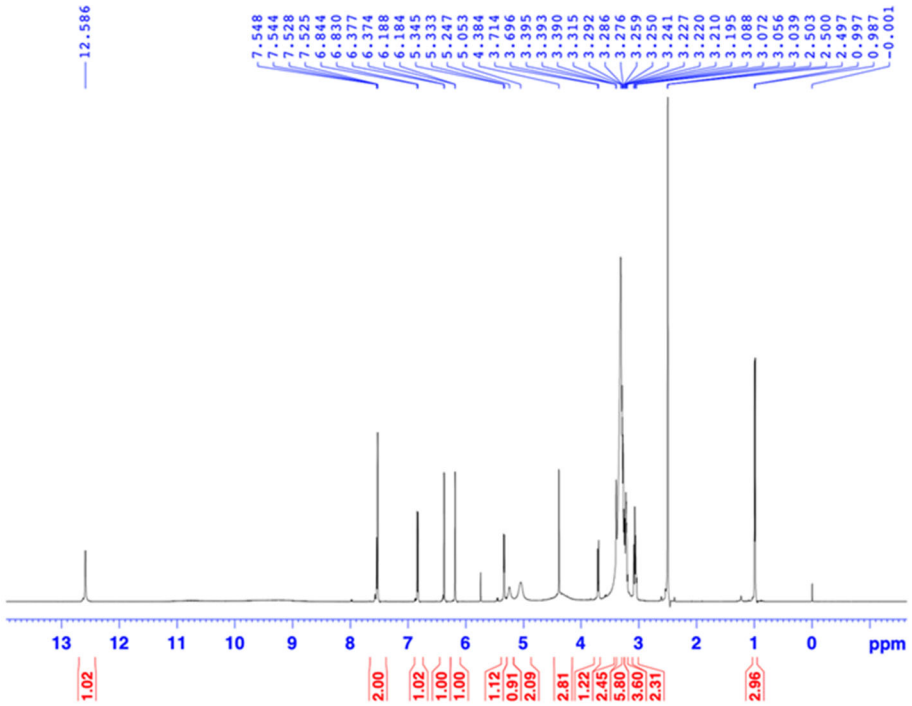


Fig S35. [1]H-NMR spectrum of compound **4**

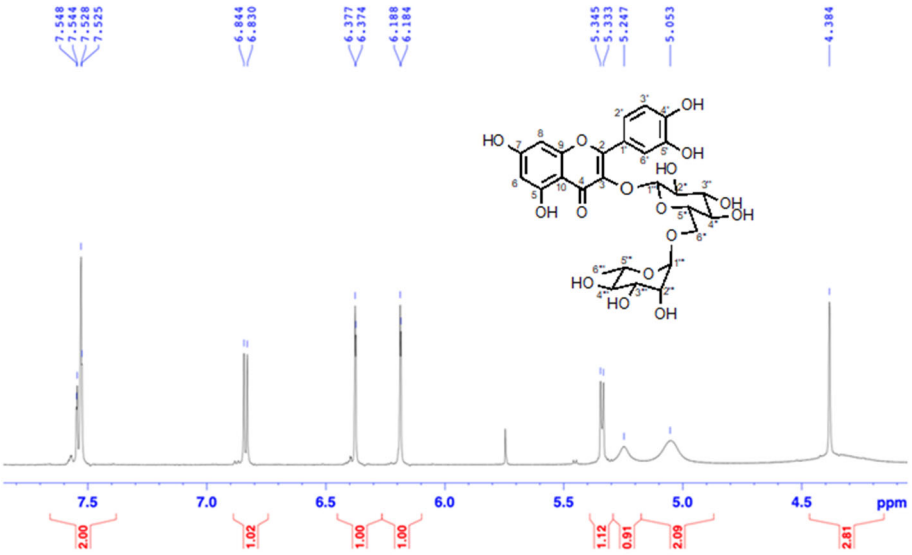


Fig S36. Expanded [1]H-NMR spectrum of compound **4**

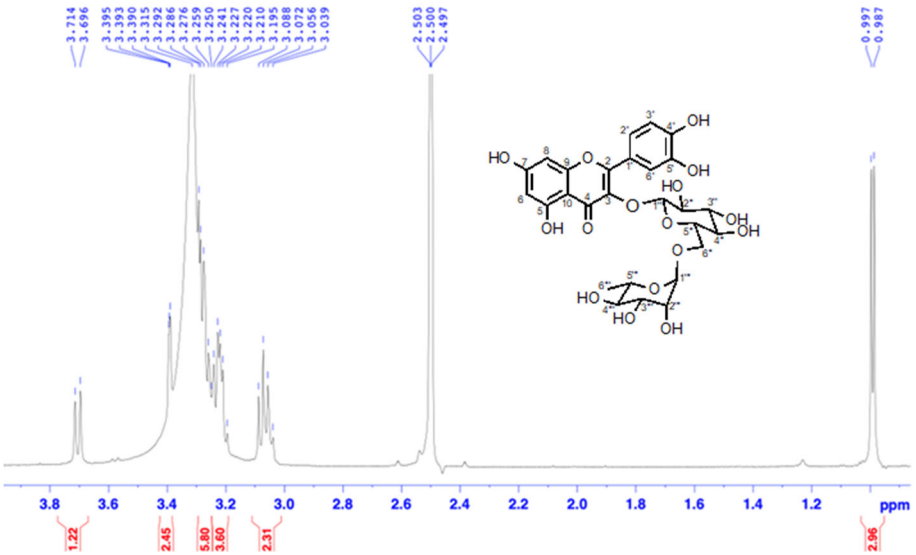


Fig S37. Expanded [1]H-NMR spectrum of compound **4**

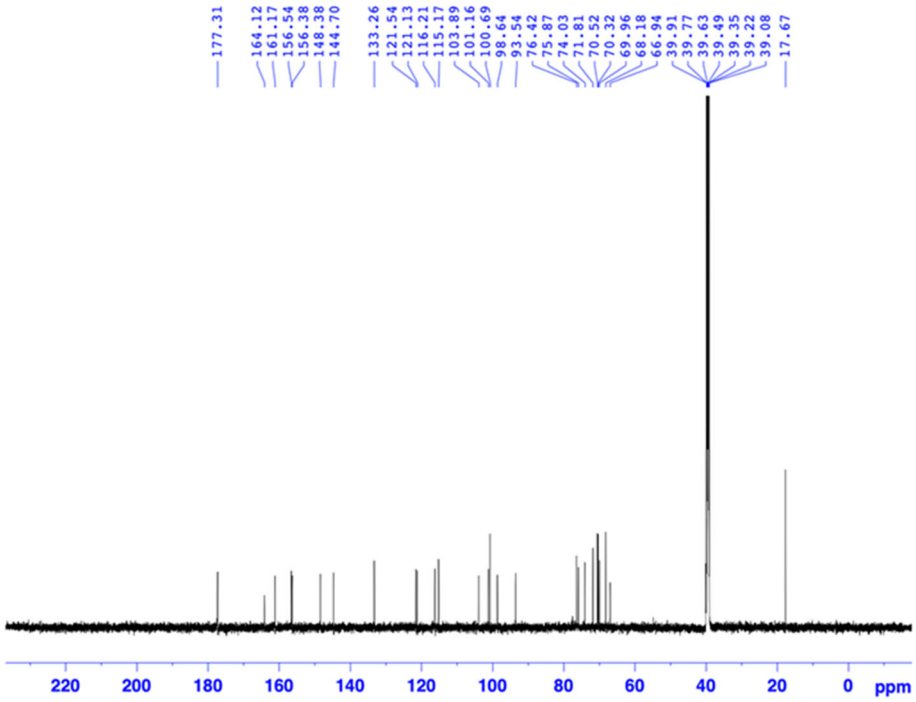


Fig S38. [13]C-NMR spectrum of compound **4**

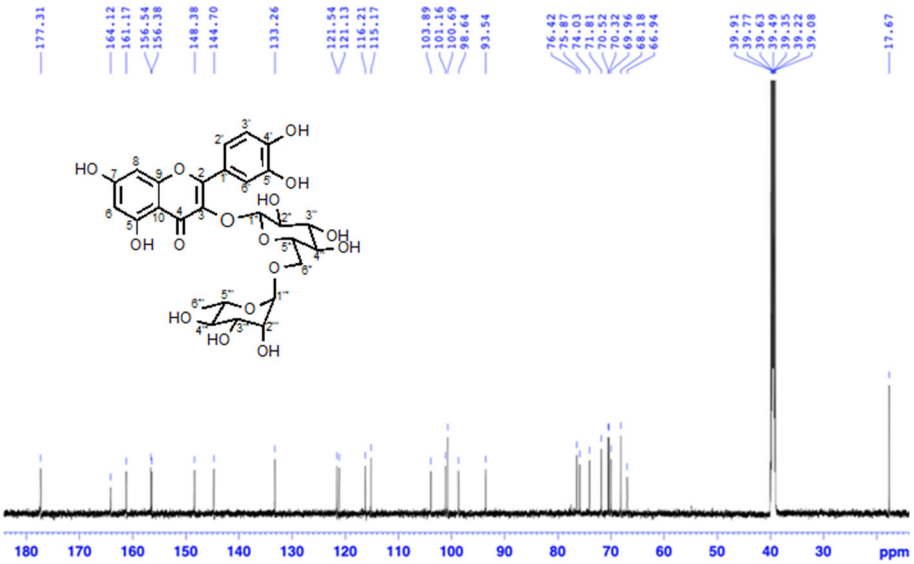


Fig S39. Expanded ^{13}C-NMR spectrum of compound **4**

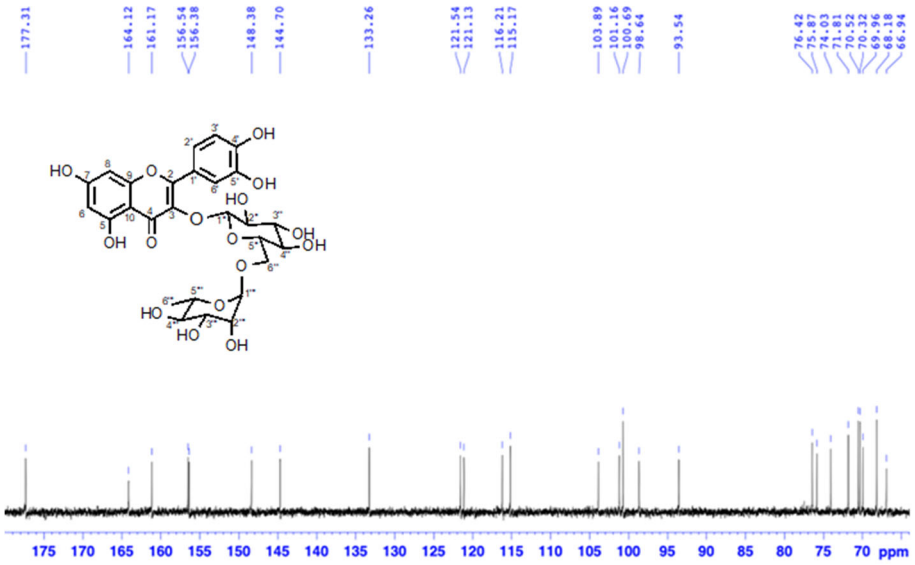


Fig S40. Expanded ^{13}C-NMR spectrum of compound **4**

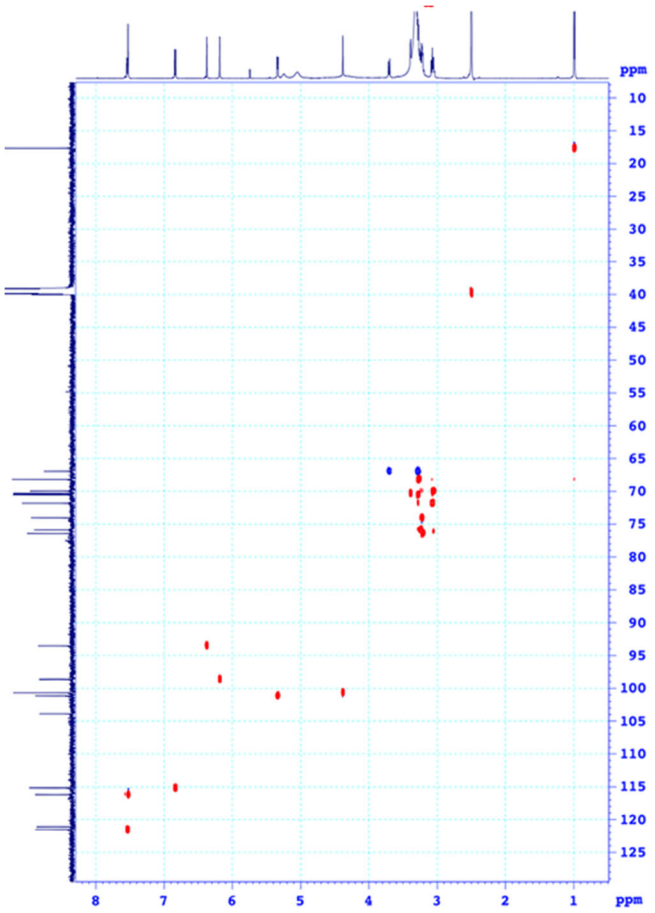


Fig S41. HSQC spectrum of compound **4**

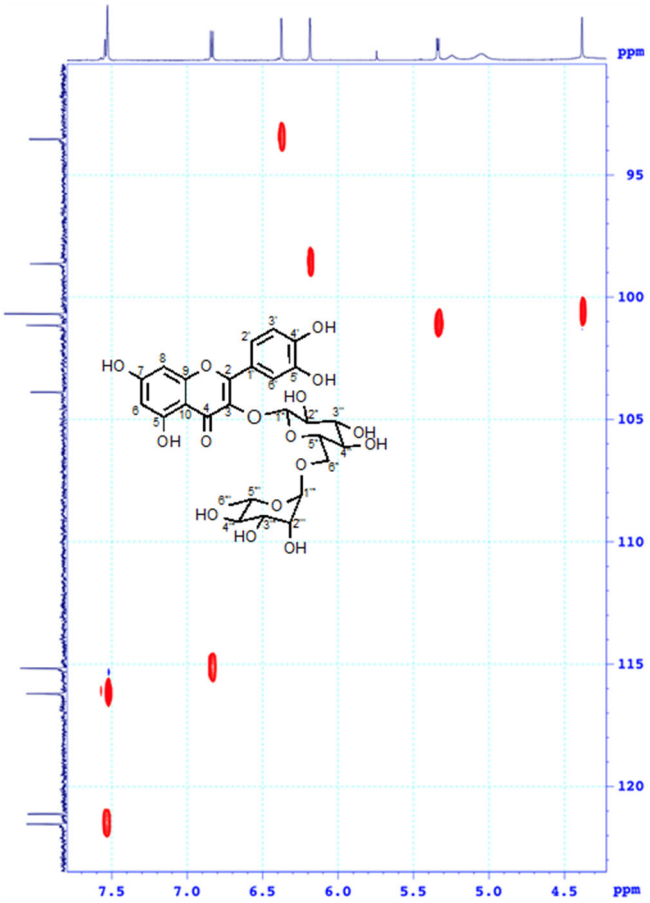


Fig S42. Expanded HSQC spectrum of compound **4**

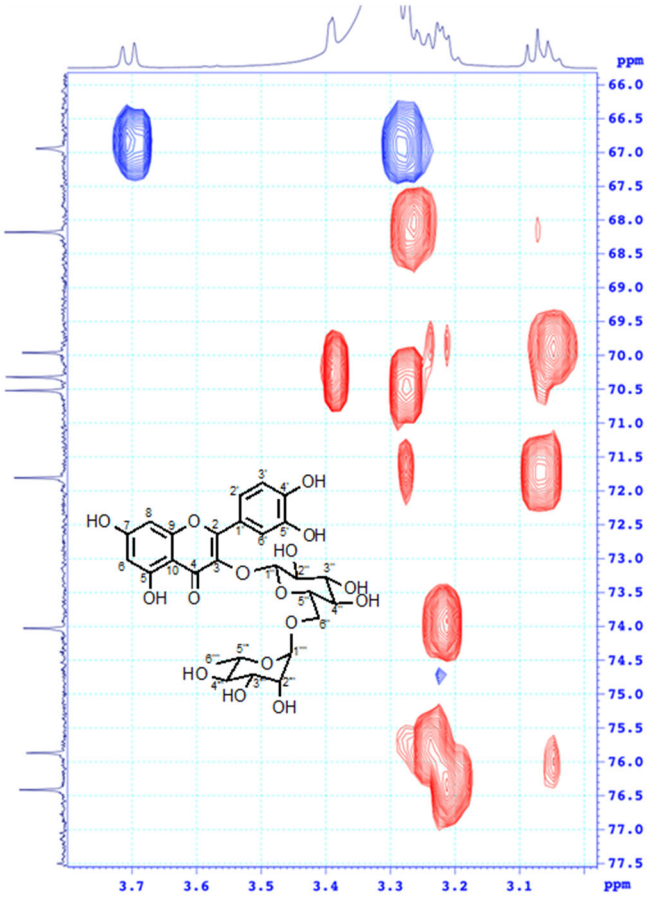


Fig S43. Expanded HSQC spectrum of compound **4**

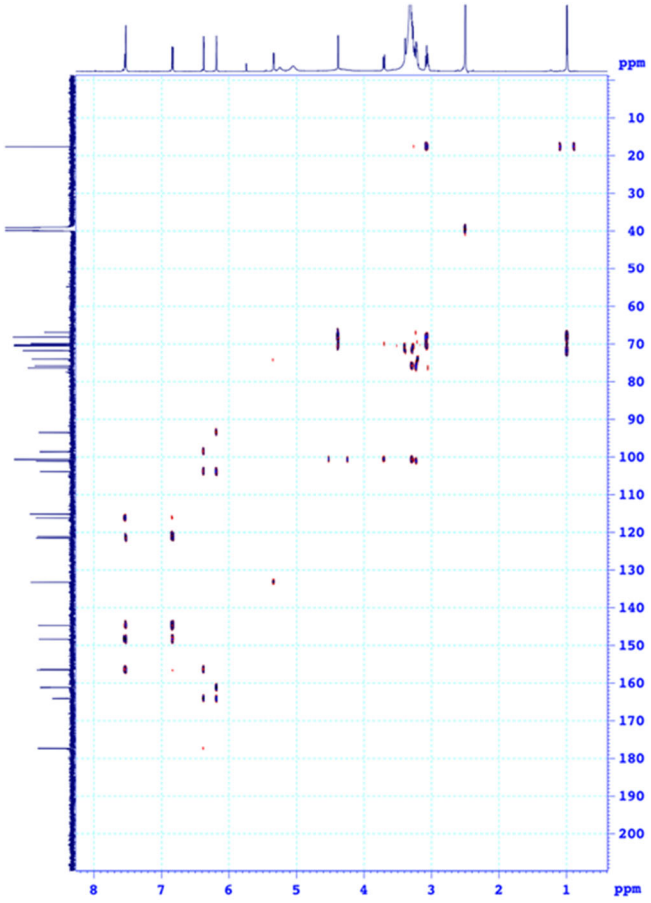


Fig S44. HMBC spectrum of compound **4**

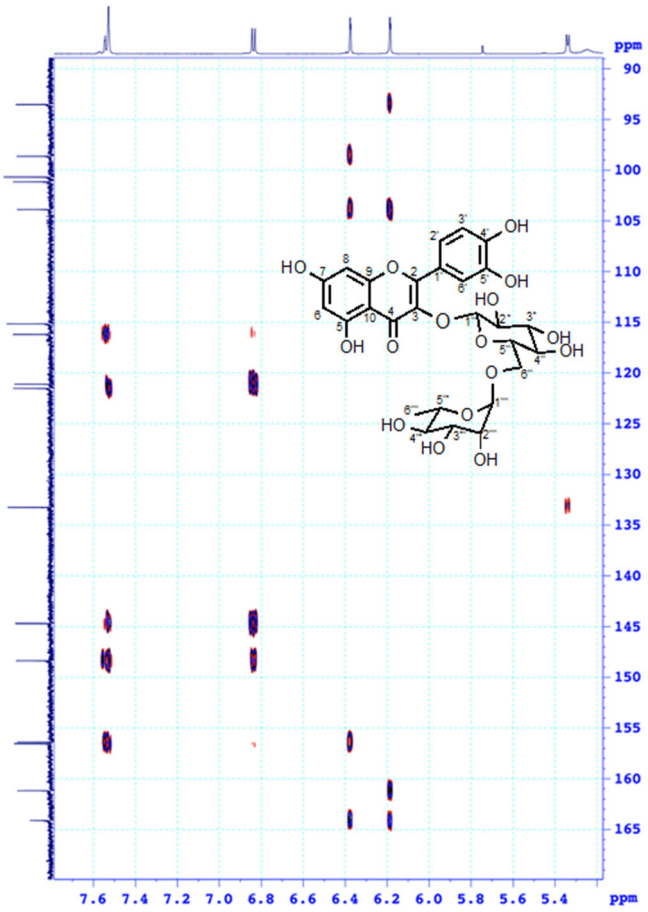


Fig S45. Expanded HMBC spectrum of compound **4**

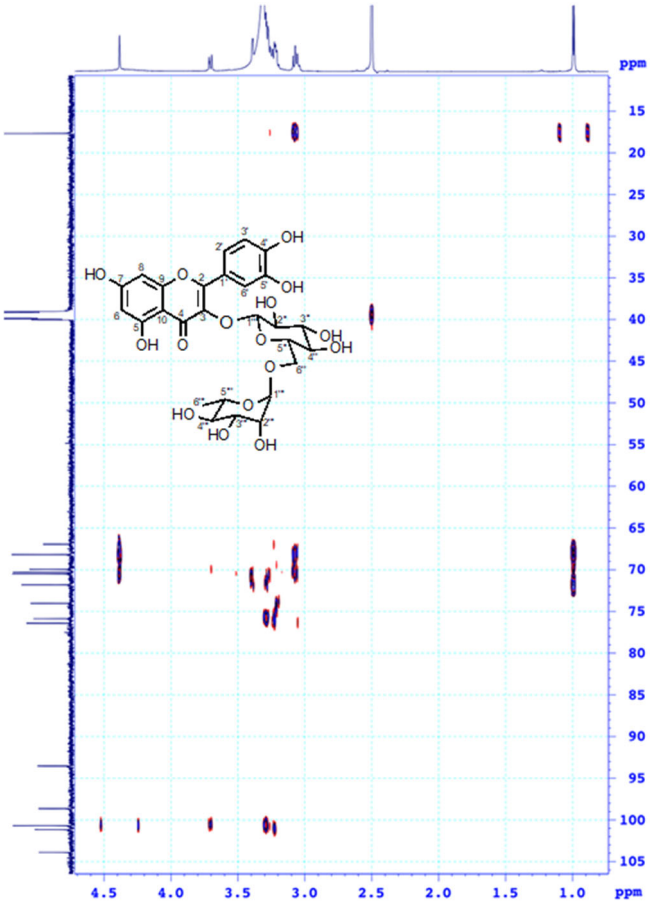


Fig S46. Expanded HMBC spectrum of compound **4**

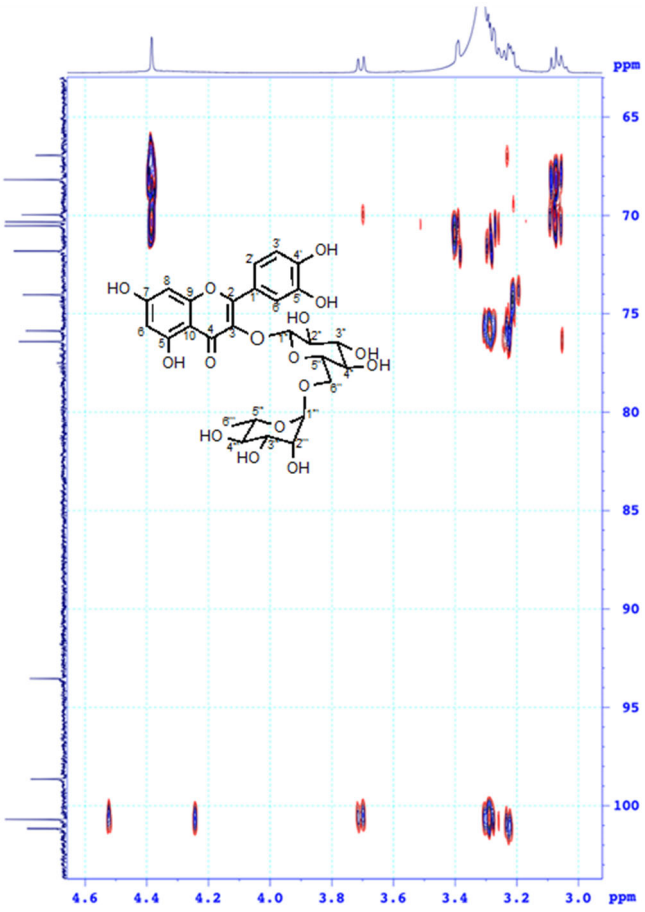


Fig S47. Expanded HMBC spectrum of compound **4**

5. Supplementary Spectroscopic Data of Compound 5

3,4-Dihydroxycinnamic acid (caffeic acid) (**5**): ^{1}H-NMR (600 MHz, MeOD), 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}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 $[M+H]^+$, 163.0391 $[M+H-H_2O]^+$, calculated $C_9H_8O_4$, *m/z* 180.0423.

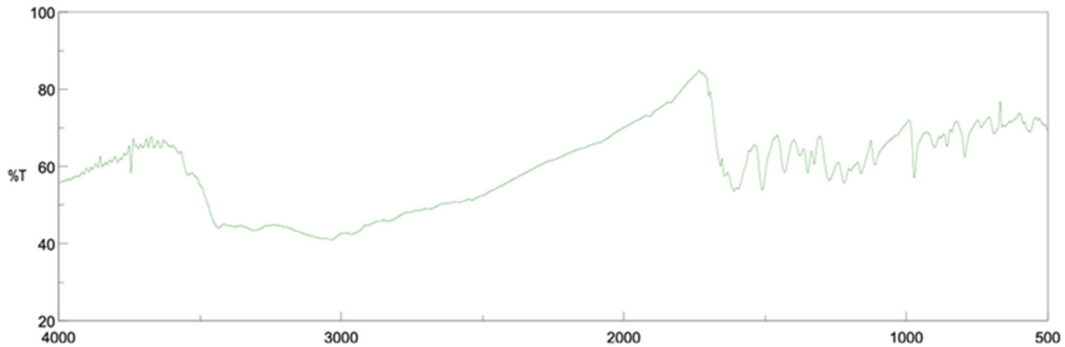


Fig S48. FTIR spectrum of compound **5**

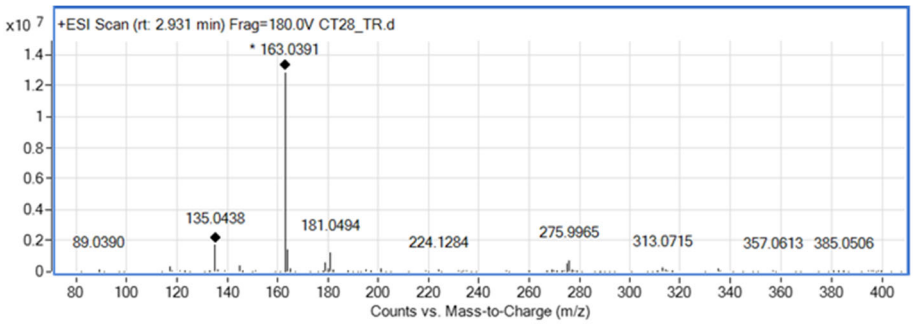


Fig S49. (+)ESI-MS spectrum of compound **5**

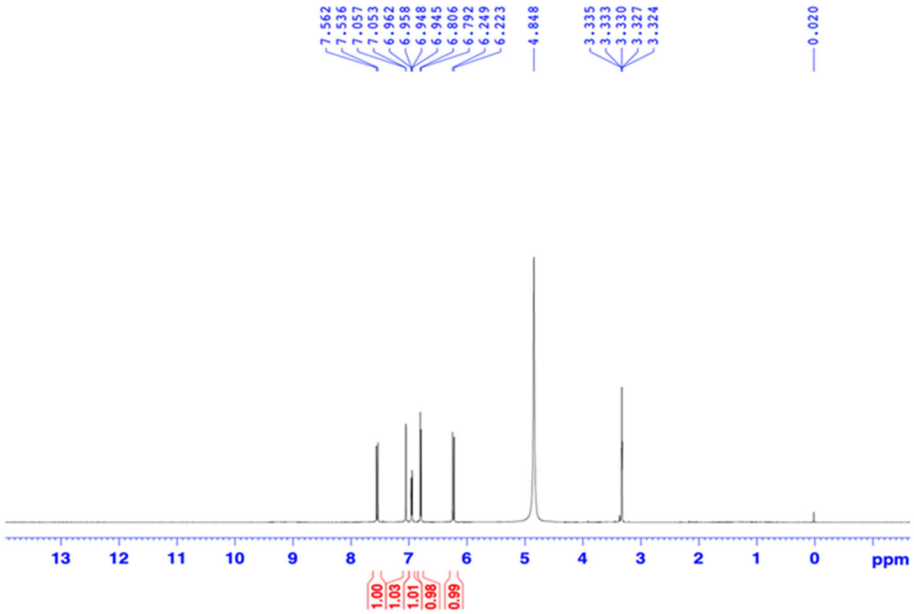


Fig S50. [1]H-NMR spectrum of compound **5**

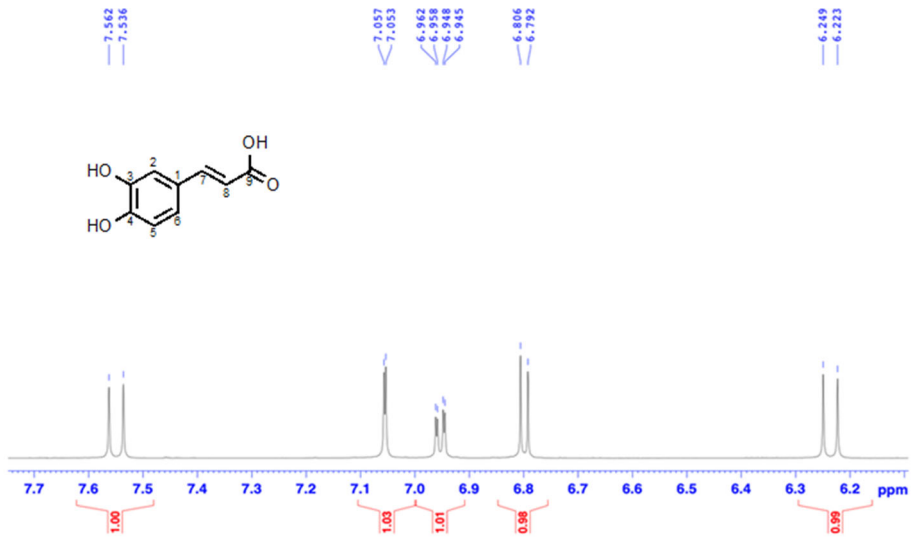


Fig S51. Expanded [1]H-NMR spectrum of compound **5**

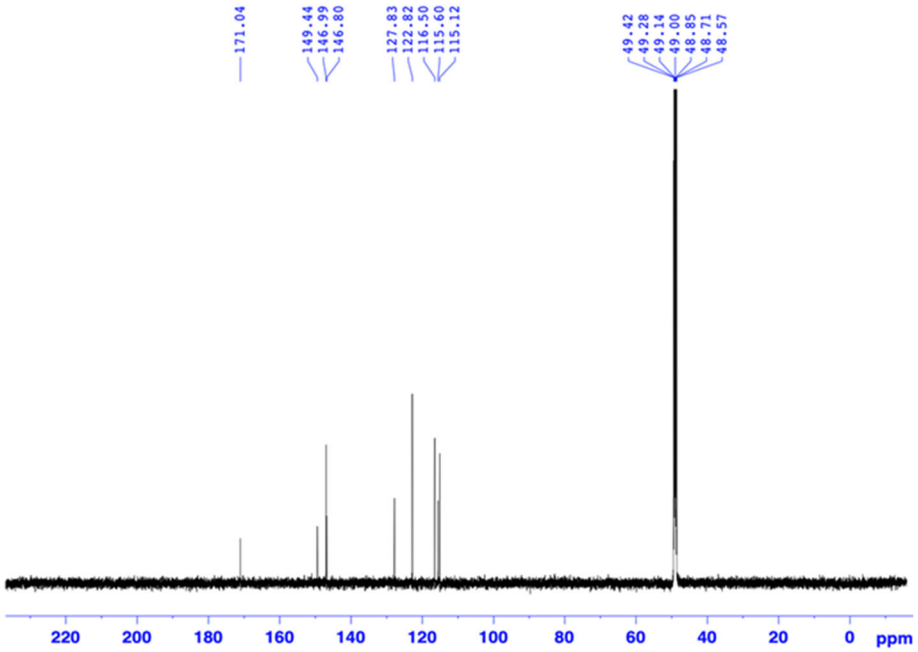


Fig S52. ^{13}C-NMR spectrum of compound **5**

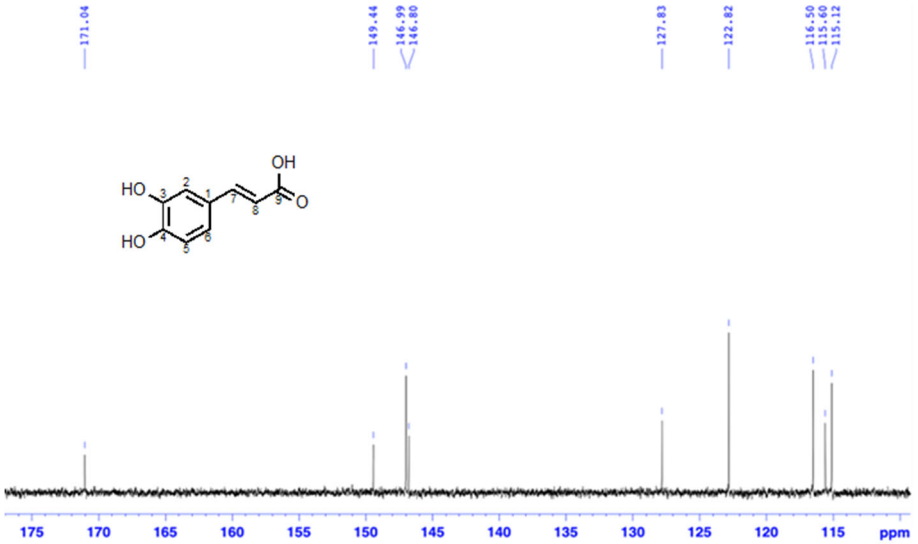


Fig S52. Expanded ^{13}C-NMR spectrum of compound **5**

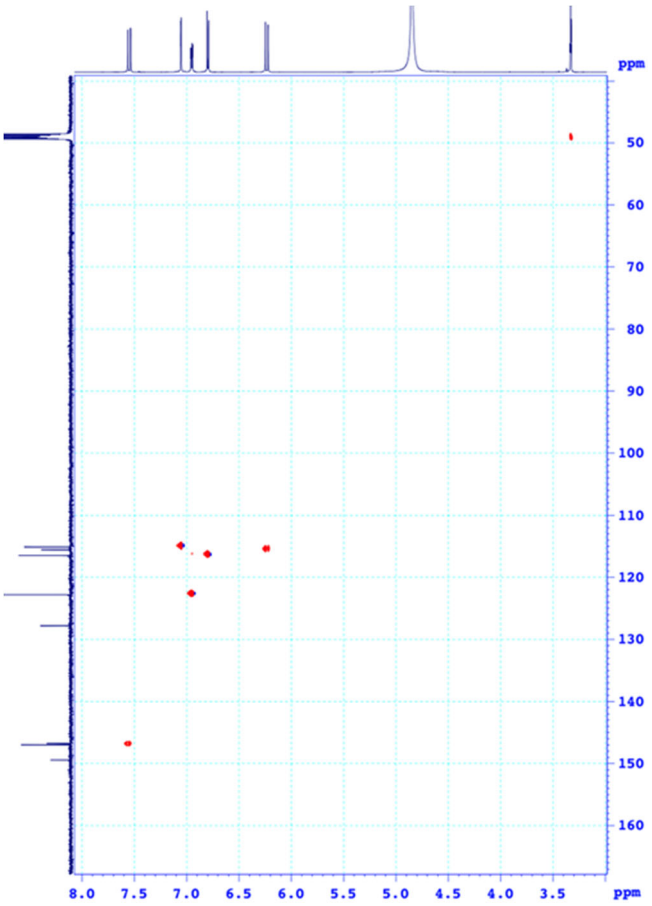


Fig S53. HSQC spectrum of compound **5**

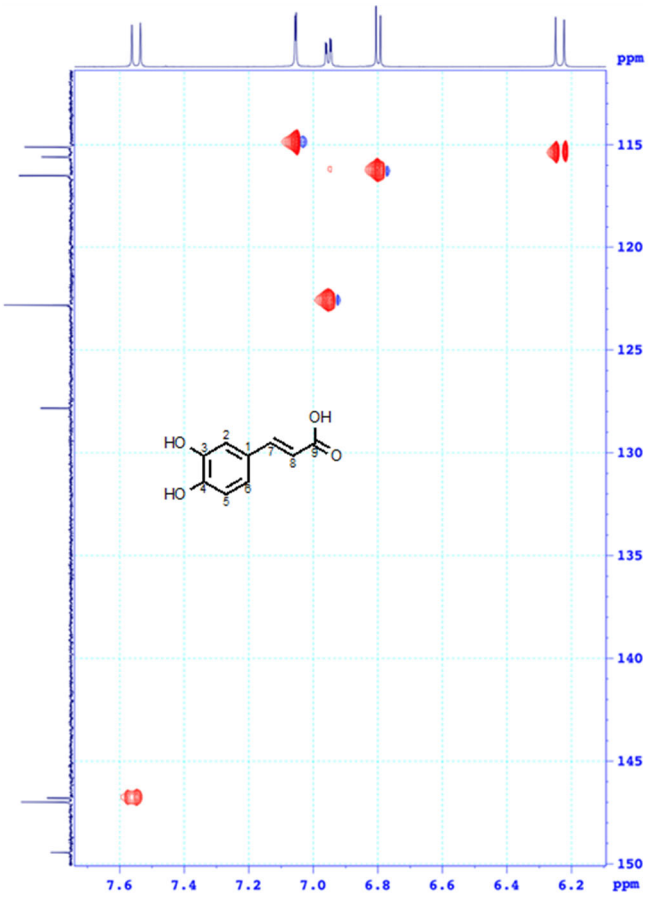


Fig S54. Expanded HSQC spectrum of compound **5**

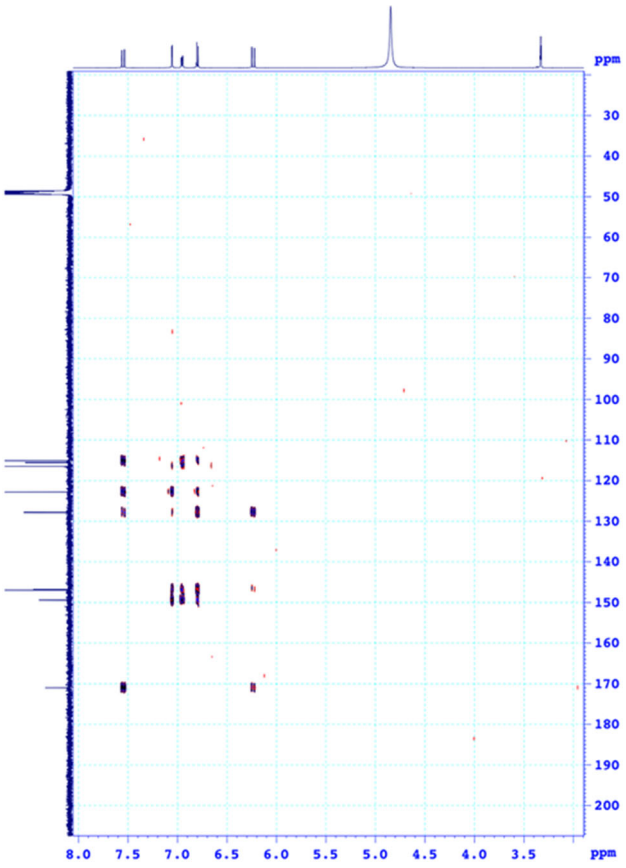


Fig S55. HMBC spectrum of compound **5**

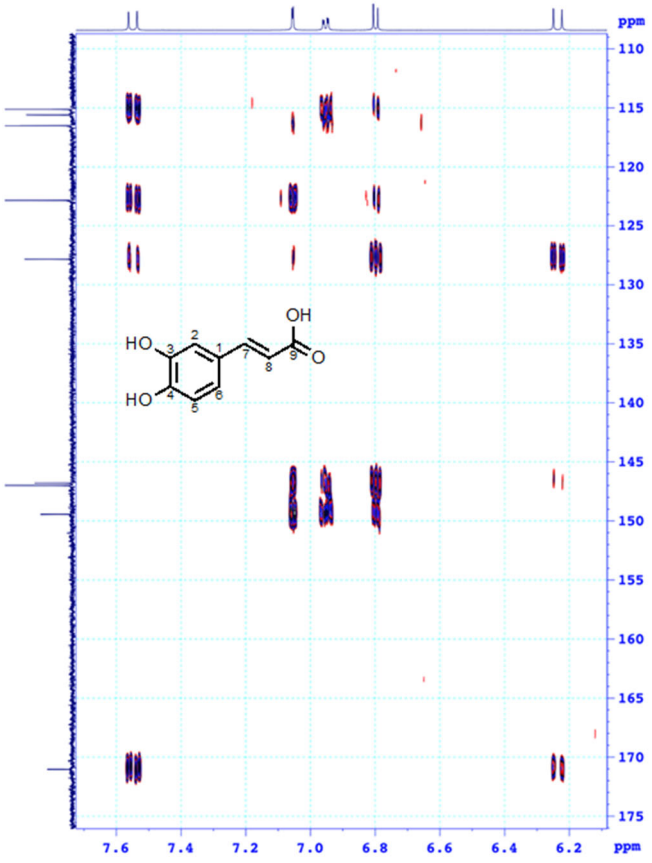


Fig S56. Expanded HMBC spectrum of compound **5**

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)(6): ^{1}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-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, $CDCl_3$), 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 $[M+H]^+$, 179.1076 $[M+H-H_2O]^+$, calculated $C_{11}H_{16}O_3$, *m/z* 196.1099.

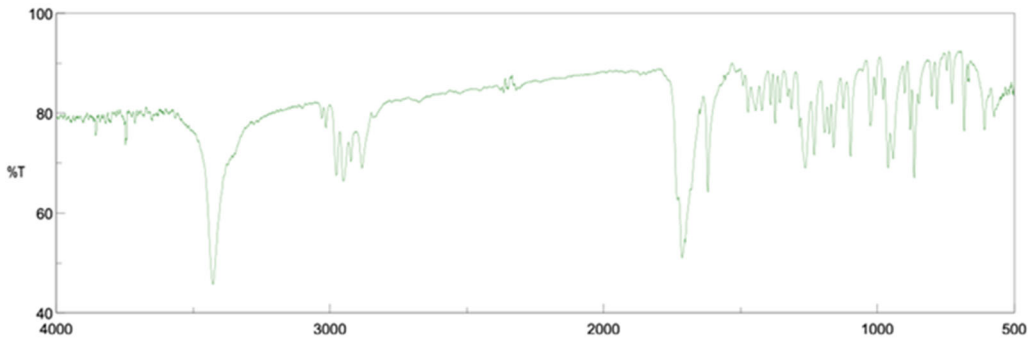


Fig S57. FTIR spectrum of compound **6**

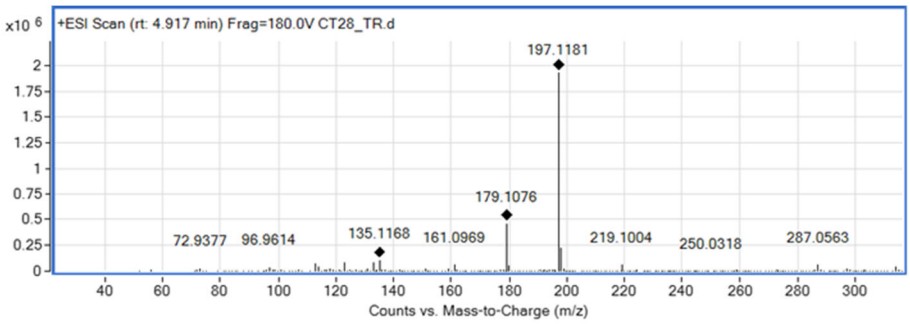


Fig S58. (+)ESI-MS spectrum of compound **6**

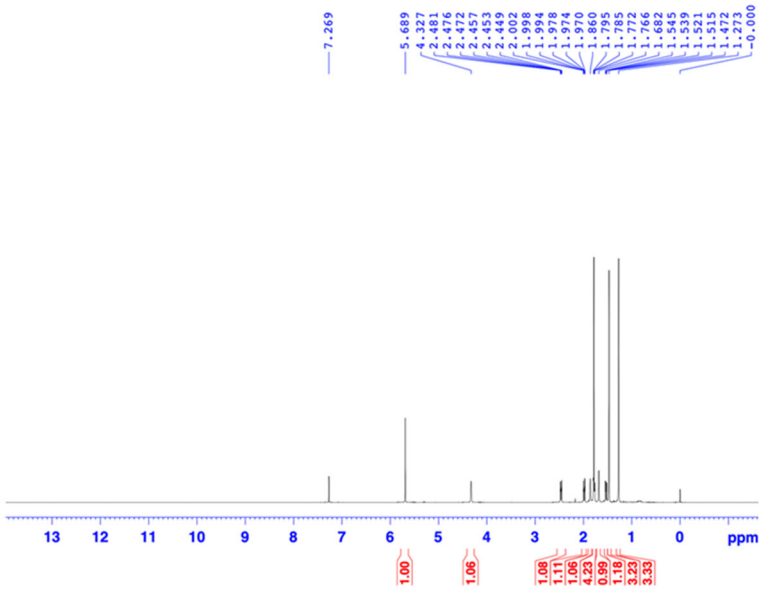


Fig S59. ^{1}H-NMR spectrum of compound **6**

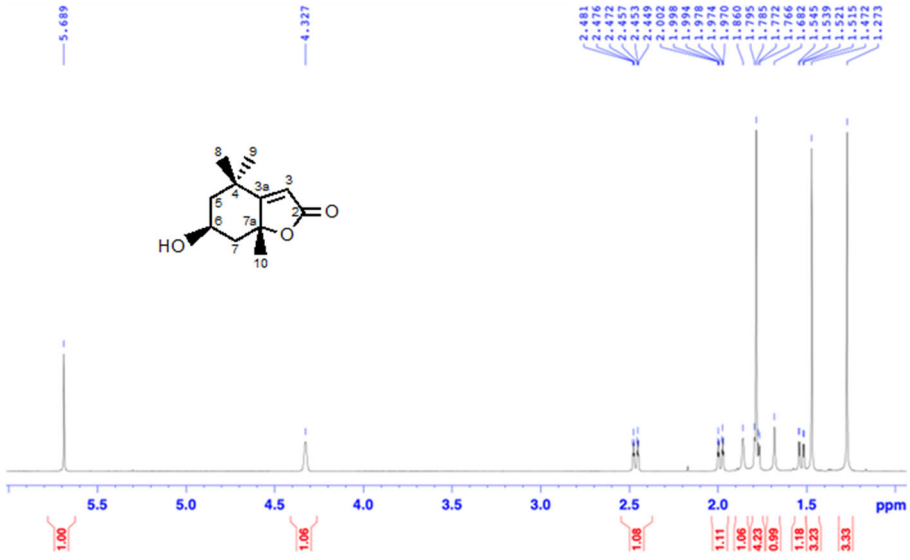


Fig S60. Expanded ^{1}H-NMR spectrum of compound **6**

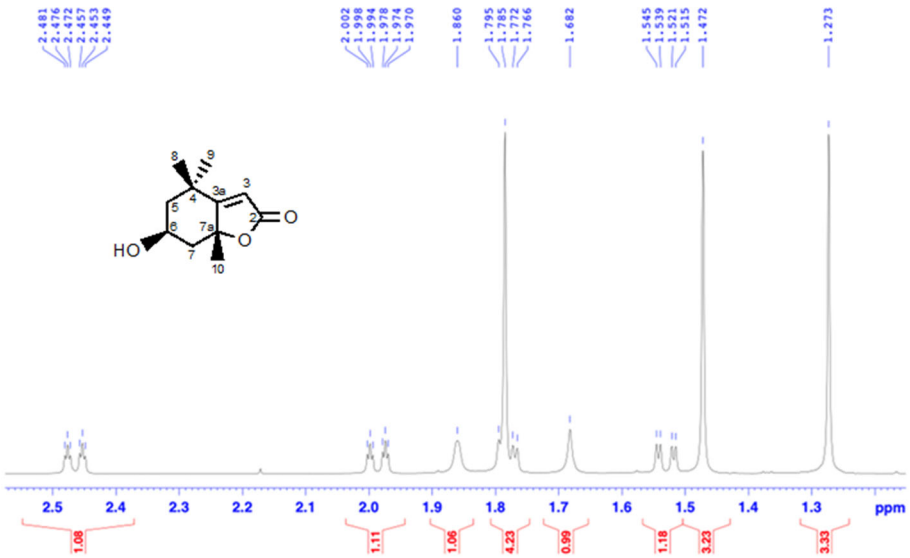


Fig S61. Expanded [1]H-NMR spectrum of compound **6**

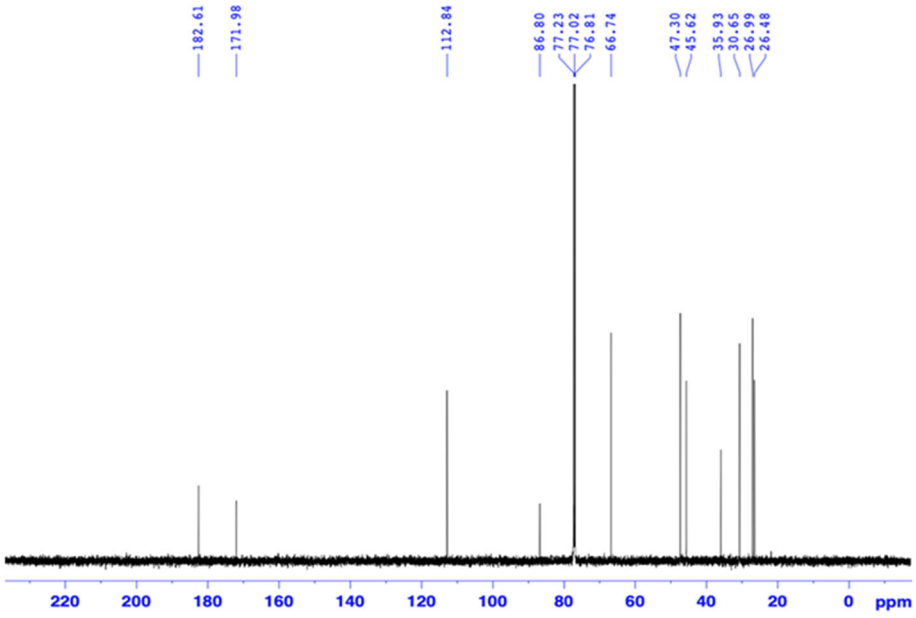


Fig S62. [13]C-NMR spectrum of compound **6**

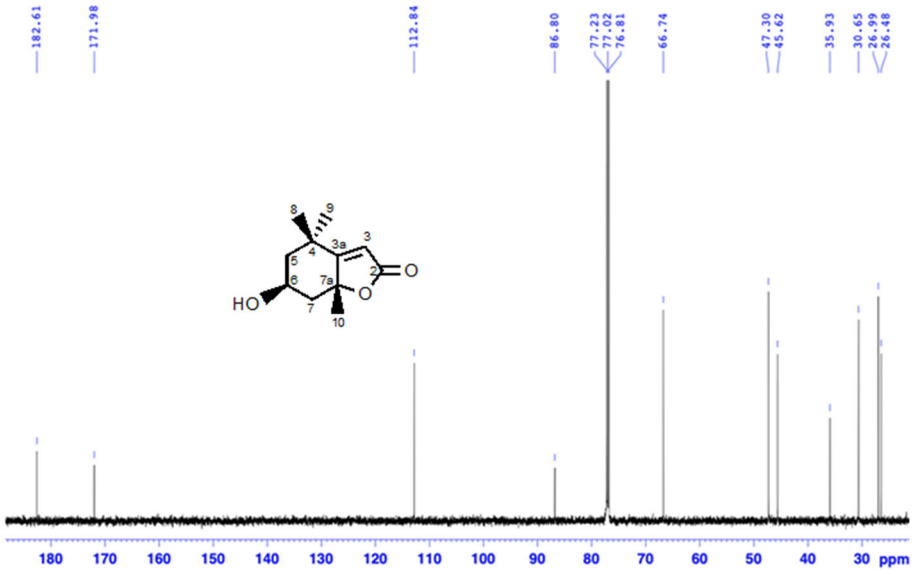


Fig S63. Expanded ^{13}C-NMR spectrum of compound **6**

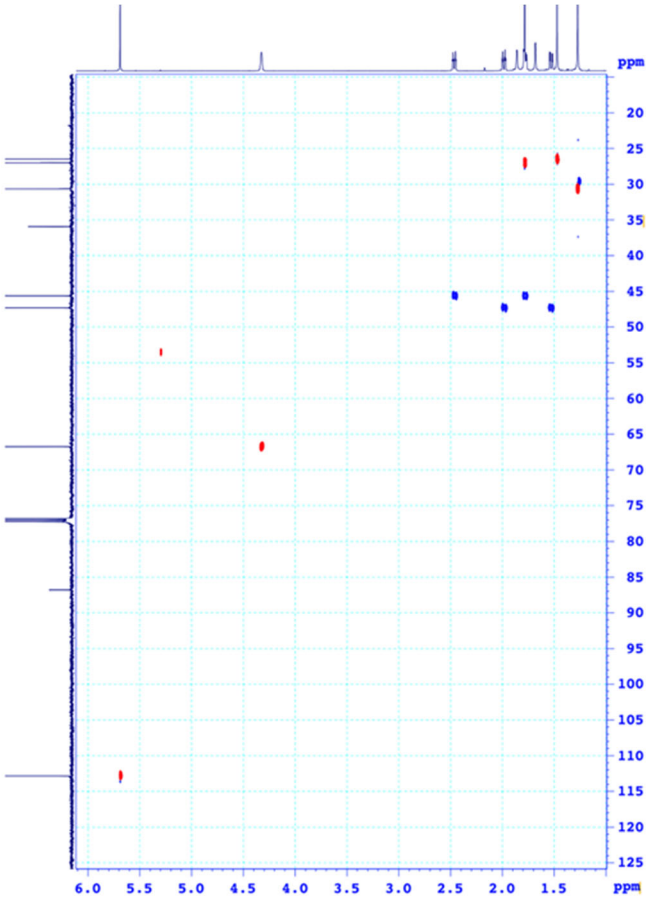


Fig S64. HSQC spectrum of compound **6**

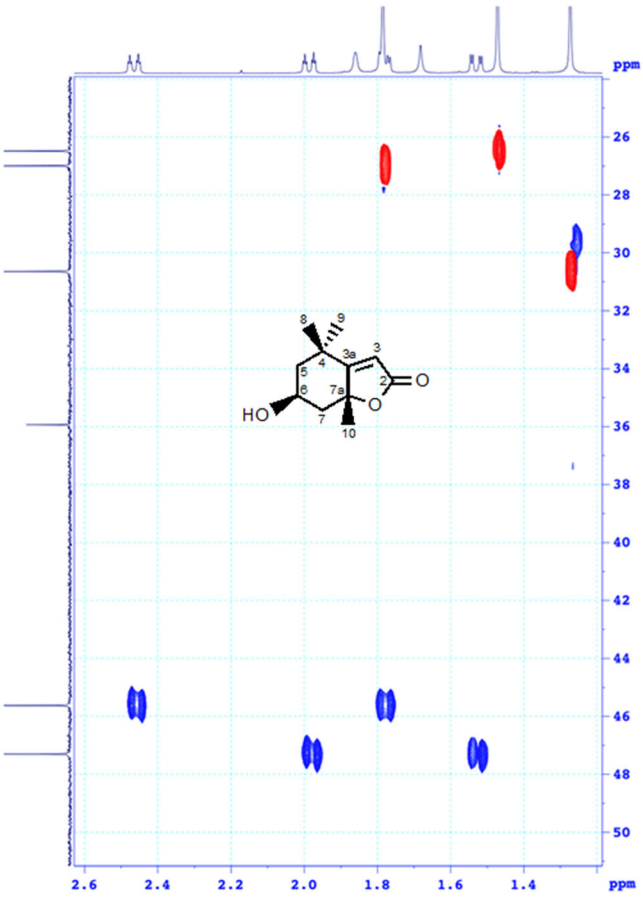


Fig S65. Expanded HSQC spectrum of compound **6**

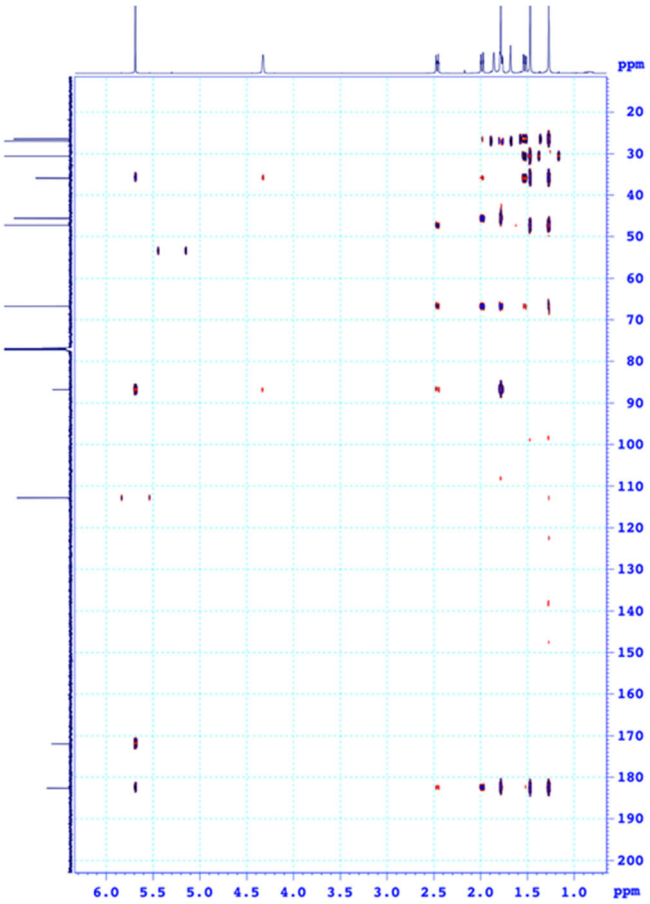


Fig S66. HMBC spectrum of compound **6**

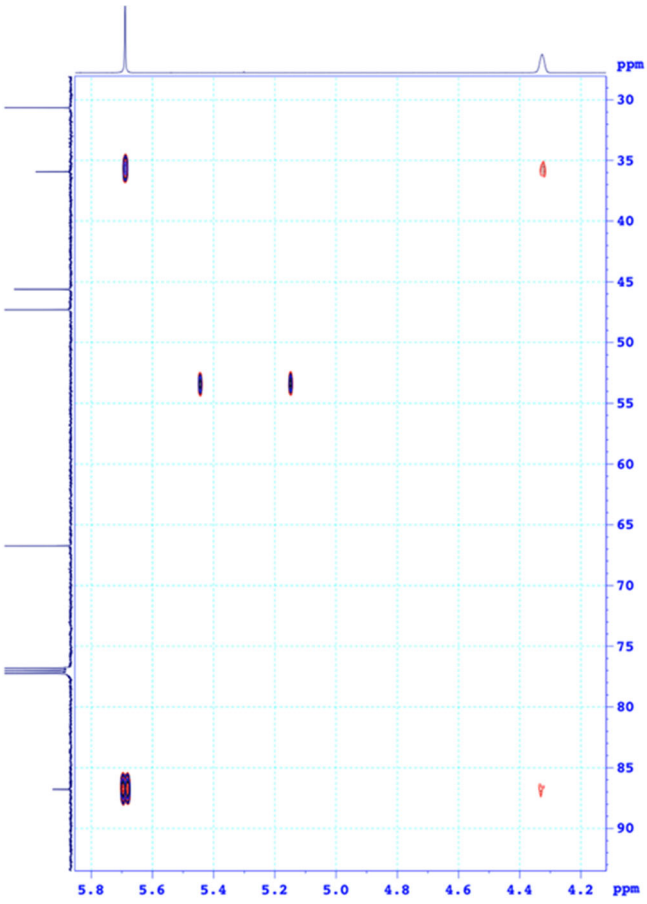


Fig S67. Expanded HMBC spectrum of compound **6**

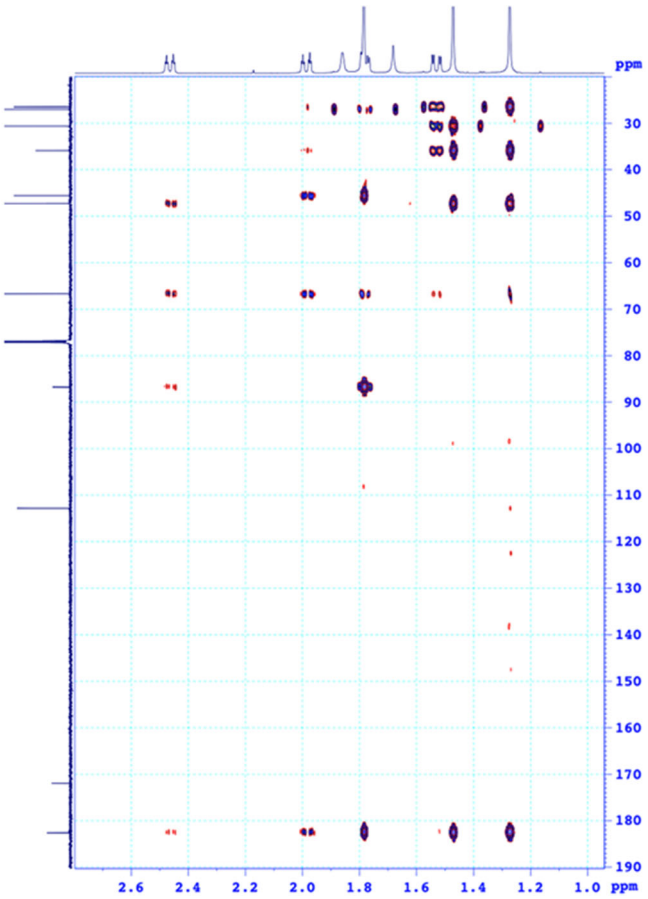


Fig S69. Expanded HMBC spectrum of compound **6**

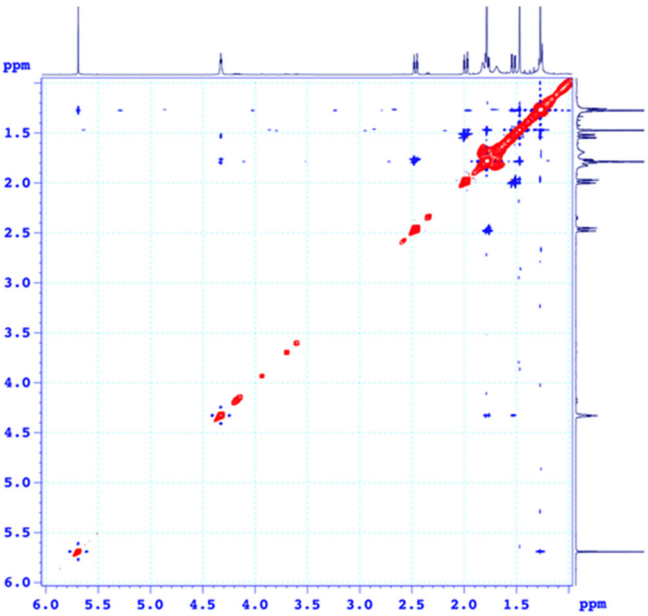


Fig S70. Complete assignment NOESY spectrum of compound **6**

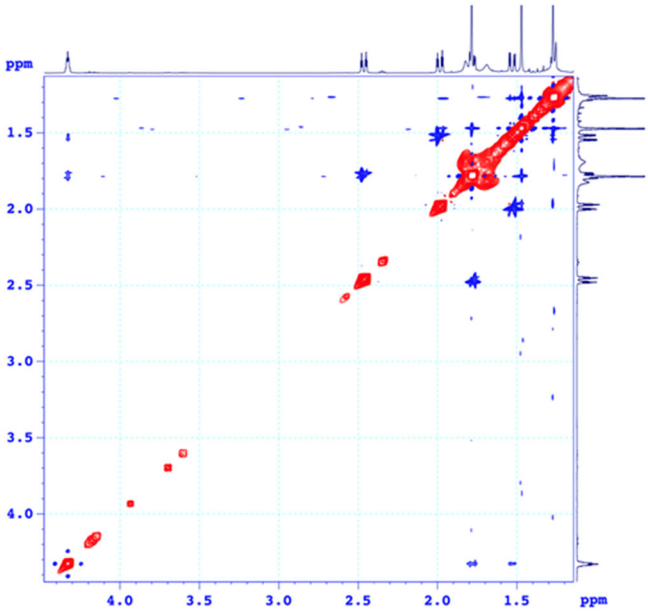


Fig S71. Expanded NOESY spectrum of compound **6**

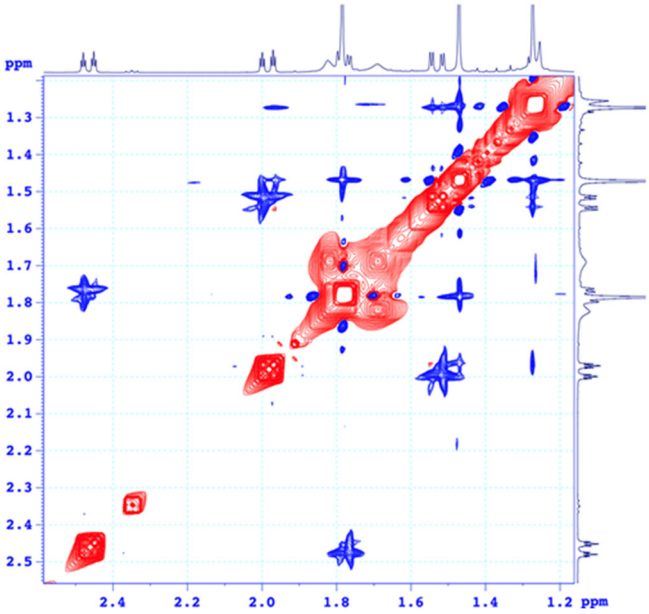


Fig S72. Expanded NOESY spectrum of compound **6**

7. Supplementary Spectroscopic Data of Compound 7

β-Sitosterol-3-O-β-D-glucopyranoside (daucosterol) (**7**): ^{1}H-NMR (600 MHz, DMSO-d_6), δ_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), 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').

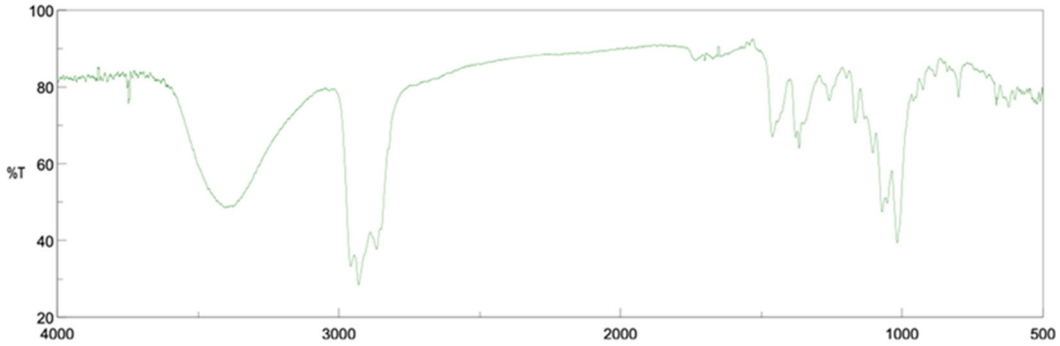


Fig S73. FTIR spectrum of compound **7**

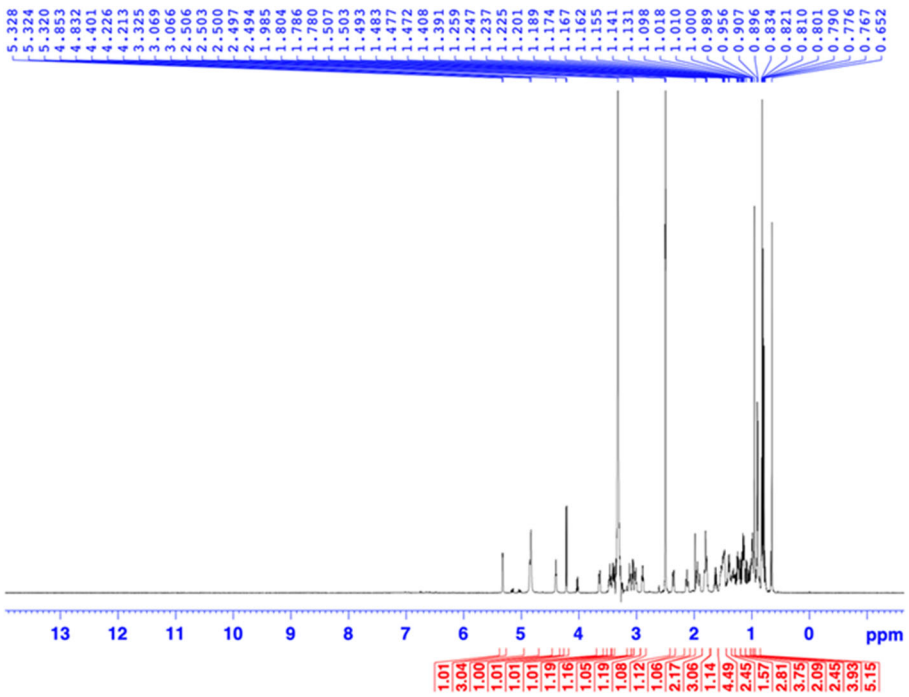


Fig S74. ^{1}H-NMR spectrum of compound **7**

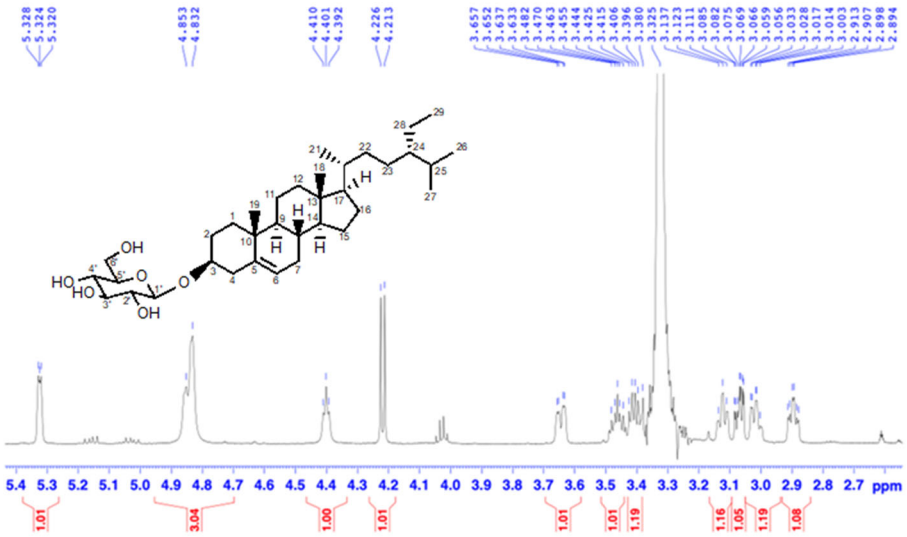


Fig S75. Expanded ^{1}H-NMR spectrum of compound **7**

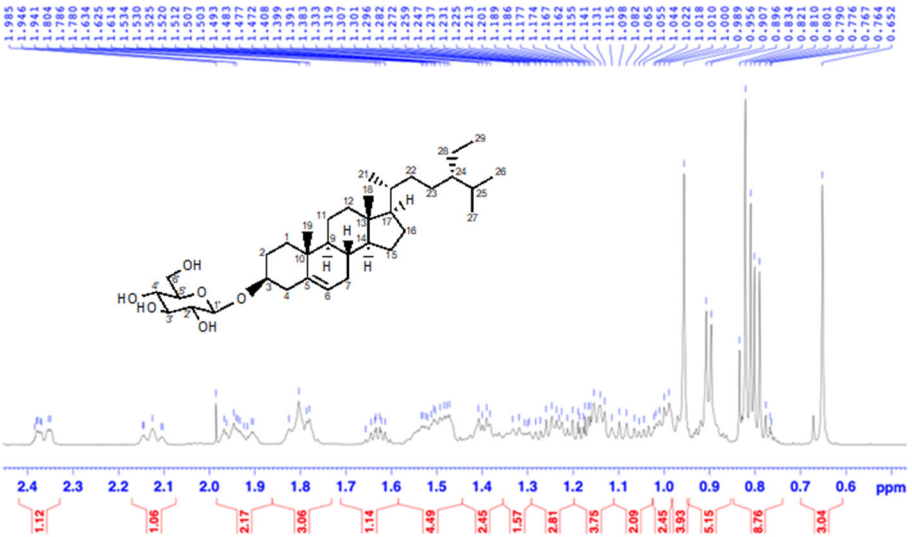


Fig S76. Expanded ^{1}H-NMR spectrum of compound **7**

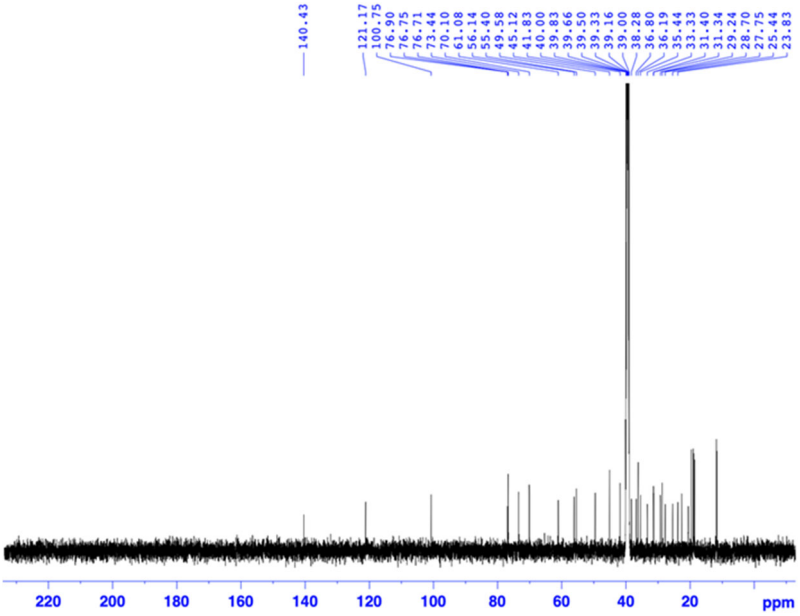


Fig S77. ^{13}C-NMR spectrum of compound **7**

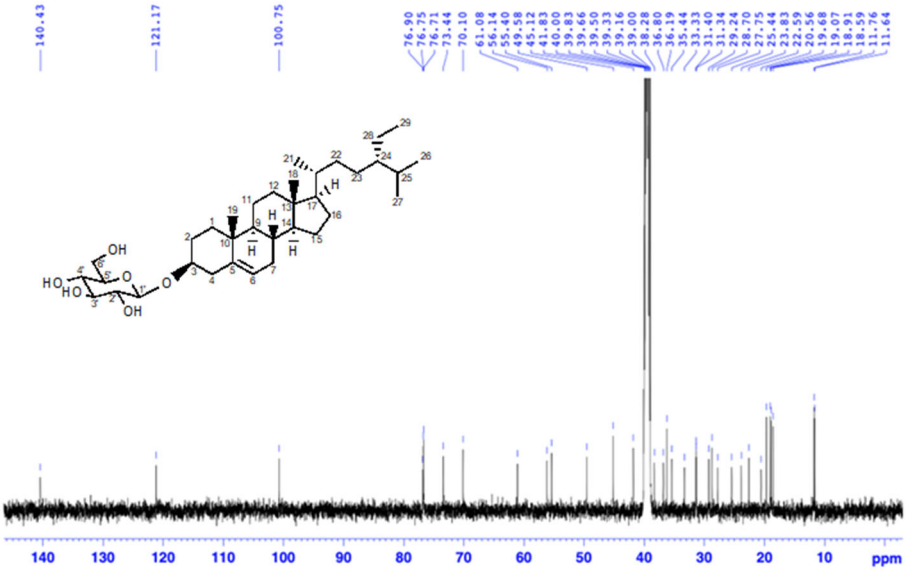


Fig S78. Expanded ^{13}C-NMR spectrum of compound **7**

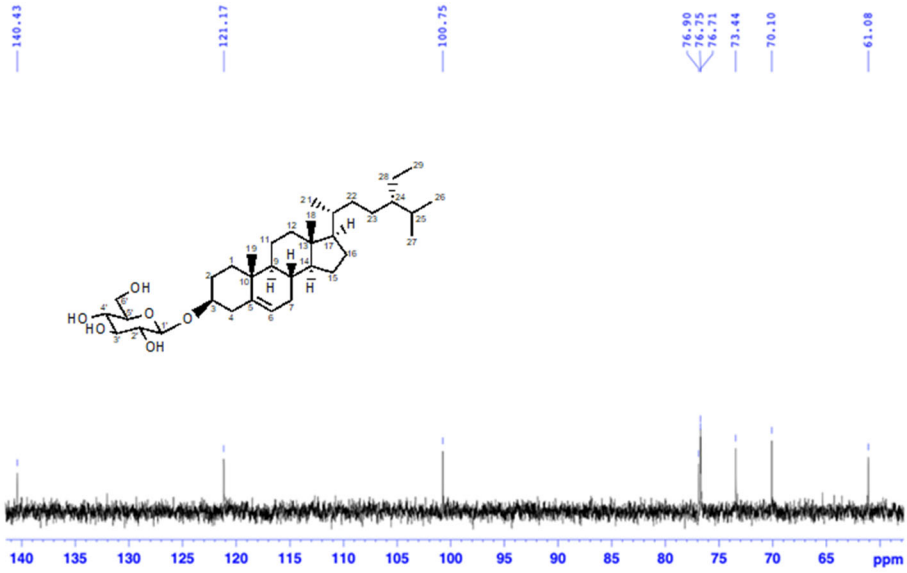


Fig S79. Expanded ^{13}C-NMR spectrum of compound **7**

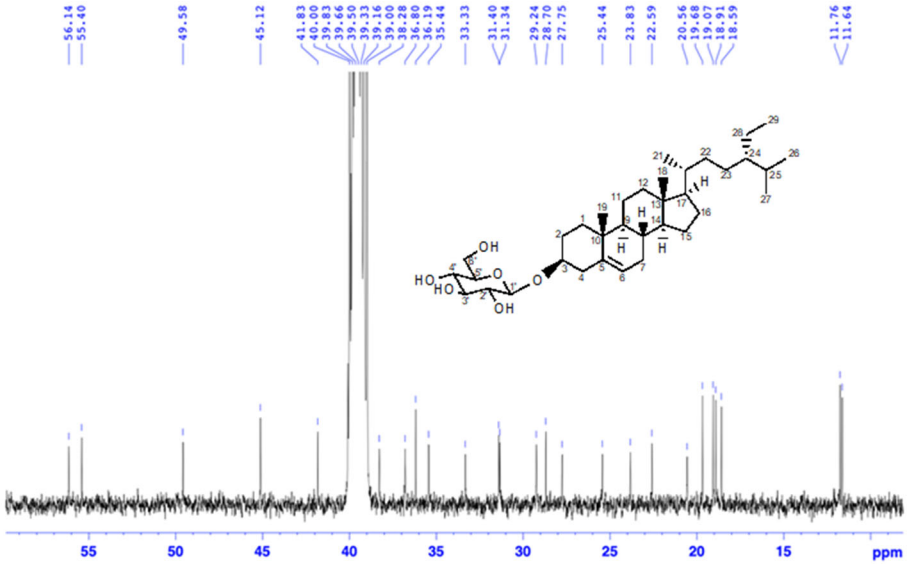


Fig S80. Expanded ^{13}C-NMR spectrum of compound **7**