

Supporting Information

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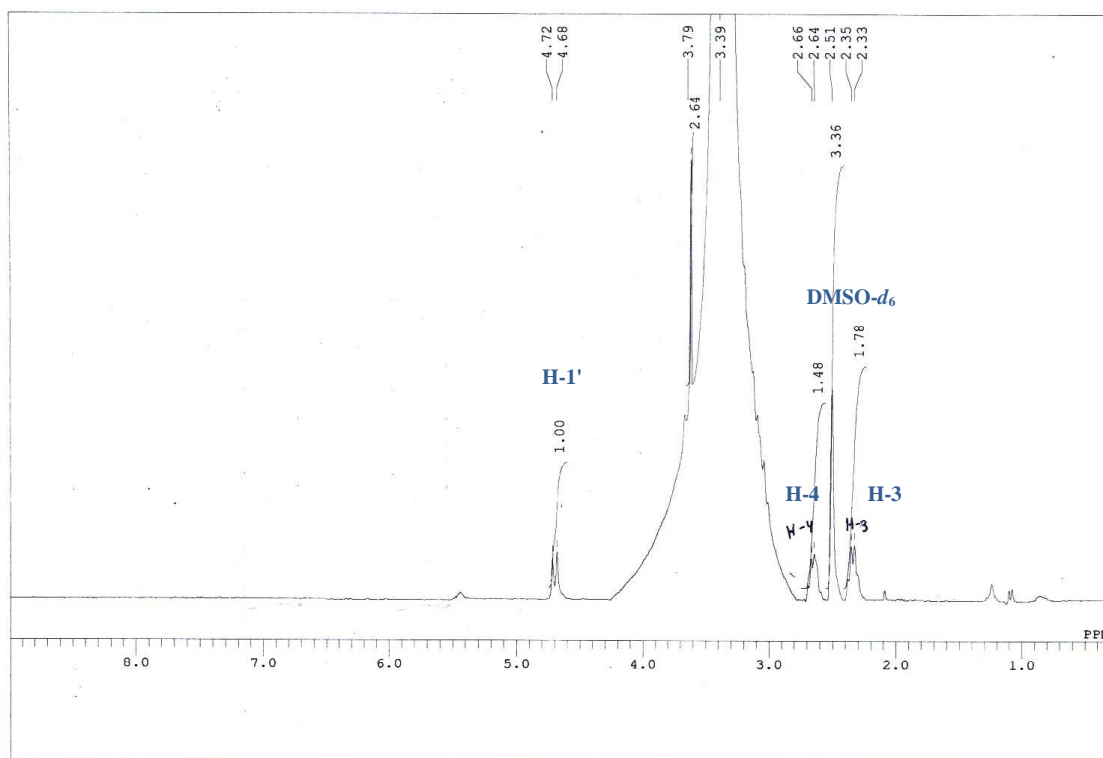
Two Cytotoxic Coumarin Glycosides from the aerial parts of *Diceratella elliptica* (DC.) Jonsell growing in Egypt.

Mona M. Marzouk*, Ahmed Elkhateeb[†], Lamyaa F. Ibrahim,
Sameh R. Hussein and Salwa A. Kawashty

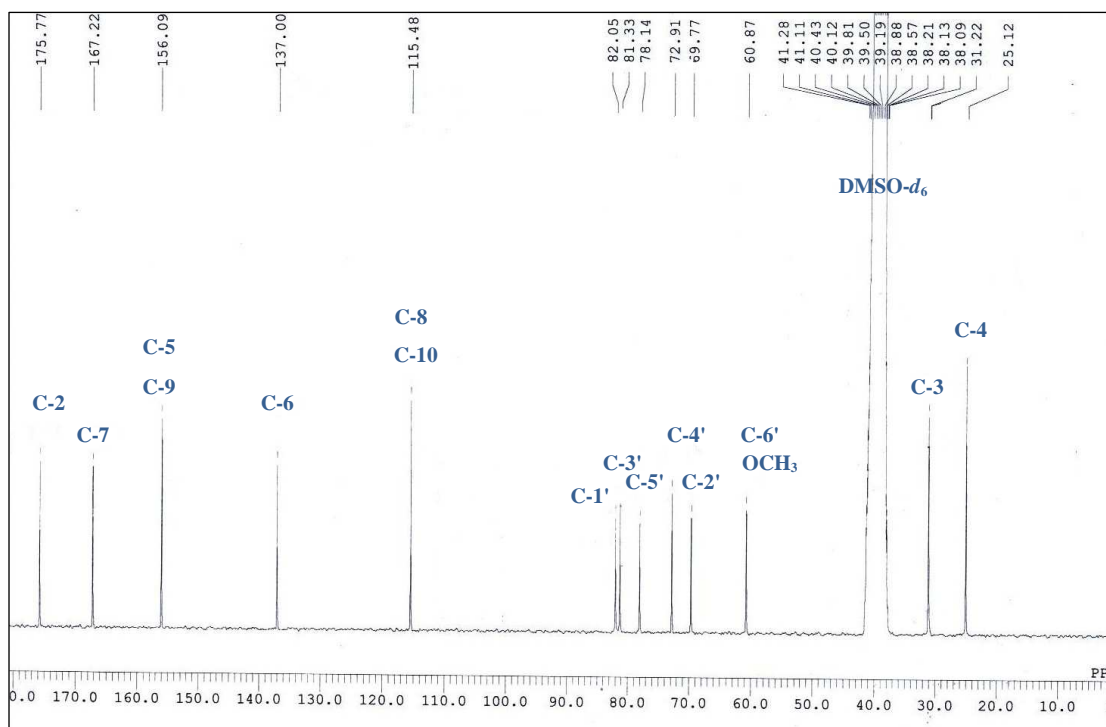
Phytochemistry and Plant Systematic Department, National Research Centre, Dokki, Giza, Egypt, 12311

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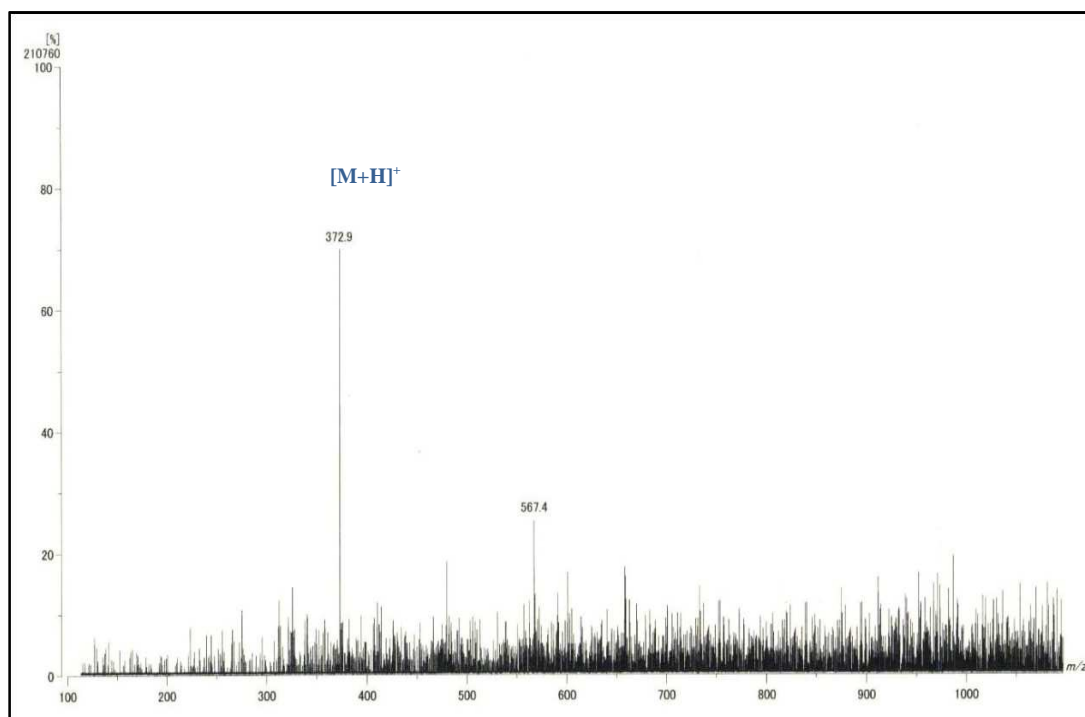
Compound (1): 6-methoxy-5,7-dihydroxy-3,4-dihydrocoumarin-8-C-glucopyranoside.



S1: ^1H NMR spectrum of compound (1), in $\text{DMSO-}d_6$, 270 MHz.

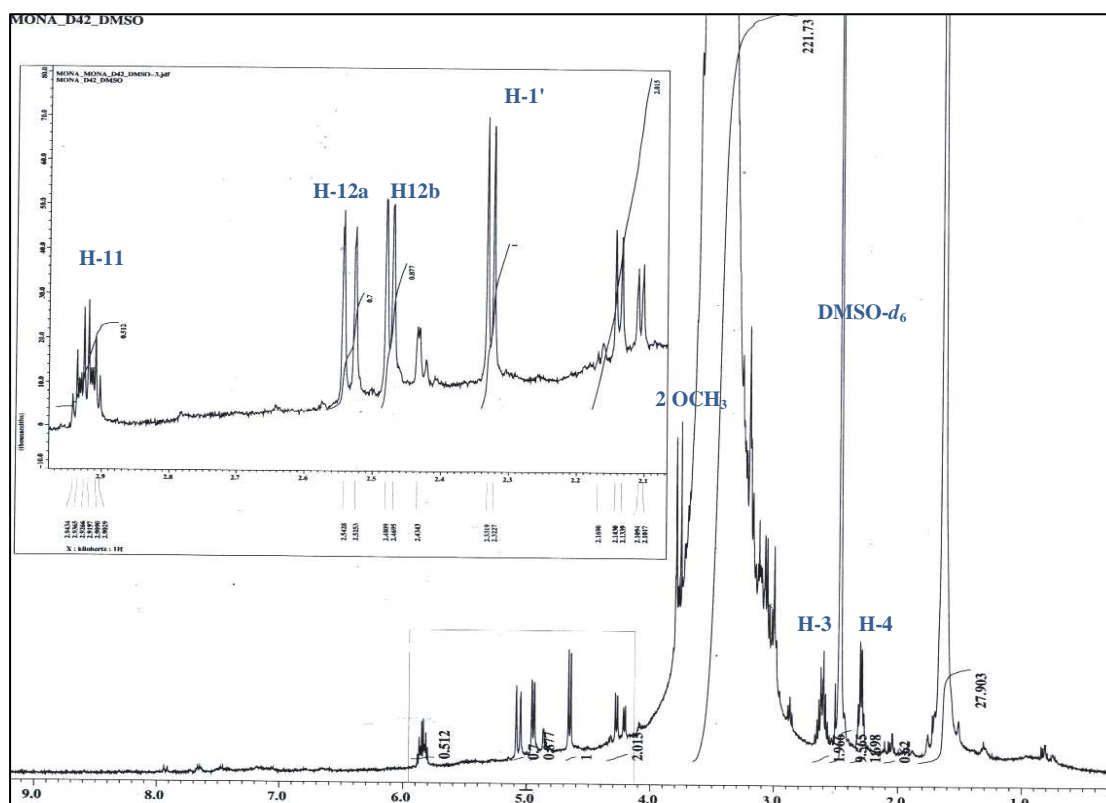


S2: ^{13}C NMR spectrum of compound (1), in $\text{DMSO-}d_6$, 67.5 MHz.

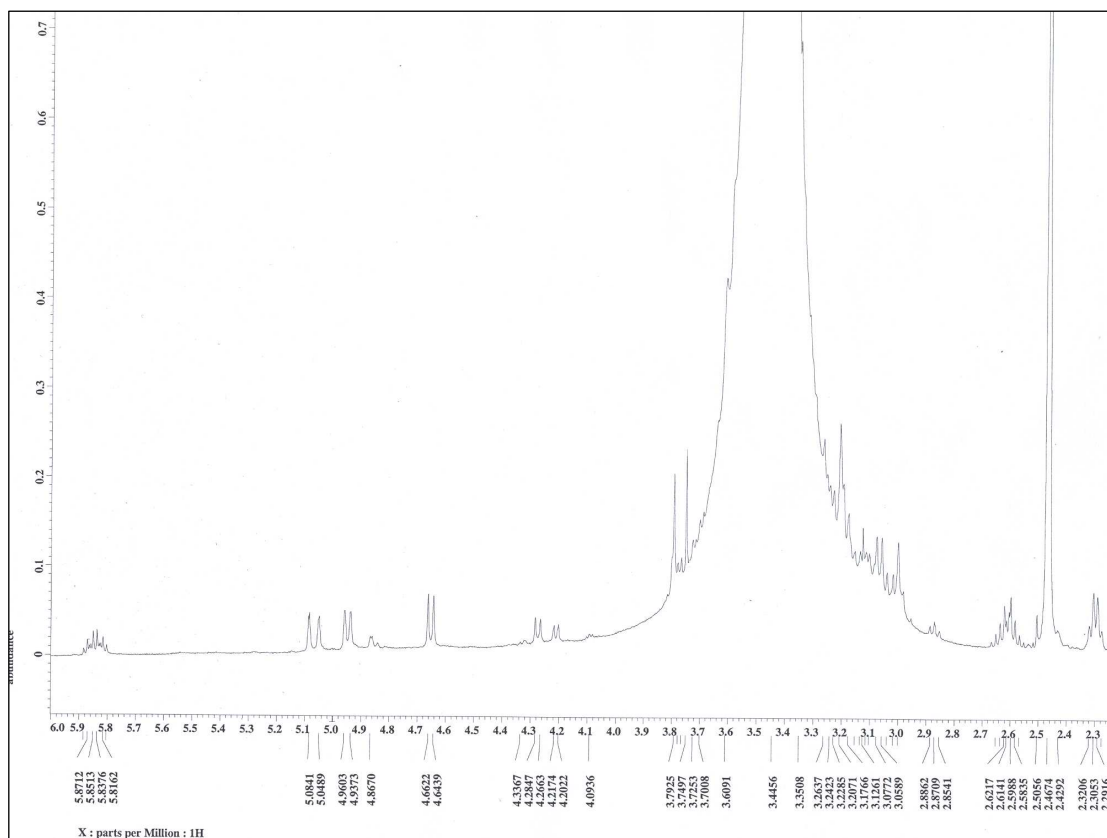


S3: Positive ion ESIMS spectrum of compound (1)

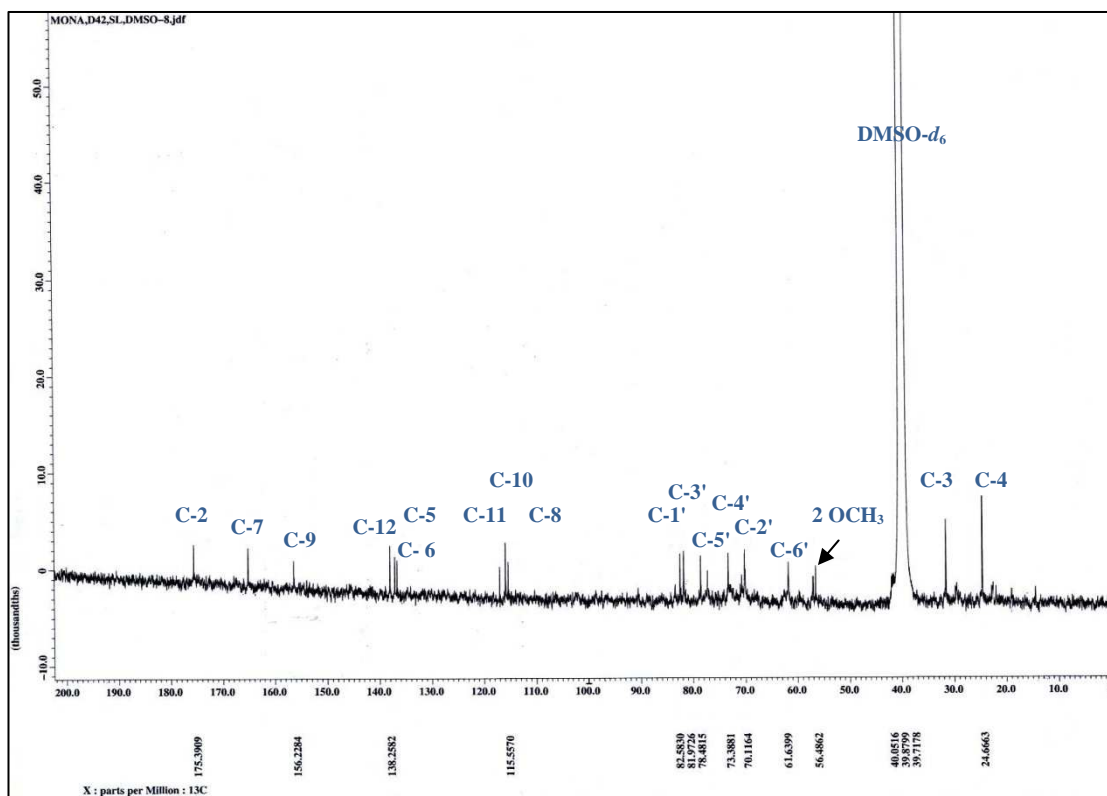
Compound (2): *5-vinyl-6,7-dimethoxy-3,4-dihydrocoumarin-8-C-glucopyranoside*.



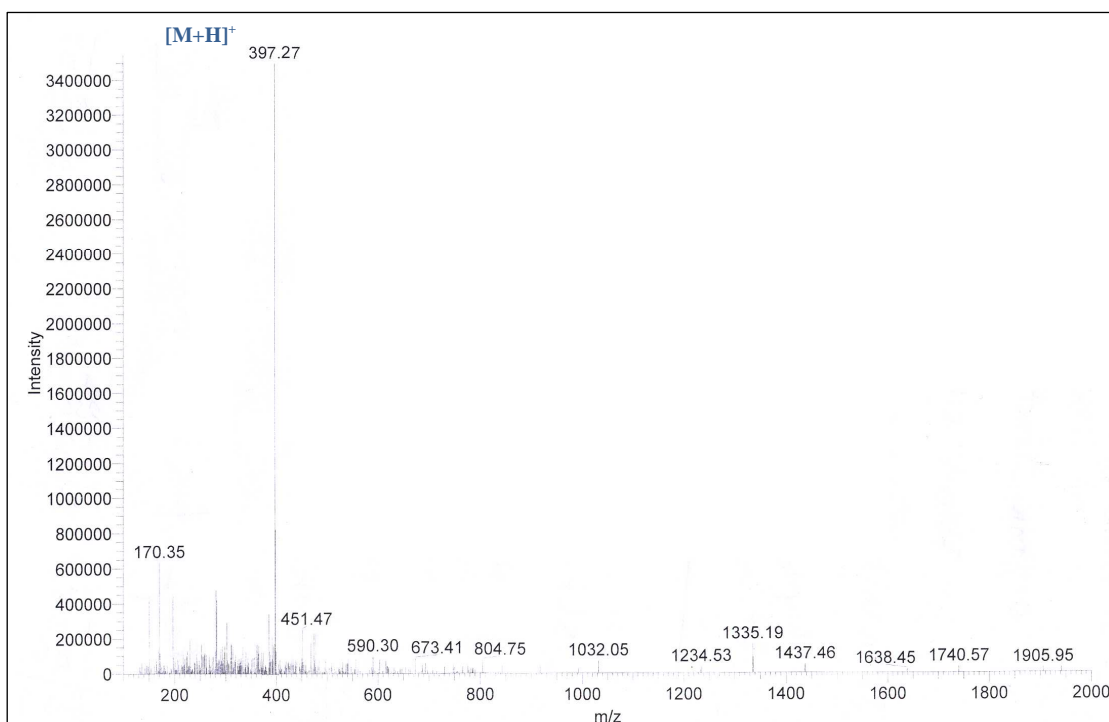
S4: ^1H NMR spectrum of compound (2), in $\text{DMSO-}d_6$, 500 MHz.



S5: Expansion of the ^1H NMR spectrum of compound (2), in $\text{DMSO-}d_6$, 500 MHz.



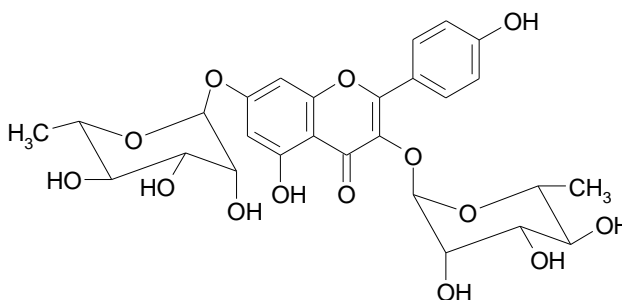
S6: ^{13}C NMR spectrum of compound (2), in $\text{DMSO-}d_6$, 125 MHz.

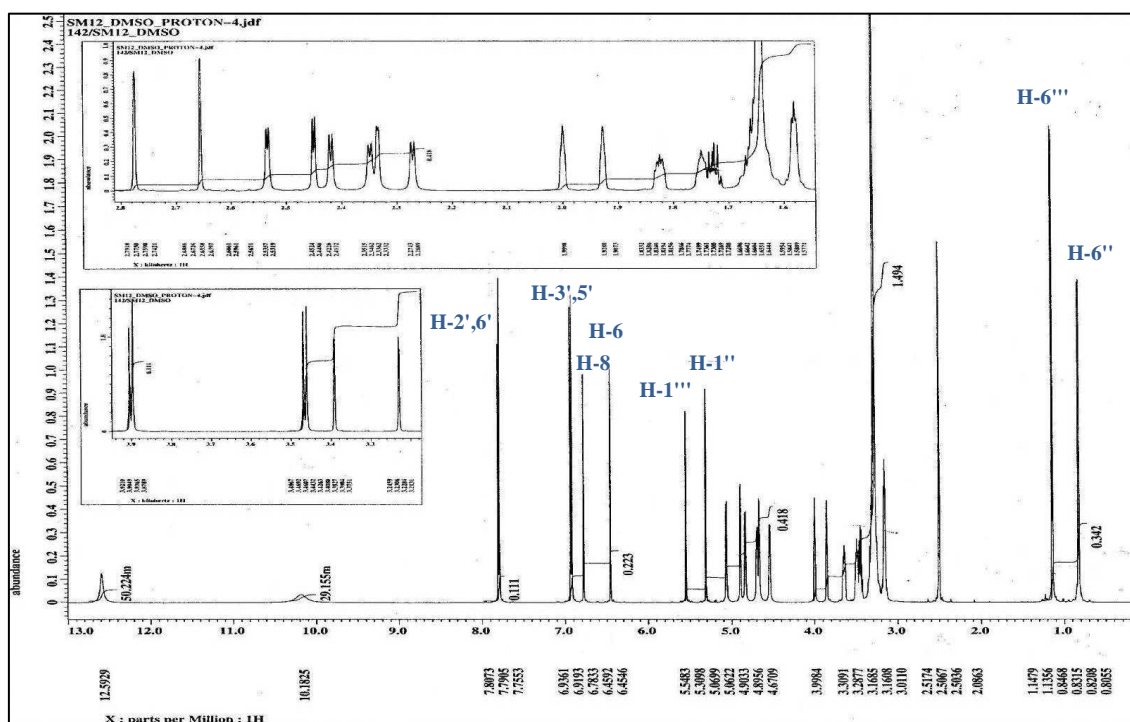


S7: Positive ion ESIMS spectrum of compound (**2**)

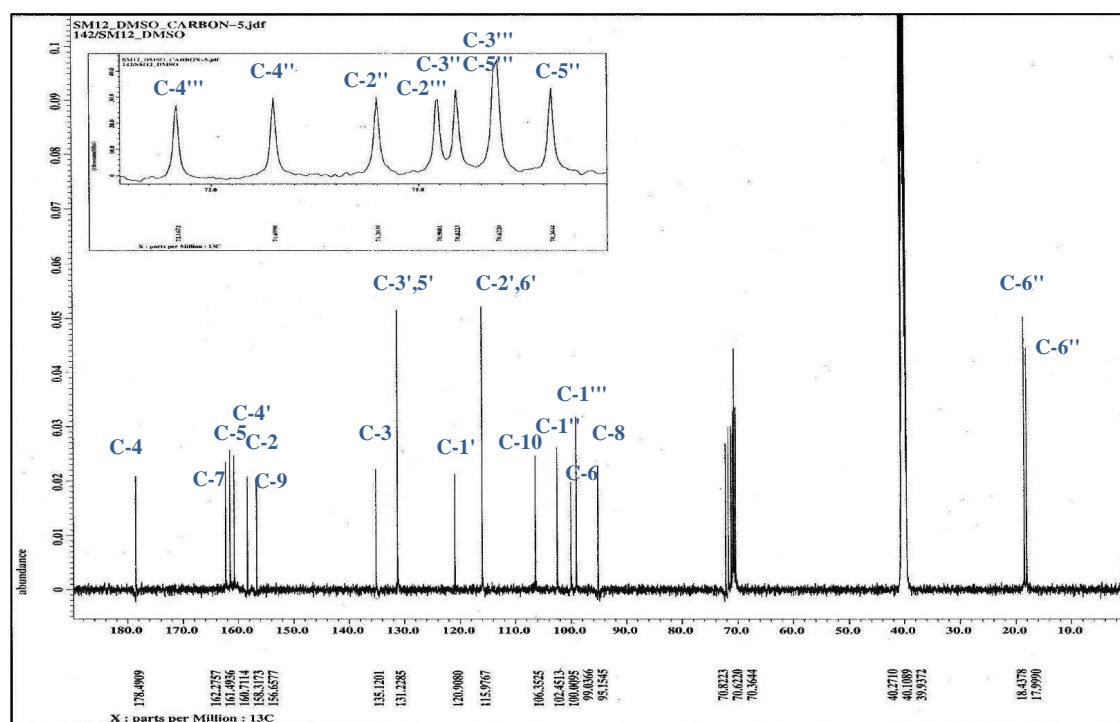
Compound (**3**) *kaempferol-3,7-di-O- α -L-rhamnopyranoside*.

Whitish yellow crystals, mp 201–205°C, *R*_f 0.62 (BAW). UV/Vis (λ_{max} , MeOH, nm): (MeOH) 266, 345; (+NaOMe) 266, 387; (+AlCl₃) 274, 300, 345, 399; (+AlCl₃/HCl) 274, 299, 341, 399; (+NaOAc) 265, 354, 389; (+NaOAc/H₃BO₃) 266, 314, 243. ¹H NMR (500 MHz, DMSO-*d*₆, δ , ppm, *J*/Hz): 7.76 (2H, d, *J* = 9.0, H-2',6'); 6.87 (2H, d, *J* = 9.0, H-3',5'); 6.66 (1H, d, *J* = 1.8, H-8); 6.35 (1H, d, *J* = 1.8, H-6); 5.5 (1H, d, *J* = 2, H-1''); 5.3 (1H, d, *J* = 2, H-1'''); 3–4 (m, sugar protons overlapped with -OH proton signals); 1.1 (3H, d, *J* = 6.0, CH₃-rhamnose at position 7); 0.8 (3H, *J* = 6.0, CH₃-rhamnose at position 3). ¹³C NMR (125 MHz, DMSO-*d*₆, δ , ppm): 178 (C-4), 162.3 (C-7); 161.5 (C-5); 160.7 (C-4'); 158.3 (C-2), 156.6 (C-9), 135 (C-3), 131.2 (C-2', C-6'), 121 (C-1'), 116 (C-3', C-5'), 106.3 (C-10), 102.4 (C-1''), 100 (C-6), 99.03 (C-1'''), 95 (C-8), 72.2 (C-4''), 71.7 (C-5''), 71.2 (C-4'''), 70.9 (C-2''), 70.8 (C-2'''), 70.6 (C-3''), 70.6 (C-3'''), 70.3 (C-5'''), 18.00 (C-6''), 18.5 (C-6'''). Negative ESIMS; *m/z* 577 [M-H]⁻

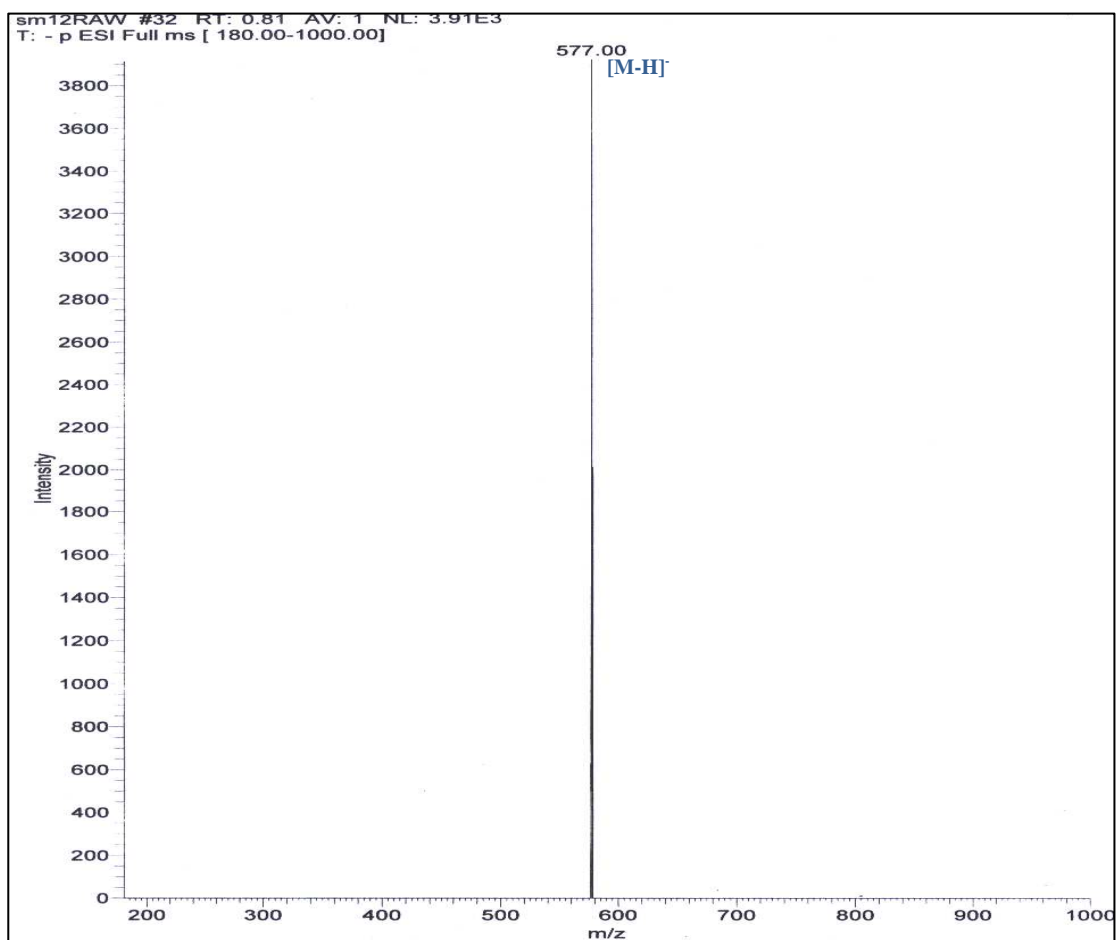




S8: ^1H NMR spectrum of compound (3), in $\text{DMSO-}d_6$, 500 MHz.



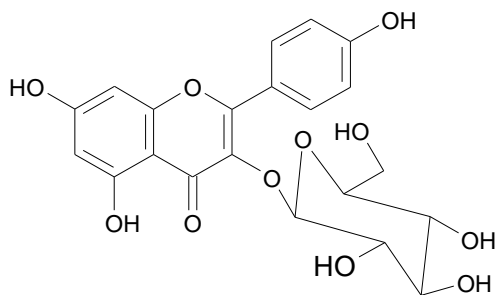
S9: ^{13}C NMR spectrum of compound (3), in $\text{DMSO-}d_6$, 125 MHz.

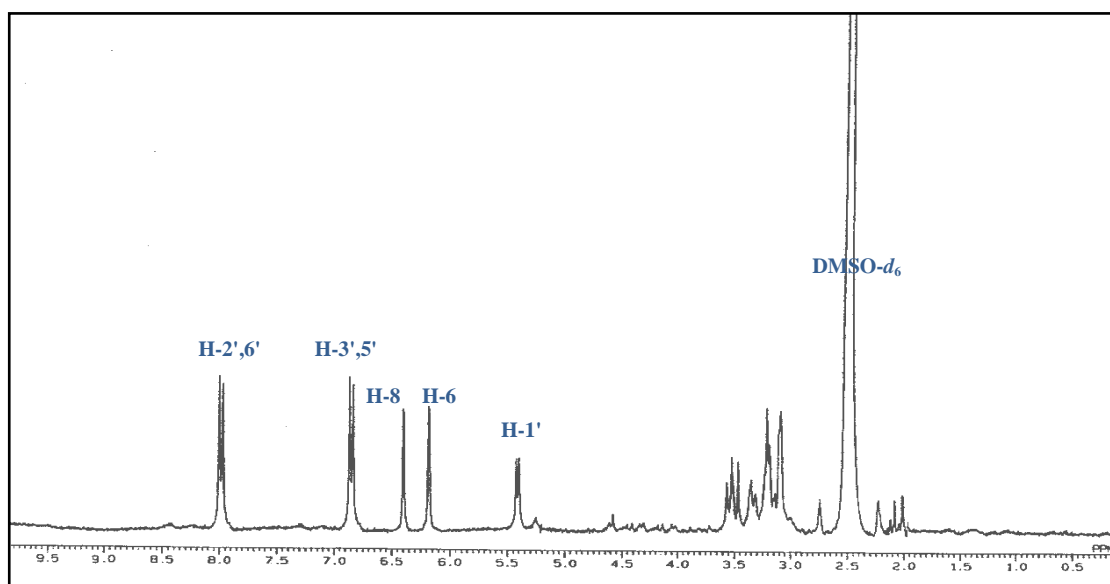


S10: Negative ion ESI-MS spectrum of compound (3).

Compound (4): *Kaempferol-3-O-β-D-glucopyranoside*

Yellow powder, R_f 0.54 (BAW). UV/Vis (λ_{max} , MeOH, nm): (MeOH) 266, 346; (+NaOMe) 274, 327 sh, 404; (+AlCl₃) 274, 302, 345, 396; (+AlCl₃/HCl) 274, 300, 344, 396; (+NaOAc) 275, 305, 393; (+NaOAc/H₃BO₃) 266, 253. ¹H NMR (270 MHz, DMSO-*d*₆, δ , ppm, J/Hz): 7.87 (2H, d, $J = 9.0$, H-2',6'); 6.86 (2H, d, $J = 9.0$, H-3',5'); 6.42 (1H, d, $J = 2.0$, H-8); 6.23 (1H, d, $J = 2.0$, H-6); 5.48 (1H, d, $J = 7.5$, H-1''), 3–4 (m, sugar protons overlapped with -OH proton signals).

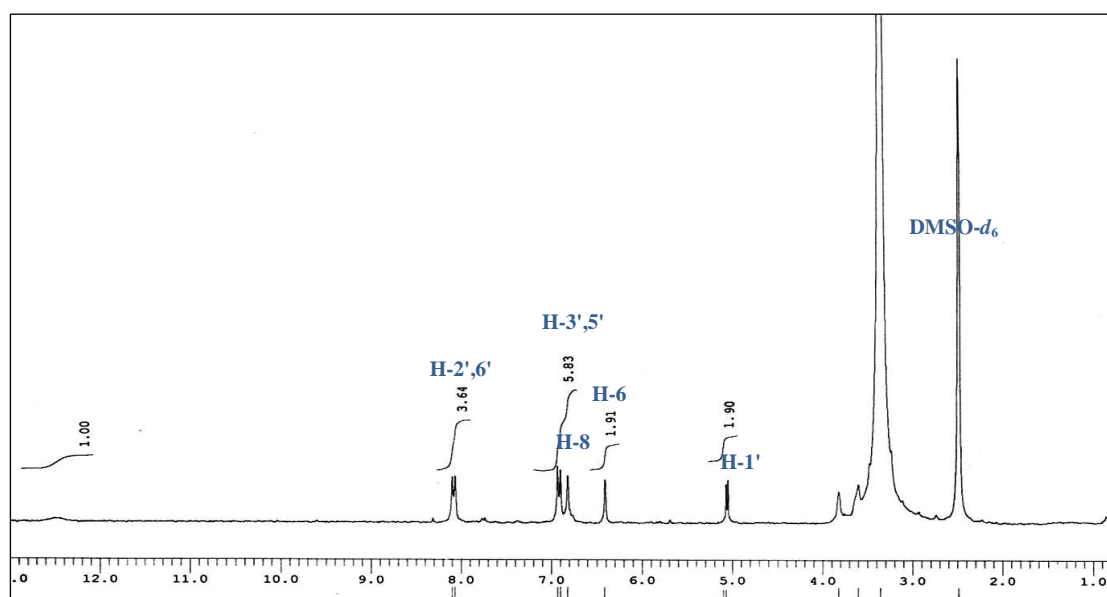
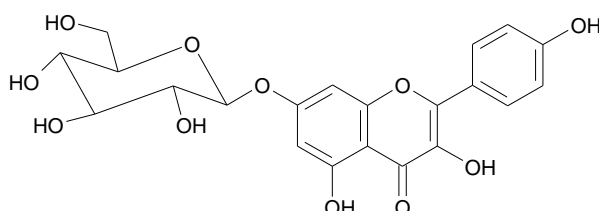




S11: ^1H NMR spectrum of compound (**4**), in $\text{DMSO-}d_6$, 270 MHz.

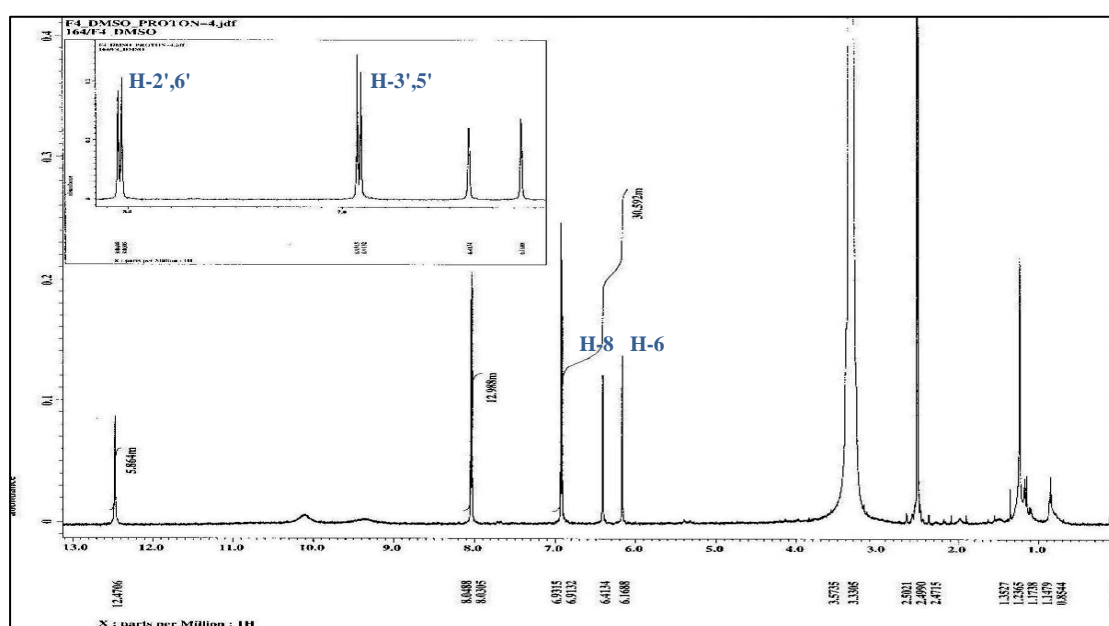
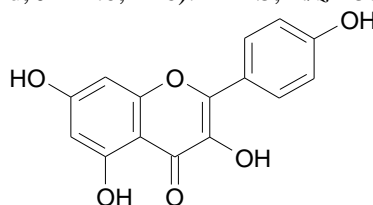
Compound (**5**): *Kaempferol 7-O- β -D- glucopyranoside*.

Yellow powder, *R_f* 0.62 (BAW). UV/Vis (λ_{max} , MeOH, nm): (MeOH) 267, 320sh, 360; (+NaOMe) 273, 450; (+AlCl₃) 278, 310, 360, 425; (+AlCl₃/HCl) 278, 309, 360, 425; (+NaOAc) 268, 360, 400; (+NaOAc/H₃BO₃) 268, 294, 360. ^1H NMR (270 MHz, $\text{DMSO-}d_6$, δ , ppm, J/Hz): 7.98 (2H, d, $J = 9.0$, H-2',6'); 6.9 (2H, d, $J = 9.0$, H-3',5'); 6.61 (1H, d, $J = 2.0$, H-8); 6.39 (1H, d, $J = 2.0$, H-6); 5.05 (1H, d, $J = 7.5$, H-1'), .

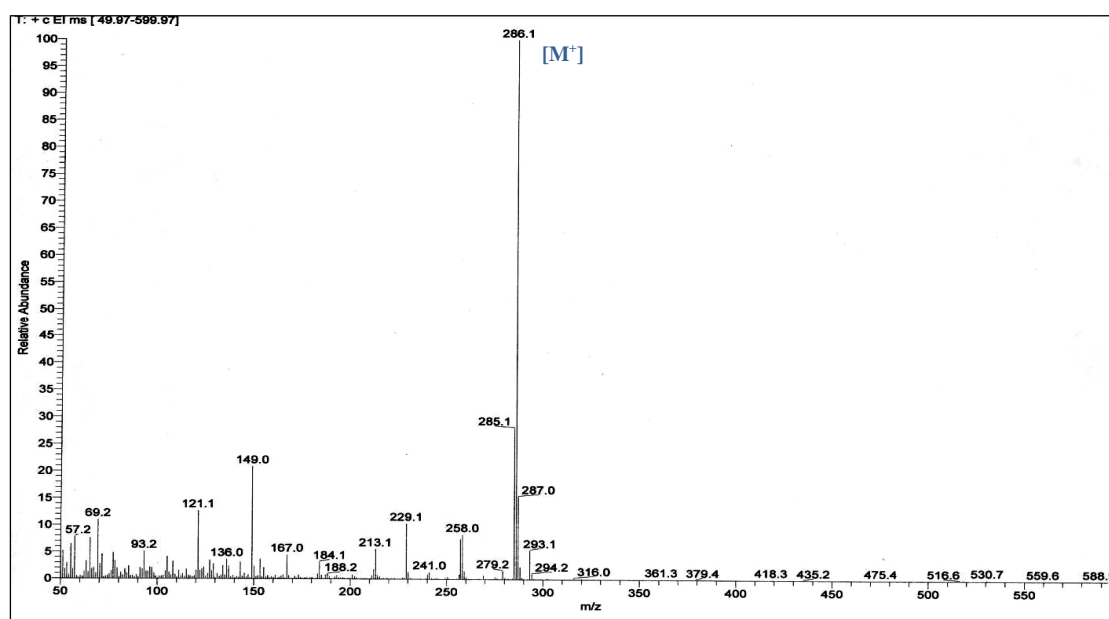


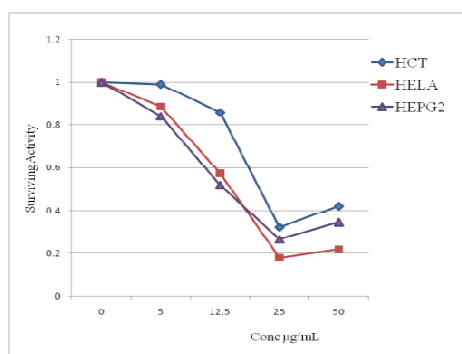
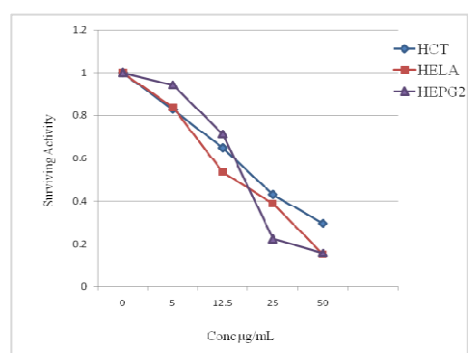
S12: ^1H NMR spectrum of compound (5), in $\text{DMSO-}d_6$, 270 MHz.
Compound (6) *Kaempferol*.

Yellow powder, R_f 0.73 (BAW). UV/Vis (λ_{max} , MeOH, nm): (MeOH) 266,292sh, 319sh, 366; (+NaOMe) 276, 320sh, 411; (+ AlCl_3) 269, 305, 350, 423; (+ AlCl_3/HCl) 267, 305, 350, 424; (+NaOAc) 274, 306, 378; (+NaOAc/ H_3BO_3) 265, 294, 319, 369. ^1H NMR (500 MHz, $\text{DMSO-}d_6$, δ , ppm, J/Hz): 8.03 (2H, d, $J = 9.0$, H-2',6'); 6.93 (2H, d, $J = 9.0$, H-3',5'); 6.41 (1H, d, $J = 2.0$, H-8); 6.17 (1H, d, $J = 2.0$, H-6). EIMS; m/z 286.1 [M^+]



S13: ^1H NMR spectrum of compound (6), in $\text{DMSO-}d_6$, 500 MHz.



S14: EI-MS spectrum of compound (6).**1****2****S15: Cytotoxic activity of compounds 1 and 2 against three human carcinoma cells lines; liver (HEPG2), colon (HCT116) and Cervix (HELA)**