

Supplementary Material

Bioassay-guided separation and identification of anticancer compounds in

***Tagetes erecta* L. flowers**

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Compound **1** (Syringic acid) ^{13}C -NMR (150 MHz, CD_3OD): δ (ppm) = 120.57 (C-1), 106.91 (C-2, C-6), 147.44 (C-3, C-5), 140.36 (C-4), 168.53 (C-7), 56.32 (O- CH_3). ^1H -NMR (600 MHz, CD_3OD): δ (ppm) = 3.82 (s, 6H, OCH_3), 7.35 (s, 2H, H-6), 12.62 (br.s, 1H, COOH).

Compound **2** (Quercetin) ^{13}C -NMR (150 MHz, CD_3OD): δ (ppm) = 146.57 (C-2), 135.81 (C-3), 175.91 (C-4), 161.09 (C-5), 97.82 (C-6), 164.14 (C-7), 93.00 (C-8), 156.81 (C-9), 103.11 (C-10), 122.74 (C-1'), 114.59 (C-2'), 144.80 (C-3'), 147.35 (C-4'), 114.81 (C-5'), 120.27 (C-6'). ^1H -NMR (600 MHz, CD_3OD): δ (ppm) = 7.75 (d, 1H, $J = 2.1$ Hz, H-2'), 6.90 (d, 1H, $J = 8.5$ Hz, H-5'), 7.64 (dd, 1H, $J = 8.5, 2.1$ Hz, H-6'), 6.40 (d, 1H, $J = 2.0$ Hz, H-8), 6.19 (d, 1H, $J = 2.0$ Hz, H-6).

Compound **3** (6-hydroxykaempferol) ^{13}C -NMR (150 MHz, CD_3OD): δ (ppm) = 146.79 (C-2), 135.37 (C-3), 176.01 (C-4), 145.46 (C-5), 128.37 (C-6), 153.24 (C-7), 92.97 (C-8), 149.77 (C-9), 103.43 (C-10), 122.54 (C-1'), 129.26 (C-2'), 114.88 (C-3'), 159.09 (C-4'), 114.88 (C-5'), 129.26 (C-6'). ^1H -NMR (600 MHz, CD_3OD): δ (ppm) = 8.11 (d, 2H, $J = 8.9$ Hz, H-2', 6'), 6.93 (d, 2H, $J = 8.9$ Hz, H-3', 5'), 6.54 (s, 1H, H-8).

Compound **4** (Protocatechuic acid) ^{13}C -NMR (150 MHz, CD_3OD): δ (ppm) = 120.09 (C-1), 116.81 (C-2), 144.66 (C-3), 150.14 (C-4), 114.44 (C-5), 122.49 (C-6), 168.67 (COOH). ^1H -NMR (600 MHz, CD_3OD): δ (ppm) = 6.90 (d, 1H, $J = 8.4$ Hz, H-5), 7.48 (dd, 1H, $J = 8.4$ Hz, H-6), 7.53 (d, 1H, $J = 2.0$ Hz, H-2).

Compound **5** (Quercetagenin) ^{13}C -NMR (150 MHz, CD_3OD): δ (ppm) = 146.71 (C-2), 135.47 (C-3), 175.96 (C-4), 146.71 (C-5), 128.34 (C-6), 153.23 (C-7), 92.90 (C-8), 149.73 (C-9), 103.40 (C-10), 122.95 (C-1'), 114.60 (C-2'), 144.80 (C-3'), 147.28 (C-4'), 114.79 (C-5'), 120.24 (C-6'). ^1H -NMR (600 MHz, CD_3OD): δ (ppm) = 7.75 (d, 1H, $J = 2.1$ Hz, H-2'), 6.90 (d, 1H, $J = 8.5$ Hz, H-5'), 7.64 (dd, 1H, $J = 8.5, 2.1$ Hz, H-6'), 6.52 (s, 1H, H-8).