Supporting Information

***Rec. Nat. Prod*. 11:5 (2017) 479-484**

Flavonoid Derivatives from the Aerial Parts of *Trifolium trichocephalum* M. Bieb. and Their Antioxidant and Cytotoxic Activity

Gülin Renda[1*], Ufuk Özgen[1], Zeynep Ünal[2], Suna Sabuncuoğlu[2], Erhan Palaska[3] and İlkay Erdoğan Orhan[4]

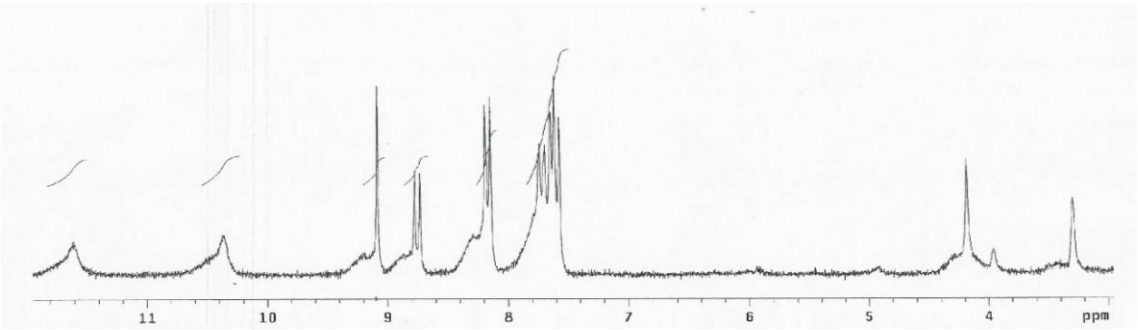
[1]Karadeniz Technical University, Faculty of Pharmacy, Department of Pharmacognosy, Trabzon, Türkiye

[2]Hacettepe University, Faculty of Pharmacy, Department of Toxicology, Ankara, Türkiye

[3]Hacettepe University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Ankara, Türkiye

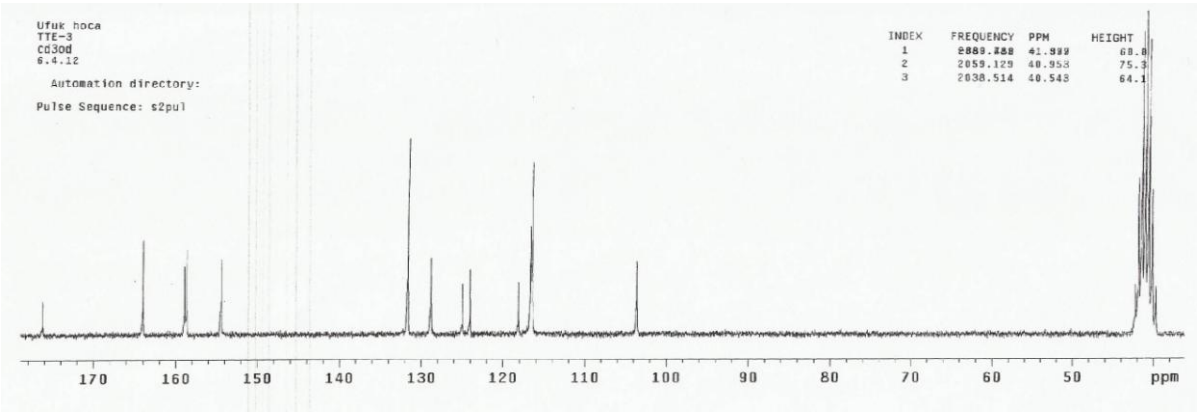
[4]Gazi University, Faculty of Pharmacy, Department of Pharmacognosy, Ankara, Türkiye

Table of Contents **Page**

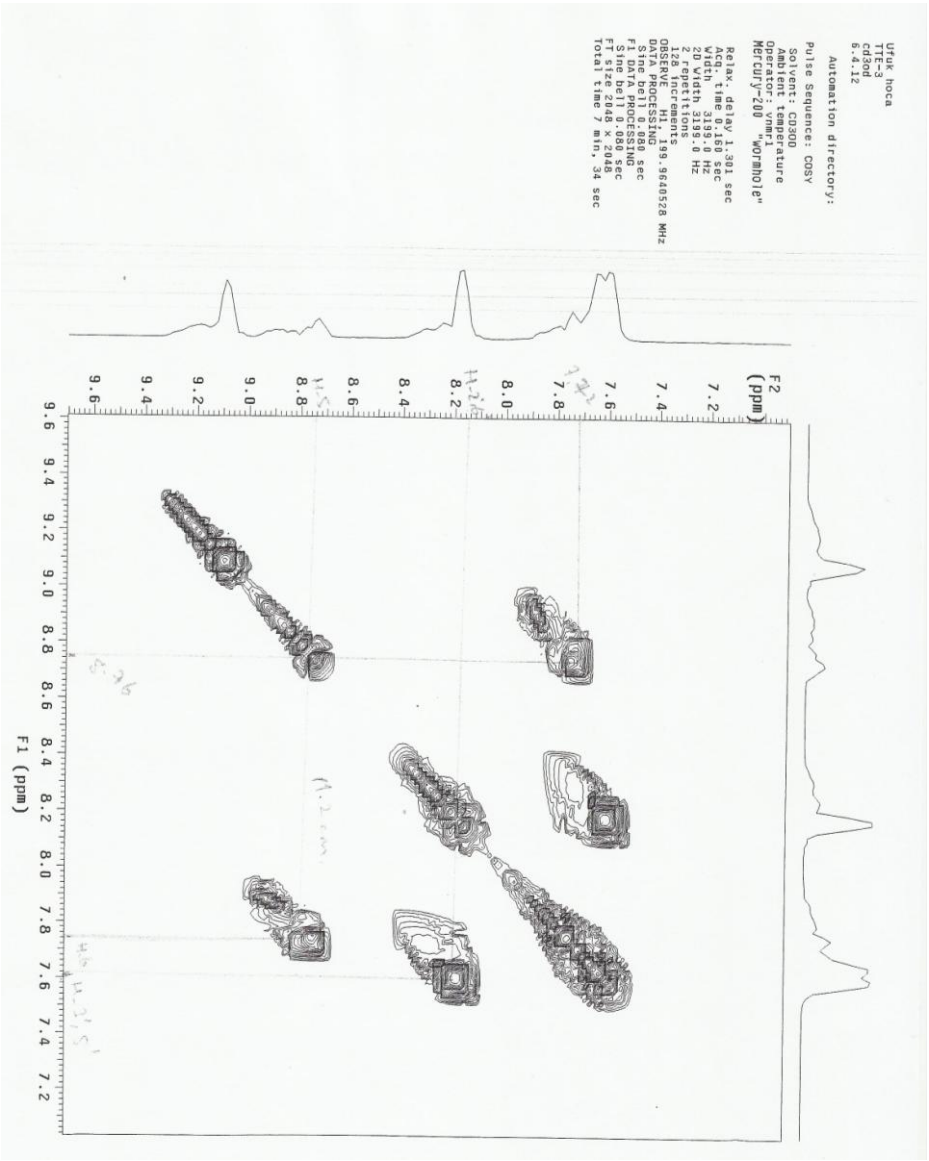


S1: ^{1}H-NMR (200 MHz, $CDCl_3$) Spectrum of Compound **1** (daidzein)

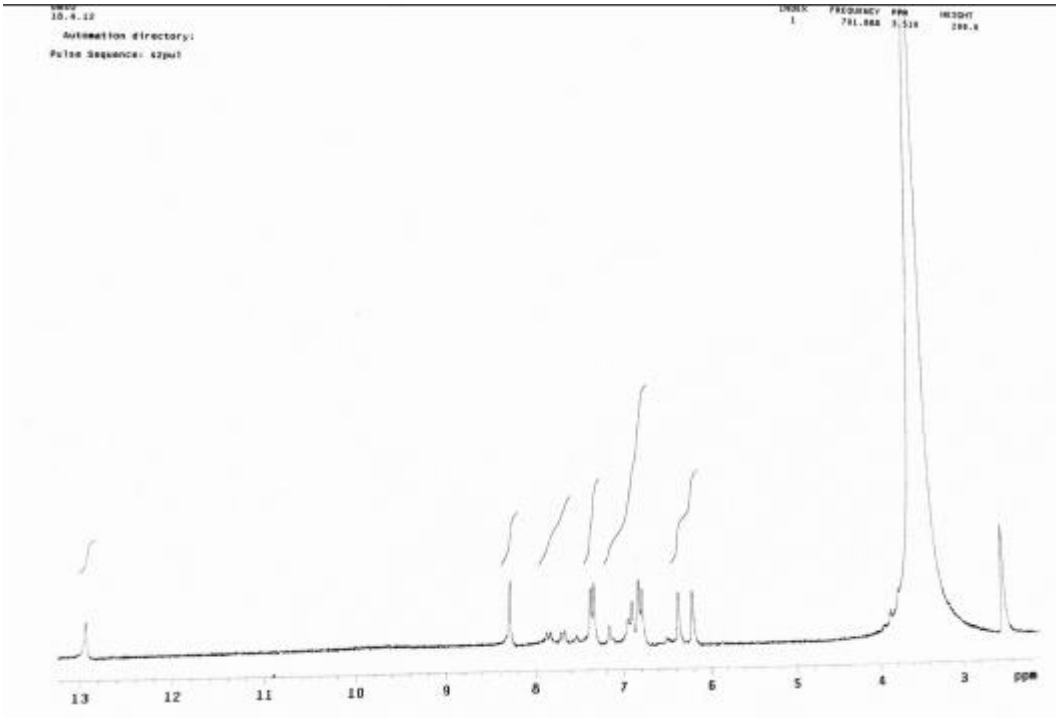
Daidzein (**1**): ^{1}H NMR (200 MHz, CD_3OD) δ: 8.28 (1H, H-2, s), 7.95 (1H, H-5, d, *J*= 9.0 Hz), 7.36 (2H, H-2',6', d, *J*= 8.2 Hz), 6.91 (1H, H-6, d, *J*= 8.6 Hz), 6.85 (1H, H-8, s), 6.79 (2H, H-3',5', d, *J*= 8.6 Hz); ^{13}C NMR (50 MHz, CD_3OD) δ: 176.2 (C-4), 164.0 (C-7), 158.9 (C-9), 158.7 (C-4'), 154.4 (C-2), 131.6 (x2C) (C-2',6'), 128.8 (C-5), 125.0 (C-1'), 124.0 (C-3), 118.1 (C-10), 116.6 (C-6), 116.4 (x2C) (C-3',5').



S2: ^{13}C-NMR (50 MHz, $CDCl_3$) Spectrum of Compound **1** (daidzein)

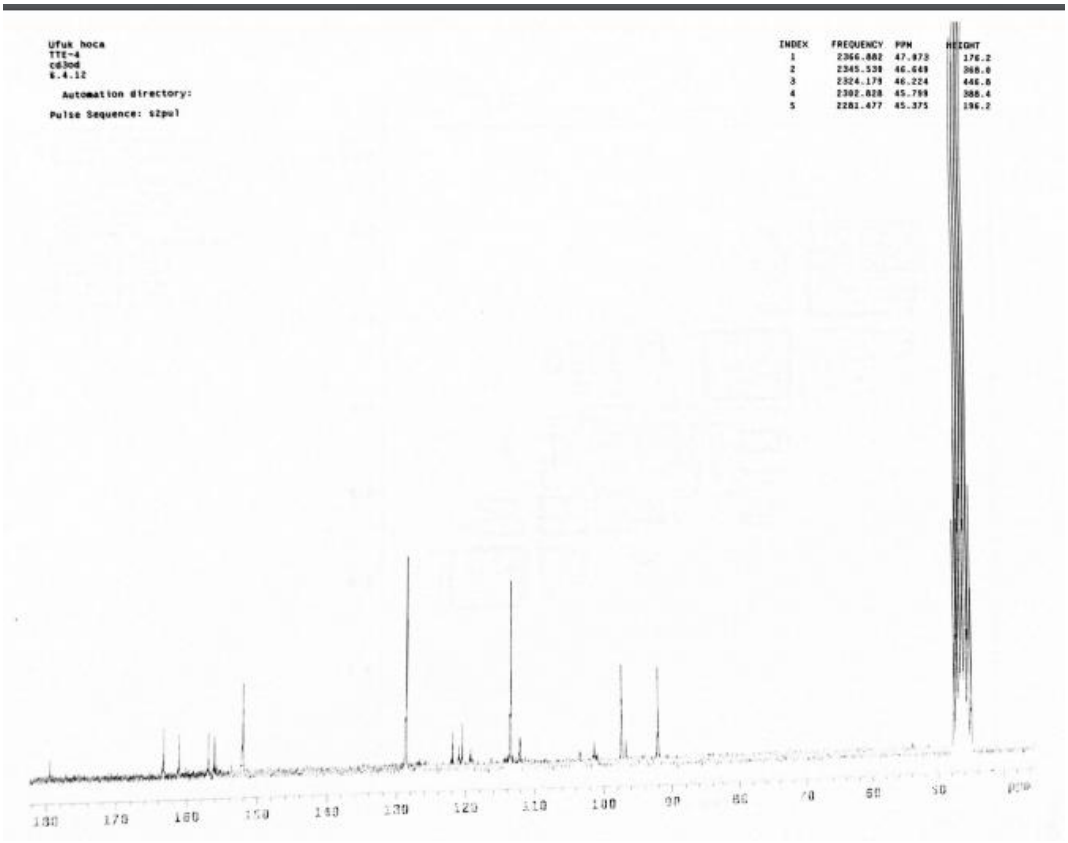


S3: COSY (200 MHz) Spectrum of Compound **1** (daidzein)



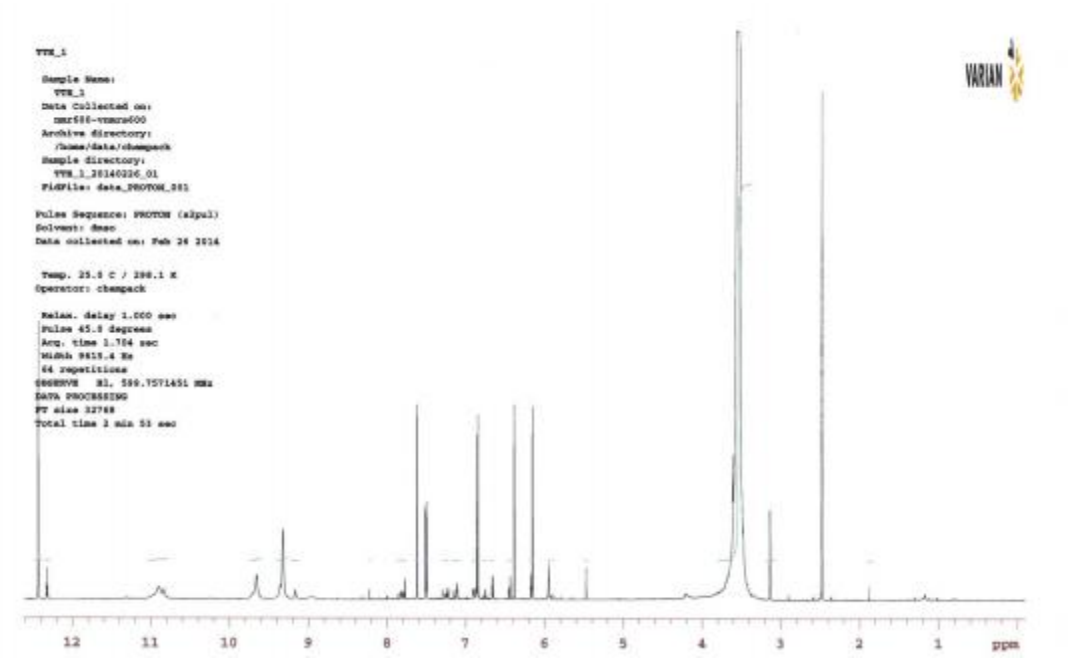
S4: ^{1}H-NMR (200 MHz, $CDCl_3$) Spectrum of Compound **2** (genistein)

Genistein: ^{1}H NMR (200 MHz, CD3OD): d 8.10 (1H, H-2, s), 7.38 (2H, H-2',6', d, J= 8.2 Hz), 6.86 (2H, H-3',5', d, J=8.2 Hz), 6.34 (1H, H-8, s), 6.22 (1H, H-6, s); ^{13}C NMR (50 MHz, CD3OD): d 179.4 (C-4), 169.2 (C-7), 161.0 (C-5), 156.9 (C-9), 156.0 (C-4'), 152.0 (C-2), 128.6 (x2C) (C-2',6'), 121.9 (C-3), 120.5 (C-1'), 113.4 (x2C) (C-3', 5'), 101.3 (C-10), 97.3 (C-6), 92.0 (C-8).



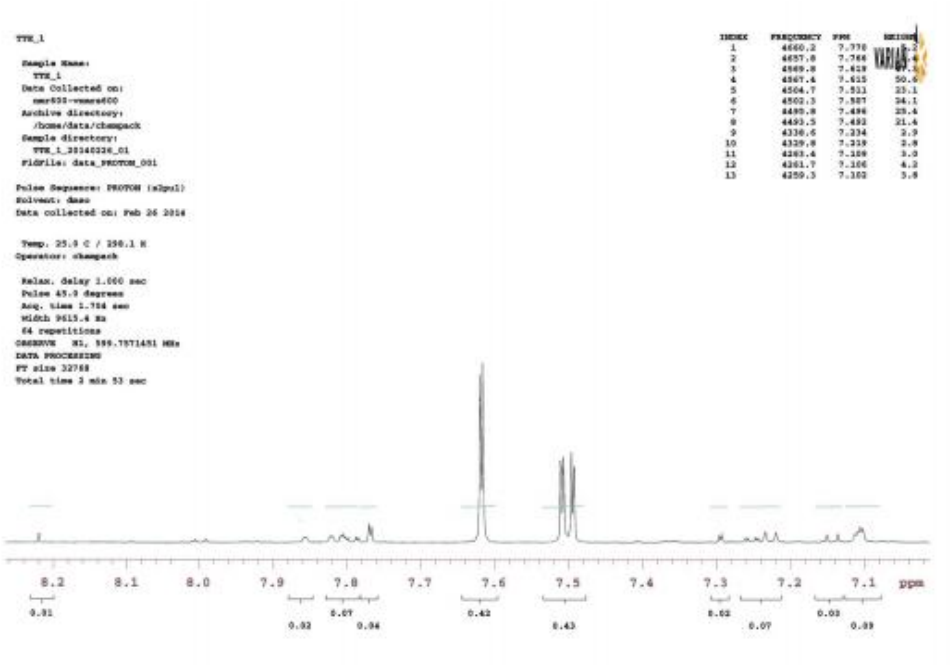
S5: ^{13}C-NMR (50 MHz, $CDCl_3$) Spectrum of Compound **2** (genistein)

S6: COSY (200 MHz) Spectrum of Compound **2** (genistein)

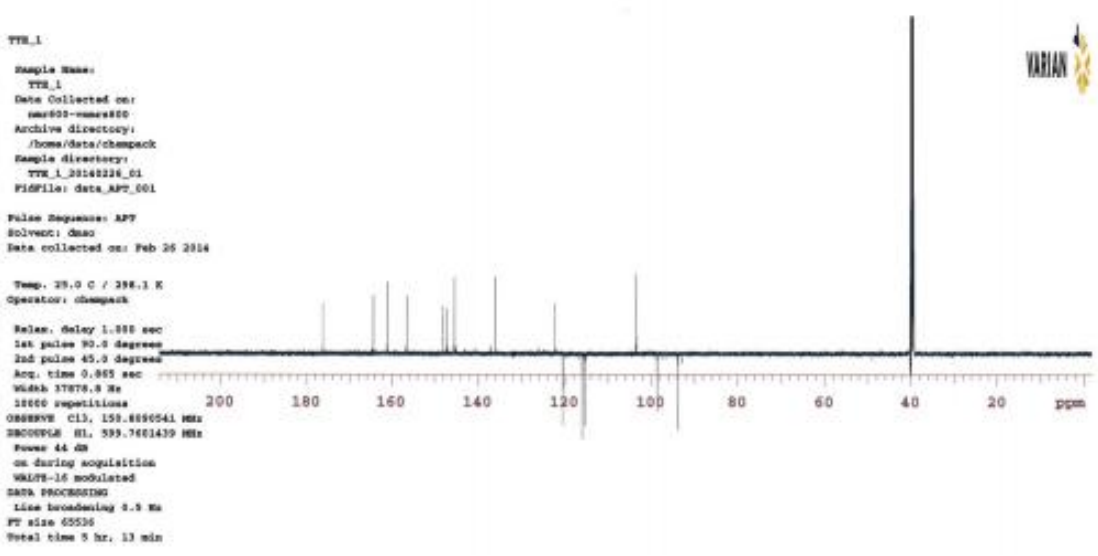


S7: ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of Compound **3** (quercetin)

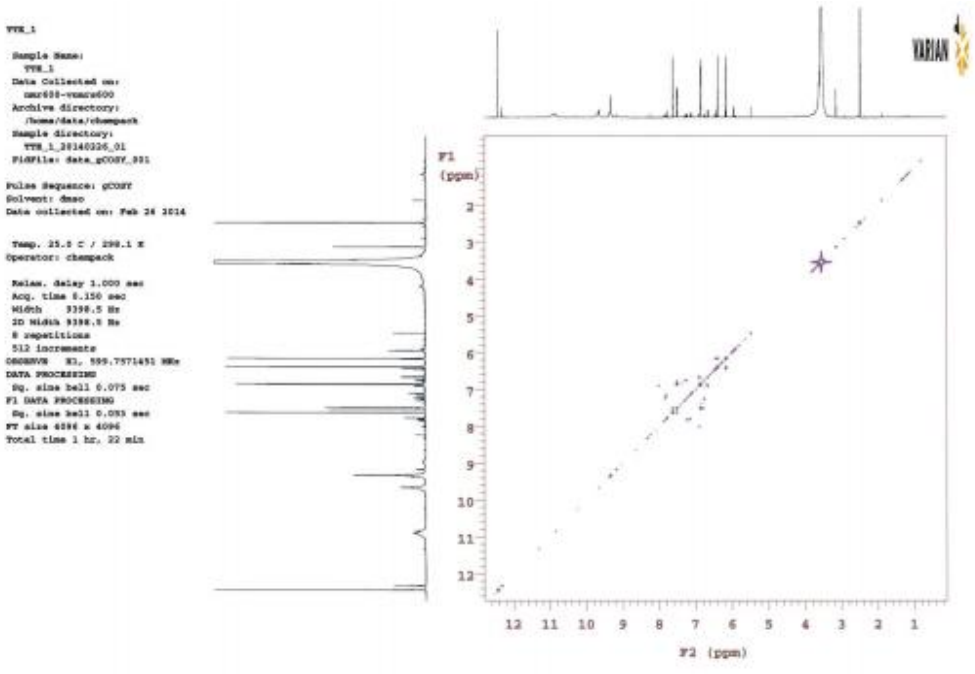
Quercetin: ^{1}H NMR (600 MHz, DMSO-d6) d: 7.61 (1H, H-2', d, J=2.4 Hz), 7.50 (1H, H-6', dd, J=2.4, 8.8 Hz), 6.85 (1H, H-5', d, J= 8.8 Hz), 6.38 (1H, H-8, d, J = 1.8 Hz), 6.15(1H, H-6, d, J = 2.3 Hz); ^{13}C NMR (125 MHz, DMSO d6): d 176.2 (C-4), 164.3 (C-7), 161.1 (C-5), 156.6 (C-9), 148.1 (C-4'), 147.2 (C-2), 145.5 (C-3'), 136.1 (C-3), 122.4 (C-1'), 120,5 (C-6'), 116.0 (C-5'), 115.4 (C-2'), 103.4 (C-10), 98.6 (C-6), 93.8 (C-8).



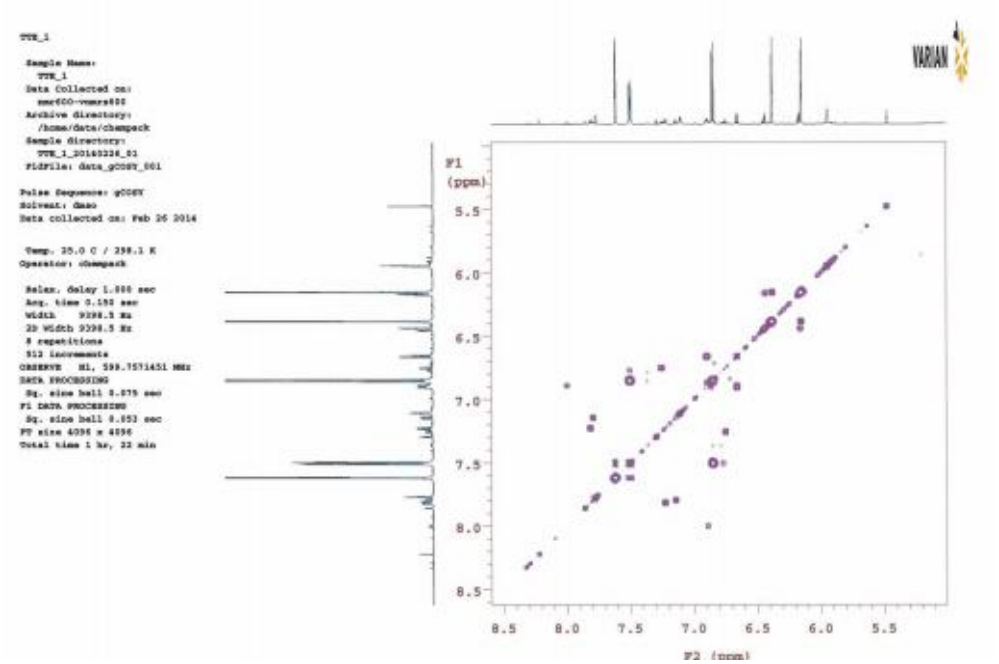
S8: Expansion of the ^{1}H-NMR Spectrum of Compound **3** (quercetin)



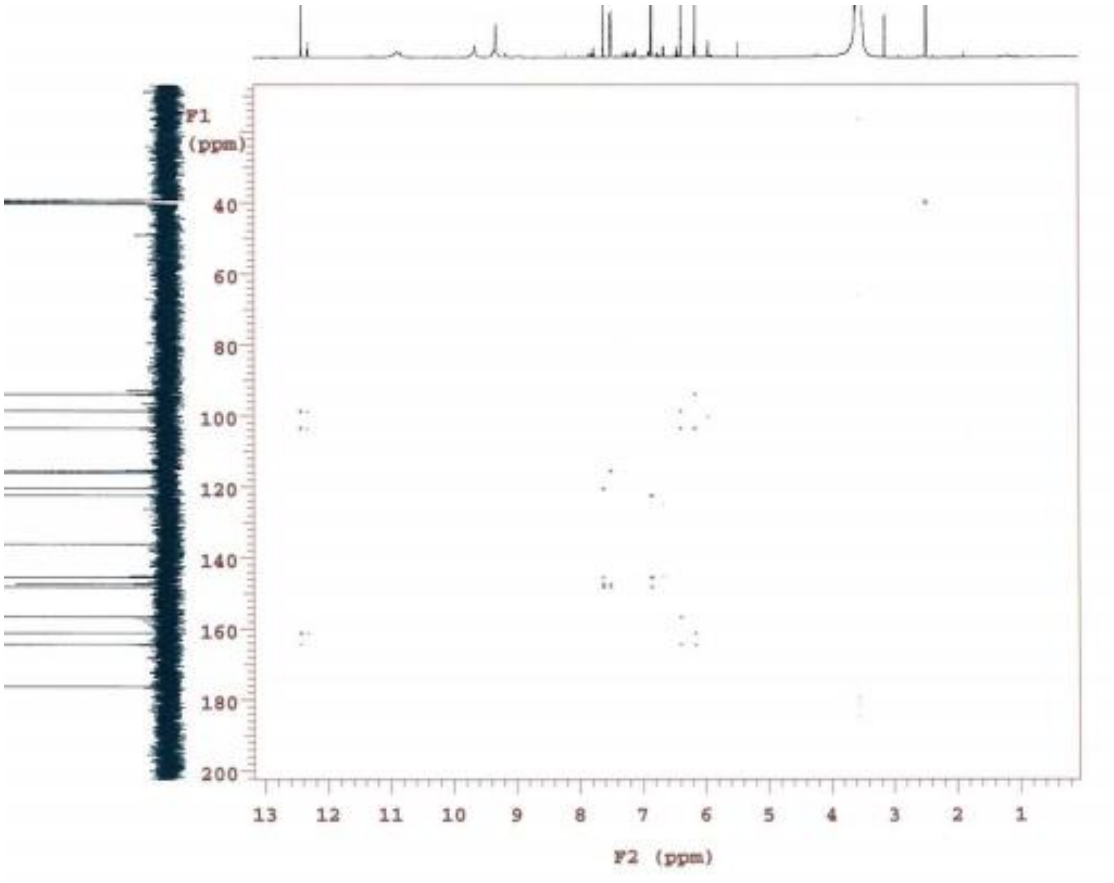
S9: ^{13}C-NMR + DEPT (125 MHz, $CDCl_3$) Spectrum of Compound **3** (quercetin)



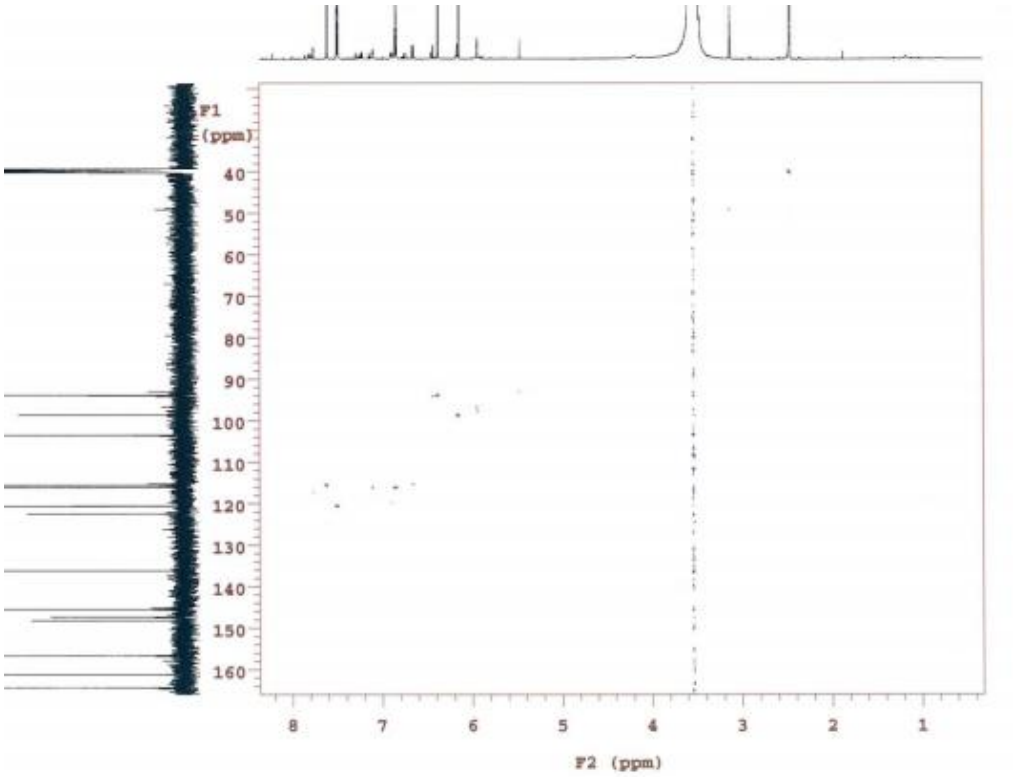
S10: COSY (600 MHz) Spectrum of Compound **3** (quercetin)



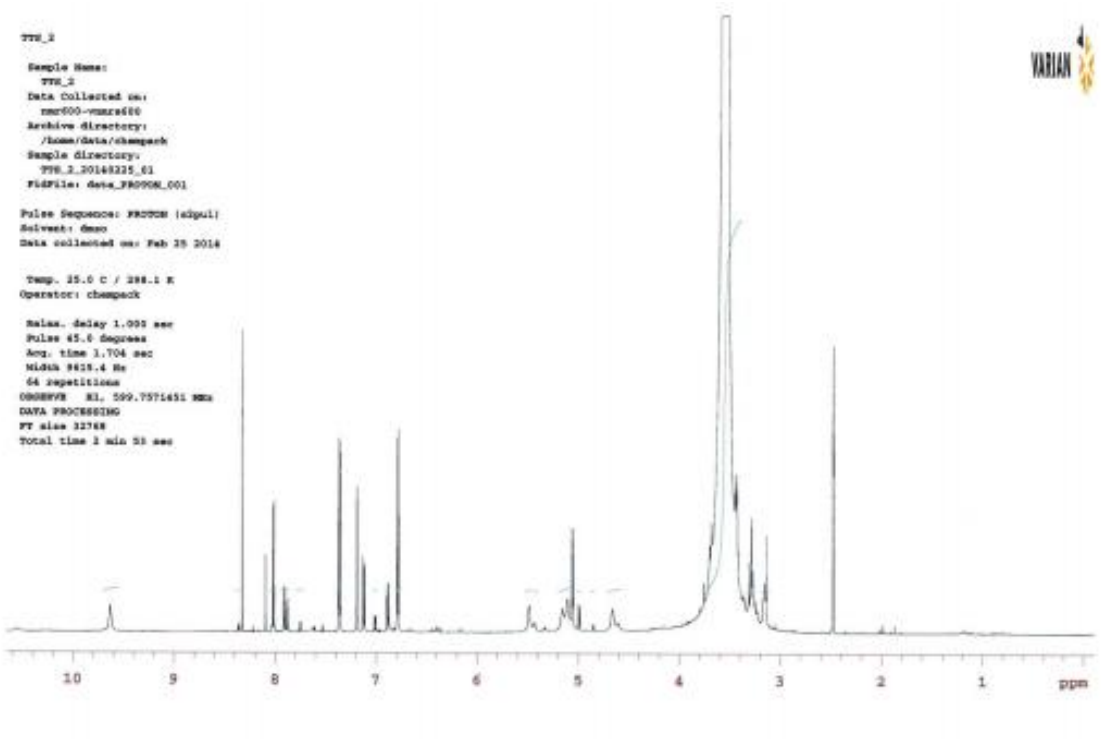
S11: Expansion of the COSY (600 MHz) Spectrum of Compound **3** (quercetin)



S12: HMBC (600 MHz) Spectrum of Compound **3** (quercetin)

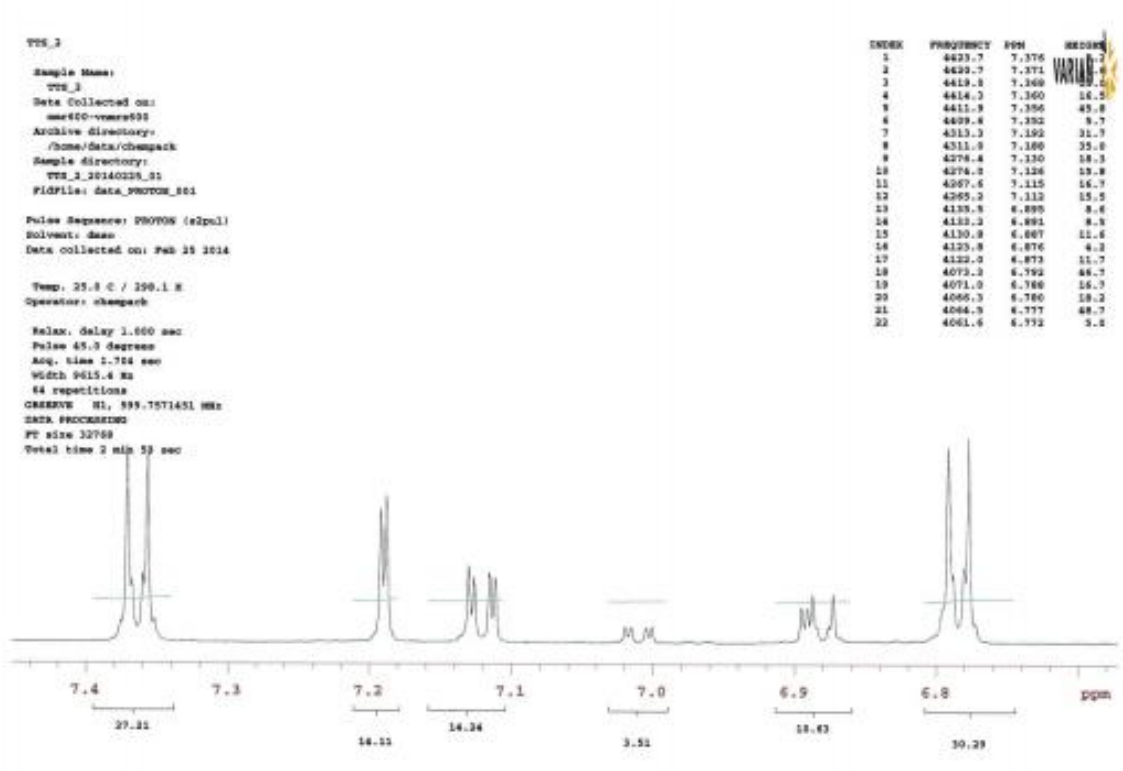


S13: HSQC (600 MHz) Spectrum of Compound **3** (quercetin)

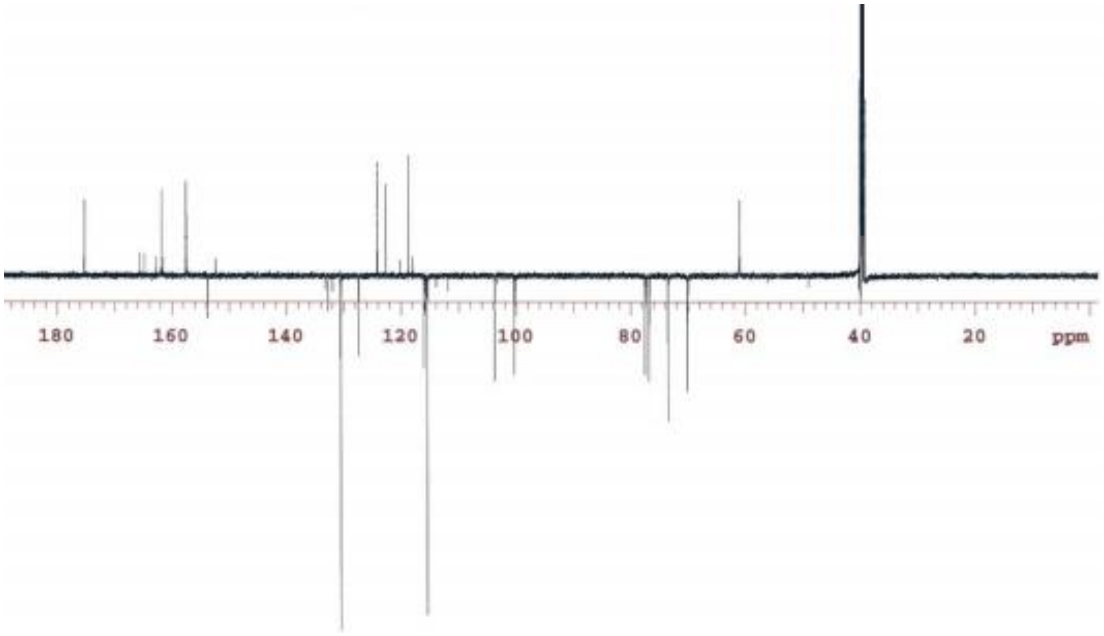


S14: ^{1}H-NMR (600 MHz, $CDCl_3$) Spectrum of Compound **4** (daidzein 4'-*O*-*β*-glucoside)

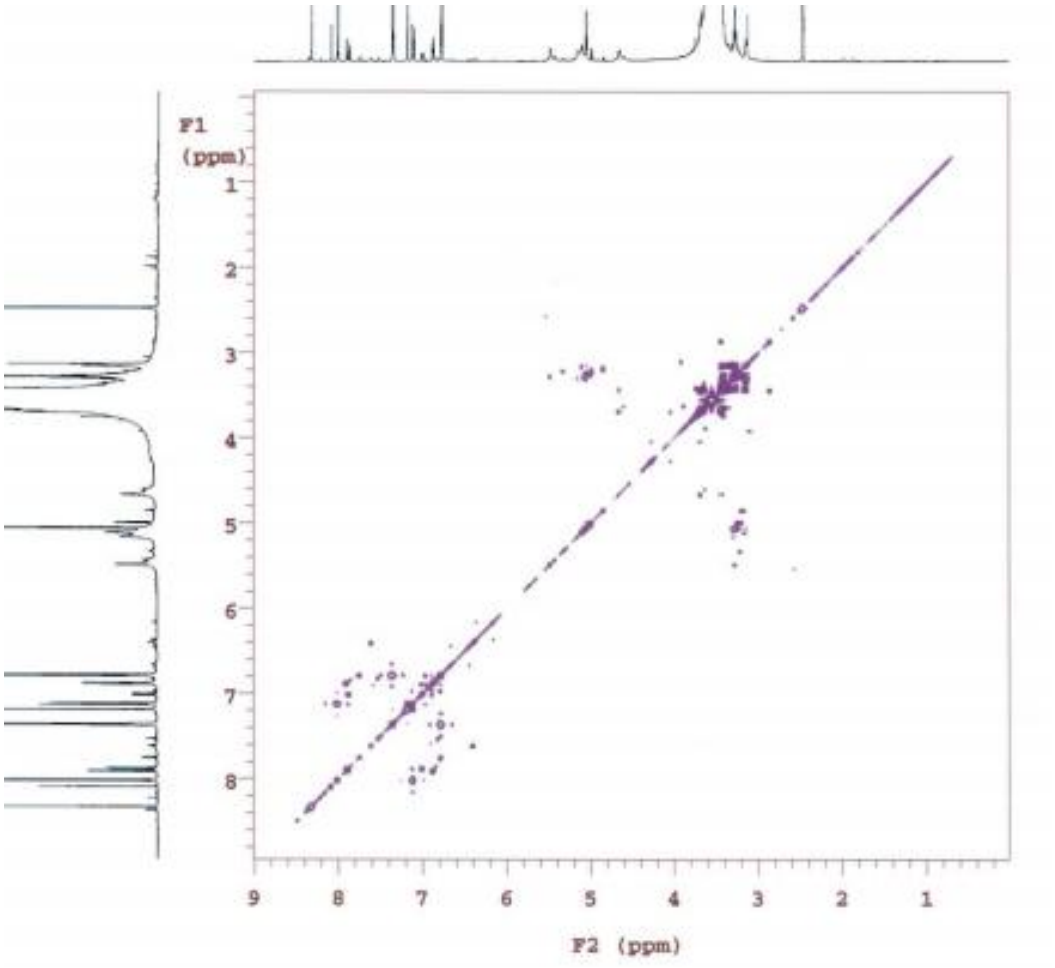
Daidzein 4'-*O*-*β*-glucoside: ^{1}H NMR (600 MHz, DMSO-d6): d 8.38 (1H, H-2, s), 8.04 (1H, H-5, d), 7.40 (2H, H-2',6', d), 7.22 (1H, H-8, s), 7.14 (1H, H-6, d), 6.81 (2H, H-3',5', d), 5.11 (1H, H-1", d), 3.68-3.18 (6H, m, sugar protons); ^{13}C NMR (125 MHz, DMSO-d6): d 180.3 (C-4), 166.8 (C-7), 162.7 (C-9), 162.5 (C-4'), 158.3 (C-2), 135.6 (x2C) (C-2',6'), 132.4 (C-5), 129.1 (C-1'), 127.7 (C-3), 123.9 (C-10), 121.1 (C-6), 120.4 (x2C) (C-3', 5'), 108.8 (C-8), 105.3 (C-1"), 82.6 (C-5"), 81.8 (C-2"), 78.5 (C-3"), 75.0 (C-4"), 66.0 (C-6").



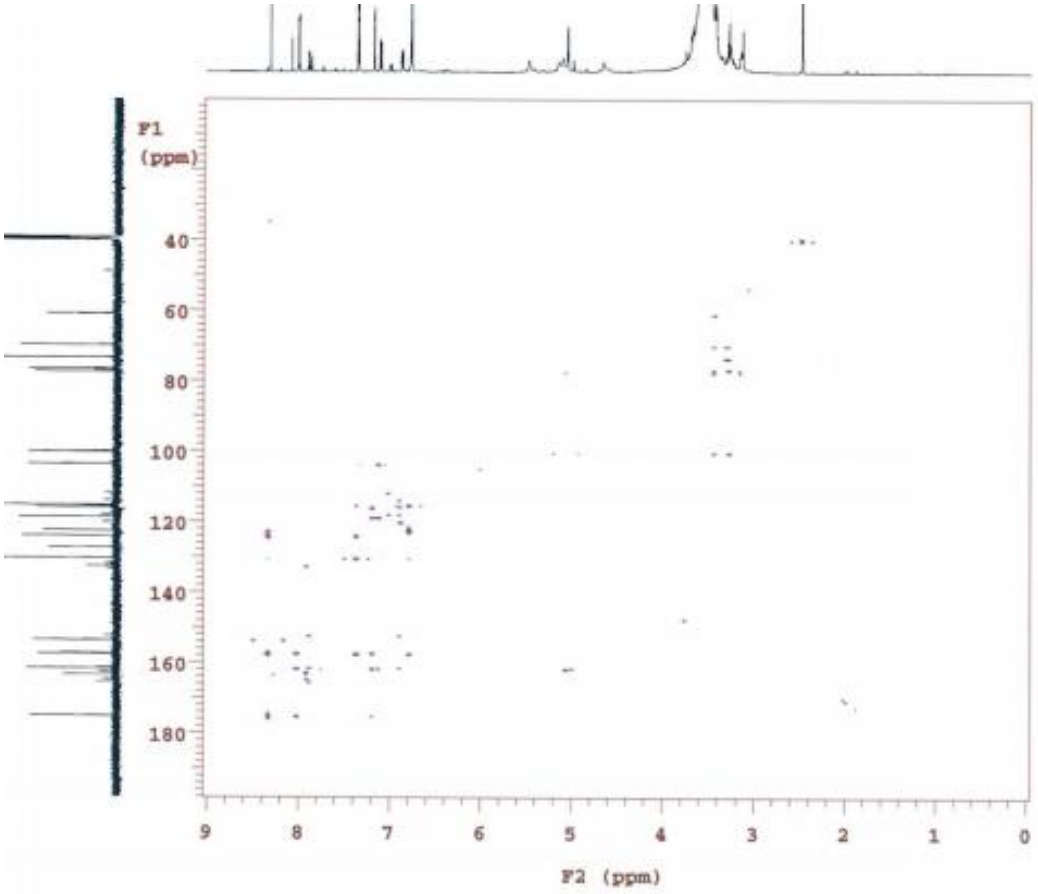
S15: Expansion of the ^{1}H-NMR Spectrum of Compound **4** (daidzein 4'-*O*-*β*-glucoside)



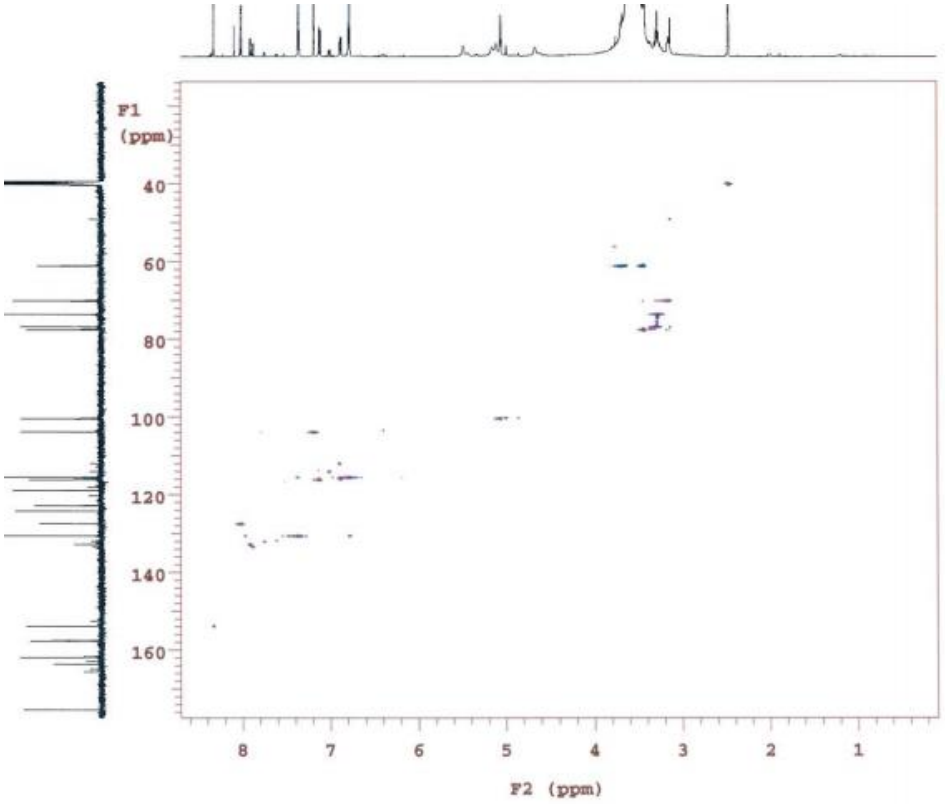
S16: ^{13}C-NMR + DEPT (125 MHz, $CDCl_3$) Spectrum of Compound **4** (daidzein 4'-*O*-*β*-glucoside)



S17: COSY (600 MHz) Spectrum of Compound **4** (daidzein 4'-*O*-*β*-glucoside)



S18: HMBC (600 MHz) Spectrum of Compound **4** (daidzein 4'-*O*-*β*-glucoside)



S19: HSQC (600 MHz) Spectrum of Compound **4** (daidzein 4'-*O*-*β*-glucoside)