

Supporting Information

Rec. Nat. Prod. 18:6 (2024) 610-617

GLUT4 translocation active flavonoids from *Caragana jubata*

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1. Characterization of Compounds

Caraganin E (1): Brown oily; $[\alpha]_D^{20} +1.4$ (*c* 0.50, MeOH); UV (MeOH); λ_{\max} (log ϵ): 225 (4.28), 280 (4.18), 350 (3.86) nm; IR ν_{KBr} max (cm^{-1}) 3225, 1654, 1616, 1519; ^1H and ^{13}C NMR spectroscopic data can be found in **Table 1**; HR-ESI-MS m/z 301.0731 $[\text{M}-\text{H}]^-$ (calcd for $\text{C}_{16}\text{H}_{13}\text{O}_6^-$, 301.0718).

(3R)-Caraganin F (2): Amorphous powder; $[\alpha]_D^{20} -5$ (*c* 0.40, MeOH); UV (MeOH); λ_{\max} (log ϵ): 225 (4.25) 300 (3.95) nm; IR ν_{KBr} max (cm^{-1}) 3410, 2916, 1620, 1338; CD (*c* 0.50, MeOH) $\lambda_{\max} (\Delta\epsilon)$ 216 (-5.88) nm, 239 (-3.84) nm, 282 (1.55) nm; ^1H and ^{13}C NMR spectroscopic data can be found in **Table 1**; HR-ESI-MS m/z 317.1020 $[\text{M}+\text{H}]^+$ (calcd for $\text{C}_{17}\text{H}_{17}\text{O}_{10}^+$, 317.1020).

7,3'-Dihydroxyl-5'-methoxyisoflavone (3): ^1H -NMR (600 MHz, CD_3OD) δ_{H} : 8.10 (1H, s, H-2), 8.02 (1H, d, $J = 8.8$ Hz, H-5), 7.01 (1H, d, $J = 1.2$ Hz, H-4'), 6.94 (2H, s, H-2', 6'), 6.91 (1H, dd, $J = 8.8, 2.3$ Hz, H-6), 6.82 (1H, d, $J = 2.3$ Hz, H-8), 3.86 (3H, s, 5'- OCH_3); ^{13}C -NMR (150 MHz, CD_3OD) δ_{C} : 178.01 (C-4), 164.76 (C-7), 159.76 (C-9), 154.85 (C-2), 149.15 (C-5'), 147.41 (C-3'), 128.51 (C-5), 126.19 (C-3), 125.77 (C-1'), 121.59 (C-6'), 118.13 (C-10), 117.38 (C-4'), 116.51 (C-6), 112.57 (C-2'), 103.24 (C-8), 56.38 (5'- OCH_3).

(6aR,11aR)-3,4-Dihydroxy-9-methoxypterocarpan (4): ^1H -NMR (600 MHz, CD_3OD) δ_{H} : 7.16 (1H, d, $J = 8.2$, H-7), 6.84 (1H, d, $J = 8.4$ Hz, H-1), 6.53 (1H, d, $J = 8.4$ Hz, H-2), 6.44 (1H, dd, $J = 8.2, 2.3$ Hz, H-8), 6.37 (1H, d, $J = 2.3$, H-10), 5.48 (1H, d, $J = 6.5$ Hz, H-11a), 4.34 (1H, m, H_{α} -6), 3.73 (3H, s, 9- OCH_3), 3.56 (1H, s, H_{β} -6), 3.52 (1H, m, H-6a); ^{13}C -NMR (150 MHz, CD_3OD) δ_{C} : 162.59 (C-9), 162.02 (C-10a), 147.14 (C-3), 145.81 (C-4a), 134.32 (C-4), 125.98 (C-7), 122.11 (C-1), 120.73 (C-6b), 113.75 (C-11b), 110.40 (C-2), 107.22 (C-8), 97.51 (C-10), 80.29 (C-11a), 67.91 (C-6), 55.88 (9- OCH_3), 40.99 (C-6a).

(6aR,11aR)-3,8-Dihydroxy-9-methoxypterocarpan (5): ^1H -NMR (600 MHz, CD_3OD) δ_{H} : 7.25 (1H, dd, $J = 8.4$ Hz, H-1), 6.76 (1H, s, H-7), 6.46 (2H, m, H-2, 10), 6.28 (1H, d, $J = 2.4$ Hz, H-4), 5.38 (1H, d, $J = 6.8$ Hz, H-11a), 4.19 (1H, dd, $J = 10.6, 4.6$, H-6), 3.78 (3H, s, 9- OCH_3), 3.51 (1H, t, $J = 10.6$ Hz, H_{α} -6), 3.44 (1H, m, H-6a); ^{13}C -NMR (150M, CD_3OD) δ_{C} : 160.00 (C-3), 158.00 (C-4a), 154.06 (C-10a), 149.51 (C-9), 141.61 (C-8), 133.14 (C-1), 119.42 (C-6b), 113.08 (C-11b), 112.44 (C-7), 110.65 (C-2), 104.04 (C-4), 96.22 (C-10), 79.54 (C-11a), 67.51 (C-6), 56.62 (MeO-9), 41.61 (C-6a).

Lespedezol D₁ (6): ^1H -NMR (600 MHz, $\text{DMSO}-d_6$) δ_{H} : 7.24 (1H, d, $J = 8.4$ Hz, H-1), 6.98 (1H, s, H-7), 6.46 (1H, dd, $J = 8.4, 2.4$ Hz, H-2), 6.28 (1H, s, H-10), 6.26 (1H, d, $J = 2.4$ Hz, H-4), 5.43 (1H, d, $J = 6.8$, H-11a), 4.22 (1H, m, H-6 α), 3.70 (3H, s, 8- OCH_3), 3.54 (2H, m, H-6 β , 6a); ^{13}C -NMR (150 MHz, $\text{DMSO}-d_6$) δ_{C} : 158.60 (C-3), 156.27 (C-4a), 153.33 (C-10a), 147.39 (C-9), 141.91 (C-8), 132.09 (C-1), 116.31 (C-6b), 111.51 (C-11b), 110.41 (C-7), 109.58 (C-2), 102.77 (C-4), 98.18 (C-10), 77.47 (C-11a), 65.91 (C-6), 56.81 (8- OCH_3), 40.11 (C-6a).

Pinoresinol (7): ^1H -NMR (600 MHz, CD_3OD) δ_{H} : 6.95 (2H, d, $J = 1.9$ Hz, H-2, 2'), 6.81 (2H, dd, $J = 8.0, 1.9$ Hz, H-6, 6'), 6.77 (2H, d, $J = 8.0$ Hz, H-5, 5'), 4.70 (2H, d, $J = 4.6$ Hz, H-7, 7'), 4.23 (2H, dd, $J = 9.0, 6.9$ Hz, H-9a, 9a'), 3.85 (6H, s, 3, 3'- OCH_3), 3.83 (2H, m, H-9b, 9b'), 3.14 (2H, m, H-8, 8'); ^{13}C -NMR (150M, CD_3OD) δ_{C} : 149.11 (C-3, 3'), 147.30 (C-4, 4'), 133.78 (C-

1, 1'), 120.05 (C-6, 6'), 116.06 (C-5, 5'), 110.93 (C-2, 2'), 87.51 (C-7, 7'), 72.59 (C-9, 9'), 56.37 (3, 3'-OCH₃), 55.36 (C-8, 8').

kaempferol (**8**): ¹H-NMR (600 MHz, CD₃OD) δ_H: 8.08 (2H, d, *J* = 8.8 Hz, H-2', 6'), 6.89 (2H, d, *J* = 8.8 Hz, H-3', 5'), 6.38 (1H, d, *J* = 1.8 Hz, H-8), 6.17 (1H, d, *J* = 1.8 Hz, H-6); ¹³C-NMR (150 MHz, CD₃OD) δ_C: 177.41 (C-4), 165.60 (C-7), 162.54 (C-5), 160.57 (C-4'), 158.26 (C-9), 148.05 (C-2), 137.19 (C-3), 130.68 (C-2', 6'), 123.74 (C-1'), 116.30 (C-3', 5'), 104.54 (C-10), 99.25 (C-6), 94.44 (C-8).

Liquiritigenin (**9**): ¹H-NMR (600 MHz, CD₃OD) δ_H: 7.71 (1H, d, *J* = 8.7 Hz, H-5), 7.30 (2H, d, *J* = 8.5 Hz, H-2', 6'), 6.80 (2H, d, *J* = 8.5 Hz, H-3', 5'), 6.48 (1H, dd, *J* = 8.7, 2.3 Hz, H-6), 6.33 (1H, d, *J* = 2.3 Hz, H-8), 5.36 (1H, dd, *J* = 13.1, 2.8 Hz, H-2), 3.30 (1H, dd, *J* = 16.9, 13.1 Hz, H-3b), 2.67 (1H, dd, *J* = 16.9, 2.9 Hz, H-3a); ¹³C-NMR (150 MHz, CD₃OD) δ_C: 193.56 (C-4), 166.82 (C-7), 165.58 (C-5), 158.98 (C-4'), 131.34 (C-1'), 129.86 (C-5), 129.02 (C-2', 6'), 116.30 (C-3', 5'), 114.96 (C-10), 111.75 (C-6), 103.81 (C-8), 81.05 (C-2), 44.95 (C-3).

Erycibenin D (**10**): ¹H-NMR (600 MHz, CD₃OD) δ_H: 7.73 (1H, d, *J* = 8.7 Hz, H-5), 7.13 (1H, d, *J* = 1.9 Hz, H-2'), 6.99 (1H, dd, *J* = 8.1, 1.9 Hz, H-6'), 6.84 (1H, d, *J* = 8.1 Hz, H-5'), 6.54 (1H, dd, *J* = 8.7, 2.2 Hz, H-6), 6.34 (1H, d, *J* = 2.2 Hz, H-8), 5.01 (1H, d, *J* = 11.9 Hz, H-2), 4.58 (1H, d, *J* = 11.9 Hz, H-3), 3.89 (3H, s, 3'-OCH₃); ¹³C-NMR (150 MHz, CD₃OD) δ_C: 194.50 (C-4), 166.88 (C-7), 165.07 (C-9), 148.90 (C-3'), 148.28 (C-4'), 130.10 (C-1'), 130.03 (C-5), 122.20 (C-6'), 115.94 (C-5'), 113.46 (C-10), 112.42 (C-2'), 112.13 (C-6), 103.71 (C-8), 85.74 (C-2), 74.54 (C-3), 56.43 (3'-OCH₃).

Quercetin 3-O-β-glucopyranoside (**11**): ¹H-NMR (600 MHz, DMSO-*d*₆) δ_H: 7.57 (2H, m, H-2', 5'), 6.83 (1H, d, *J* = 9.0 Hz, H-6'), 6.38 (1H, s, H-6), 6.17 (1H, s, H-8), 5.47 (1H, d, *J* = 7.3 Hz, Glc-1), 3.21 (6H, m, Glc-2-Glc-6); ¹³C-NMR (150 MHz, DMSO-*d*₆) δ_C: 177.36 (C-4), 164.87 (C-7), 161.24 (C-5), 156.41 (C-2), 156.07 (C-9), 148.63 (C-4'), 144.92 (C-3'), 133.26 (C-3), 121.60 (C-6'), 121.12 (C-1'), 116.18 (C-5'), 115.25 (C-2'), 103.73 (C-10), 100.90 (Glc-1), 98.88 (C-6), 93.63 (C-8), 77.61 (Glc-5), 76.53 (Glc-3), 74.12 (Glc-2), 69.94 (Glc-4), 60.98 (Glc-6).

Calycosin (**12**): ¹H-NMR (600 MHz, DMSO-*d*₆) δ_H: 8.28 (1H, s, H-2), 7.96 (1H, d, *J* = 8.8 Hz, H-5), 7.04 (1H, d, *J* = 1.6 Hz, H-2'), 6.94 (2H, m, H-5', 6'), 6.93 (1H, m, H-6), 6.85 (1H, d, *J* = 2.2 Hz, H-8), 3.79 (3H, s, 4'-OCH₃); ¹³C-NMR (150 MHz, DMSO-*d*₆) δ_C: 174.63 (C-4), 162.76 (C-7), 157.46 (C-9), 153.11 (C-2), 147.52 (C-4'), 146.04 (C-3'), 127.34 (C-5), 124.73 (C-1'), 123.38 (C-3), 119.74 (C-6'), 116.59 (C-10), 116.46 (C-2'), 115.27 (C-6), 111.95 (C-5'), 102.14 (C-8), 55.68 (4'-OCH₃).

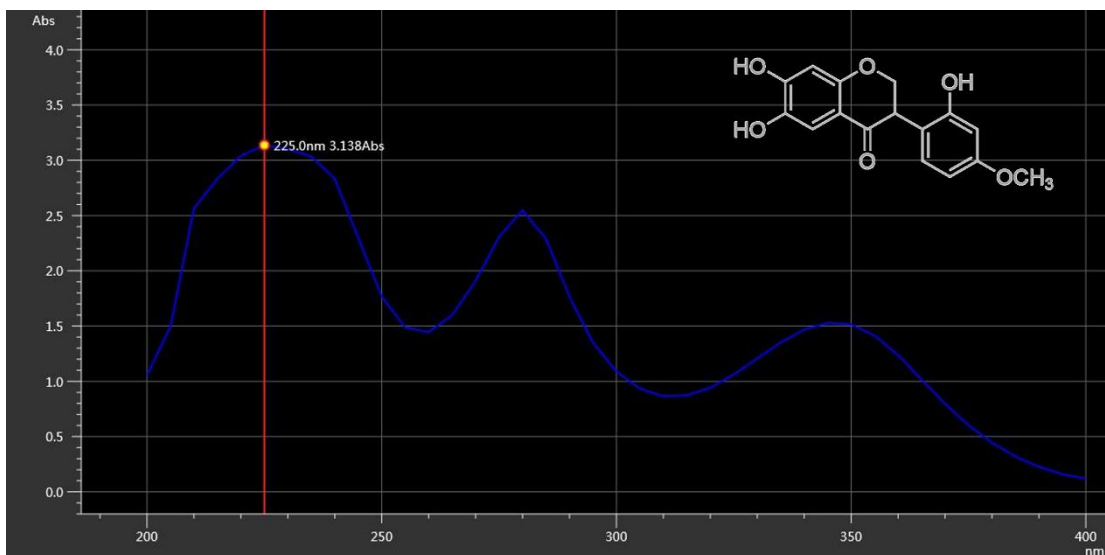


Figure S1: UV spectrum of Compound 1

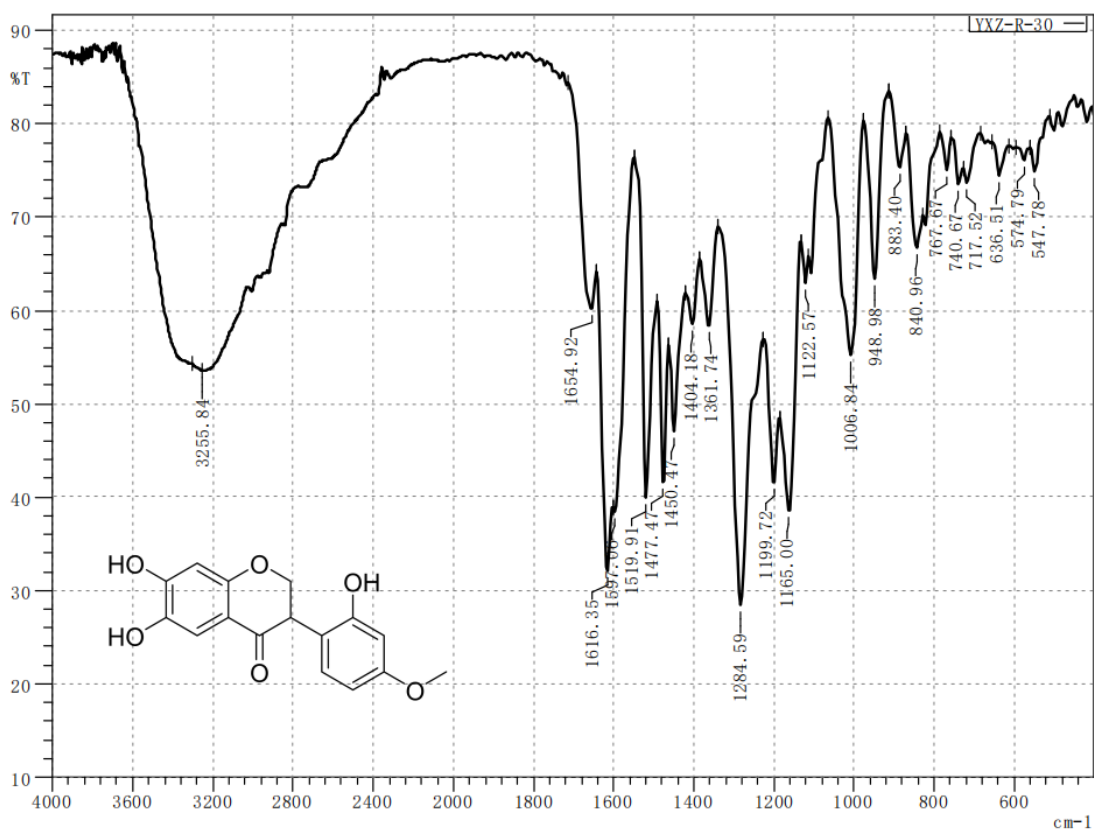


Figure S2: IR spectrum of Compound 1

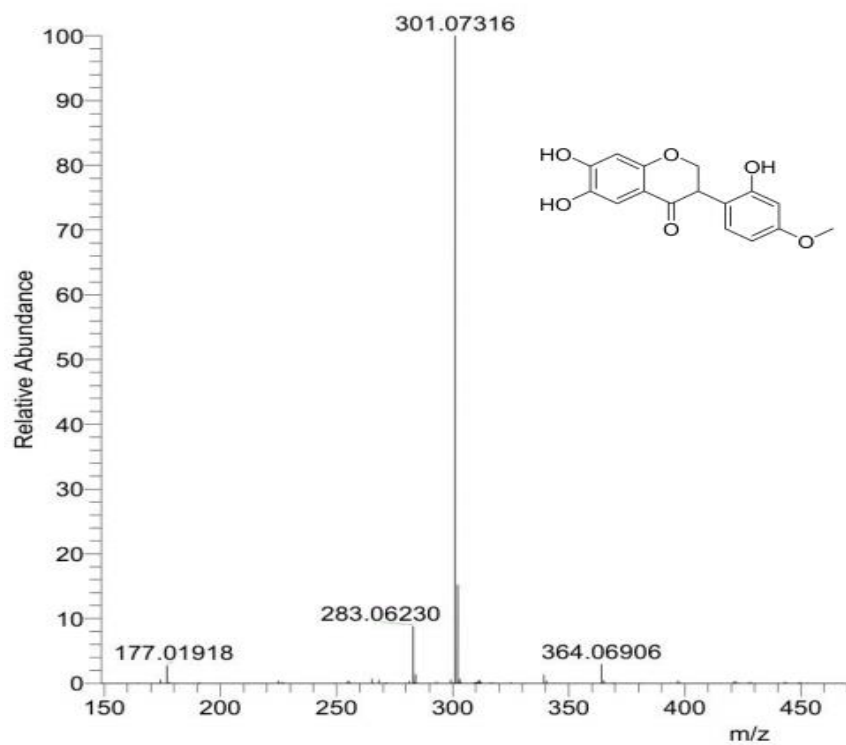


Figure S3: HR-ESI-M of Compound 1

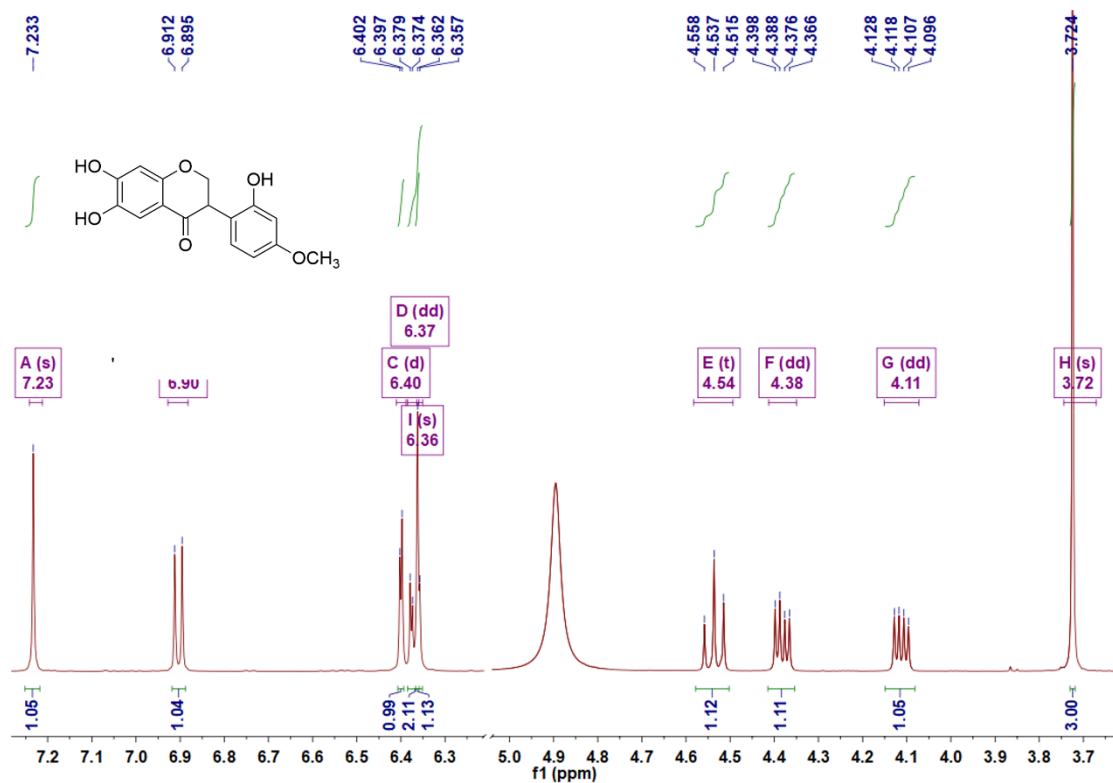


Figure S4: ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of Compound 1

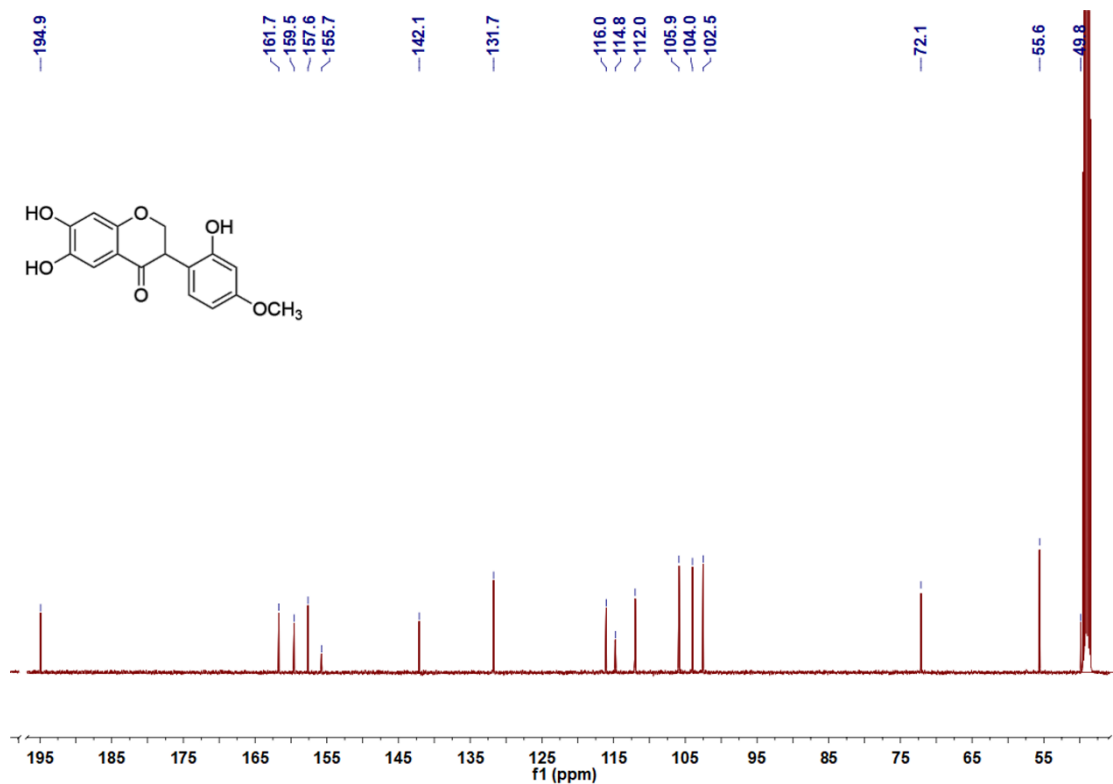


Figure S5: ^{13}C NMR spectrum (150 MHz, DMSO- d_6) of Compound 1

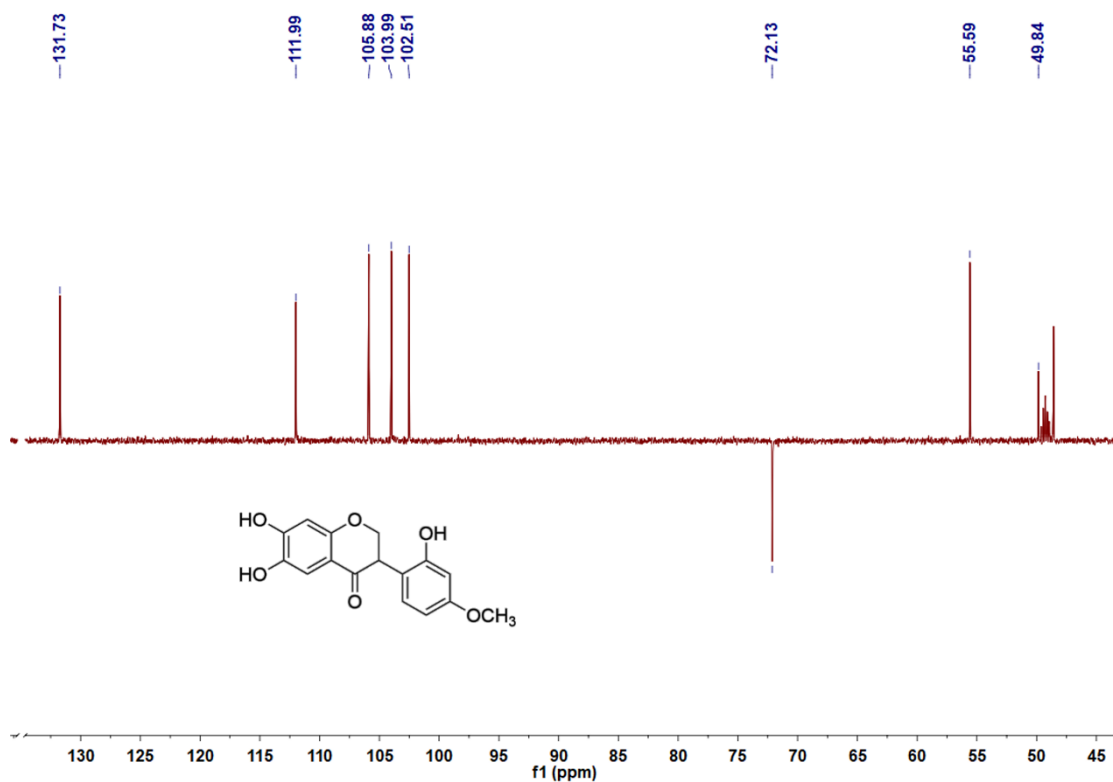


Figure S6: DEPT 135° spectrum (150 MHz, DMSO- d_6) of Compound 1

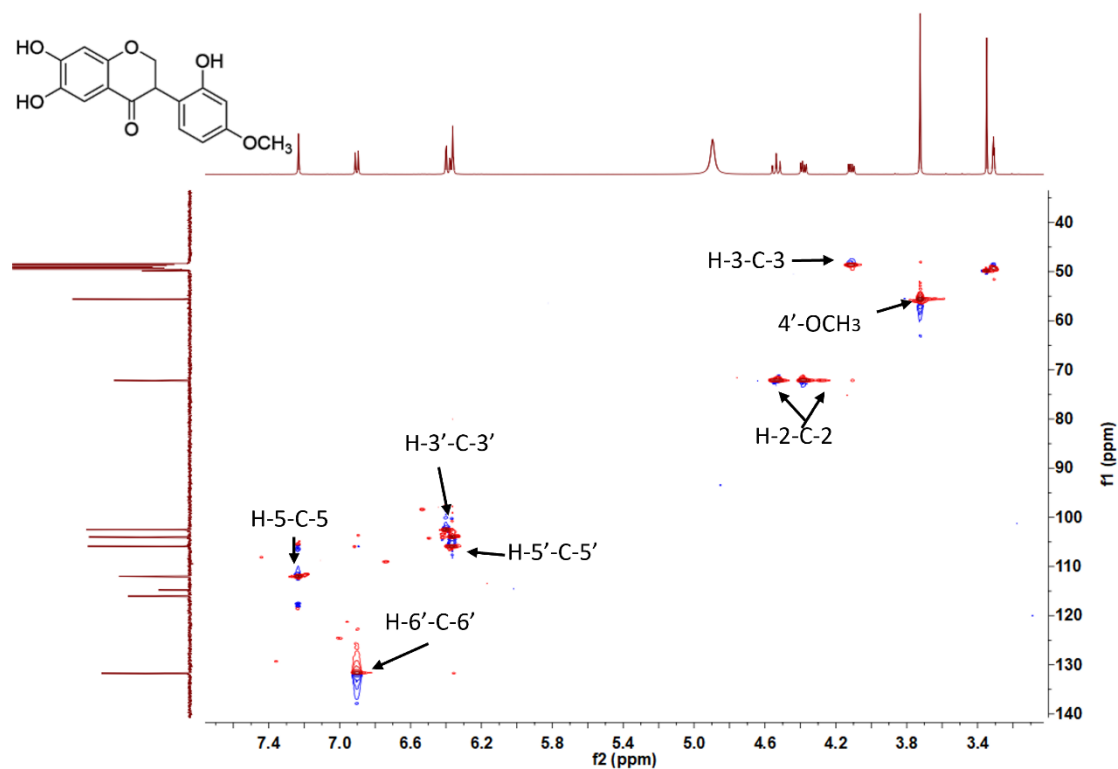


Figure S7: HSQC spectrum of Compound **1**

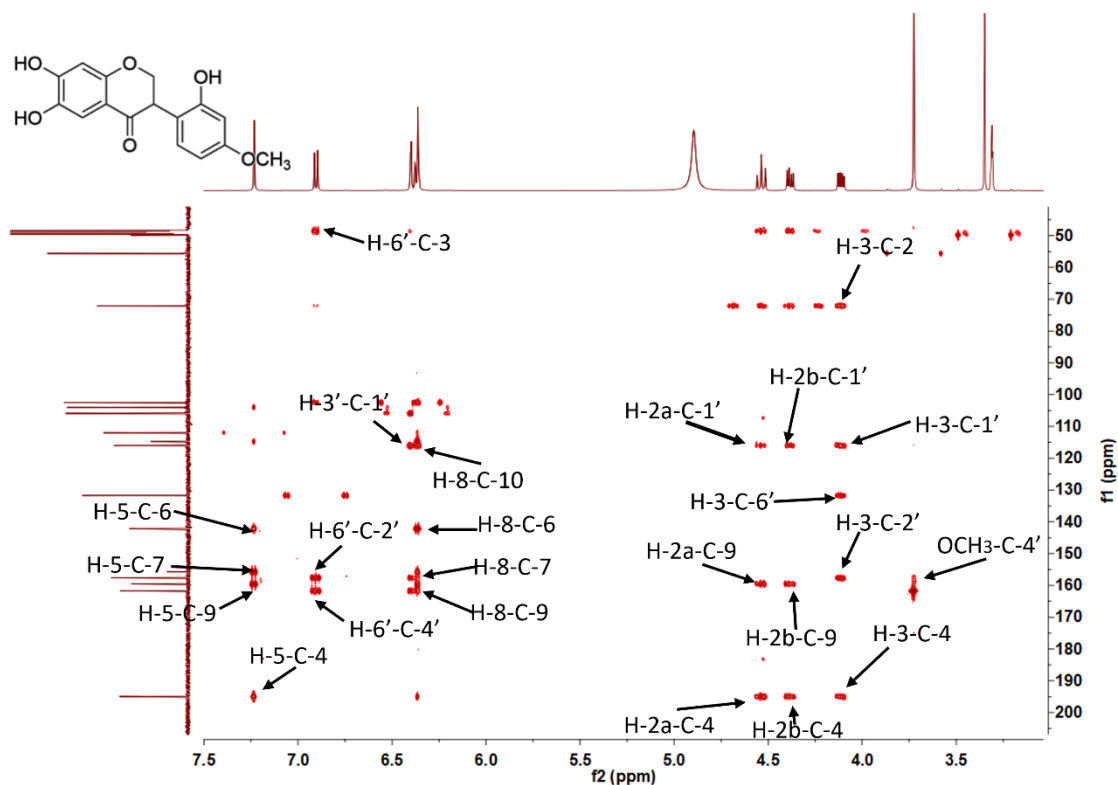


Figure S8: HMBC spectrum of Compound **1**

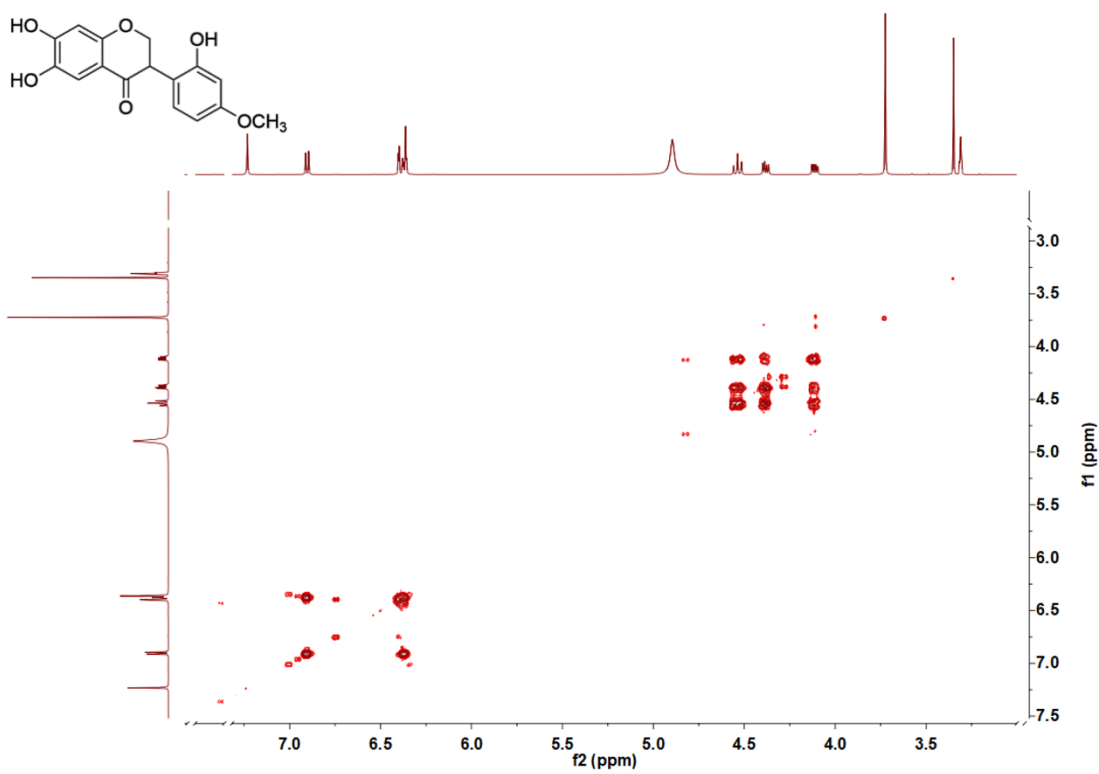


Figure S9: ^1H - ^1H COSY spectrum of Compound 1

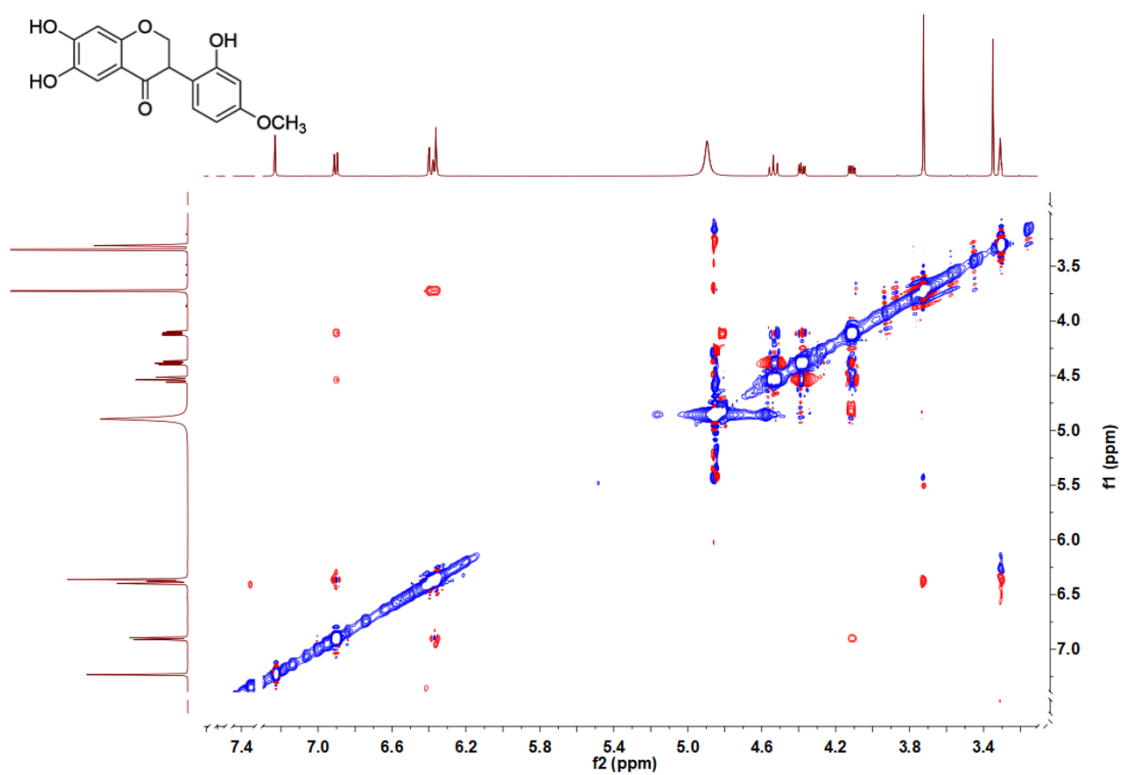


Figure S10: ROESY spectrum of Compound 1

Figure S11. CD spectrum of Compound 1

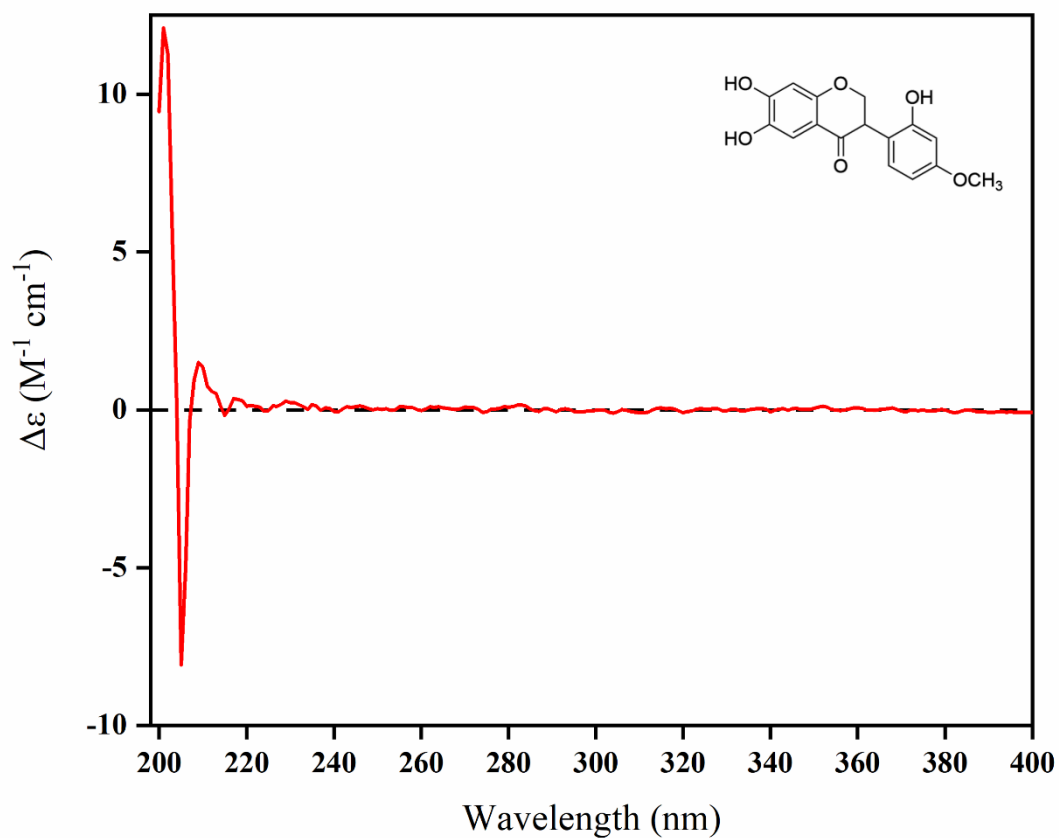


Figure S11: CD spectrum of Compound 1

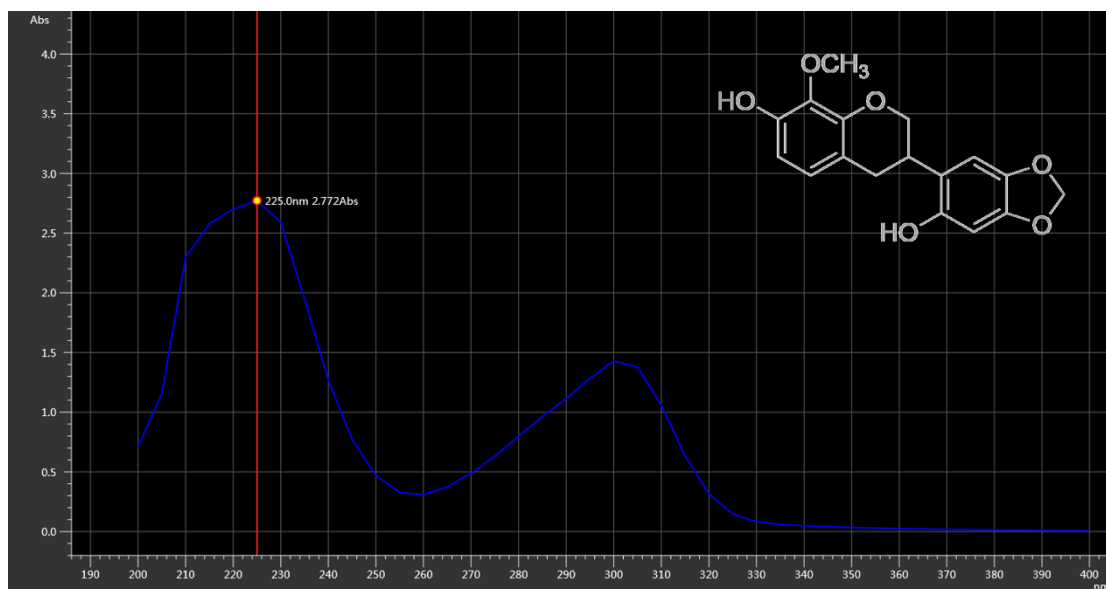


Figure S12: UV spectrum of Compound 2

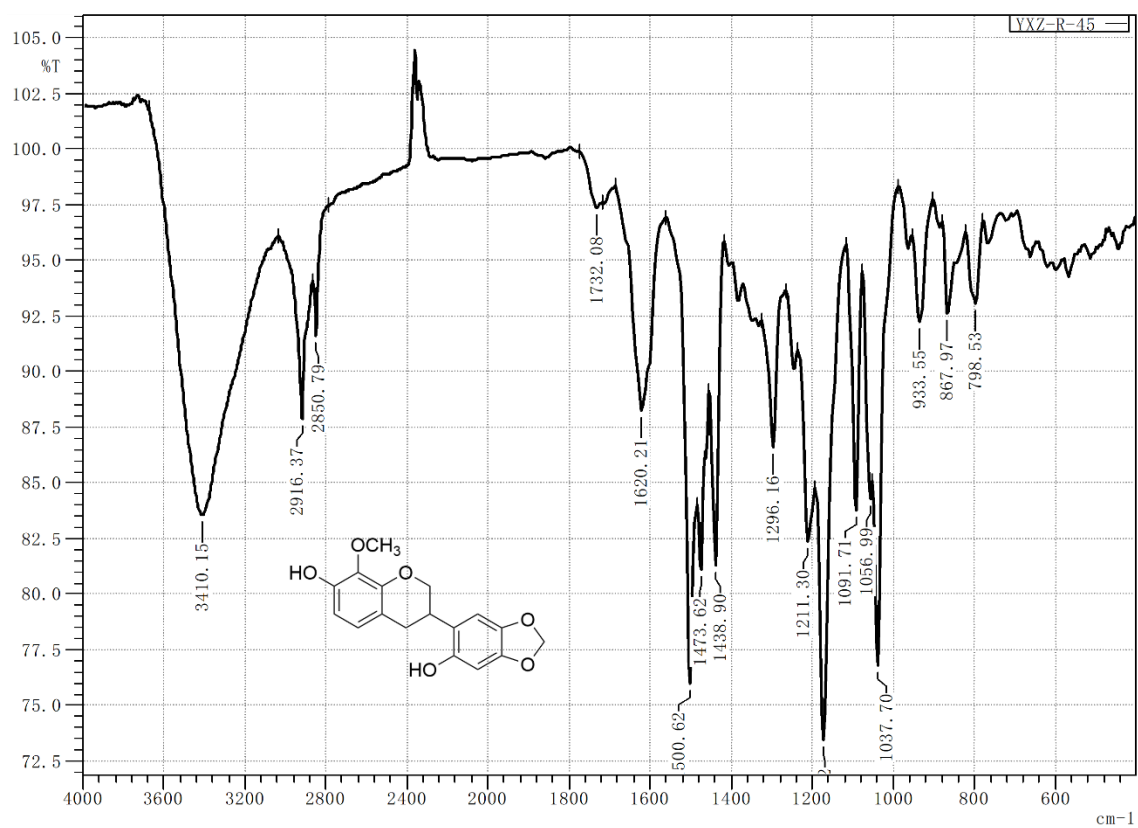


Figure S13: IR spectrum of Compound 2

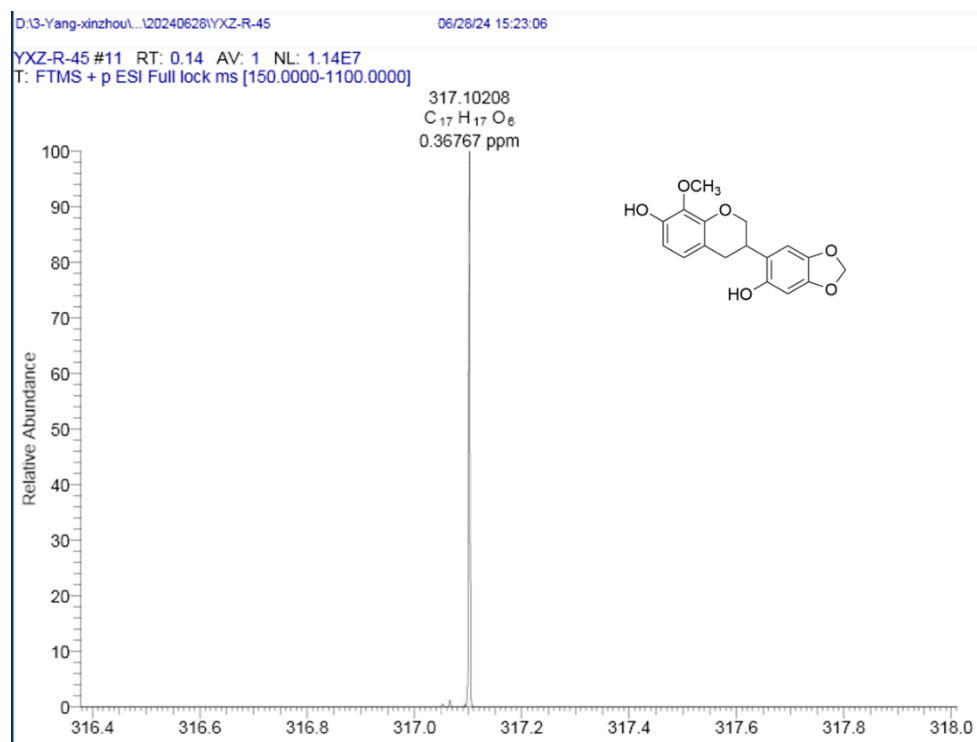


Figure S14: HR-ESI-M of Compound 2

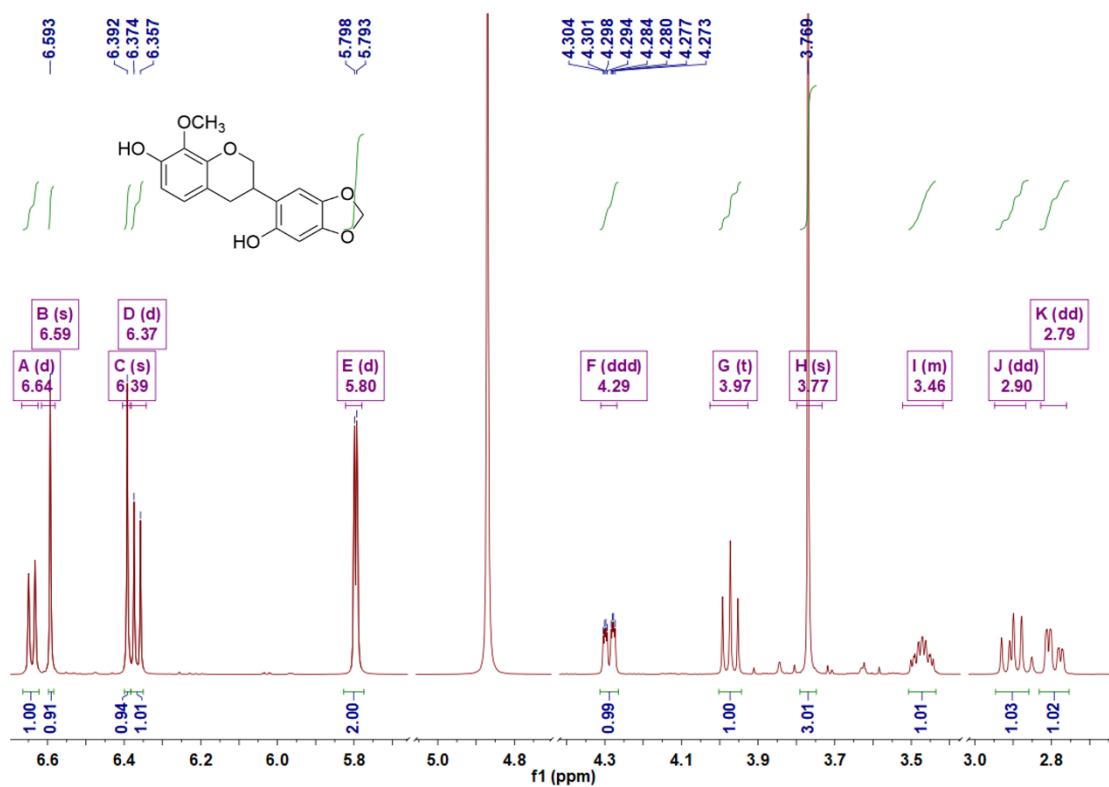


Figure S15: ^1H NMR spectrum (600 MHz, $\text{DMSO-}d_6$) of Compound 2

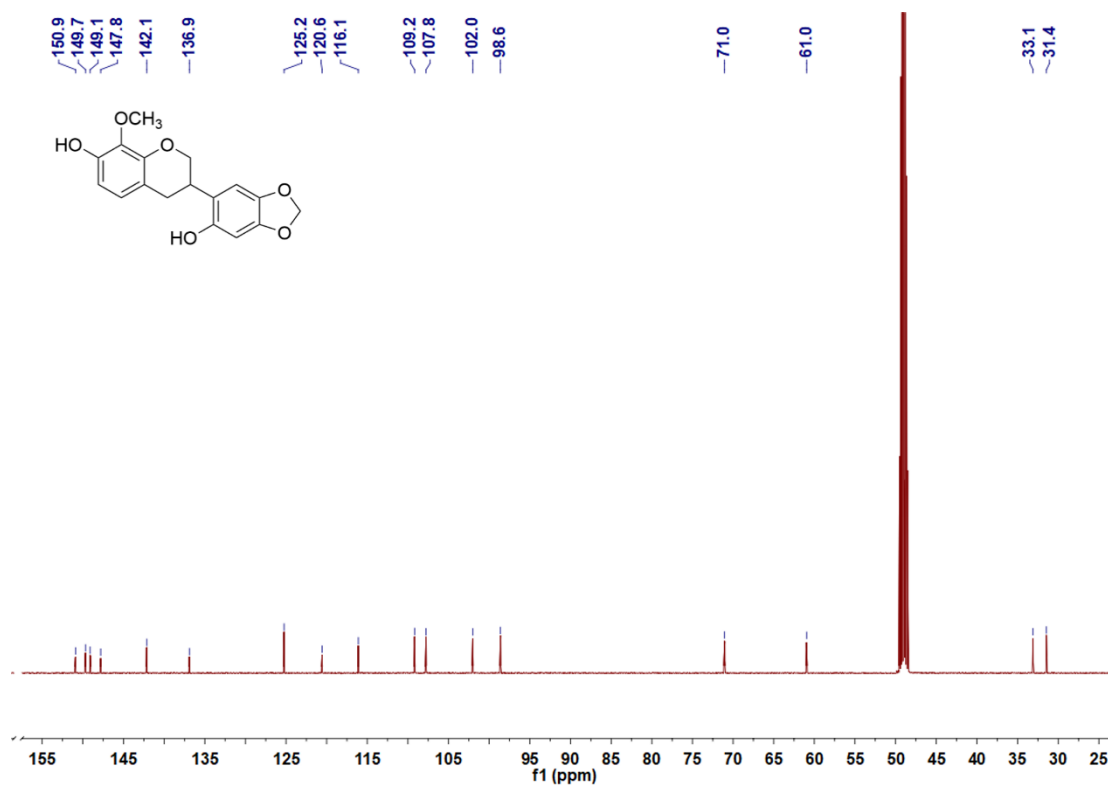


Figure S16: ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$) of Compound 2

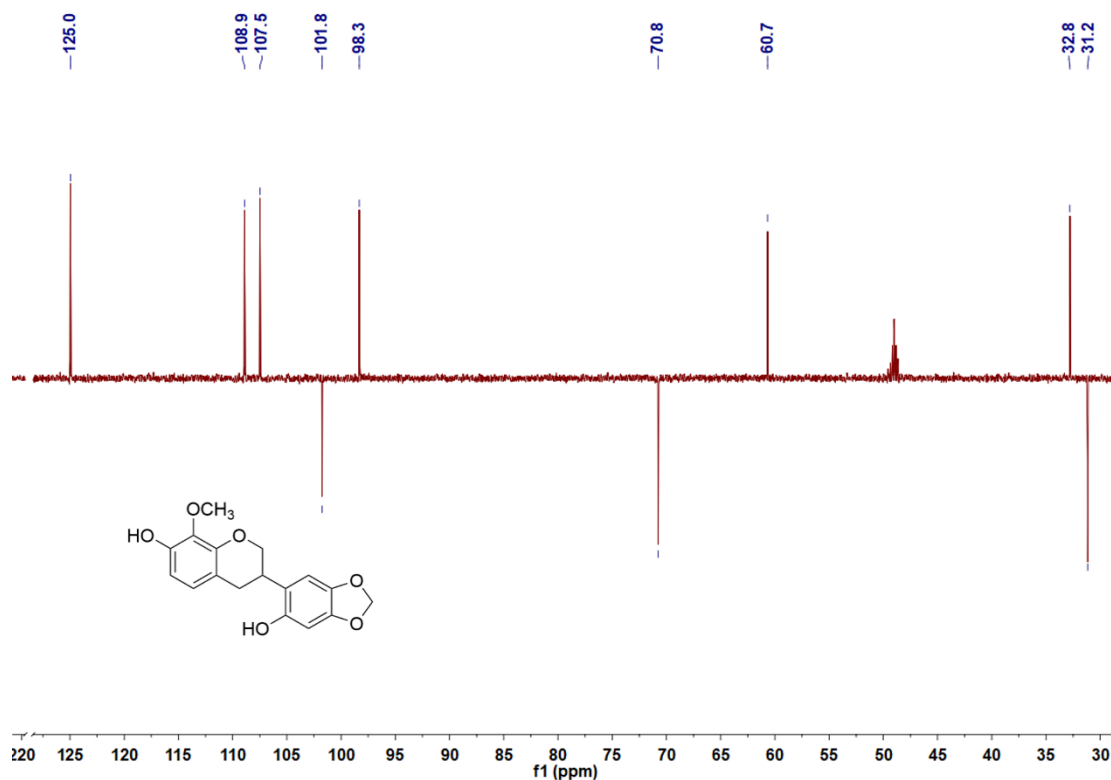


Figure S17: DEPT 135° spectrum (150 MHz, DMSO-*d*₆) of Compound 2

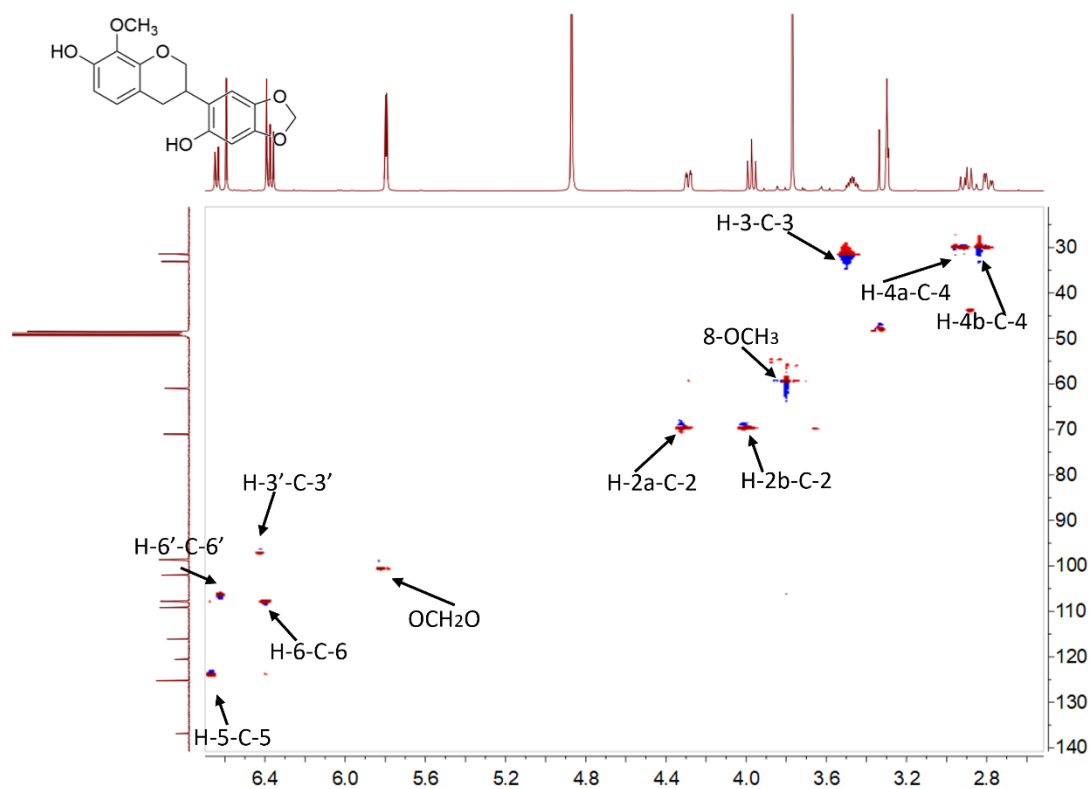


Figure S18: HSQC spectrum of Compound 2

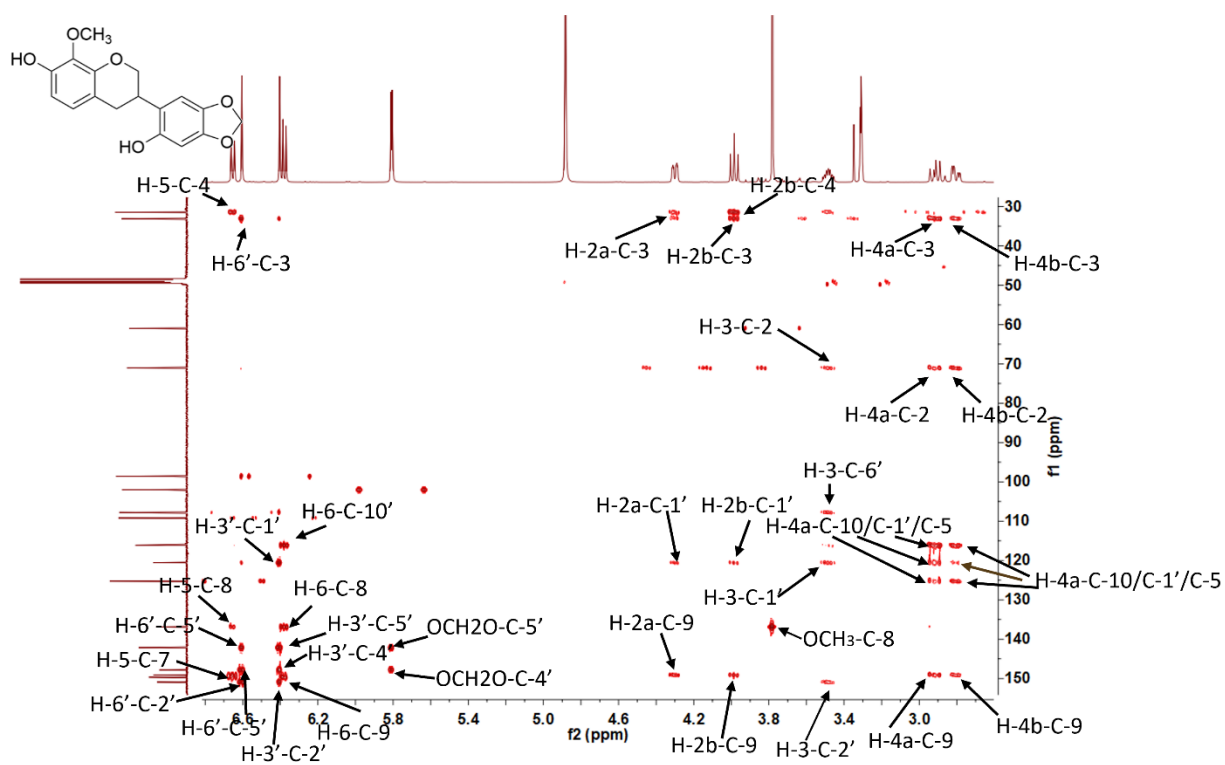


Figure S19: HMBC spectrum of Compound 2

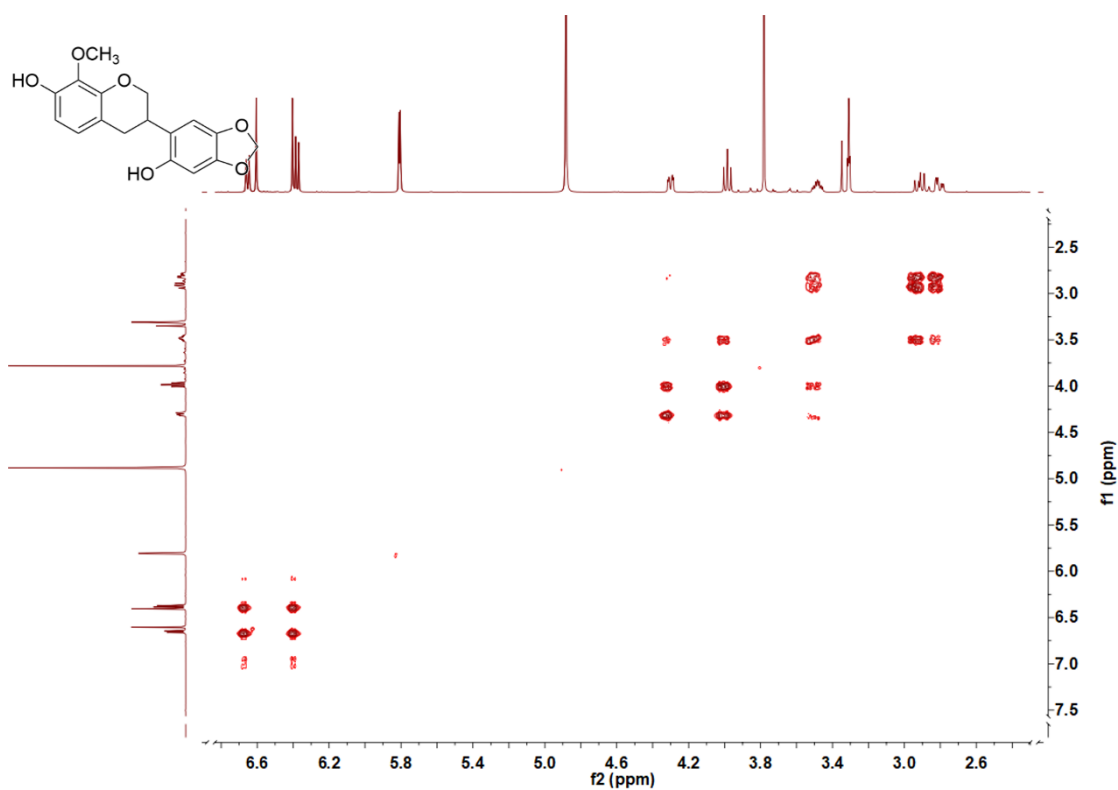


Figure S20: ^1H - ^1H COSY spectrum of Compound 2

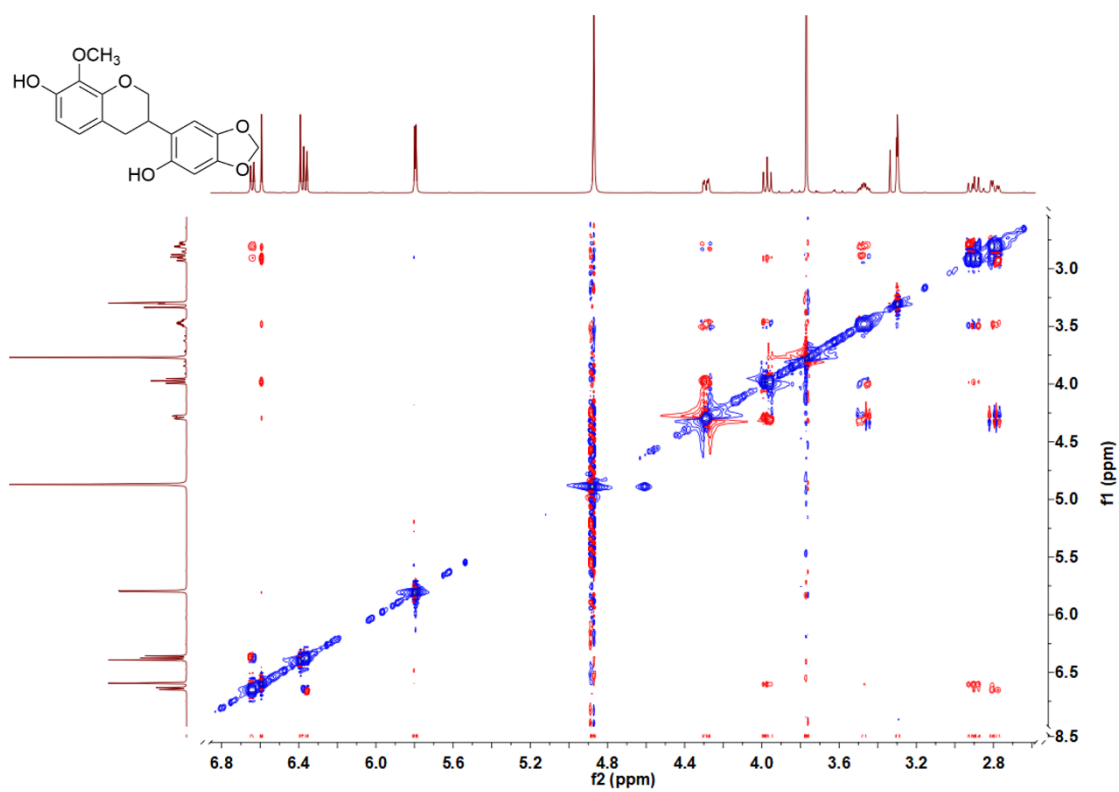


Figure S21: ROESY spectrum of Compound **2**

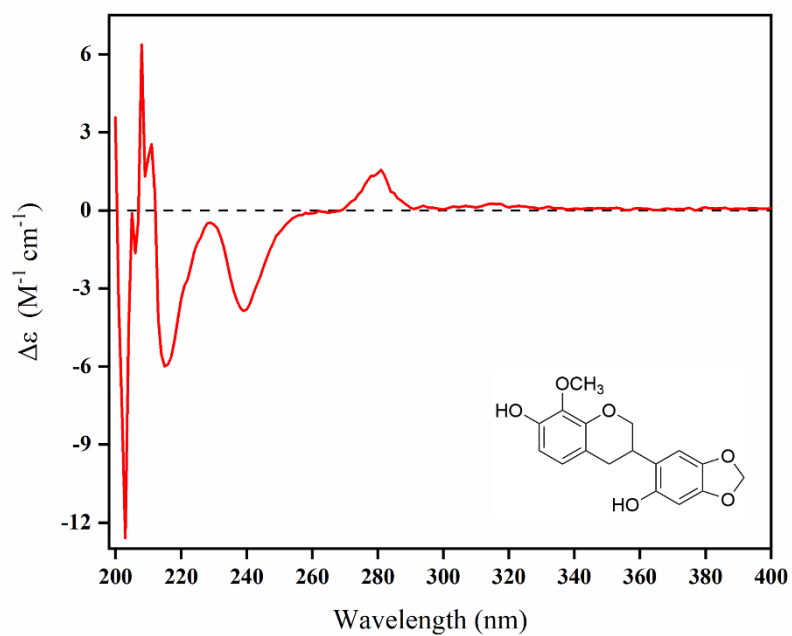
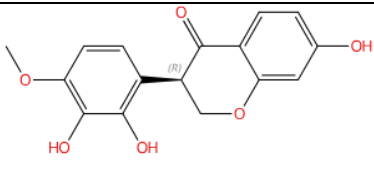
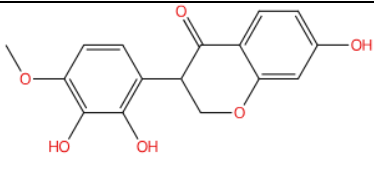
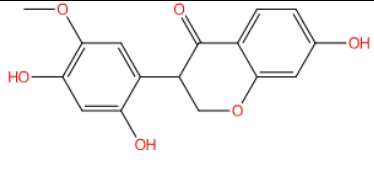
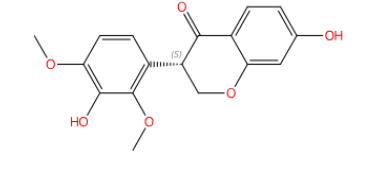
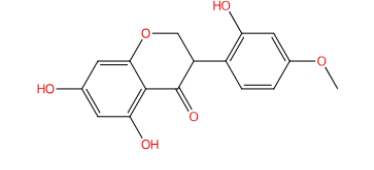
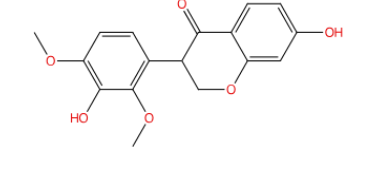
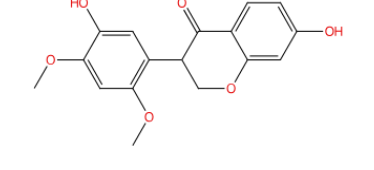
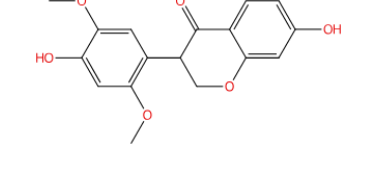


Figure S22: CD spectrum of Compound **2**

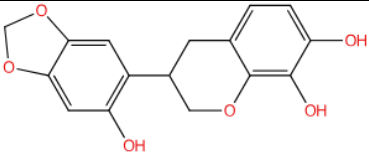
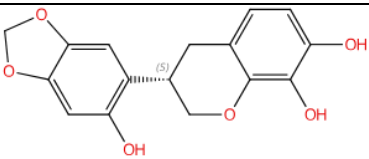
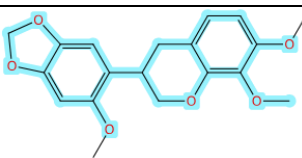
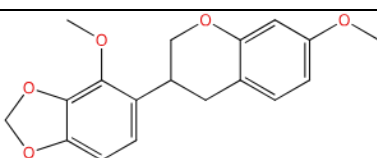
Table S1: SciFinder searches for the ten compounds most similar to Compound 1 in the report

No.	structure	similarity
1		97%
2		97%
3		97%
4		96%
5		96%
6		96%
7		96%
8		96%

9		96%
10		96%

Table S2: SciFinder searches for the ten compounds most similar to Compound 2 in the report

No.	structure	similarity
1		98%
2		98%
3		97%
4		97%
5		97%
6		96%

7		96%
8		96%
9		95%
10		95%