

1 **Supplementary material**

2 Tetrahydronethoxychalcone (1): Yellow powder. HR-ESI-MS m/z:
3 303.0859 [M+H]⁺. ¹H-NMR (DMSO-*d*₆, 400 MHz)δ_{ppm}: 7.80(1H, d,
4 *J*=15.6 Hz, H-β), 7.62(1H, d, *J*=15.6Hz, H-α), 7.54 (1H, dd, *J*=8.3, 1.9 Hz,
5 H-6'), 7.48(1H, d, *J*=1.9 Hz, H-2'), 7.30 (1H, d, *J*= 8.6 Hz, H-6), 6.85 (1H,
6 d, *J*=8.3 Hz, H-5'), 6.63 (1H, d, *J*=8.5 Hz, H-5), 3.77 (3H, s, -OCH₃). ¹³C-
7 NMR (DMSO-*d*₆, 100 MHz)δ_{ppm}: 187.21(C=O), 150.50 (C-4'), 149.46 (C-
8 4), 148.46 (C-1), 145.36 (C-3'), 138.29 (C-3), 137.90 (C-β), 129.98 (C-1'),
9 121.59 (C-6'), 119.51 (C-1), 119.15 (C-α), 118.53 (C-6), 115.23 (C-2'),
10 115.06 (C-5'), 111.62 (C-5), 60.66 (-OCH₃).

11 7,4'-Dihydroxyflavone (2): Yellow powder. HR-ESI-MS m/z: 255.0670
12 [M+H]⁺. ¹H-NMR (DMSO-*d*₆, 400 MHz) δ_{ppm}: 7.92 (2H, d, *J*=8.7 Hz, H-
13 2', H-6'), 7.87 (1H, d, *J*=8.7 Hz, H-5), 6.97 (2H, d, *J*=2.0 Hz, H-3', H-5'),
14 6.93 (1H, m, H-3', H-8), 6.90 (2H, d, *J*=2.0 Hz, H-6), 6.73 (1H, s, H-3).
15 ¹³C-NMR (DMSO-*d*₆, 100 MHz)δ_{ppm}: 176.23(C=O), 162.49(C-7), 162.40
16 (C-2), 160.64 (C-1), 157.33 (C-9), 128.08 (C-2', C-6'), 126.42 (C-5),
17 121.75 (C-1'), 116.08 (C-3'), 115.85 (C-5'), 114.73 (C-6), 104.44 (C-3),
18 102.43 (C-8).

19 Licochalcone B (3): Yellow powder. HR-ESI-MS m/z: 287.0938 [M+H]⁺.
20 ¹H-NMR (DMSO-*d*₆, 400 MHz)δ_{ppm}: 8.01 (2H, d, *J*=8.7Hz, H-2', H-6'),
21 7.85 (1H, d, *J*=15.6 Hz, H-β), 7.68 (1H, d, *J*=15.6 Hz, H-α), 7.34 (1H, d,

22 $J=8.6$ Hz, H-6), 6.94 (2H, d, $J=8.7$ Hz, H-3', H-4'), 6.64 (1 H, d, $J=8.6$ Hz,
23 H-5), 3.77 (3H, s, -OCH₃). ¹³C-NMR (DMSO-*d*₆, 100 MHz) δ_{ppm} : 187.14
24 (C=O), 161.81 (C-4'), 149.53 (C-2), 148.49 (C-4), 138.26 (C- β), 138.09
25 (C-3), 130.81 (C-2'), 129.49 (C-6'), 119.48 (C-1), 119.04 (C- α), 118.44 (C-
26 6), 115.27 (C-3', C-5'), 111.61 (C-5), 60.72 (-OCH₃).

27 Liquiritigenin (4): White powder. HR-ESI-MS m/z : 257.0840 [M+H]⁺. ¹H-
28 NMR (DMSO-*d*₆, 400 MHz) δ_{ppm} : 7.65 (1H, d, $J=8.7$ Hz, H-5), 7.33 (2H,
29 d, $J=8.5$ Hz, H-2', H-6'), 6.79 (2H, d, $J=8.5$ Hz, H-3', H-5'), 6.50 (1H, dd,
30 $J=8.7, 2.1$ Hz, H-6), 6.33 (1H, d, $J=2.1$ Hz, H-8), 5.44 (1H, dd, $J=12.9, 2.6$
31 Hz, H-2), 3.12 (1H, dd, $J=16.7, 13.0$ Hz, H-3), 2.62 (1H, dd, $J=16.8, 2.8$
32 Hz, H-3). ¹³C-NMR (DMSO-*d*₆, 100 MHz) δ_{ppm} : 190.08 (C=O), 164.58 (C-
33 9), 163.14 (C-7), 157.58 (C-4'), 129.28 (C-5), 128.37 (C-2'), 128.23 (C-6'),
34 115.09 (C-3', C-5'), 113.50 (C-10), 110.45 (C-6), 102.52 (C-8), 78.93 (C-
35 2), 43.13 (C-3).

36 Echinatin (5): Yellow powder. HR-ESI-MS m/z : 271.0933 [M+H]⁺. ¹H-
37 NMR (DMSO-*d*₆, 400 MHz) δ_{ppm} : 10.33 (1H, s, 4-OH), 10.15 (1H, s, 4'-
38 OH), 7.99 (2H, d, $J=8.6$ Hz, H-2', H-6'), 7.92 (1H, d, $J=15.6$ Hz, H- β), 7.77
39 (1H, d, $J=8.4$ Hz, H-6), 7.66 (1H, d, $J=15.6$ Hz, H- α), 6.87 (2H, d, $J=8.7$
40 Hz, H-3', H-5'), 6.47 (1H, s, H-3), 6.44 (1H, d, $J=8.5$ Hz, H-5), 3.84 (3H,
41 s, -OCH₃). ¹³C-NMR (DMSO-*d*₆, 100 MHz) δ_{ppm} : 187.15 (C=O), 161.72 (C-
42 4'), 161.52 (C-4), 159.96 (C-2), 137.87 (C- β), 130.76 (C-2', C-6'), 130.04

43 (C-6), 129.58 (C-1'), 117.97 (C- α), 115.23 (C-3', C-5'), 114.52 (C-1),
44 108.12 (C-5), 99.00 (C-3), 55.48 (2-OCH₃).

45 Isoliquiritigenin (6): Yellow powder. HR-ESI-MS m/z: 257.0839 [M+H]⁺.

46 ¹H-NMR (DMSO-*d*₆, 400 MHz) δ_{ppm} : 13.61(1H, s, 2'-OH), 10.64(1H, s, 4'-

47 OH), 10.16 (1H, s, 4-OH), 8.14 (1H, d, *J*=8.9 Hz, H-6'), 7.76 (4H, m, H-2,

48 H-6, H- β , H- α), 6.84 (2H, d, *J*=8.9 Hz, H-3, 5), 6.41 (1H, dd, *J*=8.9, 2.2

49 Hz, H-5'), 6.28 (1H, d, *J*=2.2 Hz, H-3'). ¹³C-NMR (DMSO-*d*₆, 100

50 MHz) δ_{ppm} : 191.50(C=O), 165.76 (C-4'), 164.92 (C-2'), 160.24 (C-4),

51 144.24 (C- β), 132.82 (C-6'), 131.91 (C-2, C-6), 125.72 (C-1), 117.38 (C-

52 α), 115.81 (C-3, C-5), 112.97 (C-1'), 108.06 (C-5'), 102.55 (C-3') .

53 Inflacoumarin A (7): White powder. HR-ESI-MS m/z: 323.1290 [M+H]⁺.

54 ¹H-NMR(DMSO-*d*₆, 400 MHz) δ_{ppm} : 10.86(1H, s, 7-OH), 10.25(1H, s, 4-

55 OH), 7.90 (2H, d, *J*=8.7 Hz, H-3', H-5'), 7.67 (1H, s, H-5), 6.98 (1H, s, H-

56 8), 6.92 (2H, d, *J*=8.7 Hz, H-2', H-6'), 6.71 (1H, s, H-3), 5.33 (1H, t, *J*=7.3

57 Hz, H-2''), 3.30 (1H, d, *J*=7.3 Hz, H-1''), 1.74 (1H, s, H-4''), 1.69 (1H, s,

58 H-5''). ¹³C-NMR (DMSO-*d*₆, 100 MHz) δ_{ppm} : 176.22 (C-4), 162.18 (C-2),

59 160.55 (C-4'), 160.35 (C-7), 155.62 (C-9), 132.38 (C-3''), 128.00 (C-2', C-

60 6'), 127.23 (C-6), 124.54 (C-5), 121.85 (C-1'), 121.76 (C-1''), 115.84 (C-

61 3', C-5'), 115.76 (C-10), 104.43 (C-3), 101.73 (C-8), 27.50 (C-1''), 25.56

62 (C-4''), 17.60 (C-5'').

63 Licochalcone D (8): Yellow powder. HR-ESI-MS m/z : 355.1538 $[M+H]^+$.

64 $^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 400 MHz) δ_{ppm} : 7.85(1H, d, $J=8.4$ Hz, H-6'), 7.81(1H,

65 d, $J=15.6$ Hz, H- β), 7.65 (1H, d, $J=15.6$ Hz, H- α), 7.31 (1H, d, $J=8.6$ Hz,

66 H-6), 6.90 (1H, d, $J=8.4$ Hz, H-5'), 6.64 (1H, d, $J=8.5$ Hz, H-5), 5.36 (1H,

67 m, H-2''), 3.77 (3H, s, $-\text{OCH}_3$), 3.29 (1H, d, $J=7.2$ Hz, H-1''), 1.70 (3H, s,

68 4''- CH_3), 1.70 (3H, s, 5''- CH_3). $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$, 100 MHz) δ_{ppm} :

69 187.34 (C=O), 159.61 (C-4'), 148.45 (C-2), 149.52 (C-4), 138.29 (C- β),

70 138.01 (C-3), 131.69 (C-1'), 130.13 (C-6'), 129.46 (C-3''), 127.82 (C-2'),

71 122.39 (C-2'), 119.48 (C-1), 119.20 (C- α), 118.57 (C-6), 114.56 (C-5'),

72 111.60 (C-5), 60.65 ($-\text{OCH}_3$), 28.01 (C-1''), 25.50 (C-4''), 17.67 (C-5'').

73 Licochalcone E (9): Yellow powder. HR-ESI-MS m/z : 339.1593 $[M+H]^+$.

74 $^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 400 MHz) δ_{ppm} : 7.97 (2H, d, $J=8.7$ Hz, H-2', 6'), 7.89

75 (1H, d, $J=15.6$ Hz, H- β), 7.58 (1H, d, $J=15.6$ Hz, H- α), 7.47 (1H, s, H-6),

76 6.88 (2H, d, $J=8.7$ Hz, H-3', H-5'), 6.53 (1H, s, H-3), 4.82 (2H, s, H-3''),

77 3.83 (3H, s, $-\text{OCH}_3$), 3.68 (1H, m, H-1''), 1.62 (3H, s, 5''- CH_3), 1.31 (3H,

78 d, $J=7.1$ Hz, H-4''). $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$, 100 MHz) δ_{ppm} : 187.24(C=O),

79 161.70 (C-4'), 158.07 (C-4), 148.54 (C-2''), 138.52 (C- β), 130.73 (C-2', C-

80 6'), 129.58 (C-1'), 127.92 (C-6), 123.84 (C-5), 117.80 (C- α), 115.25 (C-3',

81 C-5'), 114.20 (C-1), 109.62 (C-3''), 98.76 (C-3), 55.43 ($-\text{OCH}_3$), 37.30 (C-

82 1''), 21.80 (C-5''), 18.96 (C-4'').

83 Licochalcone A (10): Orange powder. HR-ESI-MS m/z: 339.1595 [M+H]⁺.
84 ¹H-NMR(DMSO-*d*₆, 400 MHz)δ_{ppm}: 7.97(2H, d, *J*=8.7 Hz, H-2', H-6'),
85 7.90 (1H, d, *J*=15.6Hz, H-β), 7.60 (1H, s, H-6), 6.88 (2H, d, *J*=8.6 Hz, H-
86 3', H-5'), 6.52 (1H, s, H-3), 6.29 (1H, dd, *J*=17.8, 10.3 Hz, H-2''), 4.95 (1H,
87 d, *J*=2.3 Hz, H-3''b), 4.92 (1H, d, *J*=2.2 Hz, H-3''a), 3.83 (3H, s, -OCH₃),
88 1.45 (6H, s, -CH₃). ¹³C-NMR (DMSO-*d*₆, 100 MHz)δ_{ppm}: 187.25 (C=O),
89 161.67 (C-4), 159.69 (C-4'), 158.26 (C-2), 147.47 (C-2''), 138.70 (C-β),
90 130.73 (C-1'), 129.62 (C-6), 127.74 (C-5), 117.76 (C-α), 115.25 (C-1),
91 113.50 (C-3', C-5'), 110.02 (C-3''), 99.90 (C-3), 55.43 (-OCH₃), 26.97 (C-
92 4'', C-5'').

93 Glabrone (11): Yellowish powder. HR-ESI-MS m/z: 337.1096 [M+H]⁺. ¹H-
94 NMR (DMSO-*d*₆, 400 MHz)δ_{ppm}: 8.27 (1H, s, H-2), 7.99 (1H, d, *J*=8.8, H-
95 5), 6.97 (1H, dd, *J*=8.8, 2.1 Hz, H-6), 6.93 (1H, d, *J*=8.3 Hz, H-6'), 6.91
96 (1H, d, *J*=2.1 Hz, H-8), 6.68 (1H, d, *J*=10 Hz, H-4''), 5.69 (1H, d, *J*=10 Hz,
97 H-3''), 1.38 (6H, s, H-5'', H-6''). ¹³C-NMR(DMSO-*d*₆, 100 MHz) δ_{ppm}:
98 176.01 (C=O), 162.78 (C-7), 157.55 (C-8a), 155.16 (C-2), 153.55 (C-4'),
99 151.34 (C-2'), 131.00 (C-6'), 128.84 (C-3''), 127.25 (C-5), 122.06 (C-3),
100 117.03 (C-4''), 116.21 (C-4a), 115.36 (C-6), 112.75 (C-1'), 110.06 (C-3'),
101 107.62 (C-5'), 102.03 (C-8), 75.44 (C-2''), 27.48 (C-5'', C-6'').

102 Licoisoflavone B (12): Yellow powder. HR-ESI-MS m/z: 353.1009
103 [M+H]⁺. ¹H-NMR (DMSO-*d*₆, 400 MHz)δ_{ppm}: 8.19 (1H, s, H-2), 6.89 (1H,

104 d, $J=8.1$ Hz, H-6'), 6.67 (1H, d, $J=10.0$ Hz, H-1''), 6.39 (1H, d, $J=1.7$ Hz,
105 H-8'), 6.33 (1H, d, $J=8.2$ Hz, H-5'), 6.22 (1H, d, $J=1.7$ Hz, H-6), 5.69 (1H,
106 d, $J=10.0$ Hz, H-2''), 1.67 (6H, s, H-4'', H-5''). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100
107 MHz) δ_{ppm} : 180.53 (C=O), 164.50 (C-7), 161.78 (C-5), 157.73 (C-9),
108 1505.65 (C-4'), 153.57 (C-2), 151.20 (C-2'), 131.36 (C-6'), 128.83 (C-2''),
109 120.46 (C-3), 116.97 (C-1''), 111.24 (C-1'), 109.73 (C-3'), 107.38 (C-5'),
110 98.96 (C-6), 93.69 (C-8), 75.39 (C-3''), 27.45 (C-4'', C-5'').

111 Glycyuralin R (13): White powder. HR-ESI-MS m/z : 391.1889 $[\text{M}+\text{H}]^+$.

112 $^1\text{H-NMR}$ (DMSO- d_6 , 400 MHz) δ_{ppm} : 10.81 (1H, s, 7-OH), 10.19 (1H, s, 4-
113 OH), 7.74 (1H, d, $J=2.0$ Hz, H-2'), 7.66 (1H, s, H-5), 6.97 (1H, s, H-8), 6.67
114 (1H, s, H-3), 5.33 (1H, m, H-2''), 3.30 (2H, d, $J=7.3$ Hz, H-1''), 3.30 (2H,
115 d, $J=7.3$ Hz, H-1'''), 1.74 (3H, s, H-5''), 1.72 (3H, s, H-4'''), 1.72 (3H, s, H-
116 5'''), 1.69 (3H, s, H-4''). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100 MHz) δ_{ppm} : 176.19 (C-
117 4), 162.38 (C-2), 160.32 (C-7), 158.33 (C-4'), 155.59 (C-9), 132.38 (C-3''),
118 131.76 (C-3'''), 128.36 (C-3'), 127.43 (C-2'), 127.18 (C-6), 125.41 (C-6'),
119 124.55 (C-6'), 122.33 (C-4), 121.76 (C-2'), 115.77 (C-10), 115.29 (C-5'),
120 104.33 (C-3), 101.70 (C-8), 28.05 (C-1'''), 27.49 (C-1''), 25.56 (C-5''),
121 25.50 (C-5'''), 17.68 (C-4'''), 17.60 (C-4'').

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129 **Table S1** The linear range, precision and recovery of compounds.

Compound	Linear range (mg/L)	R^2	LOQ (mg/L)	LOD (mg/L)	Precision RSD (%)		Recovery yield (%)
					Intraday	Interday	
Licochalcone B	4.2-66.6	0.9997	1.21	0.36	2.19	2.98	97.84
Terahydronethoxychalcone	4.9-79.3	0.9997	2.54	0.76	2.56	2.22	98.75
Echinatin	5.2-83.3	0.9997	0.94	0.28	2.35	2.94	98.68
Isoliquiritigenin	7.3-115.3	0.9996	1.07	0.32	2.60	3.02	97.47
Licochalcone D	5.3-86.0	0.9998	2.11	0.63	2.35	2.87	97.74
Licochalcone E	6.2-98.7	0.9996	3.60	1.08	2.33	2.67	96.86
Licochalcone A	4.7-74.7	0.9997	1.47	0.44	2.99	2.46	95.68

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