

Supporting Information

Matrix-Assisted ^1H DOSY Applied to Flavonoid Analysis in *Scutellaria baicalensis*

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Mass spectrometry analysis and test conditions

Chromatographic column: Extend-C₁₈ column (150 mm × 4.6 mm i.d., 5 μm; Agela Technologies); connected C₁₈ guard column (4.0 mm × 3.0 mm i.d., 5 μm; Phenomenex). Liquid phase conditions: aqueous solution containing 0.1% formic acid was used as the A phase and acetonitrile was used as the B phase; the gradient elution conditions used were: 0-22 min: 10%-90% B; 22-24 min: 90%-10% B; the flow rate was set to 1 mL/min and the column temperature was set to 25 °C.

Mass spectrometry parameters: Mass spectrometry was performed in positive ion mode, and the instrument was calibrated by external standard method with mass accuracy less than 3 ppm. Ionization voltage was set to 4.0 kV, capillary temperature was set to 320 °C, and nitrogen was used as sheath gas (40 units) and auxiliary gas (5 units). The resolution of primary full scan of the instrument was set to 15000, and the resolution of secondary full scan was set to 7500. The [M + H]⁺ or [M+NH₄]⁺ ions were used as parent ions were dissociated in the high-energy cleavage (HCD) mode at 50% of the normalized collision energy, with a separation width of 3 Da and a reaction time of 30 ms.

Table S1

The results obtained by mass spectrometric analysis of total flavonoid extract of *S. baicalensis* for compound search.

No.	Name	Formula	Molecular Weight
1	(2R,3S,4S,5R,6R)-5- {[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl) oxolan-2-yl] oxy } -2-(hydroxymethyl)-6-[2-(4-hydroxyphenyl) ethoxy] oxane-3,4-diol	C ₁₉ H ₂₈ O ₁₁	449.18974
2	(2S,3S,4S,5R,6S)-3,4,5-trihydroxy-6-[(5-hydroxy-8-methoxy-4-oxo-2-phenyl-4H-chromen-7-yl) oxy] oxane-2-carboxylic acid	C ₂₂ H ₂₀ O ₁₁	460.1007
3	2-(3,4-Dihydroxyphenyl) ethyl 3-O-(6-deoxy-β-L-mannopyranosyl)-6-O-[(2E)-3-(3,4-dihydroxyphenyl)-2-propenoyl]-β-D-glucopyranoside	C ₂₉ H ₃₆ O ₁₅	641.23198
4	3-C-Methyluteolin 5-rhamnoside	C ₂₂ H ₂₂ O ₁₀	446.11965
5	5,2'-Dihydroxy-6,7,8,6'-tetramethoxyflavone	C ₁₉ H ₁₈ O ₈	374.10058
6	5,3',4',5'-Tetrahydroxy-6,7-dimethoxyflavone	C ₁₇ H ₁₄ O ₈	346.06914
7	5,6,7-trihydroxy-2-(4-methoxyphenyl)-4H-chromen-4-one	C ₁₆ H ₁₂ O ₆	300.06352
8	5,7-dihydroxy-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl]-8-(3,4,5-trihydroxyoxan-2-yl)-4H-chromen-4-one	C ₂₆ H ₂₈ O ₁₃	548.15318
9	5,7-dihydroxy-3-(4-hydroxyphenyl)-6-methoxy-4H-chromen-4-one	C ₁₆ H ₁₂ O ₆	300.06352
10	5,7-dihydroxy-3,8-dimethoxy-2-phenyl-4H-chromen-4-one	C ₁₇ H ₁₄ O ₆	314.08037
11	5,7-Dihydroxy-4'-methoxy-3-O-acetylflavanone	C ₁₈ H ₁₆ O ₇	344.09108
12	5-hydroxy-2-(4-hydroxyphenyl)-6-methoxy-7- {[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl] oxy } -4H-chromen-4-one	C ₂₂ H ₂₂ O ₁₁	462.11574
13	6-O-Methylscutellarin	C ₂₂ H ₂₀ O ₁₂	476.09508
14	Adenosine	C ₁₀ H ₁₃ N ₅ O ₄	267.09722
15	Apigenin	C ₁₅ H ₁₀ O ₅	270.05282
16	Apigenin 7-O-glucuronide	C ₂₁ H ₁₈ O ₁₁	446.0847
17	Aureusin	C ₂₁ H ₂₀ O ₁₁	448.10068
18	Baicalin	C ₂₁ H ₁₈ O ₁₁	446.08476
19	Chrysin	C ₁₅ H ₁₀ O ₄	254.05831
20	Cirsiliol	C ₁₇ H ₁₄ O ₇	330.07454
21	D - (+)-Maltose	C ₁₂ H ₂₂ O ₁₁	364.09786
22	DL-Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	204.08978
23	Eupatilin	C ₁₈ H ₁₆ O ₇	344.08934
24	Genistin	C ₂₁ H ₂₀ O ₁₀	432.10558

25	Genistein	C ₁₅ H ₁₀ O ₅	270.05318
26	Apigenin	C ₂₁ H ₂₀ O ₁₀	432.10558
27	Isovitexin 2"-O-rhamnoside	C ₂₇ H ₃₀ O ₁₄	578.16326
28	L-Tyrosine	C ₉ H ₁₁ NO ₃	181.07367
29	Luteolin	C ₁₅ H ₁₀ O ₆	286.04799
30	Palmitic Acid	C ₁₆ H ₃₂ O ₂	273.26692
31	Pectolinarigenin 7-glucuronide	C ₂₃ H ₂₂ O ₁₂	490.11046
32	Phytosphingosine	C ₁₈ H ₃₉ NO ₃	317.29317
33	Puerarin	C ₂₁ H ₂₀ O ₉	416.11064
34	Puerarin 4'-O-glucoside	C ₂₇ H ₃₀ O ₁₄	578.16319
35	Scutellarin	C ₂₁ H ₁₈ O ₁₂	462.07961
36	Vigabatrin	C ₆ H ₁₁ NO ₂	129.07884
37	Wogonin	C ₁₆ H ₁₂ O ₅	284.06905
38	α-Lactose	C ₁₂ H ₂₂ O ₁₁	359.14327

Figure S1

The mass spectra of several compounds in *S. baicalensis* extract

