

Table S1. Optimized mass spectrometric parameters of sixteen metabolites

No	Name	CAS No	Formula	M.W.	MRM transitions(precursor tR (min) DP/V → product)			
1	liquiritin apioside	74639-14-8	C ₂₆ H ₃₀ O ₁₃	550.51	549.13/254.99	5.00	-70	-44
2	neoliquiritin	5088-75-5	C ₂₁ H ₂₂ O ₉	418.39	417.09/255.10	5.05	-150	-20
3	liquiritin	551-15-5	C ₂₁ H ₂₂ O ₉	418.39	417.08/255.06	5.23	-125	-26
4	isoliquiritin apioside	120926-46-7	C ₂₆ H ₃₀ O ₁₃	550.51	549.098/255.01	7.42	-200	-38
5	isoliquiritin	5041-81-6	C ₂₁ H ₂₂ O ₉	418.39	417.08/255.00	8.16	-165	-28
6	ononin	486-62-4	C ₂₂ H ₂₂ O ₉	430.40	475.09/267.20	8.62	-30	-18
7	neoisoliquiritin	59122-93-9	C ₂₁ H ₂₂ O ₉	418.39	417.09/254.90	8.71	-80	-22
8	licochalcone B	58749-23-8	C ₁₆ H ₁₄ O ₅	286.28	285.05/149.90	8.93	-130	-30
9	liquiritigenin	578-86-9	C ₁₅ H ₁₂ O ₄	256.25	254.99/135.00	9.73	-95	-20
10	echinatin	34221-41-5	C ₁₆ H ₁₄ O ₄	270.28	269.14/91.99	12.54	-135	-36
11	isoliquiritigenin	961-29-5	C ₁₅ H ₁₂ O ₄	256.25	255.09/119.00	14.48	-85	-32
12	glycyrrhizin	1405-86-3	C ₄₂ H ₆₂ O ₁₆	822.93	821.35/351.00	14.78	-10	-56
13	formononetin	485-72-3	C ₁₆ H ₁₂ O ₄	268.26	267.03/251.99	14.81	-140	-28
14	licoflavone A	61153-77-3	C ₂₀ H ₁₈ O ₄	322.35	320.99/266.00	14.99	-125	-32
15	licochalcone A	58749-22-7	C ₂₁ H ₂₂ O ₄	338.40	337.12/305.2	15.46	-45	-28
16	glycyrrhetinic acid	471-53-4	C ₃₀ H ₄₆ O ₄	470.68	469.28/425.00	18.07	-210	-52

Note: M.W means the molecular weight; DP means declustering potential; CE means collision energy.