

Table S1: Chemical composition of TSN.

NO.	Observed RT (min)	Component name	Formula	Neutral mass (Da)	Mass error (ppm)	ESI mode
1	5.40	Gallic acid	C ₇ H ₆ O ₅	170.02152	3.8	positive
2	24.28	Coumarin	C ₉ H ₆ O ₂	146.03678	4.4	positive
3	27.59	Tetramethylpyrazine	C ₈ H ₁₂ N ₂	136.10005	6.7	positive
4	29.35	Calycosin-7- O -β-D-glucoside	C ₂₂ H ₂₂ O ₁₀	446.12130	1.1	positive
5	33.26	4-hydroxy-3-butylphthalide	C ₁₂ H ₁₄ O ₃	206.09429	2.8	positive
6	36.44	Senkyunolide	C ₁₂ H ₁₆ O ₂	192.11503	2.7	positive
7	37.61	Ononin	C ₂₂ H ₂₂ O ₉	430.12638	1.2	positive
8	40.27	Methylnissolin	C ₁₇ H ₁₆ O ₅	300.09977	3.2	positive
9	40.27	9-O-Methylnissolin 3-O-glucoside	C ₂₃ H ₂₆ O ₁₀	462.15260	1.1	positive
10	42.08	Calycosin	C ₁₆ H ₁₂ O ₅	284.06847	3.8	positive
11	42.19	Isomucronulatol	C ₁₇ H ₁₈ O ₅	302.11542	2.5	positive

12	42.48	Quercetin	C ₁₅ H ₁₀ O ₇	302.04265	3.7	positive
13	52.42	Isoastragaloside IV	C ₄₁ H ₆₈ O ₁₄	784.46091	0.2	positive
14	54.56	Astragaloside VI	C ₄₇ H ₇₈ O ₁₉	946.51373	1.1	positive
15	56.75	Astragaloside III	C ₄₁ H ₆₈ O ₁₄	784.46091	0.6	positive
16	57.24	Astragaloside IV	C ₄₁ H ₆₈ O ₁₄	784.46091	1.1	positive
17	60.77	Astramembrannin II	C ₃₅ H ₅₈ O ₉	622.40808	-0.3	positive
18	60.82	Agroastragaloside III	C ₅₁ H ₈₂ O ₂₁	1030.53486	2.1	positive
19	61.18	Astragaloside II	C ₄₃ H ₇₀ O ₁₅	826.47147	0.4	positive
20	62.83	Astragaloside VIII	C ₄₇ H ₇₆ O ₁₇	912.50825	1.7	positive
21	68.29	Sedanolide	C ₁₂ H ₁₈ O ₂	194.13068	3	positive
22	68.32	Linolenic acid	C ₁₈ H ₃₀ O ₂	278.22458	1.3	positive
23	68.86	ligustilide	C ₁₂ H ₁₄ O ₂	190.09938	3.4	positive
24	70.45	Isoastragaloside I	C ₄₅ H ₇₂ O ₁₆	868.48204	1	positive

25	79.24	Physcion	C ₁₆ H ₁₂ O ₅	284.06847	3.4	positive
26	8.19	Protocatechuic acid	C ₇ H ₆ O ₄	154.02661	-7.6	negative
27	16.80	Sanguiin H-4	C ₂₇ H ₂₂ O ₁₈	634.08061	2.4	negative
28	16.80	d-catechin	C ₁₅ H ₁₄ O ₆	290.07904	-2.4	negative
29	17.39	caffeic acid	C ₉ H ₈ O ₄	180.04226	-7.7	negative
30	18.75	(-)-epicatechin	C ₁₅ H ₁₄ O ₆	290.07904	-5.6	negative
31	23.45	Riboflavin	C ₁₇ H ₂₀ N ₄ O ₆	376.13828	-4.5	negative
32	25.17	Ferulic acid	C ₁₀ H ₁₀ O ₄	194.05791	-11.1	negative
33	31.39	Isoquercitrin	C ₂₁ H ₂₀ O ₁₂	464.09548	1.2	negative
34	35.55	Isorhamnetin-3-glucoside	C ₂₂ H ₂₂ O ₁₂	478.11113	2.8	negative
35	41.68	Kaempferide-3-glucoside	C ₂₂ H ₂₂ O ₁₁	462.11621	-1	negative
36	42.20	isomucronulatol 7-O-glucoside	C ₂₃ H ₂₈ O ₁₀	464.16825	-1	negative
37	43.97	Chrysophanol	C ₁₅ H ₁₀ O ₄	254.05791	-4.2	negative

38	48.63	Kaempferol	C ₁₅ H ₁₀ O ₆	286.04774	-3.3	negative
39	49.12	3'-methoxy-5'-hydroxyisoflavone-7-O-β-D-glucoside	C ₂₂ H ₂₂ O ₁₀	446.1213	-3.7	negative
40	50.40	Astragaloside V	C ₄₇ H ₇₈ O ₁₉	946.51373	5.3	negative
41	54.50	Aloeemodin	C ₁₅ H ₁₀ O ₅	270.05282	-7.1	negative
42	57.44	Rhein	C ₁₅ H ₈ O ₆	284.03209	-3.7	negative
43	62.98	Agroastragaloside IV	C ₄₉ H ₈₀ O ₂₀	988.52429	5.1	negative
44	67.18	Acetylastragaloside I	C ₄₇ H ₇₄ O ₁₇	910.49260	4.7	negative
45	68.98	Tormentic acid	C ₃₀ H ₄₈ O ₅	488.35017	-1.9	negative
46	69.52	Emodin	C ₁₅ H ₁₀ O ₅	270.05282	-4	negative
47	72.60	Astragaloside I	C ₄₅ H ₇₂ O ₁₆	868.48204	4.6	negative
48	78.94	Corosolic acid	C ₃₀ H ₄₈ O ₄	472.35526	-1.9	negative
49	87.24	Linolenic acid	C ₁₈ H ₃₀ O ₂	278.22458	-5.4	negative
50	89.79	Mongholicoside I	C ₃₆ H ₆₀ O ₉	636.42373	2.1	negative

51	100	Ursolic acid	$C_{30}H_{48}O_3$	456.36035	-0.8	negative
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