

SUPPLEMENTARY DATA

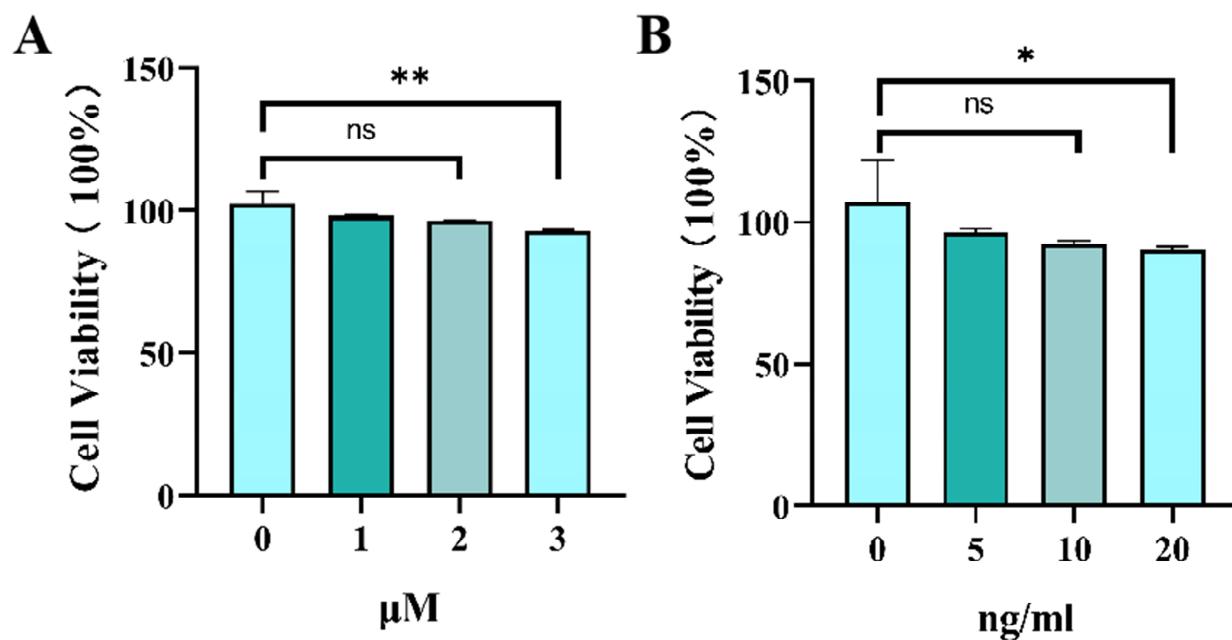


Fig. S1: Effect of SB (A) and SCC (B) alone on cell viability. n = 3. Data were shown as mean \pm SD. *p<0.05, **p<0.01 vs the 0 group.

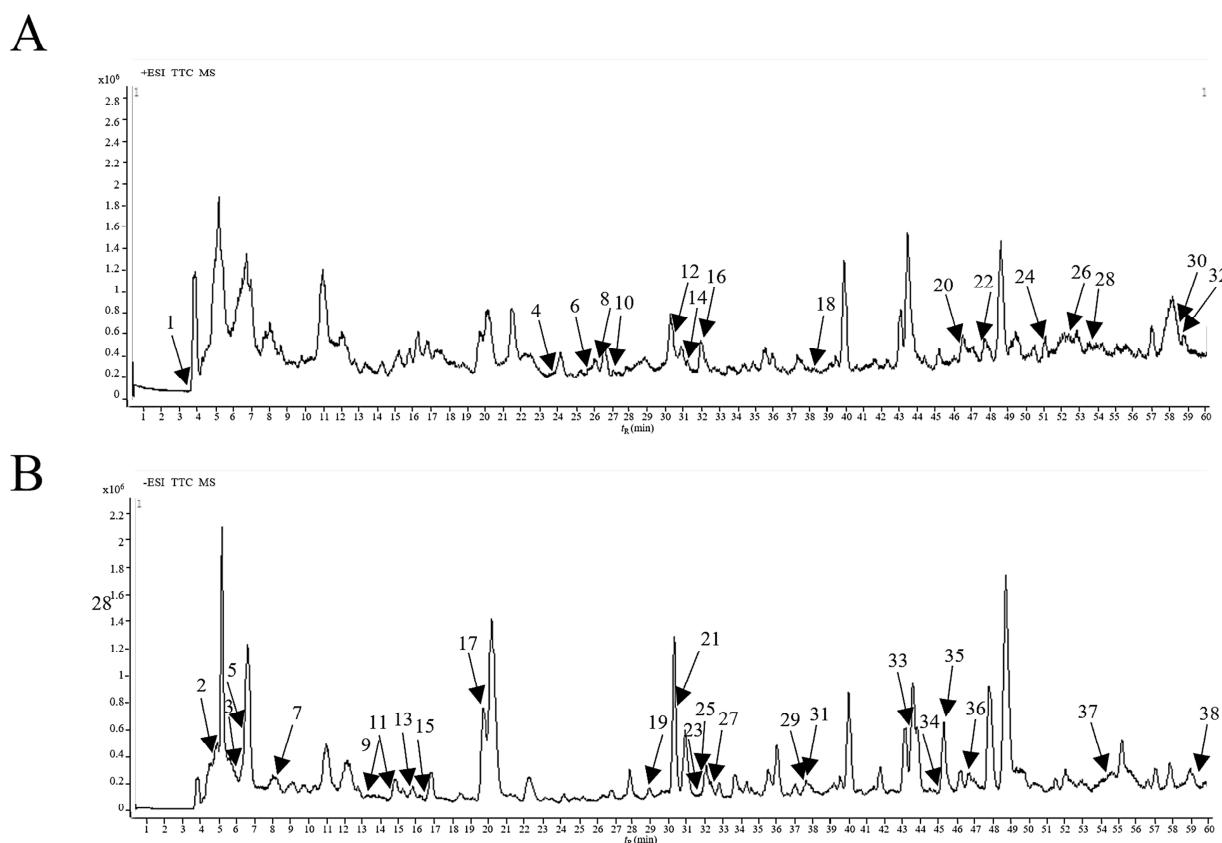


Fig. S2: Total ion chromatogram of LC-MS/MS of CYNG. (A) Positive ion. (B) Negative ion.

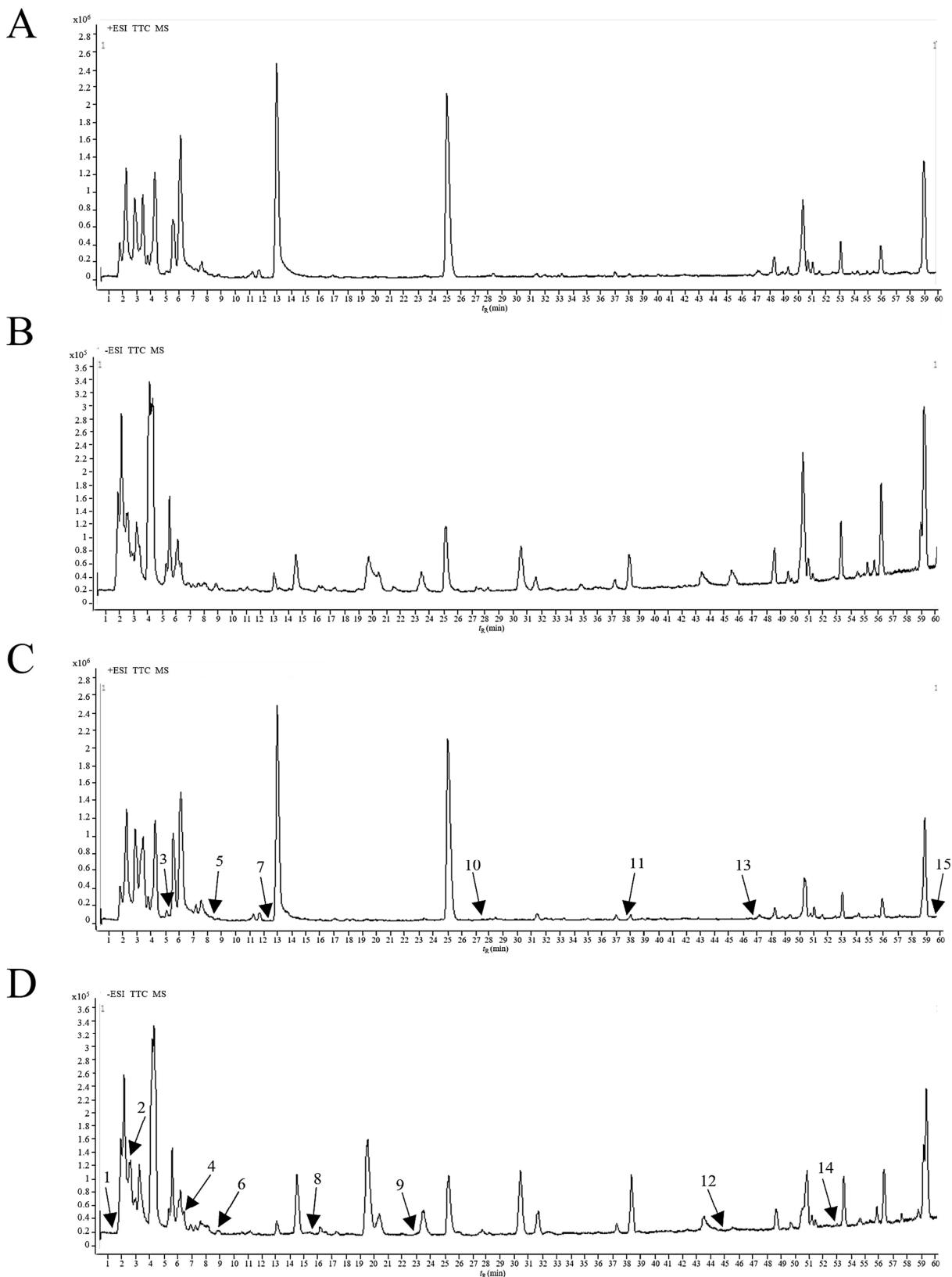


Fig. S3: Total ion chromatogram of LC-MS/MS of the serum of blank group. (A) Positive ion. (B) Negative ion. Total ion chromatogram of LC-MS/MS of the serum of CYNG group. (C) Positive ion. (D) Negative ion.

Table S1: Qualitative analysis in CYNG positive and negative ion model.

No.	t _R /min	Precursor Ion (m/z)	Theoretical mass (m/z)	Proposed formula	Proposed compounds	ion mode
1	3.463	151.0362	151.0395	C ₈ H ₆ O ₃	piperonal	pos
2	4.761	149.0079	149.0086	C ₄ H ₆ O ₆	L- (+)-tartaric acid	neg
3	6.057	115.0028	115.0031	C ₄ H ₄ O ₄	fumaric acid	neg
4	23.843	279.1567	279.1596	C ₁₆ H ₂₂ O ₄	dibutyl phthalate	pos
5	6.293	173.0448	173.0450	C ₇ H ₁₀ O ₅	shikimic acid	neg
6	25.728	166.0869	166.0868	C ₉ H ₁₁ NO ₂	phenylalanine	pos
7	8.178	161.0446	161.0450	C ₆ H ₁₀ O ₅	1,6-anhydro-beta-D-glucopyranose (levoglucosan)	neg
8	26.199	127.0396	127.0395	C ₆ H ₆ O ₃	5-hydroxymethylfurfural	pos
9	13.243	117.0189	117.0188	C ₄ H ₆ O ₄	succinic acid	neg
10	27.024	193.0893	193.0865	C ₁₁ H ₁₂ O ₃	1,3-benzodioxole,4-methoxy-6-(2-propenyl)	pos
11	14.657	175.0235	175.0218	C ₁₀ H ₈ OS	1-(1-Benzothien-3-yl) ethanone	neg
12	30.794	185.0431	185.0450	C ₈ H ₈ O ₅	methyl gallate	pos
13	15.835	125.0240	125.0239	C ₆ H ₆ O ₃	1,2,3-trishydroxybenzene	neg
14	31.265	447.1502	447.1503	C ₁₉ H ₂₆ O ₁₂	acetyl scandoside methyl ester	pos
15	16.424	389.1060	389.1084	C ₁₆ H ₂₂ O ₁₁	deacetyl as-perulosidic acid	neg
16	31.972	355.1029	355.1029	C ₁₆ H ₁₈ O ₉	chlorogenic acid	pos
17	19.723	169.0135	169.0137	C ₇ H ₆ O ₅	gallic acid	neg
18	38.334	195.0637	195.0657	C ₁₀ H ₁₀ O ₄	(E)-ferulic acid	pos
19	28.912	169.0341	167.0344	C ₈ H ₈ O ₄	2,6-dimethoxy-1,4-benzoquinone	neg
20	46.344	347.1330	347.1342	C ₁₅ H ₂₂ O ₉	2,4,6-trimethoxyphenyl β-D-glucopyranoside	pos
21	30.443	197.0448	197.0450	C ₉ H ₁₀ O ₅	ethyl gallate	neg
22	47.523	293.0307	293.0297	C ₁₃ H ₈ O ₈	brevifolin carboxylic acid	pos
23	31.621	153.0188	153.0188	C ₇ H ₆ O ₄	protocatechuic acid	neg
24	51.057	595.1679	595.1663	C ₂₇ H ₃₀ O ₁₅	nicotiflorin	pos
25	31.739	109.0290	109.0290	C ₆ H ₆ O ₂	2-furancarboxaldehyde, 5-methyl	neg
26	52.471	227.1288	227.1283	C ₁₂ H ₁₈ O ₄	12-hydroxyjasmonic acid	pos
27	32.564	315.0692	315.0716	C ₁₃ H ₁₆ O ₉	2-hydroxymethyl-5-methoxylphenyl-O-β-D-glucopyranoside	neg

Table S2: Qualitative analysis of CYNG components in blood under positive and negative ion mode.

No.	t _R /min	Precursor Ion (m/z)	Theoretical mass (m/z)	Proposed formula	Proposed compounds	ion mode
1	1.695	145.0648	145.0653	C ₁₀ H ₁₀ O	2-Propyn-1-ol, 3-(4-methylphenyl)	neg
2	2.638	175.0238	175.0218	C ₁₀ H ₈ OS	1-(1-Benzothien-3-yl) ethanone	neg
3	5.231	127.0377	127.0395	C ₆ H ₆ O ₃	5-hydroxymethylfurfural	pos
4	6.525	161.0437	161.0450	C ₆ H ₁₀ O ₅	levoglucosan	neg
5	8.530	169.0481	169.0501	C ₈ H ₈ O ₄	2,6-dimethoxy-1,4-benzoquinone	pos
6	8.999	389.1044	389.1084	C ₁₆ H ₂₂ O ₁₁	deacetyl as-perulosidic acid	neg
7	12.653	166.0869	166.0868	C ₉ H ₁₁ NO ₂	phenylalanine	pos
8	15.715	283.0635	283.0606	C ₁₆ H ₁₂ O ₅	apigenin 7,4'-dimethyl ether	neg
9	23.136	197.0408	197.0450	C ₉ H ₁₀ O ₅	Ethyl gallate	neg
10	27.850	155.0709	155.0708	C ₈ H ₁₀ O ₃	Phenol 2,6-dimethoxy	pos
11	37.863	307.0806	307.0818	C ₁₅ H ₁₄ O ₇	(2S,3R)-2-(3,4,5-Trihydroxyphenyl)-3,5,7-chromanetriol	pos
12	45.166	137.0235	137.0239	C ₇ H ₆ O ₃	Salicylic acid	neg
13	47.052	185.1159	185.1178	C ₁₀ H ₁₆ O ₃	Elsholtziol	pos
14	53.177	179.0340	179.0344	C ₉ H ₈ O ₄	caffein acid	neg
15	59.775	227.1267	227.1283	C ₁₂ H ₁₈ O ₄	12-hydroxyjasmonic acid	pos

Table S3: Prediction of key active ingredients (degree ≥ 30)

Name	Degree
12-hydroxyjasmonic acid	81.0
aesculetin	62.0
caffeic acid	54.0
Cis-4-coumaric acid	40.0
1-(1-Benzothien-3-yl) ethanone	40.0
methyl lsyringin	33.0
methyl gallate	32.0
levoglucosan	32.0
ethyl gallate	31.0

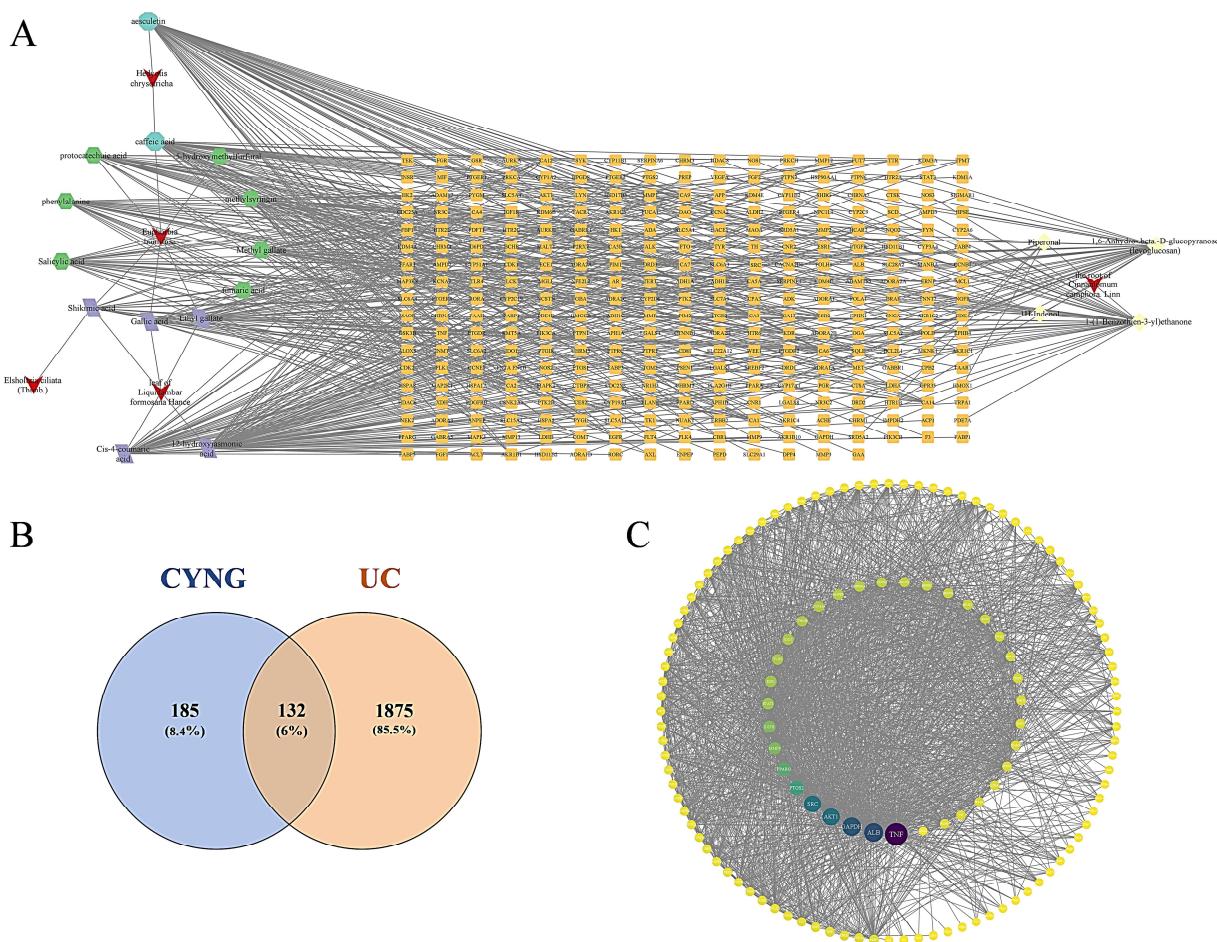


Fig. S4: Network pharmacology. (A) Component-target network. (B) Venn diagram of common UC targets and targets of CYNG components. (C) PPI network. diagram: Minimum required interaction score ≥ 0.99 .