

Table S1 Changes of metabolites of the Qi deficiency and blood stasis syndrome rat after HXC treatment

No.	Rt (min)	Ion form	m/z	Proposed compound	Mass Error (ppm)	HMDB	Formula	Trend in model	Regulated by HXC
1	0.81	M-H	130.09	Isoleucine	-3.9741	HMDB00172	C6H13NO2	↓	※
2	3.13	M-H	117.05	Methyl 3-hydroxybutyrate	1.2434	HMDB41603	C5H10O3	↑	
3	1.53	M+H	253.12	Alanine	2.1234	HMDB29098	C12H16N2O4	↑	※
4	2.70	M+H	147.11	Lysine	-2.3542	HMDB00182	C6H14N2O2	↓	※
5	0.66	M-H	148.04	L-Methionine	-8.5676	HMDB00696	C5H11NO2S	↓	※
6	0.52	M-H	146.05	DL-Glutamate	4.7270	HMDB60475	C5H9NO4	↑	
7	2.87	M+H	147.08	Glutamine	-6.2204	HMDB00641	C5H10N2O3	↑	※
8	4.77	M-H	165.04	3-Methylxanthine	4.9133	HMDB01886	C6H6N4O2	↓	※
9	2.33	M+H	348.07	Adenosine	-3.8662	HMDB11617	C10H14N5O7P	↑	※
10	1.00	M+H	181.07	Myoinositol	-2.1152	HMDB00211	C6H12O6	↑	※
11	1.22	M+H	147.06	Succinate	5.7519	HMDB33837	C6H10O4	↑	※
12	1.52	M+H	765.47	PG(16:1(9Z)/18:3(6Z,9Z,12Z))	-6.2631	HMDB10591	C40H71O10P	↓	※
13	2.57	M+H	257.22	Glycerophosphocholine	0.1283	HMDB0000086	C8H20NO6P	↑	※
14	0.53	M+H	126.02	Taurine	-5.6735	HMDB00251	C2H7NO3S	↓	※
15	1.21	M+H	174.20	Arginine	-3.7906	HMDB0003416	C6H14N4O2	↑	※
16	0.92	M+H	131.13	Creatine	2.4456	HMDB0000064	C4H9N3O2	↑	※
17	1.85	M+H	261.04	Glucose	0.6927	HMDB01586	C6H13O9P	↓	※
18	7.91	M-H	506.32	LysoPC(17:0)	-1.2722	HMDB0012108	C ₂₅ H ₅₀ NO ₇ P	↑	※
19	5.74	M+H	689.96	PE(14:0/18:1(9Z))	1.7544	HMDB0008828	C37H72NO8P	↓	※
20	5.10	M-H	566.55	Cer(d18:0/18:0)	-8.5141	HMDB0011761	C36H73NO3	↑	※
21	2.78	M-H	785.65	SM(d18:1/22:0)	-0.1004	HMDB0012103	C45H91N2O6P	↑	※
22	7.60	M+H	482.32	LysoPC(15:0)	2.8608	HMDB0010381	C23H48NO7P	↓	※
23	5.87	M+H	369.37	Tetracosanoic acid	0.3502	HMDB02003	C24H48O2	↑	※
24	4.46	M+H	316.43	Trilobinone	-1.1536	HMDB0038885	C20H28O3	↓	

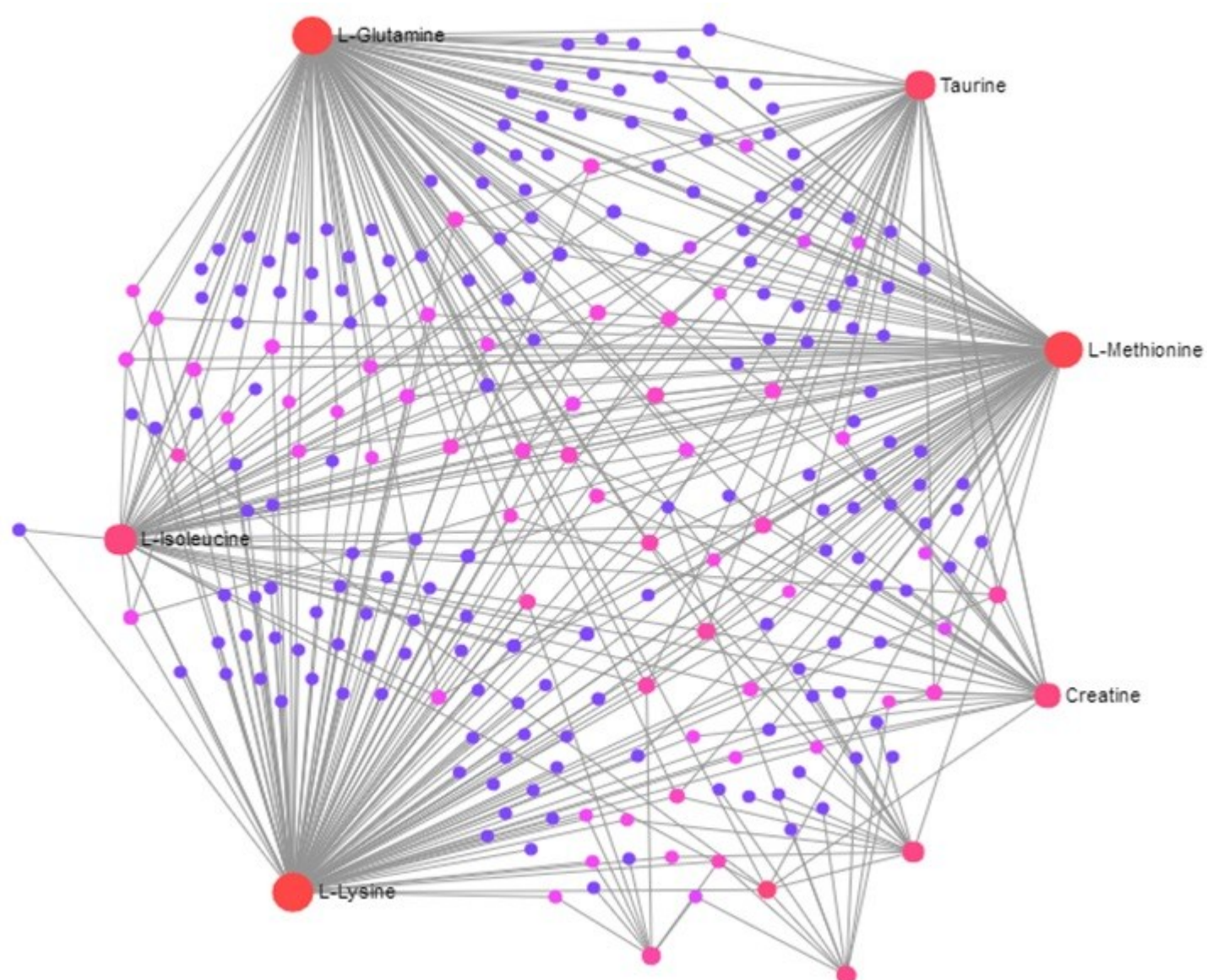


Figure S1. Metabolite-metabolite interaction network related with Huaxian capsule protective activity on the sepsis of Qi deficiency and blood stasis syndrome rat.

