

Table 1 Screening of different metabolites between groups

No.	Metabolites	Classification	Similarity [0, 1 000]	Retention time (min)	Vip value	p-value	-Lg p-value	Log ₂ Fold change	Significant	Output ID
1	Lignoceric acid	Organic acid	959	25.775 0	1.011	0.008	2.108	1.187	U	C08320
2	Palmitic acid	Organic acid	955	19.381 0	1.089	0.047	1.327	0.021	U	C00249
3	D-Talose	Saccharides	946	17.996 0	1.117	0.049	1.312	-1.837	D	C06467
4	Cerotinic acid	Organic acid	944	27.108 0	1.023	0.015	1.839	1.153	U	-
5	Benzoic acid	Organic acid	930	10.115 0	1.018	0.043	1.366	1.566	U	C00180
6	Oleic acid	Organic acid	925	20.987 0	1.250	0.048	1.318	0.901	U	C00712
7	Heptadecanoic acid	Organic acid	909	20.272 0	1.014	0.015	1.830	1.167	U	-
8	Phytol	Terpene	881	20.516 0	1.101	0.016	1.793	-1.504	D	C01389
9	Mannose	Saccharides	877	17.728 0	2.282	0.021	1.686	-2.089	D	C01662
10	Azelaic acid	Organic acid	845	16.831 0	1.002	0.039	1.405	0.933	U	C08261
11	N-Acetyl-D-galac tosamine	Saccharides	828	19.582 0	1.515	0.019	1.717	-3.723	D	C01132
12	Salicylic acid	Organic acid	825	13.532 20	1.961	0.002	2.616	4.026	U	C00805
13	3,4-dihydroxyben zoic acid	Organic acid	806	17.058 0	1.052	0.046	1.336	0.945	U	C00230

Note: Vip: The Vip value from the OPLS-DA model, the RS group is increasing relative to the HS group; -Lg p-value: The *p* value from *t*-test with a negative logarithm based on 10; Log₂ Fold change: The logarithm of the quantitative ratio of two groups of experimental substances to base; D: Decreasing of the last column in the table