

ID	Name	MS/MS score	rt	mz	Compounds category	Type	Mean AS	Mean HC	VIP	P-VALUE
1	Pyruvic acid	1	263.251	87.007985	Organic acids and derivatives	forward	0.4964835	0.3976837	1.5015746	0.0266629
2	Arachidonic acid	0.999514692	37.1885	303.23283	Lipids and lipid-like molecules	forward	2.2713397	1.2983446	1.6866259	0.0195981
3	Palmitoleic acid	0.998543231	219.253	253.21731	Lipids and lipid-like molecules	forward	0.0163886	0.019342	1.2420709	0.0410038
4	Sarcosine	0.998314538	360.156	88.03959	Organic acids and derivatives	forward	3.4072859	4.6260202	1.916151	0.0021853
5	2,3-Dihydroxybutanedioic acid	0.995710692	29.4325	149.00895	Organic oxygen compounds	forward	0.2428708	0.1054949	1.4868143	0.0210582
6	Uracil	0.994870385	76.9874	111.01926	Organoheterocyclic compound:	forward	1.4529017	0.46398	1.7039198	0.0244329
7	3-Methyl-2-oxovaleric acid	0.994417615	36.9034	129.05505	Organic acids and derivatives	forward	32.500428	52.298007	1.8263996	0.0005791
8	Adenine	0.993215923	360.166	134.04658	Organoheterocyclic compound:	forward	0.0597767	0.0808426	1.2970383	0.0304981
9	Hypotaurine	0.990013615	358.412	108.01171	Organic acids and derivatives	forward	0.0226704	0.0140825	1.4919383	0.0163634
10	Succinic acid	0.984536385	386.328	117.01865	Organic acids and derivatives	forward	1.0746449	0.4273974	2.3093178	0.0025666
11	Malonic acid	0.981726	383.9475	103.00291	Organic acids and derivatives	forward	0.1000195	0.0643635	1.5388486	0.012673
12	L-Tyrosine	0.981300231	317.02	180.0663	Organic acids and derivatives	forward	1.0305774	1.4138511	1.7297651	0.0089244
13	Ribothymidine	0.976884769	141.517	257.07798	eosides, nucleotides, and analc	forward	0.1044171	0.1379744	1.3217103	0.0366946
14	Ornithine	0.975128538	541.6245	131.08197	Organic acids and derivatives	forward	0.097607	0.1846554	1.7507919	0.001741
15	beta-Alanine	0.974484077	92.7821	88.039583	Organic acids and derivatives	forward	0.0688756	0.0544084	1.5901649	0.0123815
16	Fructose-1P	0.974130846	305.503	179.05579	Organooxygen compounds	forward	0.5671573	1.2007984	1.6499908	0.0042973
17	Hippuric acid	0.951013769	200.821	178.05059	Benzenoids	forward	1.2322435	4.0157031	1.2570812	0.0162789
18	Saccharin	0.949431231	30.7839	181.99142	Organoheterocyclic compound:	forward	0.0190364	0.1377038	1.4261756	0.0332015
19	Uric acid	0.949214231	336.2105	167.02072	Organoheterocyclic compound:	forward	2.4357743	3.9287673	1.602456	0.0162106
20	Succinic acid semialdehyde	0.947223846	383.939	101.02365	Lipids and lipid-like molecules	forward	0.5407703	0.8830932	1.7990634	0.0046334
21	Hydroxyphenyllactic acid	0.946628462	196.351	181.05026	henylpropanoids and polyketid	forward	0.5188106	0.7881247	1.7601587	0.0252262
22	Inosine	0.921620846	228.4175	267.0734	eosides, nucleotides, and analc	forward	0.1157045	0.0203505	2.099981	0.0149245
23	Isobutyrylglycine	0.920435692	190.425	144.06605	Organic acids and derivatives	forward	0.0229551	0.0281159	1.9381591	0.0002277
24	N2-gamma-Glutamylglutamine	0.919386462	435.689	274.10447	Organic acids and derivatives	forward	0.0149063	0.0248137	2.1684715	7.796E-05
25	Cyclohexanecarboxylic acid	0.908517308	335.055	127.07583	Organic acids and derivatives	forward	0.1323552	0.1654296	1.3863015	0.0212611
26	(A±)-Tryptophan	0.849128077	278.511	203.08244	Organoheterocyclic compound:	forward	1.471793	2.1698128	1.8989526	0.0008727
27	3-Sulfinato-L-alaninate	0.847247692	192.702	152.00184	Organic acids and derivatives	forward	0.1888249	0.0859926	1.378179	0.0425124
28	Pyrocatechol	0.833373	23.1999	109.02871	Benzenoids	forward	0.283076	0.5052753	1.5037116	0.0311783
29	D-Glucose	0.827613	226.128	179.05574	Organic oxygen compounds	forward	0.3734874	0.2672972	1.8183785	0.0036161
30	3-(3,4-Dihydroxy-5-methoxy)-2-propenoic acid	0.819305538	186.735	209.04546	henylpropanoids and polyketid	forward	0.0043669	0.0114	2.3513548	0.0039222
31	9,10-DHOME	0.813848462	47.13315	313.2386	Lipids and lipid-like molecules	forward	0.0228633	0.0516034	1.5954824	0.0338513
32	Ortho-Hydroxyphenylacetic acid	0.807277615	109.704	151.03956	Benzenoids	forward	0.1052897	0.0480129	1.3314575	0.0340108
33	L-Arginine	0.794383923	540.15	173.10404	Organic acids and derivatives	forward	0.0579283	0.1380524	1.8606759	0.0040376
34	Threonic acid	0.765045308	315.4975	135.02927	Organic oxygen compounds	forward	1.5213819	2.5476821	1.9054993	0.016007
35	Hypoxanthine	0.751278	174.292	135.03064	Organoheterocyclic compound:	forward	79.425346	13.536912	2.4444044	5.755E-05
36	5-Hydroxyindoleacetic acid	0.724059231	279.668	190.05073	Organoheterocyclic compound:	forward	0.0121537	0.0173944	1.5862104	0.0148341
37	Dodecanoylcarnitine	0.703063231	116.9015	342.26526	Lipids and lipid-like molecules	forward	0.0071994	0.0109164	1.1235083	0.0175325
38	3,7-Dimethyluric acid	0.661591385	376.7305	195.05074	Organoheterocyclic compound:	forward	0.1168259	0.2484489	1.985594	0.013965
39	N-Acetylarlyamine	0.660557308	200.862	134.06051	Benzenoids	forward	0.0835808	0.2961486	1.3002673	0.0143874
40	LysoPA(16:0/0:0)	0.642509692	216.959	409.23642	Lipids and lipid-like molecules	forward	0.0422554	0.046803	1.2173097	0.0323116
41	Urocanic acid	0.627231538	315.339	137.03354	Organoheterocyclic compound:	forward	0.0107158	0.0188373	1.8224233	0.0303064
42	Oxypurinol	0.608082538	175.365	151.02813	Organoheterocyclic compound:	forward	0.0052328	0.0119709	1.4467091	0.0005648
43	2-acetyl-1-alkyl-sn-glycero-3-phosphocholine	0.586633615	213.543	522.35694	Lipids and lipid-like molecules	forward	0.0042206	0.0055947	1.5152164	0.0099944
44	Ketoleucine	0.585551308	193.995	129.05508	Organic acids and derivatives	forward	0.1203969	0.1655583	1.7217763	0.0020907
45	3-Hydroxymethylglutaric acid	0.581000231	312.001	161.04507	Lipids and lipid-like molecules	forward	0.2361017	0.4630237	1.8523282	0.0041442
46	LysoPA(18:1(9Z)/0:0)	0.575933308	216.962	435.25186	Lipids and lipid-like molecules	forward	0.0221406	0.025637	1.3574015	0.0169277
47	PE(16:0/18:2(9Z,12Z))	0.551462769	168.499	714.51039	Lipids and lipid-like molecules	forward	0.0639485	0.1094615	1.5996358	0.0221944
48	fluvoxamino acid	0.531381231	185.9095	317.11453	Benzenoids	forward	0.0104571	0.0188804	1.5531146	0.0101102
49	4-hydroxy-3-[1-(4-hydroxyphenyl)-3-oxobutyl]-2H-chromen-2-one	0.512957769	185.886	323.09002	henylpropanoids and polyketid	forward	0.0020025	0.0029115	1.6783982	0.0026141
50	Dihydrolipoate	0.482846846	65.3539	207.05077	Lipids and lipid-like molecules	forward	0.0202666	0.0307198	1.3100486	0.0361652

MS/MS score: the matching score of mass spectrometry secondary ion, ranged from 0 to 1, and the greater the value, the better; Compounds category:classification information of the substance in HMDB database. Mean AS: the mean of the relative quantitative value of the AS group; Mean HC: the mean of the relative quantitative value of the HC group.