

ID	Name	MS/MS score	rt	mz	Compounds category	type	MEAN A <sup>s</sup>	MEAN HC	VIP	P-VALUE
1	Beta-Aminopropionitrile	1	351.78	71.0611	Organic nitrogen compounds	forward	1.4424	0.9723	2.06376	0.00144
2	Choline	0.999999	217.348	104.107	Organic nitrogen compounds	forward	0.12754	0.14154	1.43861	0.03382
3	1-Methylnicotinamide	0.999821231	336.8	137.071	Organoheterocyclic compounds	forward	0.07929	0.15863	1.59239	0.01472
4	Hypoxanthine	0.999624769	193.335	137.046	Organoheterocyclic compounds	forward	2.35096	0.34878	2.64121	8.9E-05
5	L-Carnitine	0.999567	369.135	162.113	Organic nitrogen compounds	forward	14.629	18.4356	1.71676	0.00525
6	threo-Syringoylglycerol	0.999247462	257.891	245.1	Benzenoids	forward	0.01406	0.00176	2.58647	0.00126
7	Quinoline	0.998993846	45.5639	130.065	Organoheterocyclic compounds	forward	0.02531	0.01262	1.32792	0.04664
8	Arabinosylhypoxanthine	0.997651615	228.305	269.088	Nucleosides, nucleotides, and analogues	forward	0.00906	0.00142	2.22104	0.04224
9	L-Gulose	0.996564615	290.868	203.053	Organic oxygen compounds	forward	0.0026	0.00667	1.69008	0.00724
10	1,7-Tetrahydro-6-hydroxy-2,3,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-dy[8a-c]necane	0.994454385	237.983	259.115	Organoheterocyclic compounds	forward	0.00417	0.00089	2.34025	0.00241
11	4-Hydroxybenzaldehyde	0.991523308	317.12	123.044	Organic oxygen compounds	forward	0.06102	0.09293	1.87187	0.00484
12	Pipecolic acid	0.991409231	547.749	130.087	Organic acids and derivatives	forward	0.19128	0.32883	1.68049	0.0079
13	L-Threonine	0.988967769	365.491	120.066	Organic acids and derivatives	forward	0.07988	0.11511	1.4007	0.04897
14	Tyrosyl-Histidine	0.988944846	270.858	319.136	Organic acids and derivatives	forward	0.00015	5.4E-05	1.86921	0.00738
15	beta-Alanine	0.988338154	359.243	90.0555	Organic acids and derivatives	forward	0.08425	0.11432	1.63753	0.03422
16	Imidazoleacetic acid	0.985918462	280.099	127.051	Organoheterocyclic compounds	forward	3.21434	2.67975	1.4131	0.0308
17	m-Aminobenzoic acid	0.983200385	301.507	138.055	Benzenoids	forward	0.12538	0.29857	1.29805	0.01585
18	Pyro-L-glutaminyL-L-glutamine	0.979788462	180.436	258.109	Organic acids and derivatives	forward	0.00074	0.00187	1.60132	7.4E-06
19	LysoPE(16:0/0:0)	0.973165846	223.102	454.293	Lipids and lipid-like molecules	forward	0.0717	0.09964	1.52695	0.01824
20	Phytosphingosine	0.969872231	63.5184	318.3	Organic nitrogen compounds	forward	0.00518	0.00119	2.78796	6E-06
21	Indoleacetaldehyde	0.966382231	263.398	160.076	Organoheterocyclic compounds	forward	0.0024	0.04158	2.24203	0.00232
22	5-Aminoimidazole	0.965251231	240.439	84.0563	Organoheterocyclic compounds	forward	0.01137	0.00419	1.67591	0.03215
23	Thiiranebutanenitrile	0.965102385	280.127	128.054	Organoheterocyclic compounds	forward	0.16275	0.13081	1.52785	0.02139
24	N6-Methyladenosine	0.954326	305.698	282.12	Nucleosides, nucleotides, and analogues	forward	0.05724	0.07952	2.20168	0.00071
25	3-Amino-2-piperidone	0.953320462	210.467	115.087	Organic acids and derivatives	forward	0.03453	0.01987	1.90611	0.00773
26	1H-Indole-3-carboxaldehyde	0.949462231	277.785	146.06	Organoheterocyclic compounds	forward	0.06164	0.09914	2.03962	0.00041
27	Thymine	0.936329692	291.645	127.051	Organoheterocyclic compounds	forward	0.18706	0.09721	1.52889	0.02732
28	Dimethylethanolamine	0.912661154	167.922	90.0918	Organonitrogen compounds	forward	0.0055	0.00825	1.80153	0.00363
29	L-Aspartic acid	0.91108	408.628	134.045	Organic acids and derivatives	forward	0.00968	0.00551	1.46795	0.03448
30	L-Kynurenine	0.901483846	279.162	209.092	Organic oxygen compounds	forward	0.01593	0.03026	1.98399	0.00498
31	Octadecylamine	0.899452769	154.179	270.316	Organonitrogen compounds	forward	0.00087	4.8E-05	2.67636	5.1E-06
32	(±)-Tryptophan	0.895806923	277.994	205.098	Organonitrogen compounds	forward	0.74067	1.09996	1.89688	0.00134
33	Trimethylaminoacetone	0.891986923	228.832	116.107	Organic oxygen compounds	forward	0.01713	0.02806	1.44917	0.0105
34	2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate	0.891442231	228.658	307.044	Phenylpropanoids and polyketides	forward	0.02007	0.00393	2.21352	0.01981
35	Theaspiron A	0.886202	447.148	209.154	Organic oxygen compounds	forward	0.00449	0.0057	1.53417	0.04447
36	L-Tyrosine	0.884292846	317.12	182.082	Organic acids and derivatives	forward	0.57266	0.84367	1.86044	0.00491
37	N-Nitroso-pyrrolidine	0.876407692	329.986	101.071	Organoheterocyclic compounds	forward	0.02752	0.01624	1.99119	0.00138
38	Triethanolamine	0.871208308	153.077	150.113	Organonitrogen compounds	forward	0.01459	0.00608	2.00065	0.0257
39	Alitame	0.849953538	235.18	332.164	Organic acids and derivatives	forward	0.0017	0.00389	1.57381	0.0057
40	Homoarecoline	0.848264	356.211	170.118	Alkaloids and derivatives	forward	0.01583	0.03703	1.88682	0.00343
41	1-(2,3-Dihydro-6,7-dimethyl-1H-pyrrolizin-5-yl)-2-hydroxy-1-propanone	0.841590769	211.723	208.133	Organoheterocyclic compounds	forward	0.02674	0.10913	1.58262	0.02799
42	Urocanic acid	0.840385769	298.744	139.05	Organic compounds	forward	0.01858	0.03054	1.56411	0.02302
43	D-1-Amino-2-pyrrolidinecarboxylic acid	0.824398692	225.494	131.082	Organic acids and derivatives	forward	0.00639	0.0044	1.35088	0.01728
44	Pivaloylcarnitine	0.808512692	260.799	246.17	Lipids and lipid-like molecules	forward	0.14294	0.22664	1.63132	0.01226
45	SM(d18:1/16:0)	0.801787615	187.507	703.574	Lipids and lipid-like molecules	forward	0.71828	0.84596	1.62377	0.01864
46	Prolylphenylalanine	0.786234769	288.012	263.139	Organic acids and derivatives	forward	0.00122	0.00265	1.16945	0.00959
47	Carzerenone	0.779733077	22.7282	231.135	Lipids and lipid-like molecules	forward	0.00498	0.00395	1.45979	0.02558
48	PC(16:0/16:0)	0.758186	38.7603	734.57	Lipids and lipid-like molecules	forward	0.11514	0.14272	1.63388	0.01331
49	2-Benzofurancarboxaldehyde	0.752976846	317.099	147.044	Organoheterocyclic compounds	forward	0.01523	0.03087	1.68325	0.00175
50	PC(20:3(8Z,11Z,14Z)/20:1(11Z))	0.741123846	156.98	838.63	Lipids and lipid-like molecules	forward	0.07993	0.12476	1.87124	0.00126
51	2,4-Diamino-6-nitrotoluene	0.739568769	339.372	168.077	Benzenoids	forward	0.0687	0.13268	1.8995	0.00931
52	2-Phenylacetamide	0.733600538	317.104	136.076	Benzenoids	forward	0.14883	0.22226	1.82253	0.00632
53	2,2,4,4,6,6-Hexamethyl-1,3,5-trithiane	0.730673077	30.7564	223.064	Organosulfur compounds	forward	0.01732	0.011	2.00349	0.00123
54	9-HOTE	0.724853154	50.108	295.227	Lipids and lipid-like molecules	forward	0.00983	0.00544	1.49347	0.03621
55	Betaine aldehyde	0.721584923	369.702	102.092	Organic nitrogen compounds	forward	0.04991	0.06395	1.59898	0.00821
56	PC(20:4(8Z,11Z,14Z,17Z)/P-18:0)	0.717308	59.3776	794.604	Lipids and lipid-like molecules	forward	0.30535	0.39677	1.34359	0.04901
57	SM(d16:1/24:1(15Z))	0.715384462	197.037	785.653	Lipids and lipid-like molecules	forward	1.02299	1.26	1.84437	0.00356
58	2-(4-(5,8,11,14,17-Eicosapentaenoyl)-1-O-hexadecylglycero-3-phosphocholine	0.711754692	36.5158	766.574	Lipids and lipid-like molecules	forward	0.08605	0.12184	1.25514	0.03704
59	DG(18:3(9Z,12Z,15Z)/20:3(5Z,8Z,11Z)/0:0)	0.698968692	30.7669	641.514	Lipids and lipid-like molecules	forward	0.00501	0.00712	1.60767	0.01676
60	trans-Hexadec-2-enoyl carnitine	0.698871692	198.998	398.327	Lipids and lipid-like molecules	forward	0.06799	0.04401	1.5652	0.02276
61	Phenylalanyl-Tryptophan	0.698820462	189.667	352.166	Organic acids and derivatives	forward	0.0009	0.00229	2.4381	4.5E-06
62	L-Cyclo(alanylglycyl)	0.692914154	339.504	129.066	Organoheterocyclic compounds	forward	0.12565	0.16873	1.69038	0.0143
63	PC(20:5(5Z,8Z,11Z,14Z,17Z)/P-18:0)	0.691202385	154.242	792.591	Lipids and lipid-like molecules	forward	0.21478	0.30071	1.77207	0.00523
64	PC(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z))	0.686595154	153.06	854.569	Lipids and lipid-like molecules	forward	0.00488	0.00938	1.55578	0.00286
65	DG(14:0/22:4(7Z,10Z,13Z,16Z)/0:0)	0.683213538	30.7838	617.514	Lipids and lipid-like molecules	forward	0.01741	0.02925	1.72943	0.02037
66	PC(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	0.675367308	36.4977	834.601	Lipids and lipid-like molecules	forward	0.17347	0.23098	1.46594	0.04334
67	N-Acetylhistidine	0.673956385	406.178	198.085	Organic acids and derivatives	forward	0.0599	0.18219	1.91297	0.01726
68	PC(22:4(7Z,10Z,13Z,16Z)/16:0)	0.671835308	60.3195	810.599	Lipids and lipid-like molecules	forward	2.66012	3.40192	1.45329	0.04
69	2-acetyl-1-alkyl-sn-glycero-3-phosphocholine	0.669880923	194.44	524.372	Lipids and lipid-like molecules	forward	0.10782	0.18153	1.68915	0.00795
70	SM(d18:1/14:0)	0.666241769	179.31	675.544	Lipids and lipid-like molecules	forward	0.01125	0.01949	1.84769	0.00454
71	PC(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	0.663807538	59.04	818.605	Lipids and lipid-like molecules	forward	0.04013	0.05366	1.67441	0.0148
72	PC(22:2(13Z,16Z)/16:1(9Z))	0.654881538	158.821	812.612	Lipids and lipid-like molecules	forward	1.0271	1.34008	1.40268	0.02298

73	SM(d17:1/24:1(15Z))	0.651156154	196.74	799.669	Lipids and lipid-like molecules	forward	0.35193	0.40388	1.41819	0.0366
74	PC(22:5(4Z,7Z,10Z,13Z,16Z)/P-18:0)	0.649539308	59.1625	820.62	Lipids and lipid-like molecules	forward	0.06017	0.0764	1.30051	0.04442
75	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z))	0.646523538	156.484	832.585	Lipids and lipid-like molecules	forward	0.13102	0.17894	1.57262	0.00892
76	Thiomorpholine 3-carboxylate	0.642427154	210.493	148.043	Organic acids and derivatives	forward	0.00736	0.01484	1.7268	0.00149
77	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:1(11Z))	0.642385308	155.293	860.615	Lipids and lipid-like molecules	forward	0.00911	0.01322	1.75428	0.0069
78	LysoPC(22:0)	0.642016846	208.198	580.434	Lipids and lipid-like molecules	forward	0.01084	0.01713	1.75549	0.01041
79	PC(P-18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	0.639919462	153.02	816.59	Lipids and lipid-like molecules	forward	0.02114	0.03064	1.98013	0.00339
80	PC(18:2(9Z,12Z)/15:0)	0.639651154	166.756	744.554	Lipids and lipid-like molecules	forward	0.12806	0.16216	1.4652	0.04019
81	SM(d18:1/20:0)	0.625838308	199.026	759.636	Lipids and lipid-like molecules	forward	0.36241	0.47956	1.9263	0.00596
82	PC(16:1(9Z)/16:1(9Z))	0.624318308	166.784	730.538	Lipids and lipid-like molecules	forward	0.10825	0.1881	1.87568	0.00187
83	PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z))	0.622864154	154.307	856.583	Lipids and lipid-like molecules	forward	0.00975	0.01454	2.23042	5.4E-05
84	PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	0.621113923	156.44	864.647	Lipids and lipid-like molecules	forward	0.00851	0.0135	1.71823	0.02252
85	LysoPC(18:1(9Z))	0.620044615	195.524	522.356	Lipids and lipid-like molecules	forward	0.02522	0.04176	1.58875	0.02586
86	Montecristin	0.618816385	30.7299	575.503	Lipids and lipid-like molecules	forward	0.01789	0.02267	1.43782	0.04612
87	DG(15:0/18:3(6Z,9Z,12Z)/0:0)	0.614711077	132.299	577.484	Lipids and lipid-like molecules	forward	0.01418	0.02953	1.5064	0.04139
88	PC(15:0/15:0)	0.608504231	52.3243	706.538	Lipids and lipid-like molecules	forward	0.00589	0.01049	1.70965	0.01427
89	PC(20:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(11Z))	0.608295385	57.955	790.573	Lipids and lipid-like molecules	forward	0.02288	0.03847	1.68433	0.01055
90	1-Phosphatidyl-1D-myo-inositol 3-phosphate	0.607852615	382.108	471.029	Organic oxygen compounds	forward	0.05986	0.03205	2.33396	1.8E-05
91	Homo-L-arginine	0.605033692	545.221	189.135	Organic acids and derivatives	forward	0.09335	0.18296	1.61918	0.03949
92	PC(18:1(11Z)/P-16:0)	0.597727846	106.254	744.59	Lipids and lipid-like molecules	forward	0.06529	0.10019	1.34795	0.03204
93	PC(20:4(8Z,11Z,14Z,17Z)/14:0)	0.593391769	72.122	754.537	Lipids and lipid-like molecules	forward	0.01299	0.02945	1.84688	0.00536
94	PC(14:0/14:0)	0.584026231	170.22	678.506	Lipids and lipid-like molecules	forward	0.0021	0.00592	1.78753	0.0032
95	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:2(11Z,14Z))	0.565939308	155.293	858.6	Lipids and lipid-like molecules	forward	0.00902	0.01389	2.41782	2E-05
96	Se-Adenosylselenohomocysteine	0.564319923	382.17	433.073	Nucleosides, nucleotides, and analogues	forward	0.01441	0.02373	2.18225	5.5E-05
97	LysoPC(20:1(11Z))	0.562204	211.636	550.387	Lipids and lipid-like molecules	forward	0.06954	0.08383	1.45803	0.02952
98	Tryptophyl-Isololeucine	0.555286923	199.052	318.181	Organic acids and derivatives	forward	0.00208	0.00108	1.95715	0.00613
99	PC(18:3(6Z,9Z,12Z)/P-18:1(11Z))	0.540542077	155.375	766.574	Lipids and lipid-like molecules	forward	0.4731	0.69658	1.56695	0.01194
100	Glaucaurubin	0.526815308	226.476	479.229	Lipids and lipid-like molecules	forward	0.00605	0.01283	1.43544	0.03408
101	Taurine	0.518577385	309.12	126.022	Organic acids and derivatives	forward	1.31077	0.78571	2.02203	0.00687
102	N,N'-Diacylhydrazine	0.516998308	277.994	117.058	Organic nitrogen compounds	forward	0.002	0.00338	2.17977	0.00033
103	LysoPC(14:0/0:0)	0.516511923	222.831	468.309	Lipids and lipid-like molecules	forward	0.30736	0.56297	1.95008	0.00187
104	LysoPC(16:1(9Z)/0:0)	0.51328	217.95	494.325	Lipids and lipid-like molecules	forward	0.42955	0.54605	1.39463	0.03521
105	S-Allylcysteine	0.509605692	258.652	162.058	Organic acids and derivatives	forward	0.00166	0.00974	1.49039	0.03397
106	Naphthalene epoxide	0.468554462	309.102	143.049	Benzenoids	forward	0.00619	0.00285	1.88189	0.00917
107	PE(P-18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	0.465040615	36.4796	750.543	Lipids and lipid-like molecules	forward	0.0179	0.0288	1.9314	0.00092
108	Octadecanamide	0.453031231	133.528	284.295	Lipids and lipid-like molecules	forward	0.00186	0.00289	1.42946	0.02928
109	PC(P-16:0/18:4(6Z,9Z,12Z,15Z))	0.449280462	156.47	738.543	Lipids and lipid-like molecules	forward	0.00743	0.01471	1.65718	0.01346
110	(R)-2-Nitro-p-mentha-1,5-diene	0.433818077	73.4438	182.118	Lipids and lipid-like molecules	forward	0.00032	0.00016	1.14507	0.04629
111	PE(20:4(8Z,11Z,14Z,17Z)/P-18:0)	0.433495769	37.514	752.559	Lipids and lipid-like molecules	forward	0.02178	0.0441	2.14478	0.00012
112	PE(P-18:1(9Z)/20:3(5Z,8Z,11Z))	0.412595615	155.362	752.558	Lipids and lipid-like molecules	forward	0.16155	0.32508	2.18953	0.0001
113	PE(P-18:1(11Z)/22:4(7Z,10Z,13Z,16Z))	0.398357308	154.294	778.575	Lipids and lipid-like molecules	forward	0.02652	0.04742	2.25541	9.6E-05
114	3beta,15alpha-Diacetoxylanosta-8,24-dien-26-oic acid	0.385740538	25.0384	557.384	Lipids and lipid-like molecules	forward	0.00041	0.0009	1.64781	0.01701
115	PE(P-16:0/20:4(5Z,8Z,11Z,14Z))	0.381521077	37.555	724.527	Lipids and lipid-like molecules	forward	0.0167	0.03225	2.12136	5.2E-05
116	PE(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	0.359927308	154.208	776.558	Lipids and lipid-like molecules	forward	0.06231	0.09781	1.97713	0.00095
117	PE(P-18:1(9Z)/18:1(9Z))	0.356409538	37.5808	728.559	Lipids and lipid-like molecules	forward	0.00609	0.01019	1.20965	0.0427
118	PE(18:3(9Z,12Z,15Z)/P-18:1(11Z))	0.331204615	158.498	724.527	Lipids and lipid-like molecules	forward	0.0795	0.15351	2.23567	3.8E-05
119	PE(P-18:1(9Z)/16:1(9Z))	0.329981769	37.6382	700.527	Lipids and lipid-like molecules	forward	0.0044	0.00921	1.30664	0.00167
120	Vitamin A	0.302557769	30.8044	269.226	Lipids and lipid-like molecules	reverse	0.00258	0.00364	2.00985	0.00082

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;