

Table S1 Mass spectrometry identification information---The fragments of MS/MS

Name	Formula	RT	Ion mode	calm/z	m/z	ppm	Fragments	Ion mode	calm/z	m/z	ppm	Fragments
Choline	C5H14NO+	1.196	M+	104.10699	104.1072	2.02	104, 60, 58, 45, 44	-	-	-	-	-
L-Carnitine	C7H15NO3	1.25	M+H	162.11247	162.11185	-3.82	162, 103, 102, 85, 60, 43	-	-	-	-	-
Allantoin	C4H6N4O3	1.317	-	-	-	-	-	M-H	157.0367	157.03571	-6.37	114, 97, 42
Lactic acid	C3H6O3	1.962	-	-	-	-	-	M-H	89.0244	89.02441	-0.11	89, 43, 41
Pyroglutamic acid	C5H7NO3	2.237	-	-	-	-	-	M-H	128.0353	128.03496	-2.81	128, 82, 42
Xanthine	C5H4N4O2	2.312	M+H	153.0407	153.04106	2.35	153, 136, 110, 81, 55	M-H	151.0262	151.02615	0.00	151, 133, 108, 80
L-Tryptophan	C11H12N2O2	7.848	M+H	205.09715	205.09691	-1.17	188, 146, 118, 115, 91	M-H	203.0826	203.08171	-4.38	203, 142, 116
Hippuric acid	C9H9NO3	8.949	M+H	180.06552	180.06555	0.17	105, 77	M-H	178.0510	178.05104	0.39	134, 77
PE(18:0/20:4)	C43H78NO8P	10.272	-	-	-	-	-	M-H	766.5392	766.53412	-6.67	303, 283
Sebacic acid	C10H18O4	10.42	-	-	-	-	-	M-H	201.1132	201.11243	-3.98	157, 139, 137
Dodecadienoic acid	C12H20O2	10.734	M+NH4	214.18016	214.18005	-0.51	214, 179, 109, 95, 81, 67	-	-	-	-	-
Prostaglandin F2a	C20H34O5	10.799	-	-	-	-	-	M-H	353.2334	353.2341	2.12	353, 317, 197, 167
Sphingosine	C18H37NO2	10.971	M+H	300.28971	300.28931	-1.33	264, 252	-	-	-	-	-
Cholic acid	C24H40O5	11.097	M+NH4	426.3214	426.32199	1.38	373, 355, 225,	M-H	407.2803	407.28055	0.61	407
Heme	C34H32FeN4O4	11.134	M+H	616.1773	616.17651	-1.28	616, 557, 498	-	-	-	-	-
LysoPE(14:0/0:0)	C19H40NO7P	11.468	-	-	-	-	-	M-H	424.2470	424.24643	-1.25	424, 227, 196
LysoPC(14:0/0:0)	C22H46NO7P	11.53	M+H	468.30847	468.30975	2.73	450, 285, 184, 104	M+FA-H	512.2994	512.29956	0.33	452, 227, 224
LysoPC(16:1/0:0)	C24H48NO7P	11.81	M+H	494.32412	494.32184	-4.61	476, 311, 184, 104	M+FA-H	538.3150	538.31183	-5.96	478, 253, 224

Palmitoylcarnitine	C23H45NO4	11.861	M+H	400.34214	400.3421	-0.10	400, 338, 85	-	-	-	-	-
LysoPE(20:4/0:0)	C25H44NO7P	11.948	M+H	502.29282	502.29123	-3.17	361, 330, 269, 203	M-H	500.2783	500.27722	-2.08	500, 303, 259, 214
LysoPE(15:0/0:0)	C20H42NO7P	11.977	M+H	440.27717	440.27667	-1.14	299, 268, 216	M-H	438.2626	438.26318	1.30	438, 241, 196
LysoPC(0:0/20:4)	C28H50NO7P	12.017	M+H	544.33977	544.34045	1.25	361, 184, 125	-	-	-	-	-
LysoPC(15:0/0:0)	C23H48NO7P	12.063	M+H	482.32412	482.32245	-3.46	464, 299, 184, 104	M+FA-H	526.3150	526.3136	-2.74	466, 241, 224
LysoPE(22:5/0:0)	C27H46NO7P	12.178	M+H	528.30847	528.30737	-2.08	387, 356	M-H	526.2939	526.2926	-2.49	526, 329, 241
LysoPC(20:4/0:0)	C28H50NO7P	12.182	M+H	544.33977	544.33972	-0.09	526, 258, 184, 104	M+FA-H	588.3307	588.33081	0.20	528, 303, 224
LysoPC(14:1/0:0)	C22H44NO7P	12.308	M+H	466.29282	466.29199	-1.78	184, 104	-	-	-	-	-
3b-Hydroxy-5-choleonoic acid	C24H38O3	12.349	M+H	375.28937	375.28864	-1.95	375, 339, 321, 221, 215	-	-	-	-	-
Deoxycholic acid	C24H40O4	12.35	M+NH4	410.32649	410.32761	2.73	357, 339, 321, 261, 247	M-H	391.2854	391.28485	-1.35	391, 345
LysoPC(17:1/0:0)	C25H50NO7P	12.398	M+H	508.33977	508.34082	2.07	490, 325, 184, 104	-	-	-	-	-
LysoPC(0:0/16:0)	C24H50NO7P	12.471	M+H	496.33977	496.33987	0.20	313, 184, 125	M+FA-H	540.3307	540.33008	-1.13	480, 255, 242
LysoPC(16:0/0:0)	C24H50NO7P	12.731	M+H	496.33977	496.33994	0.34	478, 313, 184, 104	-	-	-	-	-
LysoPE(22:4/0:0)	C27H48NO7P	12.921	M+H	530.32412	530.32587	3.30	389, 358	M-H	528.3096	528.3092	-0.68	528, 331, 287, 214
Stearoylcarnitine	C25H49NO4	12.971	M+H	428.37344	428.37277	-1.56	428, 369, 267, 8	-	-	-	-	-
LysoPE(18:1/0:0)	C23H46NO7P	13.009	M+H	480.30847	480.30746	-2.10	462, 419, 339, 308, 155	M-H	478.2939	478.29224	-3.49	478, 281, 196
LysoPC(22:4/0:0)	C30H54NO7P	13.028	M+H	572.37107	572.36639	-8.18	554, 387, 184	-	-	-	-	-
LysoPC(18:1/0:0)	C26H52NO7P	13.128	M+H	522.35542	522.35315	-4.35	504, 339, 184, 104	M+FA-H	566.3463	566.3432	-5.54	506, 281, 224
13-OxoODE	C18H30O3	13.306	-	-	-	-	-	M-H	293.2122	293.21335	3.85	293, 221, 113
5,6-Epoxy-8,11,14-eicosatrienoic acid	C20H32O3	13.408	-	-	-	-	-	M-H	319.2279	319.22778	-0.28	319, 257, 179, 163

LysoPE(P-18:1/0:0)	C23H46NO6P	13.467	M+H	464.31355	464.31323	-0.69	446, 390, 310, 292, 155	M-H	462.2990	462.29678	-4.80	462, 401, 265, 196, 140
LysoPC(17:0/0:0)	C25H52NO7P	13.555	M+H	510.35542	510.35587	0.88	492, 327, 184, 104	M+FA-H	554.3463	554.34332	-5.45	494, 269, 224
LysoPE(20:2/0:0)	C25H48NO7P	13.593	-	-	-	-	-	M-H	504.3096	504.30667	-5.73	504, 307, 196
LysoPC(20:2/0:0)	C28H54NO7P	13.725	M+H	548.37107	548.37427	5.84	530, 184, 104	-	-	-	-	-
LysoPE(19:1/0:0)	C24H48NO7P	13.759	M+H	494.32412	494.32303	-2.21	476, 353, 323	-	-	-	-	-
LysoPE(20:1/0:0)	C25H50NO7P	14.72	M+H	508.33977	508.34109	2.60	490, 447, 367, 336	M-H	506.3252	506.32501	-0.40	506, 309, 196
Tetradecenoylcarnitine	C21H39NO4	14.726	M+H	370.29519	370.29553	0.92	85.00	-	-	-	-	-
LysoPC(20:1/0:0)	C28H56NO7P	14.935	M+H	550.38672	550.38544	-2.33	532, 367, 184, 104	M+FA-H	594.3776	594.37714	-0.84	534, 309, 224
LysoPE(P-18:0/0:0)	C23H48NO6P	14.982	M+H	466.3292	466.33093	3.71	448, 392, 312, 294, 155	-	-	-	-	-
Linoleamide	C18H33NO	15.428	M+H	280.26349	280.26279	-2.50	263, 150, 149, 95	-	-	-	-	-
Monoelaidin	C21H40O4	17.101	M+H	357.29994	357.29993	-0.03	339, 265, 247, 135, 121	-	-	-	-	-
Dihomo-gamma-linolenic acid	C20H34O2	18.115	-	-	-	-	-	M-H	305.2486	305.24808	-1.70	305, 261, 231