

Table S1. Identified ion information of serum biomarkers in AD model rats.

No.	Rt min	M/Z Determined	M/Z Calculated	Actual_M	Scan Mode	Proposed Composition	Proposed Identity	MS/MS fragment ion (m/z)	Change Trend
1	0.56	145.0975	145.0977	146.1055	ESI ⁻	C ₆ H ₁₄ N ₂ O ₂	Lysine	145.0975[M-H] ⁻ ,128.0319[M-H ₃ N-H] ⁻ ,127.0497[M-H ₂ O-H] ⁻ ,177.0614[M+H] ⁺ ,160.0358[M-H ₃ N+H] ⁺ ,117.0300[M-CH ₄ N ₂ O+H] ⁺ ,91.0508[M-C ₂ H ₂ N ₂ O ₂ +H] ⁺	↑
2	0.57	177.0614	177.0624	176.0546	ESI ⁺	C ₄ H ₈ N ₄ O ₄	Allantoic acid	296.0859[M-H] ⁻ ,217.0600[M-CH ₅ O-H] ⁻ ,115.0395[M-C ₅ H ₅ N ₅ -H] ⁻ ,111.0320[M-C ₅ H ₇ N ₄ O-H] ⁻ ,243.0615[M+H] ⁺ ,228.0508[M-HN+H] ⁺ ,153.0426[M-C ₂ H ₄ NO ₃ +H] ⁺ ,110.0116[M-C ₅ H ₉ O ₄ +H] ⁺	↑
3	0.63	296.0859	250.094	251.1018	ESI ⁻	C ₁₀ H ₁₃ N ₅ O ₃	5'-Deoxyadenosine	189.1255[M+H] ⁺ ,128.0712[M-C ₂ H ₅ NO+H] ⁺ ,111.0684[M-C ₂ H ₆ NO ₂ +H] ⁺ ,87.0320[M-C ₅ H ₁₀ NO+H] ⁺	↑
4	0.68	243.0615	243.0617	244.0695	ESI ⁻	C ₉ H ₁₂ N ₂ O ₆	Uridine	258.1104[M+H] ⁺ ,213.0766[M-C ₂ H ₅ O+H] ⁺ ,154.0031[M-C ₅ H ₁₄ NO+H] ⁺ ,134.9847 [M-C ₅ H ₁₇ NO ₂ +H] ⁺ ,427.0059[M-H] ⁻ ,201.0413[M-	↓
5	0.70	189.1255	189.1239	188.1161	ESI ⁺	C ₈ H ₁₆ N ₂ O ₃	N6-Acetyl-L-lysine		↑
6	0.73	258.1104	258.1106	257.1028	ESI ⁺	C ₈ H ₂₀ NO ₆ P	Glycerophosphocholine		↑

8	1.11	130.0866	130.0868	131.0946	ESI ⁻	C ₆ H ₁₃ NO ₂	Leucine	C ₉ H ₅ N ₄ O ₂ -H] ⁻ ,146.9847[M- C ₆ H ₉ N ₄ O ₇ P-H] ⁻ ,128.0348[M- C ₅ H ₇ N ₃ O ₈ P ₂ -H] ⁻ 427.0059[M-H] ⁻ ,113.0841[M-HO-H] ⁻ ,87.0320[M-C ₃ H ₇ -H] ⁻ ,85.0891[M- CHO ₂ -H] ⁻	↓
9	1.14	164.0357	164.0348	165.0426	ESI ⁻	C ₈ H ₇ NO ₃	Formylanthranilate	164.0357[M-H] ⁻ ,147.0320[M-HO-H] ⁻ ,103.0184[M-CH ₃ NO ₂ -H] ⁻ ,91.0422 [M-C ₂ HO ₃ -H] ⁻	↓
10	2.54	136.0626	136.0623	135.0545	ESI ⁺	C ₅ H ₅ N ₅	Adenine	136.0626[M+H] ⁺ ,107.0358[M- CH ₃ N+H] ⁺ ,93.0327[M- CH ₃ N ₂ +H] ⁺ ,79.0170[M-C ₂ H ₅ N ₂ +H] ⁺ 255.0662[M+H] ⁺ ,237.0545[M- H ₂ O+H] ⁺ ,209.0596[M- CH ₂ O ₂ +H] ⁺ ,153.0096[M- C ₄ H ₈ NO ₂ +H] ⁺	↓
11	2.93	255.0662	255.0651	254.0573	ESI ⁺	C ₇ H ₁₄ N ₂ O ₆ S	5-L-Glutamyl-taurine	514.2831[M+H] ⁺ ,205.0535[M- C ₁₈ H ₂₉ NO ₃ +H] ⁺ ,106.9439[M- C ₂₅ H ₄₃ NO ₃ +H] ⁺ ,79.956[M- C ₂₆ H ₄₂ NO ₄ +H] ⁺ , 213.0147[M-H] ⁻ ,197.0215[M-O-H] ⁻ ,116.0473[M-H ₂ O ₄ P-H] ⁻ ,79.9663[M- C ₅ H ₉ O ₄ -H] ⁻	↑
12	3.63	514.2831	514.2838	513.2760	ESI ⁺	C ₂₆ H ₄₃ NO ₇ S	Sulfolithocholyglycine	157.0609[M+H] ⁺ ,141.0664[M- OH+H] ⁺ ,129.0426[M-	↓
13	4.02	213.0147	213.0164	214.0242	ESI ⁻	C ₅ H ₁₁ O ₇ P	Deoxyribose 5-phosphate		↑
14	4.13	157.0609	157.0613	156.0535	ESI ⁺	C ₆ H ₈ N ₂ O ₃	4-Imidazolone-5-propionic acid		↓

15	4.28	464.3004	464.3012	465.3090	ESI ⁻	C ₂₆ H ₄₃ NO ₆	Glycocholic acid	CH ₂ N+H] ⁺ ,116.0473[M-CHN ₂ +H] ⁺ 464.3004[M-H] ⁻ ,446.2906 [M-H ₂ O- H] ⁻ ,420.3114[M-CO ₂ -H] ⁻ ,288.2089[M-C ₇ H ₁₄ NO ₄ -H] ⁻	↑
16	4.29	448.3064	448.3063	449.3141	ESI ⁻	C ₂₆ H ₄₃ NO ₅	Glycoursodeoxycholic acid	448.3064[M-H] ⁻ ,464.2906[M-H ₂ O- H] ⁻ ,436.3114[M-CO ₂ -H] ⁻ ,341.2531[M-C ₃ H ₉ NO ₅ -H] ⁻	↑
17	4.34	369.2257	369.2277	370.2355	ESI ⁻	C ₂₀ H ₃₄ O ₆	Thromboxane B2	369.2257[M-H] ⁻ ,317.1753[M-CH ₄ -H] ⁻ ,285.1491[M-C ₂ H ₈ O-H] ⁻ ,205.0865[M- C ₈ H ₁₆ O-H] ⁻	↑
18	4.42	159.1015	159.1021	160.1099	ESI ⁻	C ₈ H ₁₆ O ₃	3-Hydroxyoctanoic acid	159.1015[M-H] ⁻ ,141.0916[M-H ₂ O- H] ⁻ ,115.0395[M-C ₃ H ₈ -H] ⁻	↑
19	4.42	353.2306	353.2328	354.2406	ESI ⁻	C ₂₀ H ₃₄ O ₅	Prostaglandin F2a	,113.0954[M-CH ₂ O ₂ -H] ⁻ 353.2306[M-H] ⁻ ,335.2222 [M-H ₂ O- H] ⁻ ,309.2430[M-CO ₂ -H] ⁻	↑
20	4.47	165.0542	165.0552	166.0630	ESI ⁻	C ₉ H ₁₀ O ₃	Homovanillin	,111.0446[M-C ₁₄ H ₂₆ O ₃ -H] ⁻ 165.0542[M-H] ⁻ ,149.0239[M-CH ₄ -H] ⁻ ,136.0524[M-CHO-H] ⁻ ,133.0290[M- CH ₄ O-H] ⁻	↓
21	4.50	241.1319	241.1301	240.1222	ESI ⁺	C ₁₀ H ₁₆ N ₄ O ₃	Anserine	241.1319[M+H] ⁺ ,225.1113[M- H ₂ N+H] ⁺ ,155.0821[M- C ₃ H ₆ N ₂ O+H] ⁺ ,121.0640[M- C ₄ H ₁₀ NO ₃ +H] ⁺	↑
22	4.52	295.2253	295.2273	294.2195	ESI ⁺	C ₁₈ H ₃₀ O ₃	9-OxoODE	295.2253[M+H] ⁺ ,279.1960[M- CH ₄ +H] ⁺ ,196.1099[M-	↑

23	4.53	185.1174	185.1178	186.1256	ESI ⁻	C ₁₀ H ₁₈ O ₃	3-Oxodecanoic acid	C ₇ H ₁₅ +H] ⁺ ,181.1229[M-C ₇ H ₁₄ O+H] ⁺ 185.1174[M-H] ⁻ ,167.1072[M-H ₂ O- H] ⁻ ,155.0708[M-C ₂ H ₆ -H] ⁻ ,113.0239[M-C ₅ H ₁₂ -H] ⁻ 343.1254[M+H] ⁺ ,312.1057[M- CH ₃ O+H] ⁺ ,284.1107[M- C ₂ H ₃ O ₂ +H] ⁺ ,181.0712[M- C ₆ H ₁₀ O ₅ +H] ⁺	↓
24	4.54	343.1254	343.124	342.1162	ESI ⁺	C ₁₂ H ₂₂ O ₁₁	Epimelibiose	151.0383[M-H] ⁻ ,136.0524[M-O-H] ⁻ ,121.0290[M-CH ₂ O-H] ⁻ ,108.0211[M- C ₂ H ₃ O-H] ⁻ 249.1123[M-H] ⁻ ,233.0814[M-CH ₄ -H] ⁻ ,205.0865[M-C ₂ H ₄ O-H] ⁻ ,111.0082[M- C ₉ H ₁₄ O-H] ⁻ 407.2796[M-H] ⁻ ,389.2692[M-H ₂ O- H] ⁻ ,C ₂₄ H ₃₅ O ₃ [M-H ₄ O ₂ -H] ⁻ ,289.2168[M-C ₅ H ₁₀ O ₃ -H] ⁻ 321.2061[M+H] ⁺ ,306.1831[M- CH ₃ +H] ⁺ ,265.1440[M- C ₄ H ₈ +H] ⁺ ,251.1283[M-C ₅ H ₁₀ +H] ⁺ ,	↓
25	4.68	151.0383	151.0395	152.0473	ESI ⁻	C ₈ H ₈ O ₃	3, 4- Dihydroxyphenylacetaldeh yde	318.2987[M+H] ⁺ ,303.2752[M- CH ₃ +H] ⁺ ,286.2725 M-CH ₃ -OH+H] ⁺ 311.2194[M-H] ⁻ ,293.2117[M-H ₂ O- H] ⁻ ,195.1385[M-C ₆ H ₁₂ O ₂ -H] ⁻ ,155.0708[M-C ₁₀ H ₂₀ O-H] ⁻	↓
26	4.71	249.1123	249.1127	250.1205	ESI ⁻	C ₁₄ H ₁₈ O ₄	Ubiquinone-1		↑
27	4.72	407.2796	407.2797	408.2876	ESI ⁻	C ₂₄ H ₄₀ O ₅	Cholic acid		↑
28	4.89	321.2061	321.2066	320.1988	ESI ⁺	C ₁₉ H ₂₈ O ₄	QH2		↑
29	5.11	318.2987	318.3008	318.2987	ESI ⁺	C ₁₈ H ₃₉ NO ₃	Phytosphingosine		↓
30	5.35	311.2194	311.2222	312.2301	ESI ⁻	C ₁₈ H ₃₂ O ₄	8(R)-Hydroperoxylinoleic acid		↑

31	5.80	311.2219	311.2222	312.2301	ESI ⁻	C ₁₈ H ₃₂ O ₄	9(S)-HPODE	311.2219[M-H]-,293.2117[M-H ₂ O-H]-,267.1596[M-C ₃ H ₈ -H]-,179.1436[M-C ₆ H ₁₂ O ₃ -H]-	↑
32	5.80	333.2039	333.2066	334.2144	ESI ⁻	C ₂₀ H ₃₀ O ₄	Prostaglandin J2	333.2039[M-H]-,317.1753[M-CH ₄ -H]-,285.1491[M-C ₂ H ₆ O-H]-,273.1855[M-C ₂ H ₄ O ₂ -H]-	↑
33	5.84	269.2111	269.2117	270.2195	ESI ⁻	C ₁₆ H ₃₀ O ₃	3-Oxohexadecanoic acid	269.2111[M-H]-,253.1804[M-CH ₄ -H]-,167.1436[M-C ₅ H ₁₀ O ₂ -H]-	↓
34	5.89	303.2319	303.2324	304.2402	ESI ⁻	C ₂₀ H ₃₂ O ₂	Arachidonic acid	100.0160[M-C ₁₂ H ₂₅ -H]-,303.2319[M-H]-,286.2297[M-HO-H]-,273.1855[M-C ₂ H ₆ -H]-,151.0759[M-C ₁₁ H ₂₀ -H]-	↑
35	5.94	311.2214	311.2222	312.2301	ESI ⁻	C ₁₈ H ₃₂ O ₄	13(S)-HPODE	311.2214[M-H]-,279.1960[M-CH ₄ -H]-,155.1072[M-C ₉ H ₁₆ O-H]-,127.0759[M-C ₁₁ H ₂₀ O-H]-	↑
36	5.96	333.2035	333.2066	334.2144	ESI ⁻	C ₂₀ H ₃₀ O ₄	Prostaglandin A2	333.2035[M-H]-,317.1753[M-CH ₄ -H]-,299.1647[M-CH ₆ O-H]-,231.1021[M-C ₆ H ₁₄ O-H]-	↑
37	6.39	295.2269	295.2273	296.2351	ESI ⁻	C ₁₈ H ₃₂ O ₃	12, 13-EpOME	295.2269[M-H]-,279.1960[M-CH ₄ -H]-,155.1072[M-C ₉ H ₁₆ O-H]-,141.0916[M-C ₁₀ H ₁₈ O-H]-	↓
38	7.18	376.3205	376.3216	375.3137	ESI ⁺	C ₂₄ H ₄₁ NO ₂	Adrenoyl ethanolamide	376.3205[M+H]+,264.1964[M-C ₈ H ₁₆ +H]+,177.1643[M-C ₁₁ H ₂₁ NO ₂ +H]+,141.1154[M-C ₁₆ H ₂₇ O+H]+	↓

39	7.33	337.2356	337.2379	336.2301	ESI ⁺	C ₂₀ H ₃₂ O ₄	11H-14, 15-EETA	337.2356[M+H] ⁺ ,335.2222[M-H ₂ O+H] ⁺ ,309.2430[M-CO ₂ +H] ⁺ ,291.1960[M-C ₂ H ₆ O ₂ +H] ⁺ 300.2892[M+H] ⁺ ,282.2797[M-H ₂ O+H] ⁺ ,183.1623[M-C ₇ H ₁₇ O+H] ⁺ ,155.1310[M-C ₉ H ₂₁ O+H] ⁺ 277.2166[M-H] ⁻ ,259.2062[M-H ₂ O-H] ⁻ ,233.1542[M-C ₃ H ₈ -H] ⁻ ,189.1643[M-C ₄ H ₈ O ₂ -H] ⁻ 256.2641[M+H] ⁺ ,238.2297[M-H ₃ N+H] ⁺ ,167.1436[M-C ₅ H ₁₅ N+H] ⁺ ,116.1075[M-C ₁₀ H ₂₀ +H] ⁺ 282.2798[M+H] ⁺ ,265.2531[M-H ₃ N+H] ⁺ ,240.2327[M-C ₃ H ₆ +H] ⁺ ,114.1408[M-C ₁₀ H ₁₈ NO+H] ⁺ 279.2325[M-H] ⁻ ,261.2218[M-H ₂ O-H] ⁻ ,233.2269[M-CH ₂ O ₂ -H] ⁻ ,141.0916[M-C ₁₀ H ₁₈ -H] ⁻ 465.3033[M-H] ⁻ ,449.2726[M-CH ₄ -H] ⁻ ,381.2100[M-C ₆ H ₁₂ -H] ⁻ ,255.1749[M-C ₉ H ₂₂ O ₃ S-H] ⁻ 417.3398[M-H] ⁻ ,351.3052[M-CH ₆ O ₃ -H] ⁻ ,349.2895[M-CH ₈ O ₃ -H] ⁻ ,283.2062[M-C ₇ H ₁₈ O ₂ -H] ⁻ 393.2974[M+H] ⁺ ,329.2844[M-	↑
40	7.40	300.2892	300.2903	299.2824	ESI ⁺	C ₁₈ H ₃₇ NO ₂	Sphingosine		↓
41	7.47	277.2166	277.2168	278.2246	ESI ⁻	C ₁₈ H ₃₀ O ₂	Gamma-Linolenic acid		↓
42	7.74	256.2641	256.264	255.2562	ESI ⁺	C ₁₆ H ₃₃ NO	Palmitic amide		↓
43	7.92	282.2798	282.2797	281.2719	ESI ⁺	C ₁₈ H ₃₅ NO	Oleamide		↓
44	7.97	279.2325	279.2324	280.2402	ESI ⁻	C ₁₈ H ₃₂ O ₂	Linoleic acid		↓
45	8.69	465.3033	465.3039	466.3117	ESI ⁻	C ₂₇ H ₄₆ O ₄ S	Cholesterol sulfate		↑
46	9.10	417.3398	417.3369	418.3447	ESI ⁻	C ₂₇ H ₄₆ O ₃	17a, 20a-Dihydroxycholesterol		↑

48	10.9 4	864.6223	864.6235	863.6156	ESI ⁺	C ₄₆ H ₈₉ NO ₁₁ S	Sulfatide	CH ₄ O ₃ +H] ⁺ ,149.0966[M- C ₁₄ H ₂₈ O ₃ +H] ⁺ ,121.1017 [M- C ₁₅ H ₂₈ O ₄ +H] ⁺ 864.6223[M+H] ⁺ ,662.3938[M- C ₃ H ₈ O+H] ⁺ ,283.2147[M- C ₂₀ H ₃₉ O ₈ S+H] ⁺ ,171.0895[M- C ₂₈ H ₅₅ O ₈ S+H] ⁺	↑
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↑ or ↓ represents the level of compound in serum that was increased or decreased in the AD model group compared with the control group, respectively.