Electronic Supplementary Material (ESI) for Analyst.

Table S1 Potential biomarkers and related metabolic pathways between the atherosclerosis and control rats based on fecal metabolic profiling(ESI- mode)

No	t_R(min)	Mass	Metabolites	MS\MS	Related pathway	Level in ASG (FC)*	Level in DBZG (FC)#	Level in SVTG (FC)#
1	2.73	301.2987	Sphinganine[c]	282,268,253, 239,58	Sphingolipid metabolism	↑(10)		
2	3.25	188.1074	Nonanedioic acid[a]	169,143,125,97, 80,57	Fatty acid oxidation	↑(11)		
3	3.27	266.0527	UN			↑(14)	↓(9)	↓(13)
	3.28	181.0754	Tyrosine[b]	163,119,93,72	Tyrosine metabolism	↑(17)		
5	3.29	400.1063	UN			↑(14)	↓(8)	
6	3.64	188.1174	UN			↑(17)		
7	15.86	180.055	UN			↑(14)	↓(14)	↓(14)
8	15.69	204.0914	L-tryptophan[b]	142,116,74	Tryptophan metabolism	↑(18)		
9	15.79	430.1653	Gln Gln Arg[c]			↑(15)		
10	16.04	186.0475	UN			↑(3)		
11	16.08	228.1491	3,5-Dinitrosalicylic acid[a]	183,113,69		↑(9)		
12	16.38	161.0486	UN			↑(18)	↓(10)	
13	16.27	270.1601	UN			↑(15)	↓(15)	

14	16.40	306.1695	UN			↑(14)	↓(13)	↓(14)
15	16.84	287.1865	UN			↑(16)	↓(8)	
16	17.43	170.05	UN	58		↑(3)	↓(3)	
17	17.53	196.0749	Homoveratric acid[a]	151,136,121,93,65,41		↑(15)	↓(15)	↓(12)
18	17.59	122.0371	4-hydroxybenzaldehyde[a]	92,65,41	Phenylpropanoids	↑(11)	↓(8)	
19	17.97	439.1348	UN			↑(14)	↓(11)	
20	18.21	196.0749	UN			↑(15)	↓(5)	↓(14)
21	18.62	249.103	UN			↑(6)	↓(4)	
22	18.66	230.1537	Dodecanedioic acid[a]	211,185,167,139	Fatty acid oxidation	↑(12)	↓(3)	
23	19.28	314.1181	UN			↑(10)	↓(9)	
24	19.28	350.095	UN			↑(12)	↓(9)	
25	19.29	145.0533	Indole-3-carboxyaldehyde[a]	126,115,66		↑(12)	↓(7)	
26	19.42	382.201	UN			↑(15)	↓(10)	↓(13)
27	19.78	425.3518	Elaidic carnitine[c]		Fatty acid oxidation	↓(14)	↓(13)	
28	20.76	174.0877	Suberic acid[a]	111,83,67,57,41	Fatty acid oxidation	↑(19)	↓(14)	↓(17)
29	21.45	298.1233	Enterolactone[a]	253,189,165,145,133,121,107,79	mammalian phytoestrogens	↑(18)	↓(10)	
30	21.61	254.227	UN			↑(15)	↓(12)	
31	22.07	202.1227	Sebacic acid[a]	183,139,111,57	Fatty acid oxidation	↑(9)	↓(7)	
32	22.96	408.2899	1α,3α,7α-					

			Trihydroxy-5β-cholan-24-oic Acid[c]					
33	23.06	212.1429	7-Oxo-11-dodecenoic acid[c]	193,169,113,97, 57,41		↑(15)		
34	24.89	460.2602	Lys TrpLys[c]			↑(12)		
35	26.37	346.2185	21-Deoxycortisol[c]	327,309,267,173,145,119,95,41		↓(14)		
36	27.01	302.1517	Enterodiol[a]	283,271,253,241,146,133,106	mammalian phytoestrogens	↑(5)	↓(3)	
37	27.36	258.0899	3',4',7-Trihydroxy-Isoflavan[c]			↑(13)		
38	27.39	406.274	3-Oxocholic acid[c]		Bile acidsbiosynthesis	↑(14)	↓(5)	↓(13)
39	27.52	490.3278	UN			↑(13)	↓(13)	↓(12)
40	27.84	454.2962	UN			↑(15)	↓(12)	↑(14)
41	29.06	449.3148	Glycoursodeoxycholic acid[c]		Bile acidsbiosynthesis	↑(14)	↓(12)	
42	29.52	158.1315	UN			↑(12)	↓(10)	
43	30.18	408.29	Cholic acid[b]	343,289,251,95, 69,43	Bile acids biosynthesis	↑(15)	↓(12)	
44	30.28	444.2646	3-(O-Geranylgeranyl)-sn-glycerol 1-phosphate[c]		Glycerophospholipid metabolism	↑(15)	↓(12)	↓(14)
45	30.38	312.2326	9(S)-HPODE[a]	293,197,183, 125, 79,58	Linoleic acid metabolism	↑(13)	↓(11)	
46	30.58	392.2951	Deoxycholic acid[c]	373,355,345,	Bile acids	↑(15)	↓(10)	

				327,311,69	biosynthesis			
47	31.01	312.233	13(S)-HPODE[a]	293,275,249, 223,205,195,183,167,139,113	Linoleic acid metabolism	↑(13)	↓(11)	
48	31.30	314.2485	12,13-DiHOME [a]	295,277,195, 183,129,99,58	Linoleic acid metabolism	↑(13)	↓(10)	
49	31.25	802.5411	PA(19:0/22:4(7Z,10Z,13Z,16Z))[c]		Glycerophospholipid metabolism	↑(13)	↓(7)	↑(13)
50	31.58	822.5411	PG(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[c]		Glycerophospholipid metabolism	↑(15)	↓(13)	
51	31.71	390.2796	7-Oxolithocholic acid[c]		Bile acids biosynthesis	↑(4)	↓(3)	
52	32.09	460.2827	Trp Lys Lys[c]			↑(14)		
53	32.10	392.2957	Hyodeoxycholic Acid[c]	373,283,266, 134,45	Bile acids biosynthesis	↑(13)	↓(3)	
54	32.89	391.2855	UN			↑(17)	↓(14)	↓(16)
55	34.21	806.5724	PA(19:0/22:2(13Z,16Z))[c]		Glycerophospholipid metabolism	↑(15)	↓(9)	↑(14)

a Identified tentatively by comparing accurate molecular weights, the fragment ions in conjunction with the metabolomics databases.

b Identified based on retention time and MS^n spectrum of an authentic standard.

[C] Identified by comparing the extract mass as described in the literatures for atherosclerosis using LC-MS metabolomics as well.

* Compared to HCG

Compared to SVG

UN: unknown.

(↓) down-regulated and (↑) up-regulated.