

Table S1. Identified metabolites in rats plasma

NO	Retention time	Metabolites	Level of identification	metabolic pathway
1	9.923	Cyclopentanecarboxylic acid	Monocarboxylic acids	energy metabolism
2	10.394	Propanedioic acid	Di-carboxylic acids	energy metabolism
3	10.512	Lactic acid	Monocarboxylic acids	energy metabolism
4	10.655	Alanine	Amino acids and derivatives	Amino acid
5	10.718	3-hydroxybutyrate	Hydroxyl acids	energy metabolism
6	11.105	Cystathionine	Amino acids and derivatives	Amino acid
7	11.356	5-hydroxybutyrate	Hydroxyl acids	energy metabolism
8	11.492	4-Hydroxycyclohexylacetic acid	Hydroxyl acids	energy metabolism
9	11.481	L-Valine	Amino acids and derivatives	Amino acid
10	11.744	Glycine	Amino acids and derivatives	Amino acid
11	12.318	Ethanedioic acid	Monocarboxylic acids	Energy
12	12.401	Butanoic acid	Monocarboxylic acids	Energy
13	12.464	Ethanamine	Other N-compounds	Carbohydrate
14	12.559	4-Hexenoic acid	Di-carboxylic acids	Energy
15	13.206	Benzoic acid	Monocarboxylic acids	Energy
16	13.29	d-(+)-Glyceric acid	Hydroxyl acids	Carbohydrate
17	13.374	leucine	Amino acids and derivatives	Amino acid
18	13.426	4-Hydroxybutyric acid	Hydroxyl acids	Carbon metabolism
19	13.499	Gluconic acid	Carbohydrates and derivatives	Carbohydrate
20	13.522	Hexanoic acid	Monocarboxylic acids	Energy
21	14.116	Propanedioic acid	Monocarboxylic acids	Energy
22	14.168	Isobutyric acid	Monocarboxylic acids	Energy
23	14.263	Aspartic acid	Amino acids and derivatives	Amino acid
24	14.388	Methionine	Amino acids and derivatives	Amino acid
25	14.430	1H-Indole-2,3-dione	-	-
26	14.775	D-Erythro-Pentonic acid	Carbohydrates and derivatives	Carbohydrate
27	14.869	2-Oxiranecarboxylic acid	Monocarboxylic acids	Carbohydrate
28	14.956	1,3 Propanediol	Polyols	Carbohydrate
29	15.110	1,3-Octanediol	Polyols	Carbohydrate
30	15.423	5-O-Methyl-d-gluconic acid dimethylamide	Carbohydrates and derivatives	Carbohydrate
31	15.497	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrate
32	16.072	Cyclohexanecarboxylic acid	Monocarboxylic acids	Energy
33	16.124	Methoxyacetic acid	Monocarboxylic acids	Energy
34	16.438	glycylglycine	Amino acids and derivatives	Amino acid
35	16.845	Glycylvaline	Amino acids and derivatives	Amino acid
36	17.201	Urea	Other N-compounds	Amino acid
37	17.358	D-Ribonic acid	Carbohydrates and	Carbohydrate

			derivatives	
38	17.421	Methy6-O-1-methylpropyl- α -d-galactopyranoside	Carbohydrates and derivatives	Carbohydrate
39	17.630	2-Aminobutyric acid	Other N-compounds	Energy
40	17.975	Methoxyacetic acid	Monocarboxylic acids	Energy
41	18.424	Internal standard docosanoic	-	-
42	19.031	α -D-Glucopyranoside	Carbohydrates and derivatives	Carbohydrate
43	19.805	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid	Hydroxyl acids	Energy
44	21.241	Methoxyacetic acid, 4-tetradecyl ester	Fatty acid methyl ester	lipid
45	21.341	α -N-Acetyl neuraminic acid	Carbohydrates and derivatives	Carbohydrate
46	21.980	α -DL-Lyxopyranose	Carbohydrates and derivatives	Carbohydrate
47	23.611	α -D-Glucopyranoside	Carbohydrates and derivatives	Carbohydrate
48	24.165	α -DL-Arabinopyranose	Carbohydrates and derivatives	Carbohydrate
49	24.249	Tetradecanoic acid	Long chain monocarboxylic acids	Lipid
50	24.312	D-Mannitol	Carbohydrates and derivatives	Carbohydrate
51	24.594	D-glucose	Carbohydrates and derivatives	Carbohydrate
52	24.709	α -D-Glucopyranoside, methyl	Carbohydrates and derivatives	Carbohydrate
53	24.793	N-Acetyl glucosamine	Carbohydrates and derivatives	Carbohydrate
54	25.086	Glucitol	Carbohydrates and derivatives	Carbohydrate
55	25.363	Arabinitol	Carbohydrates and derivatives	Carbohydrate
56	26.068	linoleic acid	Fatty acid methyl ester	Lipid
57	27.773	9,12-(Z,Z)-Octadecadienoic acid	Long chain monocarboxylic acids	Lipid
58	27.919	Hexadecanoic acid,	Long chain monocarboxylic acids	Lipid
59	28.223	(E)-9- Hexadecenoic acid	Long chain monocarboxylic acids	Lipid
60	28.693	scyllo-inositol	Polyols	Lipid (Inositol metabolism)
61	29.979	(9E)-9-octadecenoate	Fatty acid methyl ester	Lipid
62	30.575	2-Dodecenedioic acid	Long chain monocarboxylic acids	Lipid

63	31.799	11-cis-Octadecenoic acid	Long chain monocarboxylic acids	Lipid
64	31.956	9,12-Octadecadienoic acid (Z,Z)-	Long chain monocarboxylic acids	Lipid
65	32.060	Hexadecanoic acid	Long chain monocarboxylic acids	Lipid
66	33.688	9,12,15-Octadecatrienoic acid	Long chain monocarboxylic acids	Lipid
67	33.134	oleic acid	Long chain monocarboxylic acids	Lipid
68	34.894	arachidonate	Fatty acid methyl ester	Lipid
69	36.870	3-Hydroxyspirost-8-en-11-one	Sterols	Lipid
70	39.209	Docosahexaenoic Acid	Long chain monocarboxylic acids	Lipid
71	40.269	9-Octadecenoic acid (Z)-, methyl ester	Long chain monocarboxylic acids	Lipid
72	42.230	Cholesterol	Sterols	Lipid (Sterol/Steroid)

Table S2 Identified metabolites in liver tissue homogenate

NO	Retention time	Metabolites	Level of identification	metabolic pathway
1	9.805	Cyclopentanecarboxylic acid	Monocarboxylic acids	Energy
2	10.352	leucine	Amino acids and derivatives	Amino acids
3	10.456	isoleucine	Amino acids and derivatives	Amino acids
4	10.508	Alanine	Amino acids and derivatives	Amino acids
5	10.624	lactic acid	Di-carboxylic acids	Energy
6	11.063	Cystathionine	Amino acids and derivatives	Amino acids
7	11.46	d-(+)-Glyceric acid	Hydroxyl acids	Energy
8	11.523	Propanoic acid	Monocarboxylic acids	Energy
9	12.304	Hexanoic acid	Monocarboxylic acids	Energy
10	12.476	Ethanedioic acid	Monocarboxylic acids	Energy
11	12.757	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrate
12	13.2	Propanoic acid	Monocarboxylic acids	Energy
13	13.416	Benzenepropanoic acid	Monocarboxylic acids	Energy
14	13.520	Threonic acid	Carbohydrates and derivatives	Carbohydrate
15	14.021	Glycine	Amino acids and derivatives	Amino acids
16	14.095	2-Hydroxybutyric acid	Hydroxyl acids	Energy
17	14.252	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrate
18	14.419	5-O-Methyl-d-gluconic acid	Carbohydrates and derivatives	Carbohydrate
19	14.764	2H-Oxireno[3,4]cyclopenta[1,2-c]furan-2-one	unknow	unknow
20	14.859	d-(+)-Glyceric acid	Glyceric acid	Lipid
21	14.953	1,2,4-Butanetriol	Polyols	Lipid
22	15.099	2-Oxiranecarboxylic acid	Monocarboxylic acids	Lipid

23	15.350	Cystathionine	Amino acids and derivatives	Amino acids and derivatives
24	15.413	Glycerol	Polyols	Lipid
25	15.486	2,2-Dimethyl-1-pentamethyldisilanyloxypropane	-	-
26	15.580	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrates
27	15.810	d-(+)-Glyceric acid	Monocarboxylic acids	Carbohydrates
28	16.072	1,3-Octanediol	Polyols	Carbohydrates
29	16.113	Cyclopentene	alkyls	-
30	16.208	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrates
31	16.400	2-Ethyl-3-hydroxypropionic acid	Hydroxyl acids	Energy
30	16.845	Adipic acid	Di-carboxylic acids	Energy
31	16.615	Proline	Amino acids and derivatives	Amino acids
32	16.730	1,3 Propanediol	Polyols	Carbohydrate
33	16.887	Adipic acid	Di-carboxylic acids	Carbohydrate
34	17.138	serine	Amino acids and derivatives	Amino acids
35	17.264	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrates
36	17.431	Benzeneacetic acid	Monocarboxylic acids	Energy
37	17.964	1-Tetradecanol	Long chain alcohols	Lipid
38	17.431	Benzeneacetic acid	Monocarboxylic acids	Energy
39	17.964	1-Tetradecanol	Long chain alcohols	Lipid
40	18.06	Arabinitol	Carbohydrates and derivatives	Carbohydrates
41	18.187	α -N-Acetylneuraminic acid	Carbohydrates and derivatives	Carbohydrates
42	18.356	Glutamic acid	Amino acids and derivatives	Amino acids
43	18.435	internal standard	-	-
44	18.487	1-Propanol	alcohol	Carbohydrate
45	19.100	Butanedioic acid	Carbohydrates and derivatives	Carbohydrate
46	19.309	α -D-Galactopyranoside	Di-carboxylic acids	Carbohydrate
47	19.731	Cyclohexanecarboxylic acid	Monocarboxylic acids	Monocarboxylic acids
48	19.745	Malic acid	Di-carboxylic acids	Energy
49	19.904	Erythro-Pentitol	Carbohydrates and derivatives	Carbohydrate
50	20.28	1-Pentadecanol	Long chain alcohols	Lipid
51	21.331	N-Acetyl glucosamine	Carbohydrates and derivatives	Carbohydrate
52	21.908	Ribonic acid	Carbohydrates and derivatives	Carbohydrate
53	24.144	2-Keto-l-gluconic acid	Carbohydrates and derivatives	Carbohydrate
54	24.552	D-Glucose	Carbohydrates and derivatives	Carbohydrate
55	24.78	mannose	Carbohydrates and derivatives	Carbohydrate
56	25.085	Galactose	Carbohydrates and derivatives	Carbohydrate
57	25.451	α -D-Glucopyranoside	Carbohydrates and derivatives	Carbohydrate
58	25.7	Glucopyranose	Carbohydrates and derivatives	Carbohydrate
59	26.079	α -N-Acetylneuraminic acid,	Carbohydrates and derivatives	Carbohydrate
60	27.909	Hexadecanoic acid	Fatty acid methyl ester	Lipid
61	28.672	Inositol	Polyols	Lipid
60	29.21	1-Monolinoleoylglycerol	Fatty acid methyl ester	Lipid

61	29.488	9,12,15-Octadecatrienoic acid	Long chain monocarboxylic acids	Lipid
62	29.979	(9Z,12Z)-9,12-Octadecadienoic acid	Long chain monocarboxylic acids	Lipid
63	30.010	(E)-9-Octadecenoic acid	Long chain monocarboxylic acids	Lipid
64	31.841	oleic acid	Long chain monocarboxylic acids	Lipid
65	32.01	Octadecanoic acid	Long chain monocarboxylic acids	Lipid
66	34.120	9,12-Octadecadienoic acid, methyl ester	Fatty acid methyl ester	Lipid
67	39.104	Unknown	-	-
68	39.200	Methyl (9E,12E,15E)-9,12,15-octadecatrienoate	Fatty acid methyl ester	Lipid
69	40.209	arachidonate	Long chain monocarboxylic acids	Lipid
70	42.230	Cholesterol	Sterols	Lipid

Table S3 Identified metabolites in rats lung

NO	Retention time	Metabolites	Level of identification	metabolic pathway
1	9.703	Lactic acid	Monocarboxylic acids	Energy
2	10.226	L-Alanine	Amino acids and derivatives	Amino acids
3	10.519	1,2,4-Butanetriol	Polyols	Krebs cycle
4	11.073	3-Hydroxybutyric acid	Hydroxyl acids	Energy
5	11.345	d-(+)-Glyceric acid	Carbohydrates and derivatives	Carbohydrate
6	11.723	Pentanoic acid	Monocarboxylic acids	Energy
7	12.359	Ethanedioic acid	Monocarboxylic acids	Energy
8	12.598	Hexanoic acid	Monocarboxylic acids	Energy
9	13.196	Propanoic acid	Monocarboxylic acids	Energy
10	13.604	Benzenepropanoic acid	Monocarboxylic acids	Energy
11	14.085	Cystathionine	Amino acids and derivatives	Amino acids
12	14.116	4-Methyl- pentanoic acid	Monocarboxylic acids	Energy
13	14.179	D-Valine	Amino acids and derivatives	Amino acids
14	14.869	2-Methylsuccinic acid	Di-carboxylic acids	Energy
15	15.047	5-O-Methyl-d-gluconic acid	Carbohydrates and derivatives	Carbohydrates
16	15.110	l-Felinine	Amino acids and derivatives	Amino acid
17	15.360	Cystathionine	Amino acids and derivatives	Amino acid
18	15.434	Glycerol	Polyols	Carbohydrate
19	15.591	Malonic acid	Di-carboxylic acids	Energy
20	15.801	2-Methylsuccinic acid	Di-carboxylic acids	Krebs cycle
21	15.957	Glutaric acid	Di-carboxylic acids	Energy
22	16.072	Trans-trans-Muconic acid	Di-carboxylic acids	Energy
23	16.124	Cyclopentene	alkyls	Energy
24	16.218	2-Ethyl-3-hydroxypropionic acid	Hydroxyl acids	Energy

25	16.438	Glycerol- 3-phosphate	Polyols	Carbohydrate
26	16.626	Proline	Amino acids and derivatives	Amino acid
27	16.845	Adipic acid	Di-carboxylic acids	Energy
28	16.943	serine	Amino acids and derivatives	Amino acid
29	17.432	Butanedioic acid	Di-carboxylic acids	Energy
30	17.734	malic acid	Di-carboxylic acids	Energy
31	17.975	Benzeneacetic acid	Di-carboxylic acids	Energy
32	18.320	Glutamic acid	Amino acids and derivatives	Amino acid
33	18.435	Internal standard docosanoic	-	-
34	18.487	α -D-Glucopyranoside	Carbohydrates and derivatives	Carbohydrate
35	19.034	α -D-Galactopyranoside	Carbohydrates and derivatives	Carbohydrate
36	19.261	Butanedioic acid	Di-carboxylic acids	Energy
37	19.731	Malic acid	Di-carboxylic acids	Energy
38	21.007	5-Hydroxyhexanoic acid	Hydroxyl acids	Energy
39	21.167	Hexanedioic acid	Di-carboxylic acids	Energy
40	21.321	α -D-Galactopyranose	Carbohydrates and derivatives	Carbohydrate
41	21.934	Ribonic acid	Carbohydrates and derivatives	Carbohydrate
42	22.643	Ribitol	Carbohydrates and derivatives	Carbohydrate
43	23.678	D-Ribo-Hexitol	Carbohydrates and derivatives	Carbohydrate
44	23.987	4- hydroxyBenzene propanoic acid	Hydroxyl acids	Energy
45	24.167	2-Keto-l-gluconic acid	Carbohydrates and derivatives	Carbohydrate
46	24.268	D-Mannitol	Carbohydrates and derivatives	Carbohydrate
47	24.587	glucose	Carbohydrates and derivatives	Carbohydrate
48	24.769	mannose	Carbohydrates and derivatives	Carbohydrate
49	25.096	Galactose	Carbohydrates and derivatives	Carbohydrate
50	25.267	Galactaric acid	Carbohydrates and derivatives	Carbohydrate
51	25.472	linoleic acid	Fatty acid ester	Lipid
52	26.068	Tetradecanoic acid	Long chain monocarboxylic acids	Lipid
53	26.905	1-Octadecanol	Long chain alcohols	Lipid
54	27.104	Unkonw	-	-
55	27.804	(9E)-9-octadecenoate	Fatty acid ester	Lipid
56	28.703	Hexadecanoic acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
57	29.854	(9Z,12Z)-9,12-Octadecadienoic acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
58	30.011	(E)-9-Octadecenoic acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
59	30.747	9,12,15-Octadecatrienoic acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
60	31.803	oleic acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
61	32.07	11-cis-Octadecenoic acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
62	39.104	Unknown	-	-

63	39.234	Docosahexaenoic Acid	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
64	39.502	Methyl cis-9-octadecenoate	Fatty acid ester	Lipid
65	40.215	arachidonate	Long chain monocarboxylic acids	Lipid (Long chain fatty acid)
66	42.109	Cholesterol t	Sterols	Lipid (Sterol/Steroid)

Table S4. Pathways associated with the inflammation 201 FDR features at (q=0.05) identified using the MetScape plugin in Cytoscape

Arachidonic acid metabolism

Bile acid biosynthesis

Butanoate metabolism

De novo fatty acid biosynthesis

Di-unsaturated fatty acid beta-oxidation

Fructose and mannose metabolism

Galactose metabolism

Glycerophospholipid metabolism

Glycine, serine, alanine and threonine metabolism

Glycolysis and Gluconeogenesis

Glycosphingolipid metabolism

Histidine metabolism

Leukotriene metabolism

Linoleate metabolism

Lysine metabolism

Omega-3 fatty acid metabolism

Omega-6 fatty acid metabolism

Pentose phosphate pathway

Phosphatidylinositol phosphate metabolism

Phytanic acid peroxisomal oxidation

Porphyrin metabolism

Propanoate metabolism

Prostaglandin formation from arachidonate

Purine metabolism

Saturated fatty acids beta-oxidation

TCA cycle

Urea cycle and metabolism of arginine, proline, glutamate, aspartate and asparagine

Valine, leucine and isoleucine degradation

Vitamin B9 (folate) metabolism