

Supplementary information

Impact of *Lycium barbarum* arabinogalactan on the fecal metabolome in a DSS-induced chronic colitis mouse model

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Figure S2 Permutation test of OPLS-DA model showing the stability of the model. (A) Permutation test of Normal vs DSS in positive model; (B) Permutation test of ASA vs DSS in positive model; (C) Permutation test of LBP-3 vs DSS in positive model; (D) Permutation test of Normal vs DSS in negative model; (E) Permutation test of ASA vs DSS in negative model; (F) Permutation test of LBP-3 vs DSS in negative model.

Figure S3 The roadmap for key metabolites and relevant intestinal species to validate their functions;
FMT, fecal microbiota transplants; AAs, amino acids; OAs, organic acids.

Table S1 HPLC-MS mobile phases for untargeted metabolomics

Time (min)	A (%)	B (%)
0	100	0
5	80	20
7	80	20
14	0	100
16	100	0
21	100	0

For positive mode, mobile phase A: 0.1% formic acid in ultrapure water, and mobile phase B: acetonitrile. For negative mode, mobile phase A: 5% ammonium acetate and 5% acetonitrile in ultrapure water, and mobile phase B: acetonitrile.

Table S2 MS parameters for untargeted metabolomics

Parameters	Setting
Ionization method	Electrospray
Ionization mode	Positive and negative
Scan type	TOF-MS
Mass range	60-1200 Da
IonSpray Voltage Floating	5500 V
Temperature	500°C
Ion Source Gas 1	50 psi
Ion Source Gas 2	50 psi
Duration	21 min
Accumulation time	0.199932 secs
Curtain Gas	35.0 psi
Declustering Potential	± 80 V
Resolution mode	High resolution
Collision Energie	± 35 V
Collision Energie Spread	15
Ion Release Delay	30
Ion Release Width	15
Data collection	IDA-MS

Table S3 HPLC-MS mobile phases for targeted metabolomics

Time (min)	A (%)	B (%)
0	15	85
3	70	30
12	98	2
15	98	2
16	15	85
25	15	85

Mobile phase A: 5% acetonitrile in 20 mM ammonium acetate buffer (pH 9.0), mobile phase B:
acetonitrile

Table S4 MS parameters for amino acids, organic acids and others

Parameters	Setting
Ionization method	Electrospray
Ionization mode	Positive and negative
Scan type	MRM
Duration	25 min
Curtain Gas	20.0 psi
Collision Gas	High (0.5 amu FWHH)
IonSpray Voltage	± 4500 V
Temperature	500°C
Ion Source Gas 1	40 psi
Ion Source Gas 2	50 psi
Interface Heater	On

Table S5 A list of MRM transitions for metabolites and their corresponding internal standards along with collision energy values

No.	Analyte	Q1 (m/z)	Q3 (m/z)	DP (V)	CE (V)
1	1-Methyladenosine	282.12	150.08	93	27
2	1-Methyl-Histidine	170.09	96.07	93	20
3	2-Aminooctanoic acid	160.00	55.30	93	21
4	2-Methylnicotinamide	137.07	94.07	93	27
5	4-Aminobutyrate	104.01	69.00	93	22
6	5'-Methylthioadenosine	298.10	136.06	93	29
7	7,8-Dihydrofolate	444.20	178.00	93	32
8	7-Methylguanosine	298.11	177.03	93	24
9	Acetoacetic acid	103.04	95.05	93	20
10	L-Acetylcarnitine	203.15	144.10	93	27
11	Acetyl-CoA	808.12	184.07	93	53
12	Acetyllysine	189.00	84.00	93	23
13	Acetylphosphate	141.00	123.06	93	24
14	Adenine	136.00	119.00	93	26
15	Adenosine	268.15	136.10	93	29
16	Aminoimidazole carboxamide ribonucleotide	339.00	110.00	93	32
17	AMP	348.15	136.00	93	23
18	Arginine	175.12	116.07	93	20
19	Argininosuccinic acid	291.13	84.08	93	37
20	Asparagine	133.06	74.02	93	20
21	Betaine	118.09	58.07	93	21
22	Betaine aldehyde	102.00	58.00	93	21
23	Carnitine	162.10	103.00	93	20
24	Choline	104.07	58.07	93	20
25	Citrulline	176.10	159.08	93	20
26	Creatine	132.08	90.06	93	20
27	Creatinine	114.07	86.07	93	20
28	Cysteine	122.03	76.06	93	20
29	Cytidinemono phosphate	324.05	112.05	93	20

30	Cytosine	112.05	70.07	93	20
31	Deoxyadenosine	252.00	136.00	93	22
32	Deoxyribose1-phosphate	215.03	72.08	93	25
33	Diiodothyronine	525.50	352.80	93	31
34	Dimethylglycine	104.11	60.08	93	21
35	D/L-Pipecolic acid	130.00	84.00	93	18
36	D-Ribulose5-phosphate	231.03	100.08	93	20
37	FAD	786.16	439.10	93	26
38	Folate	442.15	295.09	93	30
39	Glucosamine	180.00	162.00	93	12
40	Glucosamine6-phosphate	260.05	144.10	93	20
41	Glutamine	147.08	130.05	93	20
42	Glycerophosphocholine	258.10	104.00	93	16
43	Glycine	76.04	58.07	93	20
44	Guanine	152.06	135.03	93	20
45	Guanosine	284.10	152.06	93	35
46	Guanosinemono phosphate	364.07	152.06	93	21
47	Guanosinetriphosphate	524.00	184.07	93	25
48	Histidine	156.08	110.07	93	20
49	Histidinol	142.10	124.06	93	20
50	Homocysteine	136.12	90.10	93	17
51	Homoserine	120.07	103.05	93	32
52	Hydroxyproline	132.07	68.05	93	20
53	Indole	118.07	91.05	93	20
54	Isoleucine	132.10	86.10	93	20
55	Kynurenine	209.09	94.07	93	25
56	L-arginino-succinate	291.00	70.00	93	37
57	L-Carnitine	162.11	103.04	93	20
58	Leucine	132.10	86.10	93	20
59	L-methionine	150.06	104.05	93	20
60	Lysine	147.11	130.05	93	32
61	Methionine sulfoxide	166.00	74.00	93	14
62	Methylcysteine	136.04	119.05	93	20

63	Methylnicotinamide	137.00	94.00	93	20
64	N6-Acetyl-L-lysine	189.12	126.09	93	20
65	N-acetyl-glucosamine	222.00	138.00	93	18
66	N-acetyl-glutamate	190.07	130.05	93	20
67	N-acetyl-L-ornithine	175.00	115.10	93	16
68	N-acetylornithine	175.11	116.07	93	20
69	N-Acetylputrescine	131.11	114.09	93	20
70	NAD ⁺	664.10	428.00	93	32
71	NADH	664.12	136.06	93	53
72	N-carbamoyl-L-aspartate	177.05	74.00	93	19
73	Ng,NG-dimethyl-L-arginine	203.15	116.07	93	24
74	Nicotinamide	123.06	80.05	93	22
75	Ornithine	133.10	70.07	93	20
76	Phenylalanine	166.09	120.08	93	30
77	Proline	116.07	70.07	93	20
78	Propionyl-CoA	824.15	184.07	93	33
79	Purine	121.05	94.07	93	35
80	Pyridoxine	170.08	152.07	93	24
81	Ribose-5-phosphate	231.03	116.07	93	20
82	Serine	106.05	60.05	93	20
83	S-methyl-5-thioadenosine	298.00	136.00	93	29
84	Spermidine	146.17	87.04	93	20
85	Taurodeoxycholic acid	500.30	59.05	93	32
86	Thiamine	265.11	122.07	93	20
87	Tryptophan	205.10	146.06	93	20
88	Tyrosine	182.08	136.08	93	39
89	UMP	325.00	97.00	93	14
90	Uracil	113.04	70.07	93	22
91	Urea	61.04	61.04	93	21
92	Valine	118.09	72.08	93	20
93	DL-Glutamic-2,4,4- <i>d3</i> acid	151.15	107.00	93	17
94	Fructose-6-phosphate	259.03	169.00	-93	-16
95	Fucose1-phosphate	243.03	96.97	-93	-32

96	Glucose-1-phosphate	259.02	241.01	-93	-20
97	(S)-2-Hydroxyglutarate	147.03	103.06	-93	-20
98	2,3-Diphospho glyceric acid	264.95	78.96	-93	-20
99	2-Dehydro-D-gluconate	193.00	103.00	-93	-14
100	2-Hydroxy-2-methylbutanedioic acid	147.00	85.10	-93	-17
101	2-Isopropylmalic acid	175.00	115.00	-93	-19
102	2-Keto-hexanoic acid	129.06	84.94	-93	-20
103	2-Keto-isovalerate	115.05	71.05	-93	-13
104	2-Oxo-4-methylthiobutanoate	147.01	103.06	-93	-20
105	2-Phenyl-propionate	149.06	105.07	-93	-21
106	3-Methyl-phenylacetic acid	149.00	105.00	-93	-12
107	4-Hydroxy-phenyl-pyruvate	179.03	87.01	-93	-20
108	4-Pyridoxic acid	182.00	138.00	-93	-18
109	5-Phosphoribosyl-1-pyrophosphate	389.00	291.00	-93	-20
110	6-Phosphonoglucono-D-lactone	257.01	195.17	-93	-20
111	Acetoacetate	101.05	57.20	-93	-14
112	Aconitate	173.05	85.00	-93	-17
113	α -Ketoglutarate	145.00	101.00	-93	-13
114	Aminoadipic acid	160.00	116.00	-93	-18
115	Anthranilate	136.00	92.00	-93	-18
116	Ascorbic acid	175.00	87.00	-93	-19
117	Atrolactic acid	165.00	119.00	-93	-21
118	Carbamoyl phosphate	140.00	79.00	-93	-24
119	Cholesteryl sulfate	465.30	96.96	-93	-22
120	Cholic acid	407.20	345.20	-93	-32
121	Citraconic acid	129.00	85.10	-93	-13
122	Deoxycholic acid	391.20	345.20	-93	-36
123	D-Glucarate	209.03	165.02	-93	-20
124	D-Gluconate	195.00	129.00	-93	-17
125	D-Glucose 6-phosphate	259.02	96.97	-93	-20
126	D-Glucuronic acid	193.04	113.02	-93	-20
127	D-Glyceraldehyde-3-phosphate	169.05	97.00	-93	-14
128	Dihydroorotate	157.00	113.00	-93	-14

129	Gluconic acid	195.05	75.01	-93	-20
130	Guanidoacetic acid	116.00	74.30	-93	-15
131	Hydroxyisocaproic acid	131.01	85.10	-93	-16
132	Hydroxyphenylaceticacid	151.04	107.05	-93	-26
133	Hypoxanthine	135.03	92.02	-93	-20
134	Indole-3-carboxylic acid	160.00	116.00	-93	-20
135	Indole-acrylic acid	186.00	142.03	-93	-20
136	Inosine	267.07	135.03	-93	-27
137	Kynurenic acid	188.00	144.00	-93	-21
138	Lactate	89.00	43.20	-93	-16
139	L-Dihydroorotic acid	157.03	113.03	-93	-20
140	Maleic acid	115.03	71.03	-93	-13
141	Methylmalonic acid	117.00	73.10	-93	-13
142	Myo-inositol	179.06	87.01	-93	-20
143	Orotic acid	155.01	111.02	-93	-20
144	Orotidine-5-phosphate	367.00	323.00	-93	-18
145	Oxalacetic acid	131.00	87.04	-93	-20
146	Oxaloacetate	131.00	87.00	-93	-14
147	Oxoglutaric acid	145.01	101.02	-93	-20
148	p-Aminobenzoate	136.05	92.00	-93	-18
149	p-Aminobenzoic acid	136.04	92.02	-93	-20
150	Pantothenate	218.10	88.04	-93	-21
151	Phenyl-lactic acid	165.01	103.10	-93	-21
152	Phenyl-propionic acid	145.00	101.00	-93	-18
153	Phosphoenolpyruvic acid	166.01	122.09	-93	-20
154	p-Hydroxybenzoate	137.00	93.00	-93	-23
155	p-Salicylicacid	179.07	93.03	-93	-23
156	Pyroglutamic acid	128.00	82.10	-93	-19
157	Quinolinic acid	165.06	73.00	-93	-24
158	Sedoheptulose7-phosphate	289.03	96.97	-93	-27
159	Shikimate	173.05	93.03	-93	-20
160	S-ribosyl-L-homocysteine_neg	266.00	134.00	-93	-20
161	Succinate	117.02	73.03	-93	-20

162	Trans-Aconiticacid	173.01	85.03	-93	-20
163	Trehalose	341.11	142.97	-93	-20
164	Trehalose-sucrose	341.00	179.00	-93	-20
165	Uric acid	167.00	124.00	-93	-17
166	Uridine	243.06	110.02	-93	-21
167	Xanthine	151.03	108.02	-93	-23
168	Xanthosine	283.07	151.02	-93	-24
169	Xanthurenic acid	204.00	160.00	-93	-19
170	Allantoin	157.04	97.00	-93	-20
171	Taurine	124.01	79.96	-93	-20
172	Taurodeoxycholic acid	498.20	124.00	-93	-53
173	Taurocholic acid	514.28	124.01	-93	-80
174	Taurocholic acid-3-sulfate	594.24	96.96	-93	-30
175	Taurochenodeoxycholic acid	498.29	106.98	-93	-72
176	Taurohyocholic acid	514.28	106.98	-93	-80
177	Taurolithocholic acid	482.29	79.96	-93	-80
178	Tauro- β -muricholic acid	514.28	79.96	-93	-80
179	Glycolcholic acid-3-sulfate	544.26	74.02	-93	-40
180	Glycohyocholic acid	464.30	74.02	-93	-50
181	Glycolithocholic acid	432.31	74.02	-93	-50
182	Lithocholic acid	375.29	375.29	-93	-16
183	Lithocholic acid-3-sulfate	455.25	96.96	-93	-40
184	Hyocholic acid	407.28	407.28	-93	-10
185	Hyodeoxycholic acid	391.29	391.29	-93	-15
186	Tauroursodeoxycholic acid-3-sulfate	578.25	96.96	-93	-40
187	Hendecanoic acid	185.29	185.29	-93	-10
188	Nonadecanoic acid	297.50	297.50	-93	-10

Table S6 Information of differential metabolites between Normal group and DSS group

No.	Metabolites	Formula	VIP	Normal vs DSS	Mode
1	PAF (Platelet activating factor)	C26H54NO7P	2.722	↓(**)	+
2	Questin_120240	C16H12O5	1.928	↓(**)	+
3	<i>p</i> -Coumaric acid	C9H8O3	1.905	↓(**)	+
4	Lysophosphatidylcholine_16_0	C24H50NO7P	1.901	↓(**)	+
5	Norleucine	C6H13NO2	1.893	↓(**)	+
6	Phenylalanine	C9H11NO2	1.790	↓(**)	+
7	Tyrosine	C9H11NO3	1.785	↓(**)	+
8	Kaurenic acid	C20H30O2	1.565	↑(***)	+
9	Bis(2-ethylhexyl) phthalate	C24H38O4	1.270	↓(*)	+
10	Dexamethasone	C22H29FO5	1.251	↑(*)	+
11	Cucurbitacin E	C32H44O8	1.153	↓(**)	+
12	Heptelidic acid chlorohydrin_130129	C15H21ClO5	1.083	↓(**)	+
13	1-Cyclopropyl-6,7-difluoro-1,4- dihydro-8-hydroxy-4-oxo-3- quinoline-3-carboxylic acid	C13H9F2NO4	1.292	↑(***)	-
14	2-(3-(8-Hydroxyoctyl) phenoxy)-2- methylpropanoic acid	C18H28O4	1.696	↑(***)	-
15	2'-Deoxyuridine 5'-mono- phosphate	C9H13N2O8P	1.454	↓(***)	-
16	2-Oxoadipate	C6H8O5	1.140	↑(*)	-
17	3-(4-Hydroxyphenyl) lactate	C9H10O4	1.420	↓(***)	-
18	3-Dehydroshikimate	C7H8O5	1.440	↓(**)	-
19	3-Hydroxyanthranilate	C7H7NO3	1.007	↓(*)	-
20	3-Hydroxybutanoic acid	C4H8O3	1.552	↓(*)	-
21	4-Acetamidobutanoate	C6H11NO3	1.205	↑(***)	-
22	4-Imidazoleacetic acid	C5H6N2O2	1.019	↓(*)	-
23	4'-Methylgenistein	C16H12O5	1.339	↓(***)	-
24	5-Hydroxy-3,7-dimethoxy-2-(4- methoxyphenyl)-4H-chromen-4- one	C18H16O6	1.300	↑(***)	-

25	5-Oxo-D-proline	C5H7NO3	1.127	↓(**)	-
26	Butein	C15H12O5	1.081	↓(**)	-
27	Cortisol	C21H30O5	1.470	↑(****)	-
28	Cytidine 5'-diphosphate	C9H15N3O11P2	1.284	↑(***)	-
29	Deoxyuridine	C9H12N2O5	1.291	↑(***)	-
30	D-Glyceric acid	C3H6O4	1.030	↑(**)	-
31	Ferulate	C10H10O4	1.153	↑(**)	-
32	Formyl-L-methionyl peptide	C6H11NO3S	1.029	↑(*)	-
33	Fructose	C6H12O6	1.344	↓(****)	-
34	Genistein	C15H10O5	1.182	↓(*)	-
35	Glyceraldehyde	C3H6O3	1.645	↓(***)	-
36	Glycocholate	C26H43NO6	1.422	↓(*)	-
37	Homovanillate	C9H10O4	1.577	↓(**)	-
38	Inosine 5'-diphosphate	C10H14N4O11P2	1.036	↑(*)	-
39	Leucine	C6H13NO2	1.205	↓(**)	-
40	L-Histidine	C6H9N3O2	1.535	↓(**)	-
41	Linoleic acid	C18H32O2	1.423	↑(****)	-
42	Linolenic acid	C18H30O2	1.299	↑(**)	-
43	L-Lysine	C6H14N2O2	1.480	↓(***)	-
44	Myristic acid	C14H28O2	1.458	↑(****)	-
45	Palmitoleic acid	C16H30O2	1.158	↑(**)	-
46	Riboflavin	C17H20N4O6	1.623	↓(**)	-
47	Succinate	C4H6O4	1.284	↓(***)	-
48	Taurine	C2H7NO3S	1.314	↓(**)	-

Table S7 Information of differential metabolites between ASA group and DSS group

No.	ASA/DSS metabolites	Formula	VIP	ASA vs DSS	Mode
1	Phenylalanine	C ₉ H ₁₁ NO ₂	2.494	↓(**)	+
2	Norleucine	C ₆ H ₁₃ NO ₂	2.473	↓(**)	+
3	p-Coumaric acid	C ₉ H ₈ O ₃	2.410	↓(*)	+
4	Methionine	C ₅ H ₁₁ NO ₂ S	2.310	↓(**)	+
5	2-Acetoxy-6-pentadecylbenzoic acid	C ₂₄ H ₃₈ O ₄	1.263	↑(*)	-
6	3-Dehydroshikimate	C ₇ H ₈ O ₅	1.593	↓(*)	-
7	3-Hydroxyanthranilate	C ₇ H ₇ NO ₃	2.198	↑(**)	-
8	4-Imidazoleacetic acid	C ₅ H ₆ N ₂ O ₂	1.544	↓(*)	-
9	Adenine	C ₅ H ₅ N ₅	1.509	↑(*)	-
10	Azelaic acid	C ₉ H ₁₆ O ₄	1.348	↑(*)	-
11	D-Glucosamine 6-phosphate	C ₆ H ₁₄ NO ₈ P	1.900	↑(**)	-
12	Fructose	C ₆ H ₁₂ O ₆	1.398	↓(*)	-
13	L-Histidine	C ₆ H ₉ N ₃ O ₂	2.181	↓(**)	-
14	L-Lysine	C ₆ H ₁₄ N ₂ O ₂	2.352	↓(***)	-
15	Palmitoleic acid	C ₁₆ H ₃₀ O ₂	1.754	↓(***)	-
16	Thymidine	C ₁₀ H ₁₄ N ₂ O ₅	1.651	↓(**)	-

Table S8 The relative concentration of metabolites in each group

No.	Metabolites	Relative concentration (ng/mL/100 mg feces)			
		Normal	DSS	ASA	LBP-3
1	(S)-2-Hydroxyglutarate	29.58±16.71***	135.16±59.29	40.84±28.79**	27.14±18.34***
2	1D-Myo-Inositol3-phosphate	30.07±13.48	23.5±15.09	40.6±23.81	56.26±26.37*
3	2-Isopropylmalic acid	3246.9±1247.89*	8236.39±4426.79	4834.91±2740.54	3080.83±1942.11*
4	2-Keto-isovalerate	70.3±16.13	113.82±47.47	72.3±37.75	47.18±26.25*
5	2-Oxo-4-methylthiobutanoate	31.52±20.47**	97.44±45.72	83.05±54.32	52.32±31.39
6	4-Hydroxyphenylpyruvate	5.06±1.11***	38.9±13.26	65.05±44.76	42.18±25.02
7	6-Phosphonoglucono-D-lactone	255.71±145.03**	57.64±31.14	420.14±222.98***	485.51±248.22**
8	Acetoacetate	33.09±13.09	29.86±19.62	14.71±8.22	6.57±4.01**
9	α-Ketoglutarate	187.26±70.43	121.45±90.12	49.13±16.66*	129.29±81
10	Anthranilate	81.41±26.52	113.73±64.47	329.51±189.06*	106.63±56.01
11	Ascorbic acid	1406.23±511.6*	3778.98±2254.85	2128.77±1691.81	1835.35±1443.28*
12	Cholic acid	21.14±16.25*	157.66±125	60.14±56.45	164.72±234.67
13	Citraconic acid	200.3±87.57	233.46±143.8	218.09±131.35	68.34±58.23*
14	Deoxycholic acid	1694.36±628.79*	3284.37±2272.44	4457.64±1455.38	7347.83±3520.94
15	D-Glucarate	26.17±11.96	41.18±22.89	178.53±67.45***	47.03±24.72
16	D-Gluconate	105.46±72.26	241.34±123.15	172.88±144.31	137.71±73.37*
17	D-Glucose 6-phosphate	20.09±7.59	27.05±12.83	40.4±22.96	9.74±7.02**
18	Gluconic acid	187.07±90.27*	451.39±238.16	311.97±254.44	167.02±75.45*
19	Kynurenic acid	56.05±19.07**	108.83±42.79	98.97±70.38	114.75±87.02
20	Lactate	23.44±13.82**	97.14±47.36	52.93±24.44	32.22±21.07
21	Maleic acid	66.02±24.05	115.39±42.71	102.65±72.29	37.98±24.12**
22	Methylmalonic acid	387.84±98.03*	878.38±299.14	916.82±434.71	578.74±203.49
23	Myo-inositol	26.44±9.94*	67.31±35.45	88.7±38.73	40.83±21.62
24	N-Acetyl-α-D-glucosamine1-phosphate	7.68±3.42*	32.54±22.27	30.21±37.23	10.53±12.96

25	Orotidine-5-phosphate	9.02±3.43	6.01±1.93	9.74±4.55	12.7±3.56*
26	Oxalacetic acid	100.96±68.64	120.83±46.95	103.79±84.29	45.59±22.93**
27	p-Aminobenzoate	76.42±24.79	129.46±50.72	300.83±182.96*	125.76±79.48
28	p-Aminobenzoic acid	79.66±22.41	119.98±58.75	306.61±130.71*	107.73±77.78
29	Phosphoenolpyruvic acid	71.87±32.46	62.03±50.03	460.48±264.68**	280.48±170.81**
30	p-Salicylic acid	43.25±21.01	62.59±47.16	65.85±49.9	22.47±22.77*
31	Succinate	360.24±155.69**	1060.91±575.59	2061.77±1432.8	838.1±713.86
32	Taurine	2329.76±572.49*	5745.5±3184.41	4782.26±2718.09	2719.86±688.66*
33	Xanthine	47.63±21.12	91.28±85.47	13254.19±6579.66***	72.23±36.31
34	Xanthurenic acid	980.81±462.24**	316.16±290.11	430.17±280.73	141.2±121
35	Allantoin	508.02±137.07**	1079.19±462.86	831.87±541.5	1330.6±843.49
36	Deoxycholic acid-3-sulfate	14.42±9.27**	42.78±21.53	74.67±49.49	46±35.17
37	Taurocholic acid-3-sulfate	7.19±4.6**	22.83±12.33	8.53±6.25	19.1±16.82
38	Tauroursodeoxycholic acid-3-sulfate	22.53±13.83*	96.58±32.09	207.94±136.88*	53.48±38.62
39	1-Methyladenosine	18.77±14.13	45.47±25.6	61.79±31.79	11.79±6.36**
40	2-Aminooctanoic acid	3.86±1.53	2.67±1.19	9.04±7.59	26.39±16.69**
41	2-Methylnicotinamide	201.82±71.94**	86.92±36.03	280.53±105.57	86.63±83.14
42	7,8-Dihydrofolate	2.03±2.05	2.84±2.43	1.93±1.15	7.77±3.87*
43	7-Methylguanosine	2.4±0.85***	0.92±0.39	2.75±1.94	3.75±2.21**
44	Acetoacetic acid	7.88±3.79**	17.36±5.52	8.32±6.7	7.36±2.66**
45	L-Acetylcarnitine	4.39±2.19	6.13±1.65	9.15±4.51	11.43±4.12**
46	Acetylphosphate	8.27±3.01*	16.03±6.65	17.14±6.98	21.37±5.05
47	Adenine	117.61±68.93	27.16±15.04	80.03±64.24	140.27±64.83***
48	Adenosine	21.4±14.69	11.11±2.94	29.07±13.48	70.77±47.23**
49	Aminoimidazole carboxamide Ribonucleotide	1.52±0.95	2.62±1.9	3.11±1.67	8.67±5**
50	AMP	0.76±0.34	0.44±0.23	4.5±2.63**	2.09±1.42**
51	Betaine	69.57±15.96**	44.98±14.06	63.32±23.39	122.02±37.81*
52	Betaine aldehyde	22.96±3.95***	5.89±2.78	12.33±9.32	2.62±2.12
53	Cytidinemonophosphate	1.31±1.07**	0.39±0.19	1.31±1.17**	1.05±0.53**

54	Cytosine	7.25±3.16	4.46±1.52	8.35±3.27	14.44±9.57**
55	Deoxyadenosine	5.22±2.32**	1.55±1.04	2.9±1.47	4.81±1.9**
56	Deoxyribose 1-phosphate	1.9±0.67**	9.8±6.18	10.74±9.86	27.59±12.57**
57	Diiodothyronine	11.9±6.86*	4.2±1.47	9.2±4.79	28.71±18.38**
58	D-Ribulose 5-phosphate	4.74±4.14	1.68±0.7	4.73±3.89	16.29±10.08**
59	FAD	0.3±0.08	0.66±0.42	0.79±0.49	1.97±1.53*
60	Folate	3.32±1.74	2.95±1.09	4.38±2.73	7.77±2.5***
61	Glucosamine 6-phosphate	1.27±0.73	1.22±0.52	2.54±1.42	4.85±2.87**
62	Glutamine	2.89±1.26**	9.95±2.17	5.67±3.51	4.92±1.37**
63	Guanine	35.14±24.16**	6.43±2.68	8.51±5.92	11.32±4.74
64	Histidinol	5.93±7.56	5.32±1.64	5.87±2.1	14.27±5.2***
65	Homocysteine	21.1±11.56	36.61±10.52	18.26±12.09*	17.68±5.99**
66	Homoserine	196.75±80.95**	506.06±141.23	243.56±177.16*	211.05±54.91*
67	Hydroxyproline	1.27±0.35	1.22±0.37	2.87±1.78***	3.23±1.23***
68	Imidazoleacetic acid	29.04±8.74	50.45±31.18	32.7±20.21	17.12±11.4*
69	Indole	2.43±0.64	1.76±0.63	4.66±2.13**	3.89±2.56**
70	Isoleucine	15.78±7.22**	39.69±9.94	23.36±16.58	17.17±10.99**
71	Kynurenine	6.66±1.55***	1.63±0.72	2.77±0.67	5.87±2.49*
72	Leucine	19.12±7.67**	43.35±18.28	25.34±15.17	16.37±2.94**
73	Lysine	4.56±1.75*	0.65±0.38	2.25±1.71*	2.04±0.7**
74	Methionine	1.37±0.93	0.93±0.48	1.42±0.66	4.03±2.03**
75	Methylcysteine	33.21±18.22**	81.44±25.15	39.19±26	54.28±40.48
76	Methylnicotinamide	51.84±17.76**	25.81±7.3	47.33±32.3	19.16±13.67
77	N-acetyl-glucosamine	5.86±3.86	2.89±1.8	7.11±6.55	9.29±4.17**
78	NADH	1.9±0.76	1.44±0.63	4.02±1.95	6.69±4.25**
79	Nicotinamide	11.52±4.92**	34.58±10.04	24.48±15.44	56.34±25.6
80	Phenylalanine	14.29±6.57***	41.33±10.24	17.12±11.79**	16.8±5.23***
81	Purine	3.6±1.27**	10.14±4.15	7.49±7.86	6.61±2.5
82	Pyridoxine	1.89±0.58	1.48±0.92	2.5±1.72	6.58±2.15**

83	Spermidine	65.4±17.76**	125.07±41.96	122.37±21.7	184.51±88.52
84	Tryptophan	2.23±1.44*	1±0.35	0.95±0.71	4.84±1.07**
85	Tyrosine	5.66±2.9	4.13±1.13	5.99±3.51	17.51±4.97**

Differential metabolites were analysed using Student's t-test with FDR correction (* $p < 0.05$, ** $p < 0.01$ and *** $p < 0.001$ vs DSS group)

Figure S1

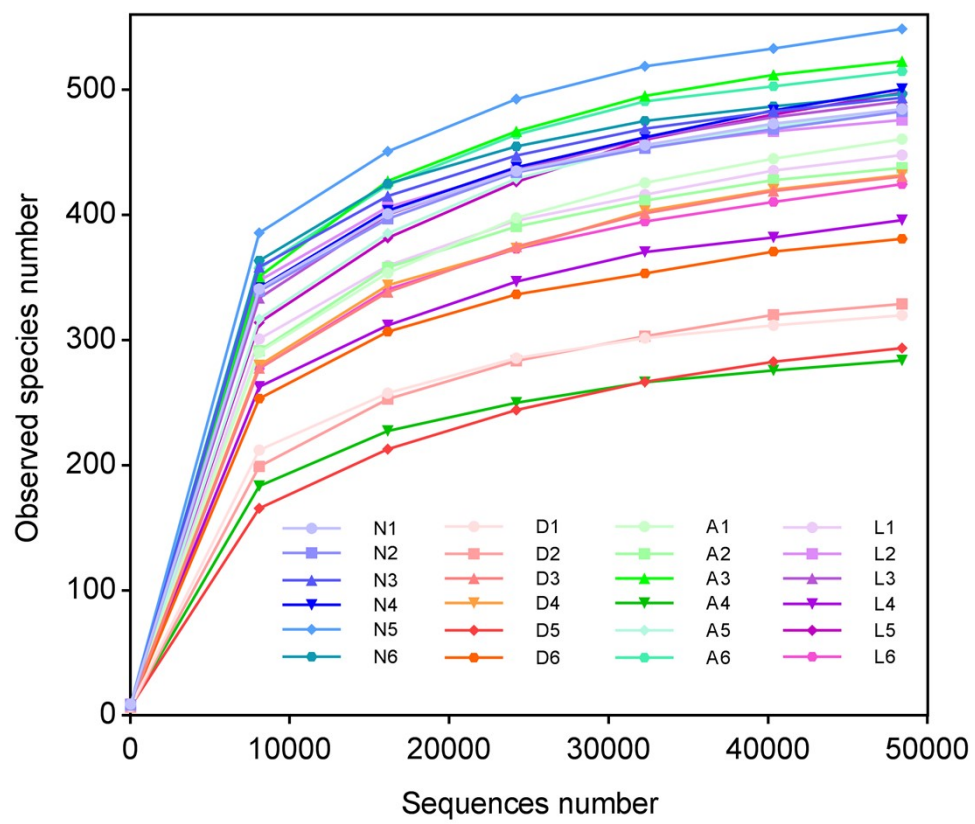


Figure S2

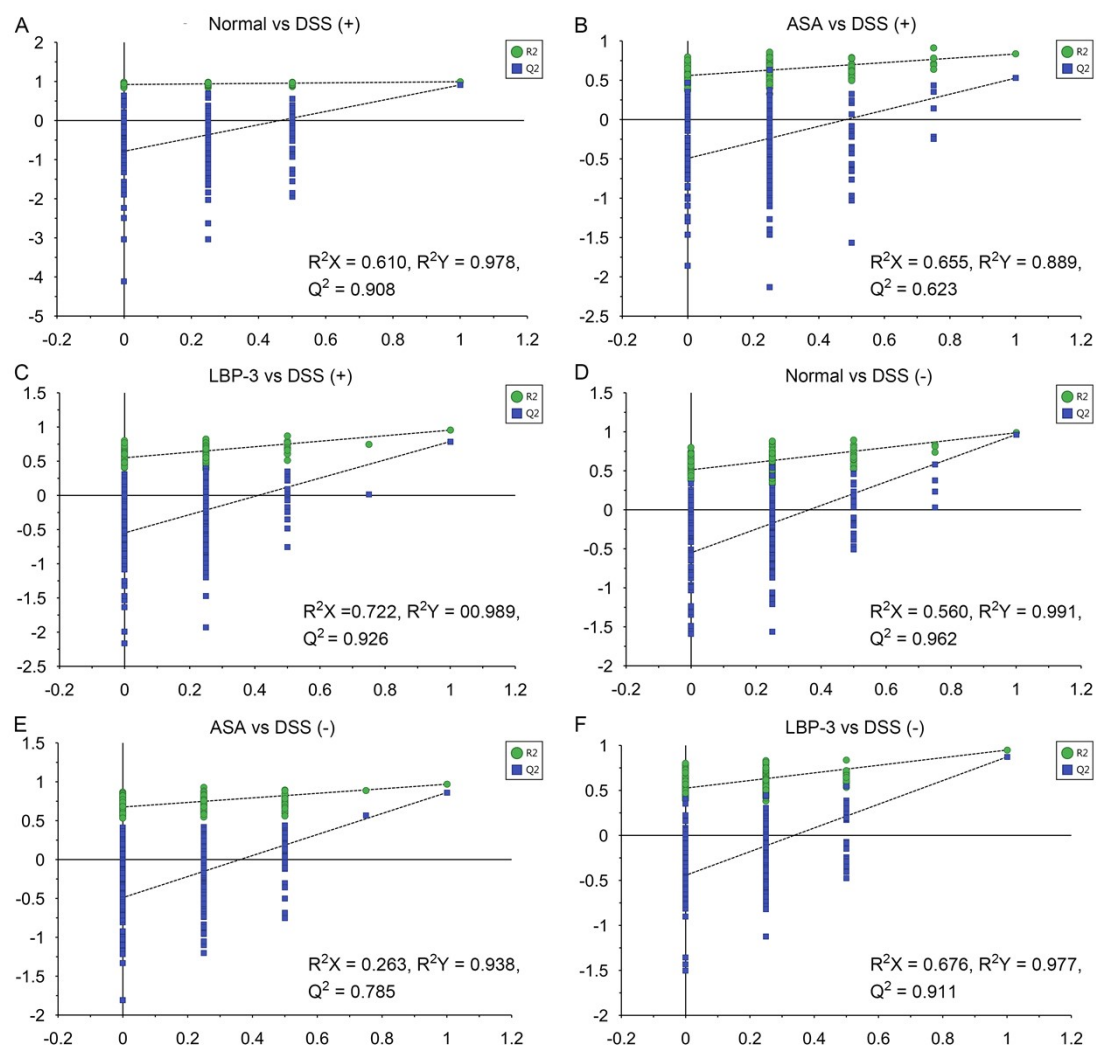


Figure S3

