Multi-omics analyses strategy reveals the molecular mechanism of the inhibition of *Escherichia coli* O157: H7 by anthocyanins from *Aronia melanocarpa* and its application

Haotian Deng[1], Li Li[1*], and Xianjun Meng[1*]

[1]College of Food Science, Shenyang Agricultural University, Shenyang, Liaoning Province, China, 110866

*Corresponding author:

Tel.: +86 186 4030 6640

E-mail address: lili1231105@126.com (L. Li)

Tel.: +86 133 9011 7107

E-mail address: mengxjsy@126.com (X. Meng)

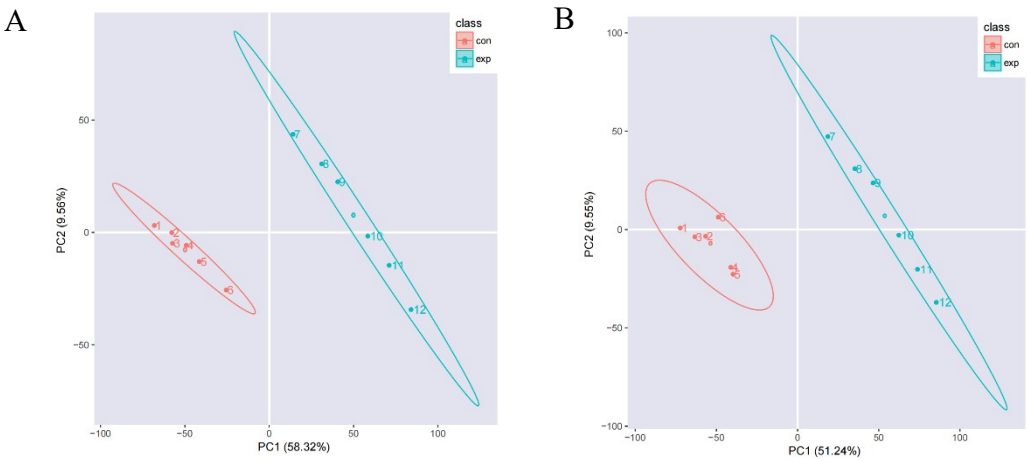

Fig. 1S (A) and (B) are the scores of PLS-DA discriminant analysis model under positive and negative ion mode respectively.

Table S1 Program setting of LC-MS.

Liquid chromatography					**Tandem mass spectrometer**			
Time (min)	Solvent A: Solvent B (v:v)	Column temperature (℃)	Flow rate (mL/min)	Injection volume (μL)	capillary voltages (Kv, positive ion mode)	capillary voltages (kV, negative ion mode)	mass range (Da)	Ion source temperature (℃)
0	95%:5%							
0.5	20%:80%							
		50	0.3	10	5	-4.5	50-1200	650
5	0%:100%							
8	95%:5%							

Table S2 Analysis and summary of differential metabolic pathways.

Pathway	Total	Expected	Hits	Raw p	-log(p)	Holm p	FDR	Impact
Galactose metabolism	39	2.76	10	0.00	3.68	0.02	0.02	0.23
Pyruvate metabolism	26	1.84	6	0.01	2.12	0.65	0.28	0.12
Citrate cycle (TCA cycle)	20	1.42	5	0.01	1.98	0.88	0.28	0.23
Glycolysis / Gluconeogenesis	29	2.05	6	0.01	1.88	1	0.28	0.47
Nicotinate and nicotinamide metabolism	15	1.06	4	0.02	1.76	1	0.30	0.10
Purine metabolism	73	5.17	10	0.03	1.56	1	0.39	0.12
Methane metabolism	26	1.84	5	0.03	1.50	1	0.39	0.42
Sphingolipid metabolism	5	0.35	2	0.04	1.37	1	0.46	0.00
Starch and sucrose metabolism	22	1.56	4	0.06	1.19	1	0.61	0.21
Glycerolipid metabolism	14	0.99	3	0.07	1.15	1	0.61	0.10
Inositol phosphate metabolism	8	0.57	2	0.10	0.98	1	0.75	0.00
Pentose phosphate pathway	26	1.84	4	0.11	0.98	1	0.75	0.26
Lysine degradation	17	1.20	3	0.11	0.95	1	0.75	0.28
Glycerophospholipid metabolism	22	1.56	3	0.20	0.70	1	1	0.07
Pentose and glucuronate interconversions	35	2.48	4	0.23	0.64	1	1	0.00

Glyoxylate and dicarboxylate metabolism	37	2.62	4	0.26	0.58	1	1	0.09
Pyrimidine metabolism	51	3.61	5	0.29	0.54	1	1	0.05
Polyketide sugar unit biosynthesis	5	0.35	1	0.31	0.51	1	1	0.00
Biosynthesis of siderophore group nonribosomal peptides	5	0.35	1	0.31	0.51	1	1	0.30
Butanoate metabolism	17	1.20	2	0.34	0.47	1	1	0.06
D-Glutamine and D-glutamate metabolism	7	0.50	1	0.40	0.39	1	1	0.00
Phenylalanine metabolism	33	2.34	3	0.42	0.38	1	1	0.00
Glycine, serine and threonine metabolism	33	2.34	3	0.42	0.38	1	1	0.09
Fructose and mannose metabolism	33	2.34	3	0.42	0.38	1	1	0.24
Aminobenzoate degradation	8	0.57	1	0.45	0.35	1	1	0.00
Alanine, aspartate and glutamate metabolism	22	1.56	2	0.47	0.33	1	1	0.00
Valine, leucine and isoleucine biosynthesis	22	1.56	2	0.47	0.33	1	1	0.13
Glutathione metabolism	22	1.56	2	0.47	0.33	1	1	0.38
Porphyrin and chlorophyll metabolism	36	2.55	3	0.48	0.32	1	1	0.13
Streptomycin biosynthesis	9	0.64	1	0.49	0.31	1	1	0.00
Pantothenate and CoA biosynthesis	24	1.70	2	0.52	0.29	1	1	0.11

Tyrosine metabolism	10	0.71	1	0.52	0.28	1	1	0.00
Propanoate metabolism	27	1.91	2	0.58	0.23	1	1	0.05
Riboflavin metabolism	13	0.92	1	0.62	0.21	1	1	0.00
Vitamin B6 metabolism	13	0.92	1	0.62	0.21	1	1	0.17
Arginine and proline metabolism	29	2.05	2	0.62	0.21	1	1	0.10
Ubiquinone and other terpenoid-quinone biosynthesis	15	1.06	1	0.67	0.17	1	1	0.00
Arginine biosynthesis	16	1.13	1	0.69	0.16	1	1	0.00
Terpenoid backbone biosynthesis	16	1.13	1	0.69	0.16	1	1	0.00
Cyanoamino acid metabolism	17	1.20	1	0.72	0.15	1	1	0.00
Peptidoglycan biosynthesis	17	1.20	1	0.72	0.15	1	1	0.07
Ascorbate and aldarate metabolism	18	1.27	1	0.74	0.13	1	1	0.00
Sulfur metabolism	20	1.42	1	0.77	0.11	1	1	0.04
Cysteine and methionine metabolism	40	2.83	2	0.79	0.10	1	1	0.00
Valine, leucine and isoleucine degradation	23	1.63	1	0.82	0.09	1	1	0.00
Phenylalanine, tyrosine and tryptophan biosynthesis	23	1.63	1	0.82	0.09	1	1	0.00

Thiamine metabolism	23	1.63	1	0.82	0.09	1	1	0.00
Folate biosynthesis	38	2.69	1	0.94	0.03	1	1	0.06
Fatty acid degradation	41	2.90	1	0.95	0.02	1	1	0.03
Amino sugar and nucleotide sugar metabolism	44	3.12	1	0.96	0.02	1	1	0.00
Aminoacyl-tRNA biosynthesis	45	3.19	1	0.97	0.02	1	1	0.00

Note: the Total is the total number of compounds in the pathway; the Hits is the actually matched number from the user uploaded data; the Raw p is the original p value calculated from the enrichment analysis; the Holm p is the p value adjusted by Holm-Bonferroni method; the FDR p is the p value adjusted using False Discovery Rate; the Impact is the pathway impact value calculated from pathway topology analysis.