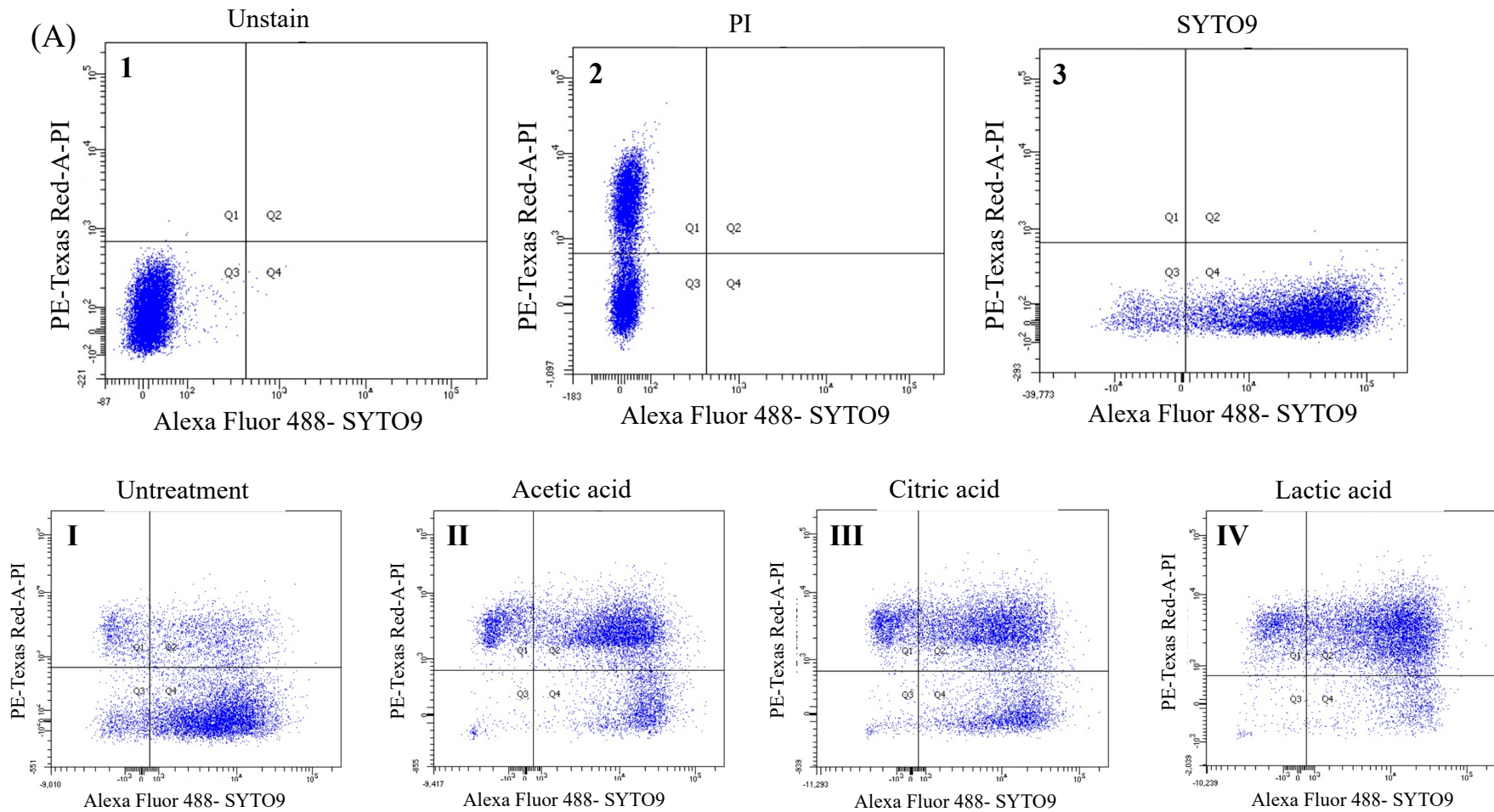


Figure S1. The flow cytometry images of ATCC 13076 (A), ATCC 14028(B) after treatments
 Note: I: control; II: acetic acid; III: citric acid; IV: lactic acid; 1-3 decide the baseline; Points in Q1: totally damaged; Q2: partly damaged



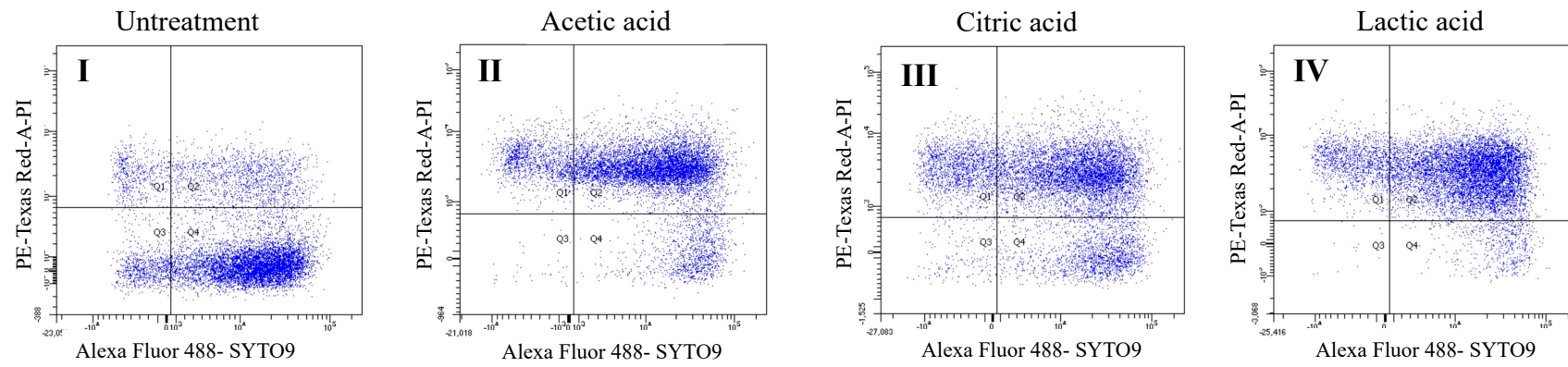
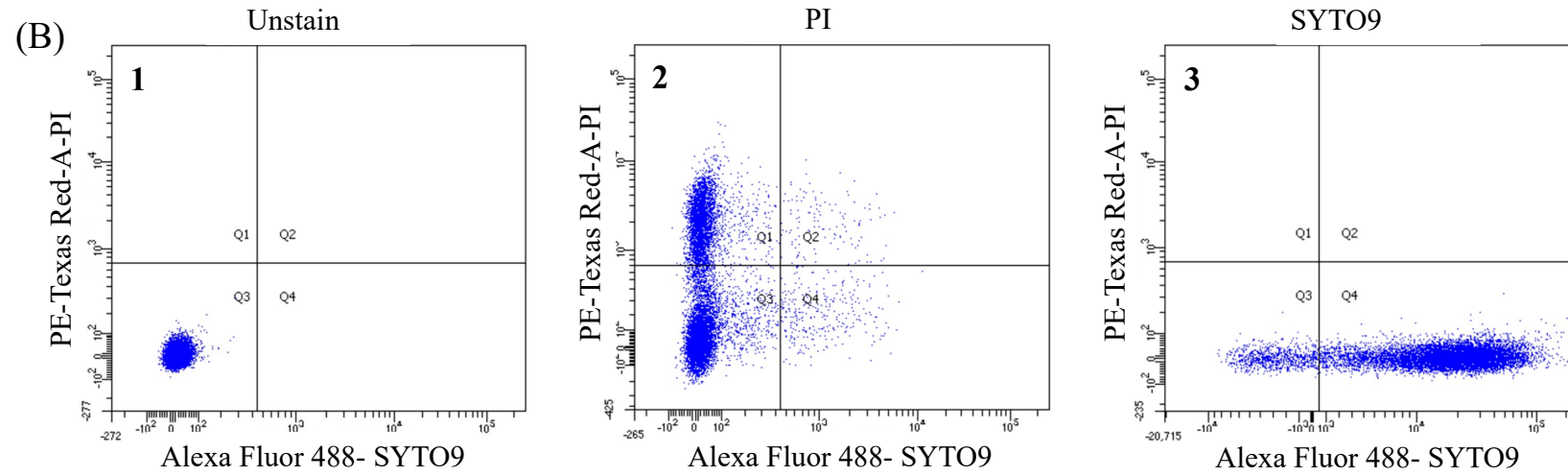
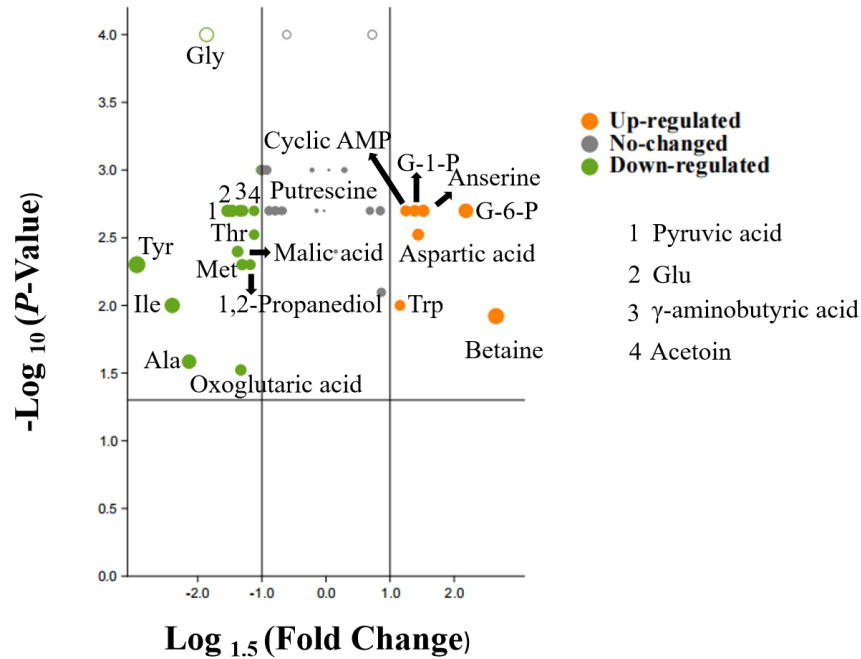


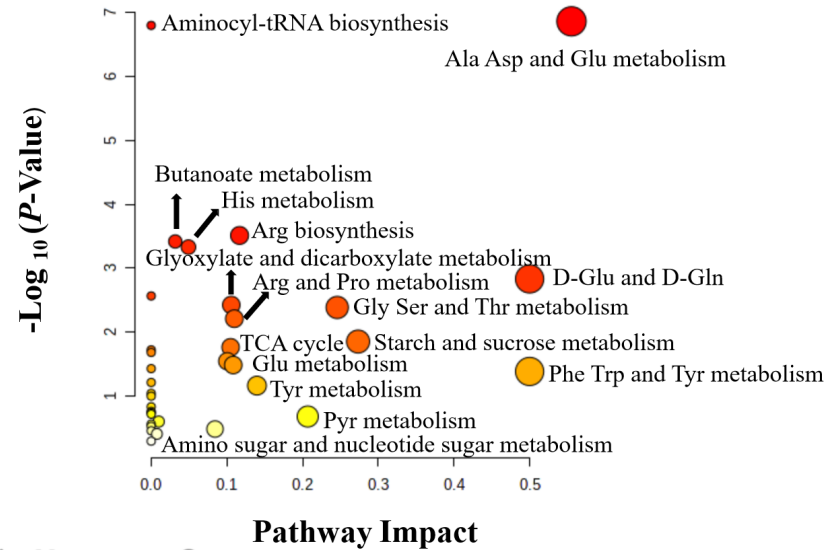
Figure S2. Volcano plots of the control and CA and LA groups (A1-F1); pathway analysis for the control and CA and LA groups (A2-F2). A-C (CA; ATCC 6962, ATCC 13076, ATCC 14028) D-F (LA; ATCC 6962, ATCC 13076, ATCC 14028)

Note: green colour in the volcano plot shows decreased amount after organic acid treatments; orange colour in the volcano plot shows increased amount after the organic acid treatments. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.

(A1)

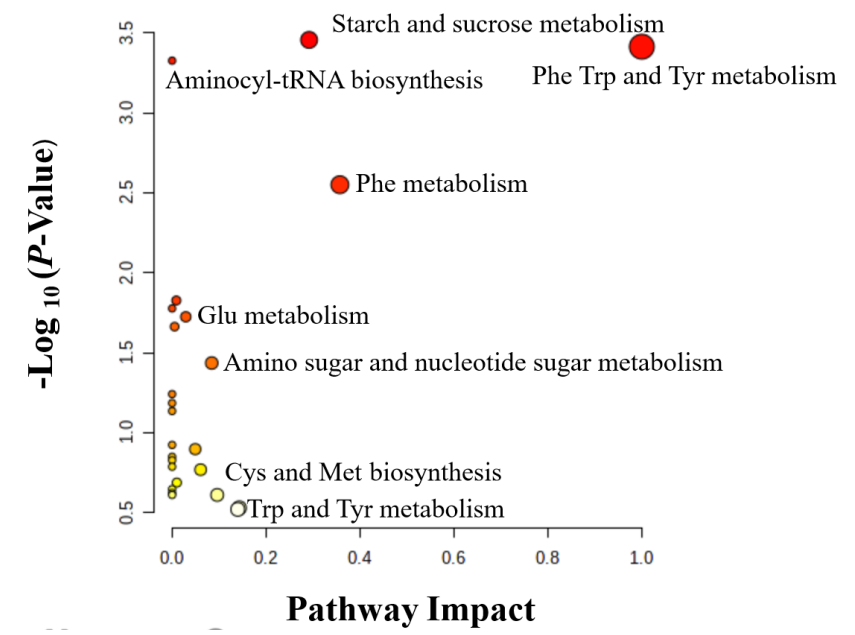
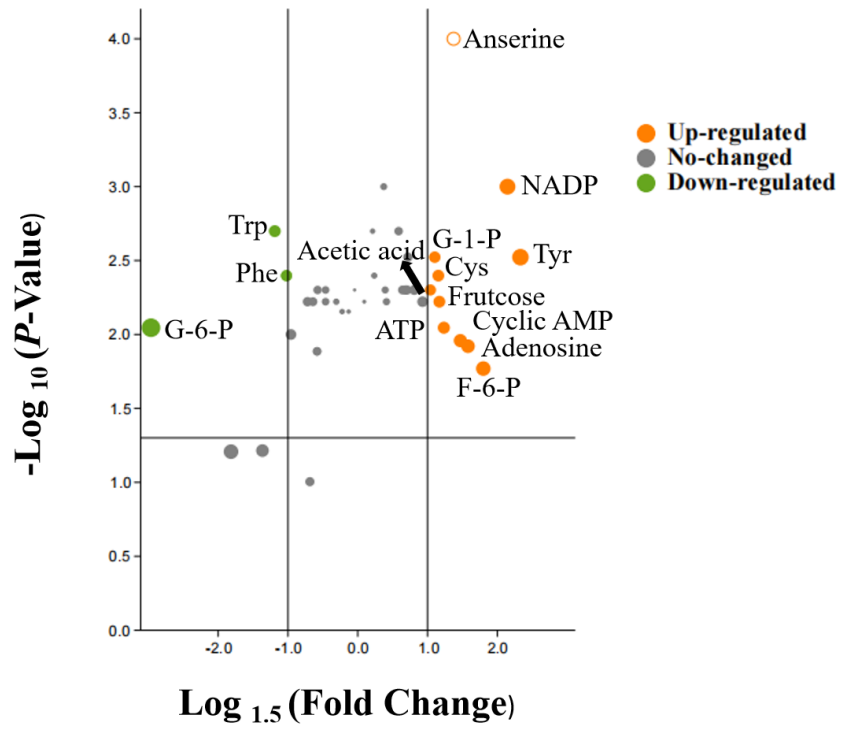


(A2)

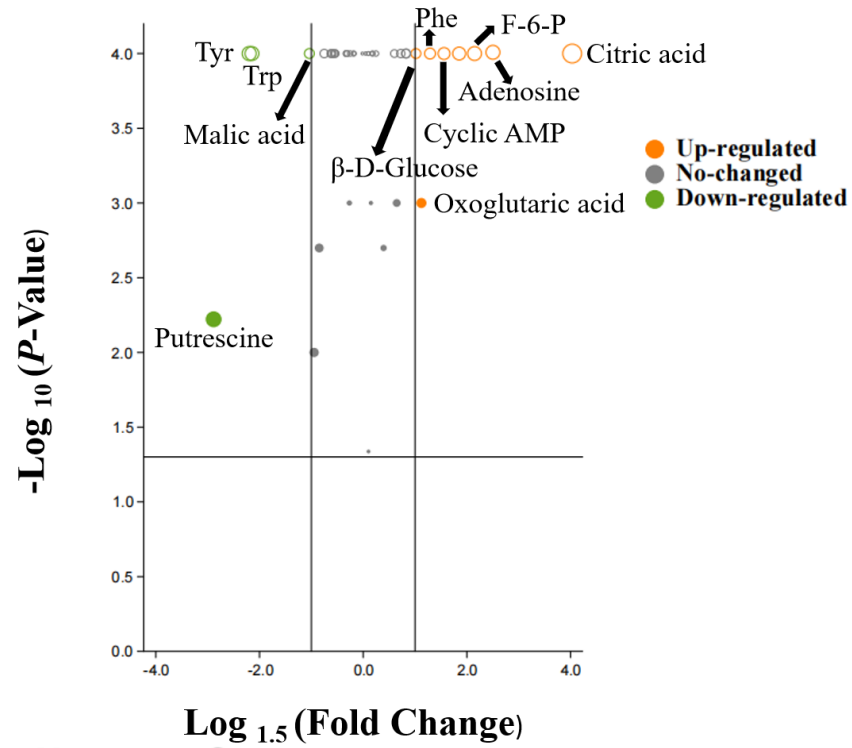


(B1)

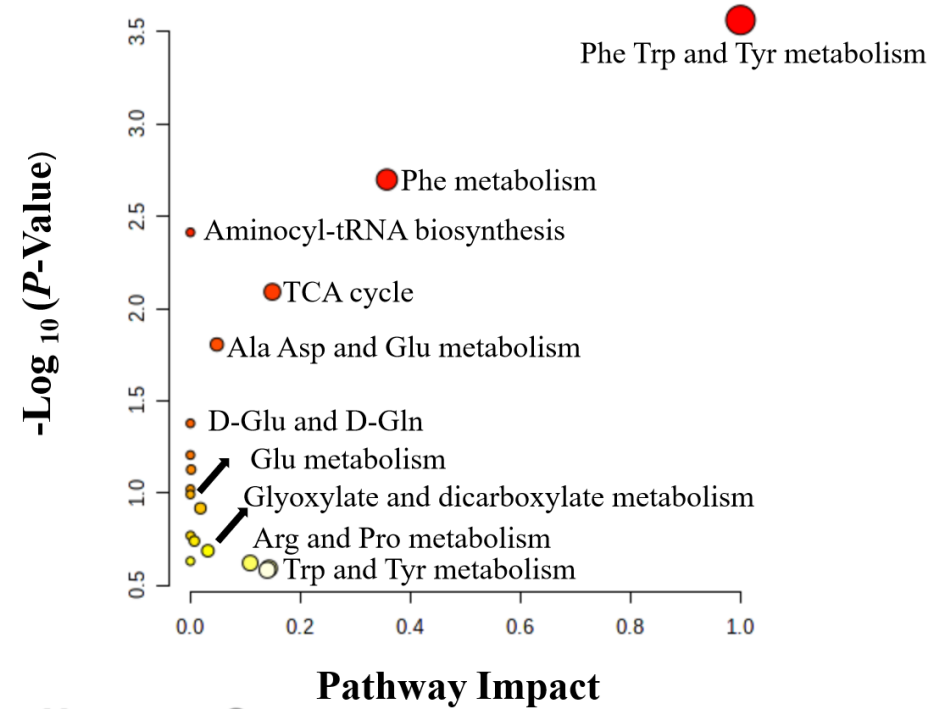
(B2)



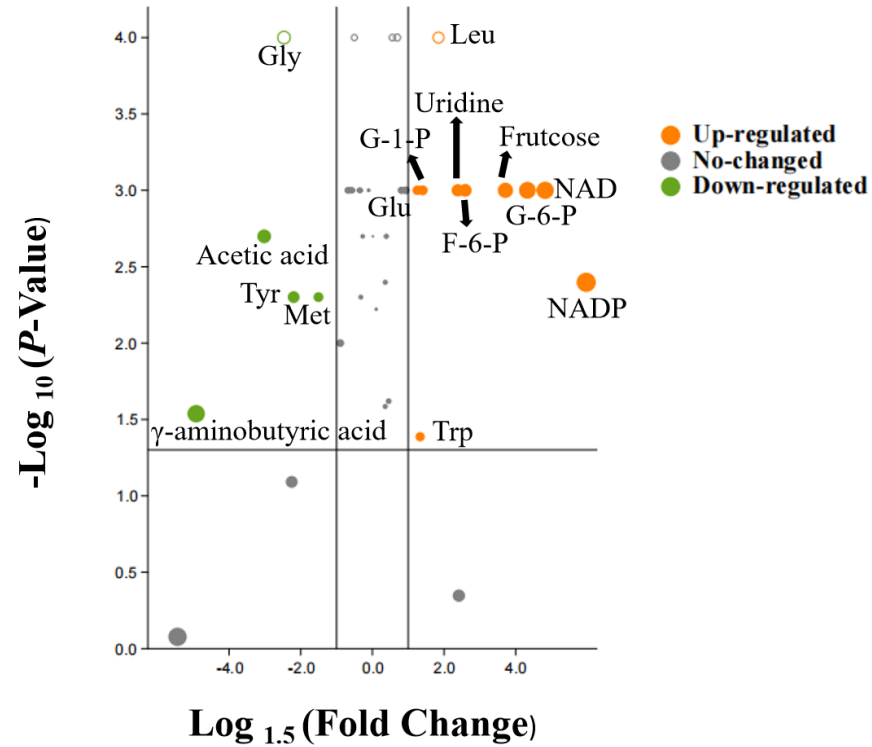
(C1)



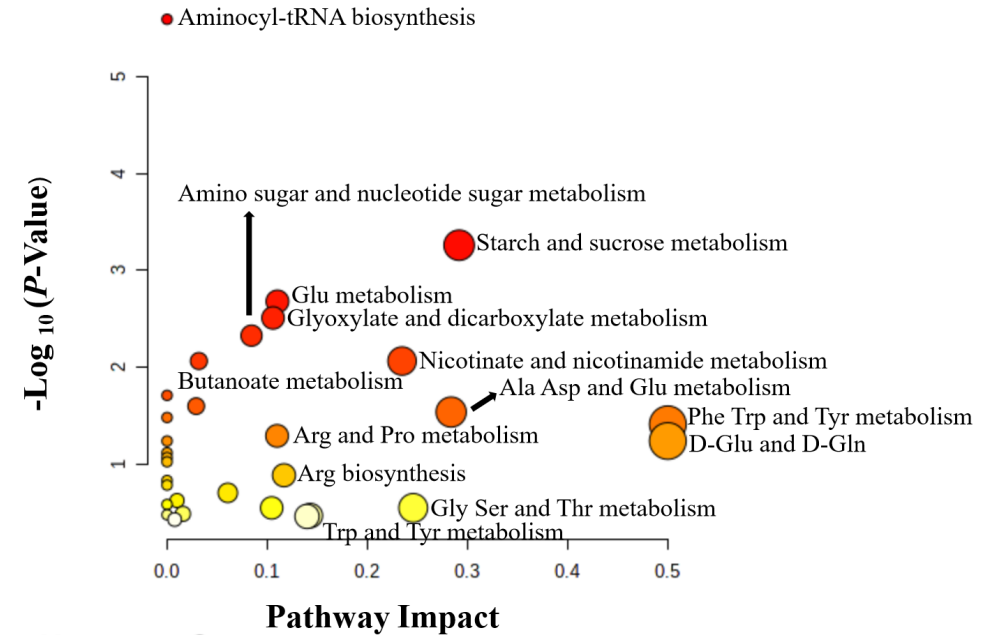
(C2)



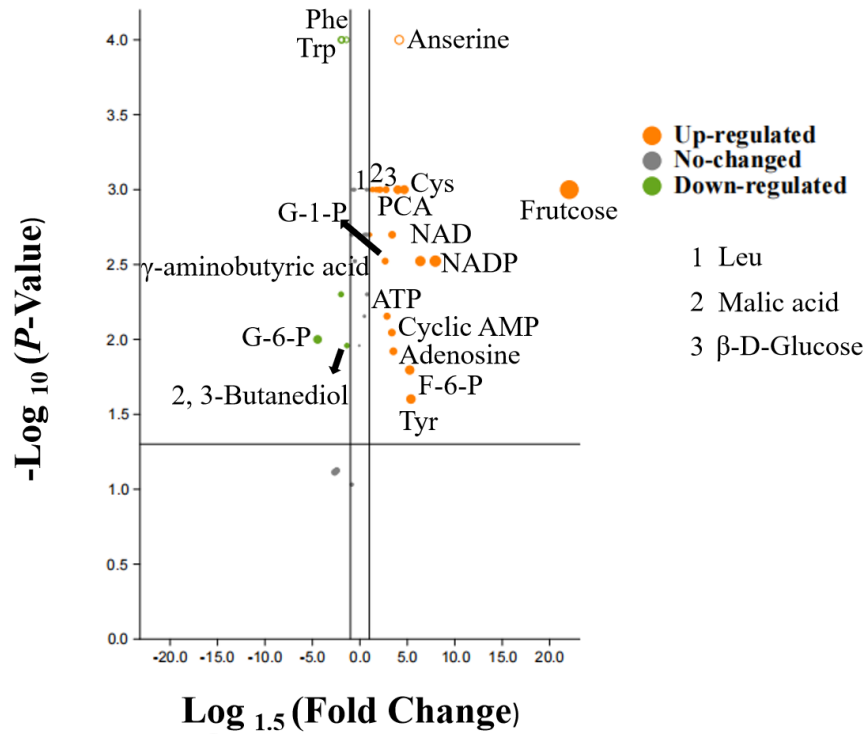
(D1)



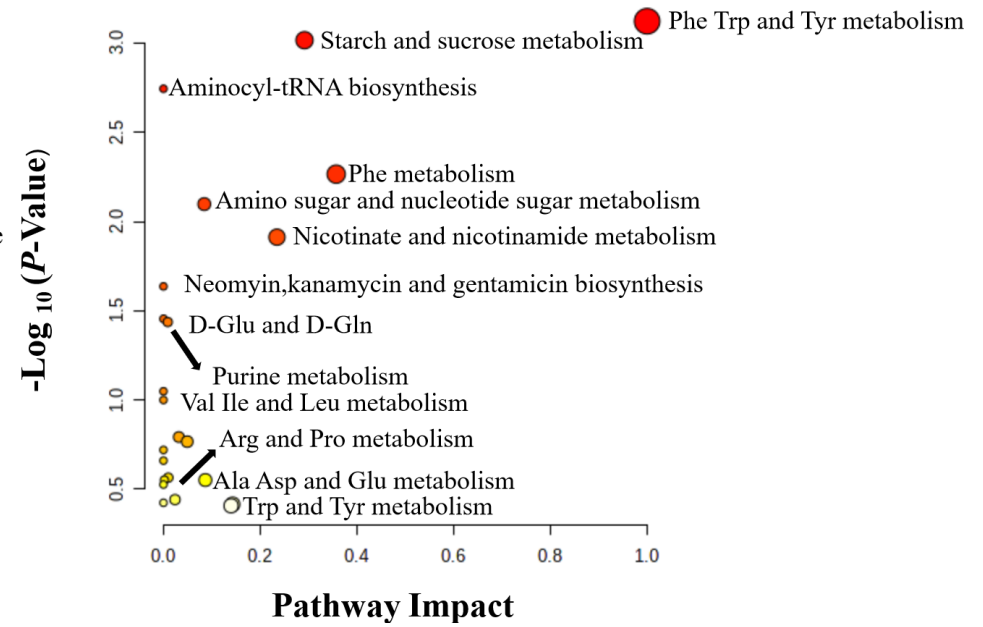
(D2)



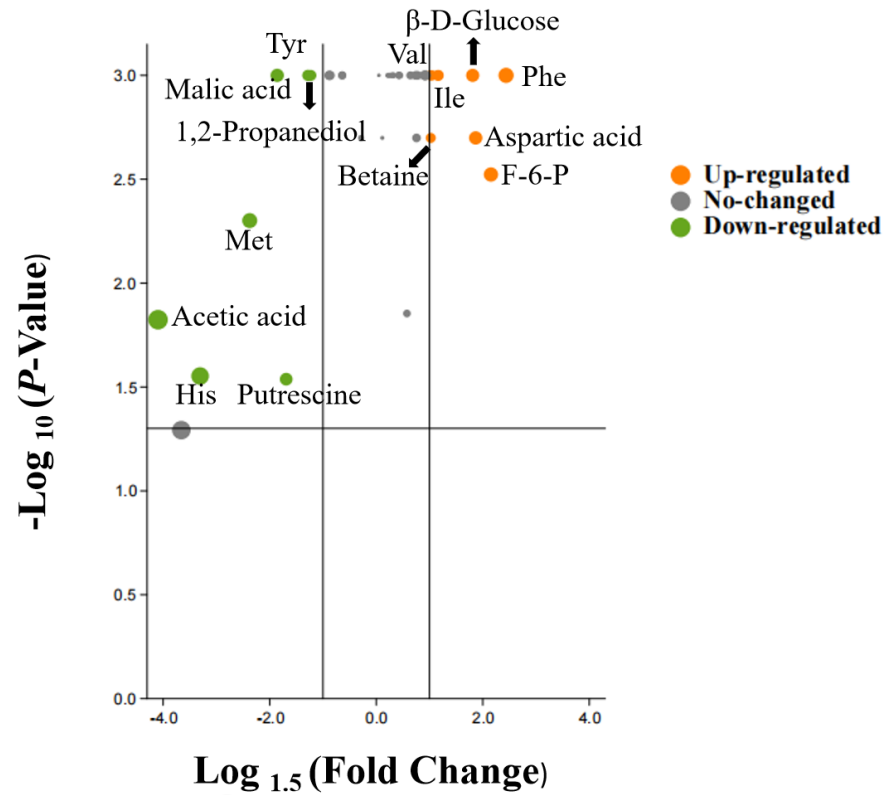
(E1)



(E2)



(F1)



(F2)

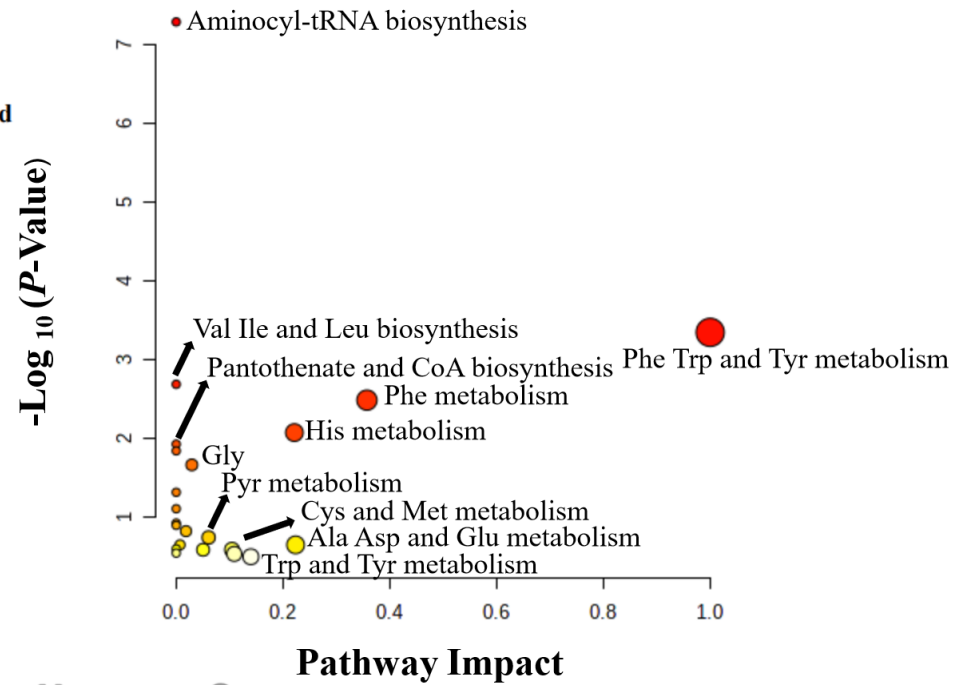


Figure S3. Three typical ^1H NMR spectra of *Salmonella* ATCC 6962, ATCC 13076 and ATCC 14028 extract in control groups. Note: I: ATCC 6962; II: ATCC 13076; ATCC 14028.

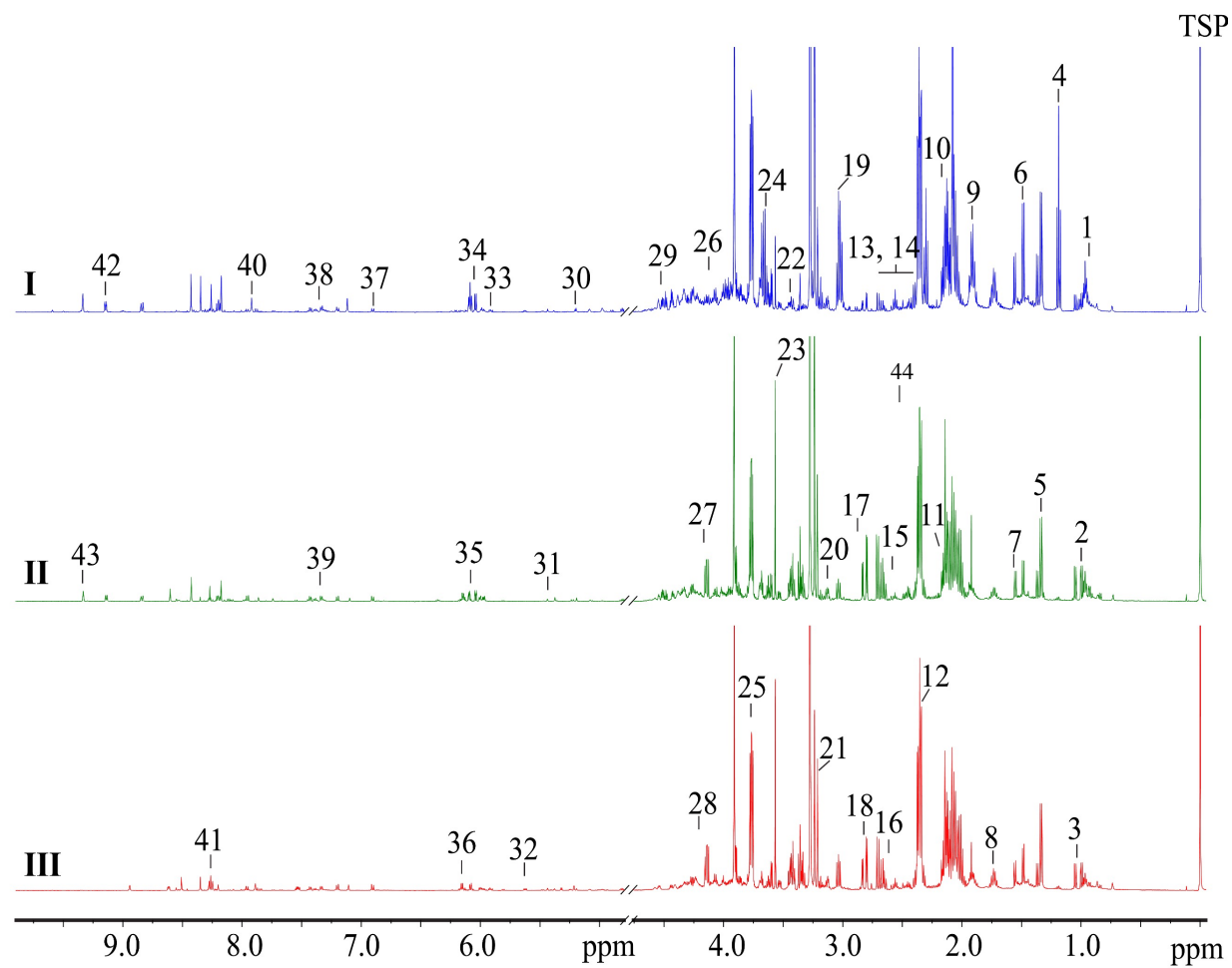


Figure S4. Nine typical ^1H NMR spectra of three *Salmonella. enterica* strains extraction after different organic acids treatments. Note: I: ATCC

6962; II: ATCC 13076; III: ATCC 14028. 1: acetic acid 2: citric acid 3: lactic acid

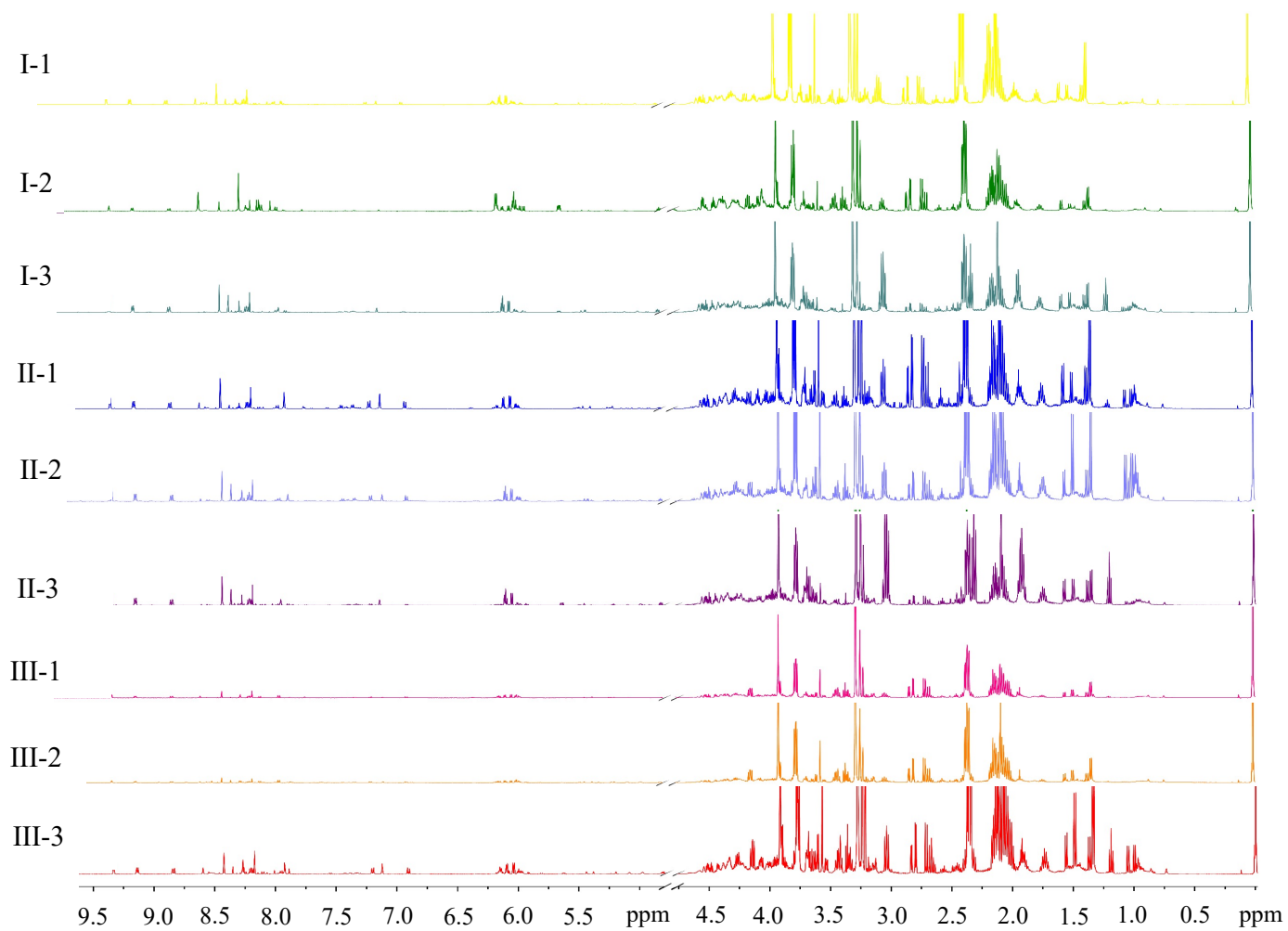


Table S1. Metabolites identified in *Salmonella*.

Metabolites	Assignments	¹ H chemical shifts (ppm)	¹³ C chemical shifts (ppm)
1 Isoleucine	α CH; β CH; γ CH ₂ ; γ' CH ₃ ; δ CH ₃	3.65 (d); 1.97 (m); 1.45 (m); 0.98 (d); 0.92 (t)	62.65; 37.79; 26.88; 17.52; 13.97
2 Leucine	α CH; β CH ₂ ; γ CH; δ CH ₃ ; δ' CH ₃	3.75 (m); 1.70(m); 1.71 (m); 0.95(t); 0.94 (t)	55.80; 42.26; 23.77; 24.76; 23.98
3 Valine	α CH; β CH; γ CH ₃ ; γ' CH ₃	3.58 (d); 2.26(m); 1.01 (d); 1.01 (d)	64.12; 32.18; 18.80; 19.48
4 Ethanol	α CH ₂ ; β CH ₃	3.66 (m); 1.19 (t)	60.22; 18.93
5 Lactic acid	α CH; β CH ₃	4.10 (q); 1.31 (d)	70.81; 21.87
6 Alanine	α CH; β CH ₃	3.77 (q); 1.50 (d)	53.60; 19.02
7 Threonine	α CH; β CH; γ CH ₃	3.57(d); 4.24 (m); 1.31(d)	62.82; 68.77; 21.89
8 Putrescine	α CH ₂ ; β CH ₂	3.04 (t); 1.75 (m)	41.11; 26.93
9 Acetic acid	CH ₃	1.91(s)	26.08
10 Methionine	α CH; β CH ₂ ; γ CH ₂ ; SCH ₃	3.85 (dd); 2.17(m); 2.63 (t); 2.10 (m)	56.45; 33.36; 31.79; 16.22
11 Acetoin	α CH ₃ ; α CH; β CH ₃	2.22(s); 4.41 (q); 1.37 (d)	28.02; 75.96; 21.04
12 Glutamate	α CH; β CH ₂ ; γ CH ₂	3.76 (m); 2.04 (m); 2.34 (m)	57.35; 32.69; 36.21
13 Succinic acid	CH ₂	2.38 (s)	37.02
14 Pyroglutamic acid	α CH; β CH ₂ ; γ CH ₂ ; γ' CH	4.16(dd); 2.49(m); 2.38 (m); 2.01(m)	60.96; 28.05; 32.39; 28.32
15 Pyruvic acid	CH ₃	2.35 (s)	29.84
16 Anserine	α CH; β CH ₂ ; CH ₃ ; NCHC; NCHN; β' CH ₂ ; β' CH ₂ N	4.49 (dd); 3.05 (d); 3.77 (s); 7.11 (s); 8.29 (s); 2.66 (m); 3.22 (m)	56.02; 27.95; 35.12; 122.58; 138.18; 35.06; 28.28
17 Cysteine	NCH; SCH ₂	3.84 (dd); 3.05(m)	58.74; 28.01
18 Aspartic acid	α CH; β CH ₂ ; γ CH ₂	3.90 (dd); 2.79 (dd); 2.71(m)	54.99; 39.44; 39.34
19 Oxoglutaric acid	α CH ₂ ; β CH ₂	2.99 (m); 2.43 (t)	38.92; 33.21
20 γ -aminobutyric acid	α CH ₂ ; β CH ₂ ; γ CH ₂	2.28 (t); 1.90 (m); 3.13 (t)	39.27; 26.33; 41.99
21 Betaine	CH ₃ ; CH ₂	3.26 (s); 3.90 (s)	55.60; 68.98
22 1,2-Propanediol	C1H ₂ ; C2H; C3H ₃	3.46(dd); 3.81(m); 1.06 (d)	69.33; 71.17; 21.17
23 Glycine	CH ₂	3.56 (s)	44.36
24 2, 3-Butanediol	CH; CH ₃	3.65 (m); 1.17 (d)	74.76; 20.23

25	Glutamine	α CH; β CH ₂ ; γ CH ₂	3.76 (t); 2.12 (m); 2.43 (m)	57.18; 29.07; 34.07
26	Fructose	C ₁ H ₂ ; C ₂ H; C ₃ H; C ₄ H; C ₆ H ₂	3.98 (m); 3.88 (m); 3.83 (m); 3.79 (d); 3.69 (d)	65.90; 65.76; 83.27; 65.45; 65.93
27	Fructose-6-phosphate	C ₁ H ₂ ; C ₂ H; C ₃ H; C ₄ H; C ₆ H ₂	4.10 (m); 4.08(m); 4.09 (t); 3.97 (m); 3.85 (m)	78.02; 78.08; 82.28; 69.44; 66.48
28	Malic acid	α CH; β CH ₂	4.28 (dd); 2.66 (dd)	73.73; 45.34
29	β -D-Glucose	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H; C ₆ H ₂	4.63 (d); 3.44 (m); 3.46 (m); 3.52 (m); 3.70 (m); 3.89(dd)	98.22; 78.84; 74.74; 74.38; 75.25; 63.64
30	α -D-Glucose	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H; C ₆ H ₂	5.21 (d); 3.67 (m); 3.81 (m); 3.33 (m); 3.93 (m); 3.86(dd)	94.88; 73.81; 773.22; 68.84; 75.35; 59.15
31	Glucose-6-phosphate	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H; C ₆ H ₂	5.22 (d); 3.56 (m); 3.72 (t); 3.56 (m); 3.96 (m); 3.98 (m)	94.71; 71.27; 75.64; 74.11; 73.26; 65.90
32	Glucose-1-phosphate	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H; C ₆ H ₂	5.45 (dd); 3.47 (m); 3.76 (m); 3.38 (t); 3.92 (m); 3.86 (m)	96.33; 75.52; 75.27; 73.15; 74.82; 63.62
33	Uridine	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H ₂ ; ¹ C ₁ H; ¹ C ₂ H	5.90 (d); 4.34 (t); 4.22 (t); 4.12 (m); 3.91 (dd); 7.87 (d); 5.88 (d)	92.05; 76.77; 72.39; 87.06; 63.54; 144.68; 104.49
34	ADP	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H ₂ ; N ¹ CHN; N ² CHN	5.94 (m); 4.57(d); 4.23 (d); 4.08 (m); 4.11 (d); 8.54 (s); 8.29 (s)	87.43; 73.45; 70.68; 65.72; 83.94; 140.42; 148.382
35	Cyclic AMP	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H ₂ ; N ¹ CHN; N ² CHN	6.13 (s); 4.75 (d); 4.54(dd); 4.34 (dd); 4.33(s); 8.17 (s); 8.19 (s)	94.22; 79.05; 69.42; 74.99; 69.10; 155.09; 142.51
36	Adenosine	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H ₂ ; N ¹ CHN; N ² CHN	6.03 (d); 4.73 (t); 4.40 (m); 4.28 (m); 3.90 (dd); 8.36 (s); 8.18 (s)	91.27; 76.43; 76.43; 88.10; 64.05; 142.97; 155.02
37	Tyrosine	C ₁ H; C ₂ H ₂ ; C ₄ H; C ₅ H	3.94 (dd); 3.17 (dd); 7.20 (d); 6.89 (d)	58.54; 37.84; 133.79;118.51
38	Tryptophan	C ₁ H; C ₂ H ₂ ; NC ₄ H; C ₆ H; C ₇ H; C ₈ H; C ₉ H	4.05 (dd); 3.46(s); 3.31 (dd); 7.31(d); 7.53 (d); 7.27 (s); 7.18 (m); 7.53(m)	58.08; 29.43; 29.31; 127.22; 114.85 124.28; 122.29; 114.85
39	Phenylalanine	C ₁ H; C ₂ H ₂ ; C ₄ H; C ₅ H; C ₆ H	3.97(m); 3.28 (m); 7.36 (m); 7.42 (m); 7.31 (m)	59.02; 39.65; 130.30; 132.50; 133.01
40	Histidine	α CH; β CH ₂ ; NCHC; NCHN	4.01 (dd); 3.20(d); 7.13 (s); 8.03 (s)	57.94; 29.20; 119.60; 138.43
41	ATP	C ₁ H; C ₂ H; C ₃ H; C ₄ H; C ₅ H ₂ ; N ¹ CHN; N ² CHN	6.14 (d); 4.81 (d); 4.65 (t); 4.38 (m); 4.30 (m); 8.54 (s); 8.24 (s)	90.04; 76.89; 74.19; 86.85; 67.57; 142.52; 155.47
42	NAD	C ₁ H; C ₂ H; C ₃ H; C ₅ H; N ¹ CHN; N ² CHN	9.33 (d); 8.19 (s); 8.86 (d); 9.20 (s); 8.12 (d); 8.41 (s)	142.17; 131.14; 147.31; 145.80; 155.32; 142.53
43	NADP	C ₁ H; C ₂ H; C ₃ H; C ₅ H; N ¹ CHN; N ² CHN	9.09 (d); 8.17 (s); 8.77 (d); 9.27 (s); 8.17 (d); 8.41(s)	144.41; 142.48; 148.75; 142.70; 131.49; 142.48
44	Citric acid	α CH; β CH ₂	2.66 (d); 2.52 (d)	48.25;48.71

Note: Bold chemical shifts indicate an identified peak in the 2D spectra.

Table S2. Fold changes of metabolites in three strains after Acetic acid treatments

Metabolites	ATCC 6962	ATCC 13076	ATCC 14028
Isoleucine	0.27±0.09 ^c	1.12±0.16 ^b	0.96±0.54 ^a
Leucine	1.24±0.07 ^b	1.48±0.21 ^a	1.08±0.05 ^b
Valine	0.96±0.18 ^b	1.46±0.20 ^a	1.16±0.05 ^a
Ethanol	0.89±0.07 ^b	0.71±0.11 ^c	1.23±0.01 ^a
Lactic acid	0.51±0.04 ^c	0.73±0.11 ^b	1.11±0.024 ^a
Alanine	1.25±0.06 ^a	1.43±0.27 ^a	1.32±0.23 ^a
Threonine	0.50±0.03 ^c	0.68±0.11 ^b	1.19±0.02 ^a
Putrescine	0.67±0.11 ^a	0.58±0.10 ^a	0.54±0.16 ^a
Acetic acid	0.78±0.06 ^c	3.41±0.58 ^a	1.69±0.03 ^b
Succinic acid	0.46±0.05 ^c	0.90±0.14 ^b	0.40±0.01 ^a
Anserine	0.66±0.07 ^c	0.99±0.06 ^a	0.91±0.07 ^b
Methionine	0.49±0.07 ^b	0.63±0.19 ^a	0.64±0.56 ^b
Cysteine	1.67±0.01 ^c	3.38±0.54 ^a	1.45±0.04 ^b
Aspartic acid	1.88±0.17 ^a	1.61±0.26 ^a	1.72±0.07 ^a
Oxoglutaric acid	0.77±0.04 ^a	1.72±0.37 ^a	0.96±0.72 ^a
Betaine	2.65±0.77 ^a	1.49±0.16 ^b	1.94±0.44 ^a
γ-aminobutyric-acid	0.32±0.04 ^b	0.56±0.11 ^a	0.25±0.15 ^b
1,2-Propanediol	0.60±0.06 ^b	0.66±0.12 ^{ab}	0.79±0.08 ^a
Glycine	0.50±0.04 ^c	3.39±0.54 ^a	1.49±0.22 ^b
Citric acid	1.40±0.24 ^a	1.75±0.39 ^a	1.49±0.35 ^a
NADP	0.88±0.40 ^b	7.54±0.07 ^a	0.81±0.06 ^b
NAD	0.79±0.06 ^b	3.38±0.49 ^a	0.81±0.06 ^b
ATP	1.14±0.19 ^b	3.52±0.59 ^a	1.04±0.06 ^b
ADP	0.95±0.15 ^b	1.64±0.25 ^a	1.14±0.09 ^b
Histidine	0.66±0.07 ^a	0.48±0.07 ^b	0.60±0.02 ^a
Phenylalanine	2.207±0.22 ^b	0.67±0.10 ^c	2.37±0.02 ^a
Tyrosine	0.23±0.01 ^b	14.29±1.21 ^a	0.53±0.05 ^b
Adenosine	2.67±0.20 ^a	1.34±0.23 ^b	1.94±0.07 ^c
G-1-P	1.55±0.17 ^b	3.27±0.48 ^a	1.45±0.16 ^b
G-6-P	2.61±0.25 ^a	0.06±0.01 ^c	1.61±0.06 ^b
β-D-Glucose	0.89±0.13 ^c	2.33±0.31 ^a	1.66±0.02 ^b
α-D-Glucose	1.24±0.11 ^b	2.35±0.37 ^a	1.43±0.08 ^b
Malic acid	0.77±0.12 ^b	0.69±0.06 ^b	1.39±0.22 ^a
F-6-P	1.72±0.21 ^b	6.21±1.41 ^a	2.10±0.05 ^b
Glutamine	0.65±0.07 ^b	1.33±0.20 ^a	0.78±0.03 ^b
Fructose	1.33±0.13 ^b	3.20±0.50 ^a	1.34±0.08 ^b

Note: The mean of different letters in the same row is significantly different ($P < 0.05$).

Table S3. Fold changes of metabolites in three strains after Citric acid treatments

Metabolites	ATCC 6962	ATCC 13076	ATCC 14028
Isoleucine	0.38±0.07 ^c	0.87±0.23 ^a	0.89±0.26 ^b
Leucine	1.31±0.17 ^a	1.25±0.13 ^a	1.28±0.14 ^a
Glutamate	0.55±0.45 ^c	1.17±0.13 ^b	0.81±0.15 ^a
Ethanol	0.92±0.07 ^b	0.71±0.11 ^c	0.78±0.13 ^a
Lactic acid	0.67±0.45 ^b	0.55±0.07 ^c	0.78±0.01 ^a
Alanine	0.42±0.12 ^c	0.95±0.12 ^b	0.68±0.12 ^a
Threonine	0.65±0.03 ^b	0.52±0.02 ^c	0.80±0.16 ^a
Putrescine	0.59±0.15 ^a	0.19±0.09 ^b	0.31±0.16 ^{ab}
Acetic acid	1.32±0.09 ^a	0.60±0.33 ^b	0.88±0.01 ^c
Succinic acid	0.55±0.45 ^b	0.53±0.31 ^b	1.02±0.02 ^a
Anserine	0.69±0.05 ^c	0.52±0.03 ^a	0.93±0.04 ^b
Pyroglutamic acid	0.75±0.06 ^b	2.34±0.31 ^a	1.07±0.03 ^b
Pyruvic acid	0.54±0.04 ^c	0.67±0.09 ^b	0.80±0.03 ^a
Acetoin	0.58±0.04 ^b	0.59±0.07 ^b	0.75±0.02 ^a
Oxoglutaric acid	0.58±0.18 ^b	1.41±0.66 ^a	1.58±0.07 ^c
Betaine	2.93±0.57 ^a	0.29±0.12 ^b	0.36±0.51 ^b
γ-aminobutyric-acid	0.59±0.05 ^b	0.42±0.07 ^b	1.04±0.40 ^a
1,2-Propanediol	0.62±0.07 ^b	0.58±0.12 ^a	0.71±0.05 ^c
Glycine	0.47±0.01 ^b	0.88±0.32 ^c	0.67±0.09 ^a
Citric acid	1.06±0.11 ^c	1.80±0.23 ^b	1.22±0.03 ^a
NADP	1.42±0.25 ^b	7.15±0.46 ^a	1.74±0.02 ^c
NAD	1.18±0.07 ^b	3.54±0.48 ^a	1.14±0.02 ^b
ATP	1.34±0.04 ^b	3.10±0.52 ^a	1.69±0.05 ^b
ADP	1.69±0.25 ^a	1.15±0.20 ^a	1.39±0.33 ^a
Histidine	0.73±0.06 ^b	0.39±0.04 ^c	0.90±0.04 ^a
Phenylalanine	1.35±0.11 ^b	1.49±0.05	1.88±0.04 ^a
Tyrosine	0.30±0.04 ^b	0.47±0.81 ^a	0.41±0.08 ^b
Tryptophan	1.59±0.28 ^a	0.34±0.03 ^a	0.42±0.07 ^b
G-1-P	1.12±0.07 ^b	2.75±0.25 ^a	1.30±0.06 ^b
Uridine	0.76±0.06 ^b	0.75±0.10 ^a	0.88±0.19 ^b
Tyrosine	0.30±0.04 ^b	8.47±0.81 ^a	0.41±0.08 ^b
Cyclic AMP	1.64±0.13 ^b	3.84±0.70 ^a	2.12±0.06 ^b
Adenosine	2.11±0.03 ^b	1.99±0.06 ^b	1.78±0.04 ^a
Malic acid	0.57±0.06 ^b	1.24±0.13 ^a	0.67±0.02 ^b
F-6-P	1.75±0.14 ^b	5.20±1.19 ^a	2.38±0.08 ^b
Fructose	1.41±0.11 ^b	2.92±0.38 ^a	1.27±0.03 ^b
Methionine	0.45±0.07 ^b	0.39±0.09 ^a	0.48±0.05 ^c
Cysteine	1.78±0.01 ^c	2.88±0.32 ^a	1.34±0.02 ^b
Aspartic acid	1.80±0.16 ^b	1.44±0.18 ^a	1.40±0.03 ^b

Note: The mean of different letters in the same row is significantly different ($P < 0.05$).

Table S4. Fold changes of metabolites in three strains after Lactic acid treatments

Metabolites	ATCC 6962	ATCC 13076	ATCC 14028
Isoleucine	1.40±0.21 ^b	1.30±0.16 ^a	1.60±0.09 ^b
Leucine	2.14±0.07 ^a	1.68±0.05 ^b	1.02±0.05 ^c
Ethanol	0.87±0.05 ^b	0.80±0.07 ^b	1.35±0.08 ^a
Lactic acid	0.86±0.04 ^b	0.73±0.11 ^b	1.18±0.08 ^a
Threonine	0.86±0.04 ^b	0.71±0.05 ^c	1.20±0.08 ^a
Methionine	0.54±0.06 ^b	0.24±0.09 ^a	0.38±0.05 ^c
Acetic acid	0.29±0.02 ^b	0.37±0.11 ^a	0.19±0.04 ^b
Succinic acid	0.80±0.04 ^a	0.71±0.40 ^a	0.45±0.08 ^a
Anserine	0.88±0.10 ^b	5.37±0.09 ^a	0.89±0.06 ^b
Cysteine	1.87±0.06 ^c	6.67±0.40 ^a	1.61±0.09 ^b
Pyruvic acid	0.64±0.04 ^c	0.59±0.09 ^b	0.72±0.03 ^a
Acetoin	0.67±0.04 ^a	0.63±0.07 ^a	0.71±0.02 ^a
Oxoglutaric acid	0.59±0.40 ^b	1.18±0.09 ^a	0.22±0.12 ^b
Betaine	3.88±3.55 ^a	0.37±0.19 ^b	1.51±0.11 ^c
γ-aminobutyric-acid	0.14±0.04 ^b	0.45±0.05 ^a	0.23±0.09 ^b
1,2-Propanediol	0.69±0.12 ^a	0.58±0.10 ^a	0.61±0.03 ^a
Glycine	0.37±0.01 ^c	6.67±0.40 ^b	1.51±0.09 ^a
Citric acid	1.51±0.44 ^a	1.29±0.10 ^a	1.36±0.11 ^a
NADP	11.27±1.16 ^b	25.14±2.52 ^a	1.77±0.04 ^c
NAD	7.07±0.34 ^b	13.25±1.21 ^a	1.75±0.02 ^c
ATP	1.39±0.09 ^b	3.19±0.46 ^a	1.02±0.05 ^b
Adenosine	1.42±0.02 ^b	1.50±0.03 ^b	1.31±0.06 ^a
ADP	1.04±0.14 ^b	1.54±0.12 ^a	1.05±0.08 ^b
Histidine	0.96±0.05 ^a	0.49±0.04 ^b	0.26±0.07 ^c
Phenylalanine	2.98±0.11 ^a	2.78±0.03 ^c	2.68±0.16 ^b
Tyrosine	0.45±0.03 ^b	5.24±0.23 ^a	0.57±0.04 ^b
Tryptophan	1.72±0.62 ^a	0.56±0.17 ^b	0.70±0.07 ^b
Glutamine	1.66±0.04 ^b	2.27±0.11 ^a	0.69±0.04 ^c
β-D-Glucose	2.17±0.09 ^c	3.06±0.12 ^b	2.08±0.12 ^a
α-D-Glucose	1.25±0.04 ^b	5.07±0.30 ^a	1.53±0.07 ^b
Cyclic AMP	1.75±0.13 ^c	3.23±0.09 ^a	2.64±0.06 ^b
Malic acid	2.40±0.14 ^b	0.40±0.14 ^a	0.48±0.02 ^a
F-6-P	2.86±0.11 ^b	8.42±1.88 ^a	2.39±0.22 ^b
Fructose	4.51±0.22 ^b	7.94±0.50 ^a	1.40±0.08 ^c
Aspartic acid	5.79±0.24 ^a	3.97±0.26 ^b	2.14±0.16 ^c

Note: The mean of different letters in the same row is significantly different ($P < 0.05$).

Table S5. List of metabolic pathway analysis for screened metabolites in ATCC 6962

Treatments	Metabolite set	Total	Hits	Raw <i>P</i>
Acetic acid	Aminoacyl-tRNA biosynthesis	48	9	0.000000
	Histidine metabolism	16	4	0.000017
	Glycine, serine and threonine metabolism	33	4	0.000334
	Starch and sucrose metabolism	18	3	0.000809
	beta-Alanine metabolism	21	3	0.001292
	Glutathione metabolism	28	3	0.003033
	Alanine, aspartate and glutamate metabolism	28	3	0.003033
	Arginine biosynthesis	14	2	0.009539
	Pantothenate and CoA biosynthesis	19	2	0.017357
	Neomycin, kanamycin and gentamicin biosynthesis	2	1	0.021822
	Glycolysis / Gluconeogenesis	26	2	0.031535
	Porphyrin and chlorophyll metabolism	30	2	0.041138
	Phenylalanine, tyrosine and tryptophan biosynthesis	4	1	0.043196
	Glyoxylate and dicarboxylate metabolism	32	2	0.046309
Cysteine and methionine metabolism	33	2	0.048981	
Citric acid	Aminoacyl-tRNA biosynthesis	48	5	0.000323
	Glutathione metabolism	28	4	0.000414
	Alanine, aspartate and glutamate metabolism	28	4	0.000414
	Nicotinate and nicotinamide metabolism	15	3	0.000879
	Phenylalanine, tyrosine and tryptophan biosynthesis	4	2	0.001033
	Starch and sucrose metabolism	18	3	0.001536
	Glycolysis / Gluconeogenesis	26	3	0.004564
	Phenylalanine metabolism	10	2	0.007372
	Amino sugar and nucleotide sugar metabolism	37	3	0.012389
	Arginine biosynthesis	14	2	0.014428
	Butanoate metabolism	15	2	0.016513
	Histidine metabolism	16	2	0.018719
	Neomycin, kanamycin and gentamicin biosynthesis	2	1	0.026922
	Citrate cycle (TCA cycle)	20	2	0.028688
beta-Alanine metabolism	21	2	0.031451	
Lactic acid	Aminoacyl-tRNA biosynthesis	48	11	0.000000
	Alanine, aspartate and glutamate metabolism	28	4	0.000275
	Glyoxylate and dicarboxylate metabolism	32	4	0.000467
	Histidine metabolism	16	3	0.000792
	Phenylalanine, tyrosine and tryptophan biosynthesis	4	2	0.000842
	Glycolysis / Gluconeogenesis	26	3	0.003400
	Valine, leucine and isoleucine biosynthesis	8	2	0.003817
	Glutathione metabolism	28	3	0.004218
	Phenylalanine metabolism	10	2	0.006045
	Amino sugar and nucleotide sugar metabolism	37	3	0.009328
	Arginine biosynthesis	14	2	0.011871

Starch and sucrose metabolism	18	2	0.019384
Pantothenate and CoA biosynthesis	19	2	0.021507
beta-Alanine metabolism	21	2	0.026030
Galactose metabolism	27	2	0.041650
Porphyrin and chlorophyll metabolism	30	2	0.050506

Table S6. List of metabolic pathway analysis for screened metabolites in ATCC 13076

Treatments	Metabolite set	Total	Hits	Raw <i>P</i>
Acetic acid	Alanine, aspartate and glutamate metabolism	28	6	0.000000
	Aminoacyl-tRNA biosynthesis	48	7	0.000000
	Arginine biosynthesis	14	3	0.000307
	Butanoate metabolism	15	3	0.000381
	Histidine metabolism	16	3	0.000466
	D-Glutamine and D-glutamate metabolism	6	2	0.001464
	Valine, leucine and isoleucine biosynthesis	8	2	0.002699
	Glyoxylate and dicarboxylate metabolism	32	3	0.003732
	Glycine, serine and threonine metabolism	33	3	0.004079
	Arginine and proline metabolism	38	3	0.006111
	Starch and sucrose metabolism	18	2	0.013886
	Citrate cycle (TCA cycle)	20	2	0.017038
	beta-Alanine metabolism	21	2	0.018719
	Neomycin, kanamycin and gentamicin biosynthesis	2	1	0.020545
	Glycolysis / Gluconeogenesis	26	2	0.028112
	Glutathione metabolism	28	2	0.032306
	Porphyrin and chlorophyll metabolism	30	2	0.036734
Phenylalanine, tyrosine and tryptophan biosynthesis	4	1	0.040694	
Citric acid	Starch and sucrose metabolism	18	3	0.000350
	Phenylalanine, tyrosine and tryptophan biosynthesis	4	2	0.000386
	Aminoacyl-tRNA biosynthesis	48	4	0.000472
	Phenylalanine metabolism	10	2	0.002815
	Purine metabolism	65	3	0.014896
	Neomycin, kanamycin and gentamicin biosynthesis	2	1	0.016709
	Glycolysis / Gluconeogenesis	26	2	0.018845
	Glutathione metabolism	28	2	0.021712
	Amino sugar and nucleotide sugar metabolism	37	2	0.036660
	Lactic acid	Phenylalanine, tyrosine and tryptophan biosynthesis	4	2
Phenylalanine metabolism		10	2	0.001999
Aminoacyl-tRNA biosynthesis		48	3	0.003864
Citrate cycle (TCA cycle)		20	2	0.008117
Alanine, aspartate and glutamate metabolism		28	2	0.015655
D-Glutamine and D-glutamate metabolism		6	1	0.041899

Table S7. List of metabolic pathway analysis for screened metabolites in ATCC 14028

Treatments	Metabolite set	Total	Hits	Raw <i>P</i>
Acetic acid	Aminoacyl-tRNA biosynthesis	48	6	0.000003
	Starch and sucrose metabolism	18	3	0.000549
	Glutathione metabolism	28	3	0.002079
	Glyoxylate and dicarboxylate metabolism	32	3	0.003075
	Amino sugar and nucleotide sugar metabolism	37	3	0.004679
	Butanoate metabolism	15	2	0.008538
	Nicotinate and nicotinamide metabolism	15	2	0.008538
	Neomycin, kanamycin and gentamicin biosynthesis	2	1	0.019267
	Glycolysis / Gluconeogenesis	26	2	0.024852
	Alanine, aspartate and glutamate metabolism	28	2	0.028584
	Porphyrin and chlorophyll metabolism	30	2	0.032529
Phenylalanine, tyrosine and tryptophan biosynthesis	4	1	0.038188	
Arginine and proline metabolism	38	2	0.050279	
Citric acid	Phenylalanine, tyrosine and tryptophan biosynthesis	4	2	0.000754
	Starch and sucrose metabolism	18	3	0.000963
	Aminoacyl-tRNA biosynthesis	48	4	0.001802
	Phenylalanine metabolism	10	2	0.005427
	Amino sugar and nucleotide sugar metabolism	37	3	0.007986
	Nicotinate and nicotinamide metabolism	15	2	0.012234
	Neomycin, kanamycin and gentamicin biosynthesis	2	1	0.023098
	Glycolysis / Gluconeogenesis	26	2	0.035115
Purine metabolism	65	3	0.036599	
Lactic acid	Aminoacyl-tRNA biosynthesis	48	7	0.000000
	Phenylalanine, tyrosine and tryptophan biosynthesis	4	2	0.000450
	Valine, leucine and isoleucine biosynthesis	8	2	0.002058
	Phenylalanine metabolism	10	2	0.003273
	Histidine metabolism	16	2	0.008461
	Pantothenate and CoA biosynthesis	19	2	0.011871
	beta-Alanine metabolism	21	2	0.014428
	Glycolysis / Gluconeogenesis	26	2	0.021761

Table S8. Loading plot table derived from principal component analysis.

Metabolite	PC1	PC2
Adenosine	-0.021	0.021
Cyclic AMP	-0.016	0.018
PCA	-0.027	0.015
Acetic acid	-0.012	0.010
G-1-P	-0.007	0.097
GABA	-0.012	0.107
Tyr	-0.002	0.005
ATP	0.006	0.228
Ethanol	0.007	0.150
α -D-Glucose	0.008	0.104
β -D-Glucose	0.006	0.119
ADP	0.012	0.078
Glu	0.012	0.007
1,2-Propanediol	0.007	0.073
Uridine	0.066	-0.009
Phe	0.004	-0.001
Thr	0.333	-0.003
Pyruvic acid	0.013	0.048
Anserine	0.075	0.009
Succinic acid	0.104	0.010
Ilu	0.066	-0.009
Gln	0.122	-0.026
His	0.068	-0.009
G-6-P	0.045	-0.016
Acetoin	0.146	-0.008
Lactic acid	0.289	-0.009