

## **Supplementary Materials**

### **Influence of Storage Conditions and Preservatives on Metabolite Fingerprints in Urine**

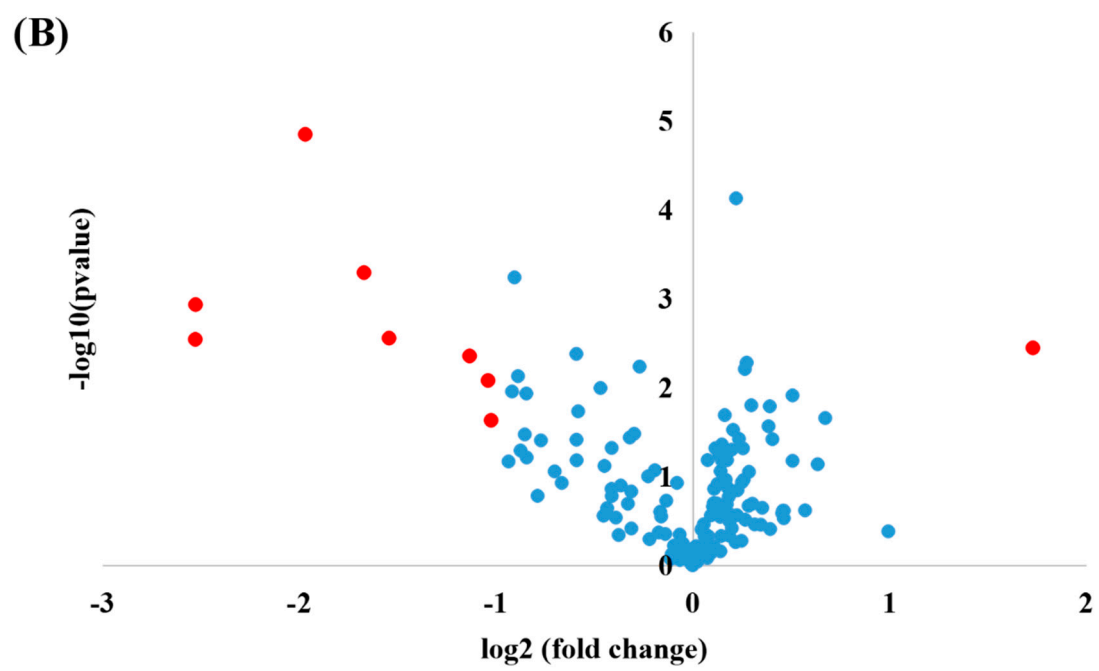
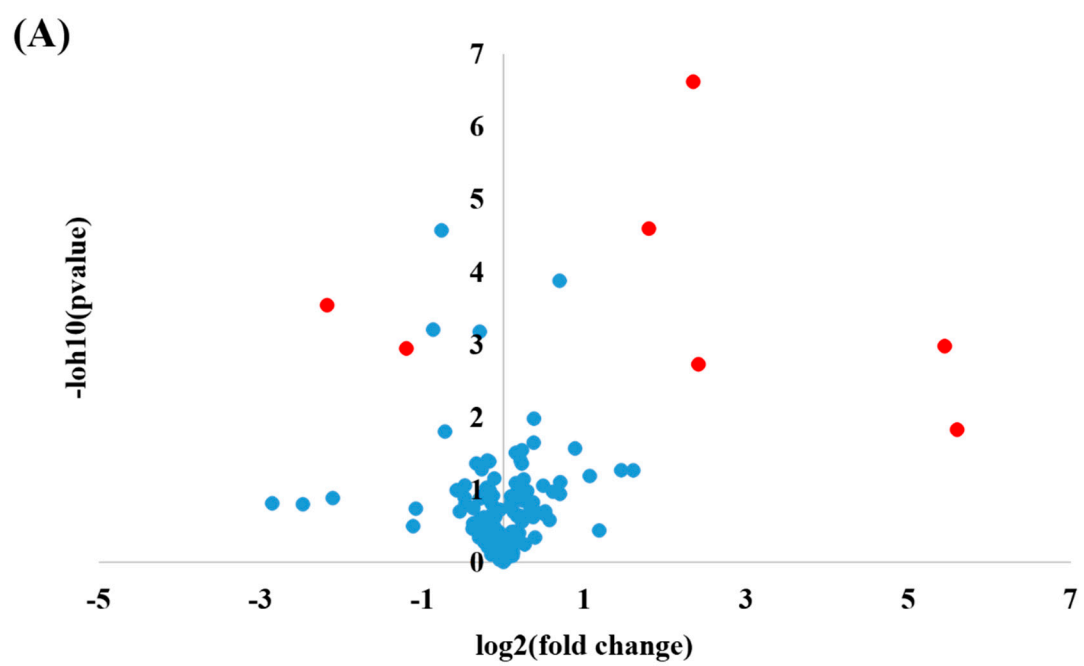
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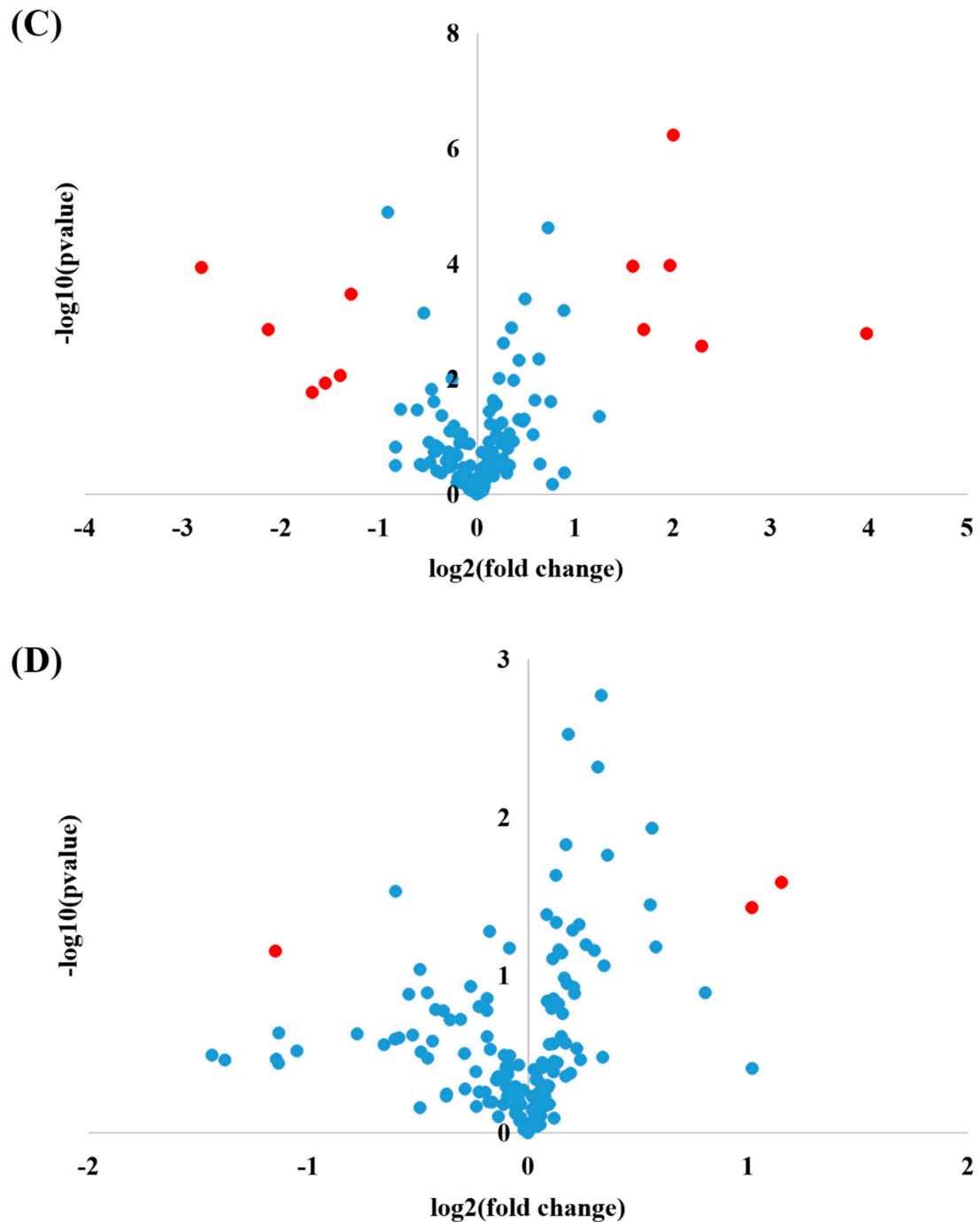
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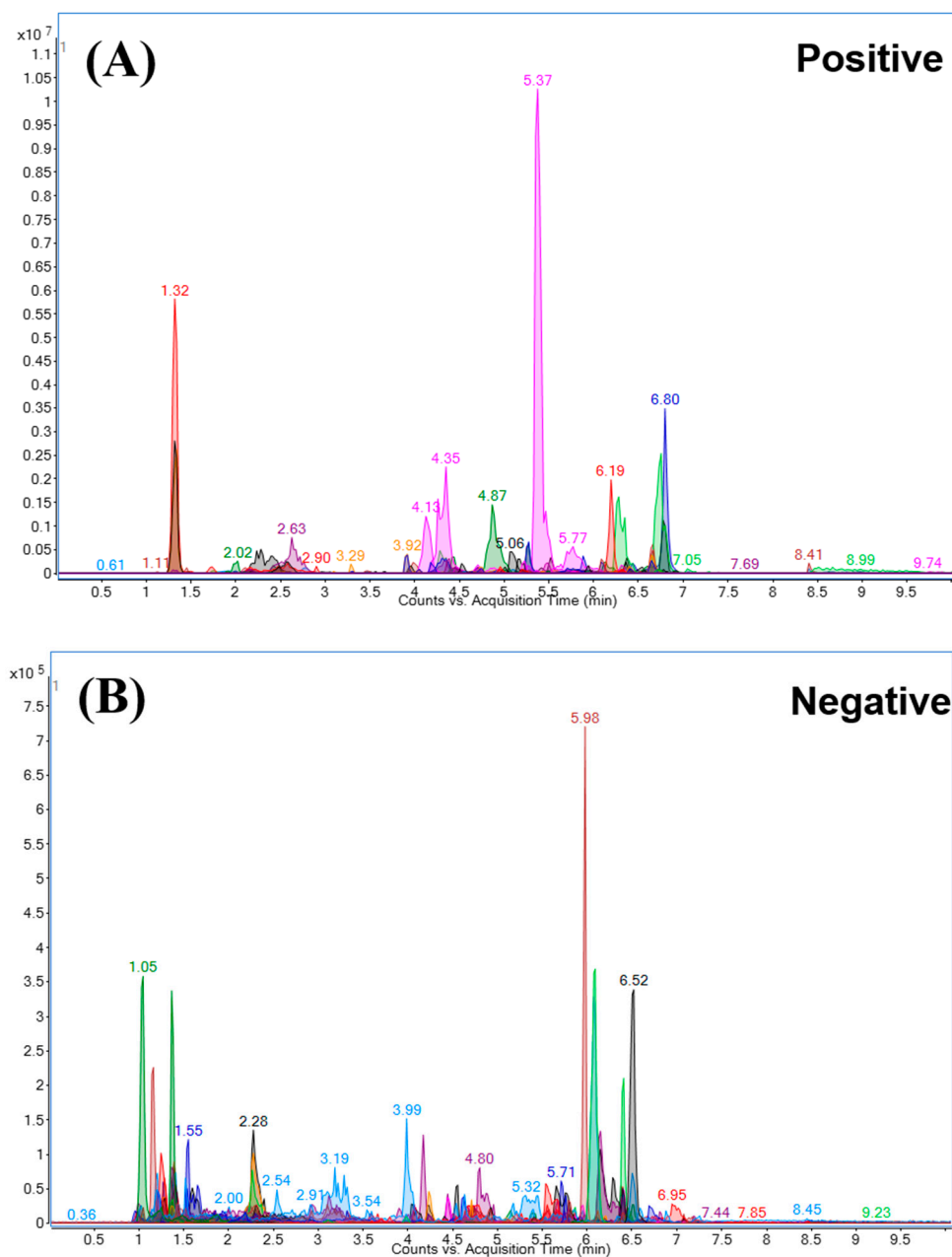
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**Supplementary Figure 1.** Volcano plots of no preservative versus preservatives for urine samples stored at  $-20^{\circ}\text{C}$ ,  $4^{\circ}\text{C}$  for 24-h/48-h, and at  $22^{\circ}\text{C}$  for 24-h **in the PABA group:** (A) no preservative versus boric acid, (B) no preservative vs. thymol; and **in the No PABA group:** (C) no preservative vs. boric acid, (D) no preservative vs. thymol. Red dots indicate metabolites with p-value  $< 0.05$  and fold change  $> 2$  or  $< 0.5$ .



**Supplementary Figure 2.** Chromatograms by targeted liquid chromatography tandem mass spectrometry (LC-MS/MS)-based metabolomics in (A) positive ion mode and (B) negative ion mode.

**Supplementary Table 1.** Significantly altered metabolites caused by boric acid and thymol compared to urine samples with No Preservative stored at -20°C, 4°C for 24-h/48-h, and at 22°C for 24-h in the PABA and No PABA Group

Metabolite	P-value	Fold Change (NP)/(BA)	Metabolite changes*
<b>PABA group</b>			
Boric Acid vs. No Preservative			
Pyridoxine	0.015	49.600	Decreased
2-Deoxyadenosine	0.001	38.289	Decreased
D-Galacturonic acid	0.002	5.054	Decreased
belta-Hydroxyisovaleric acid	<0.001	4.787	Decreased
Xanthurenic acid	<0.001	3.631	Decreased
Adenosine	<0.001	0.205	Increased
GA3P	0.001	0.428	Increased
Thymol vs. No Preservative			
3-Methyladipic acid	<0.001	3.708	Decreased
3-Hexenedioic acid	<0.001	0.176	Increased
Isovaleric acid	<0.001	0.232	Increased
Agmatine	<0.001	0.322	Increased
Dopamine	0.015	0.444	Increased
Citrulline	0.003	0.454	Increased
Alpha-KG/Adipic acid	0.016	0.465	Increased
2-Methylglutaric acid	0.030	0.473	Increased
Glutamic acid	0.044	0.494	Increased
<b>No PABA Group</b>			
Boric Acid vs. No Preservative			
2-Deoxyadenosine	<0.001	13.129	Decreased
Pyridoxine	0.003	4.909	Decreased
Adenine	0.001	3.257	Decreased
Xanthurenic acid	<0.001	4.344	Decreased
Belta-Hydroxyisovaleric acid	<0.001	3.969	Decreased

D-Galacturonic acid	<0.001	3.017	Decreased
Isovaleric acid	0.001	0.229	Increased
Adenosine	0.001	0.168	Increased
Alpha-KG/Adipic acid	<0.001	0.411	Increased
Dopamine	0.002	0.263	Increased
Pentadecanoic acid	0.002	0.380	Increased
Phenylglyoxylic acid	0.005	0.394	Increased
<hr/> Thymol vs. No Preservative <hr/>			
Tryptamine	0.009	2.013	Decreased
Anthranilic acid	0.026	2.225	Decreased
Lauric acid	0.031	0.480	Increased