

Figure S1. Inhibitory effect of 2,3,4-trihydroxybenzoic acid on the activity of α -amylase.

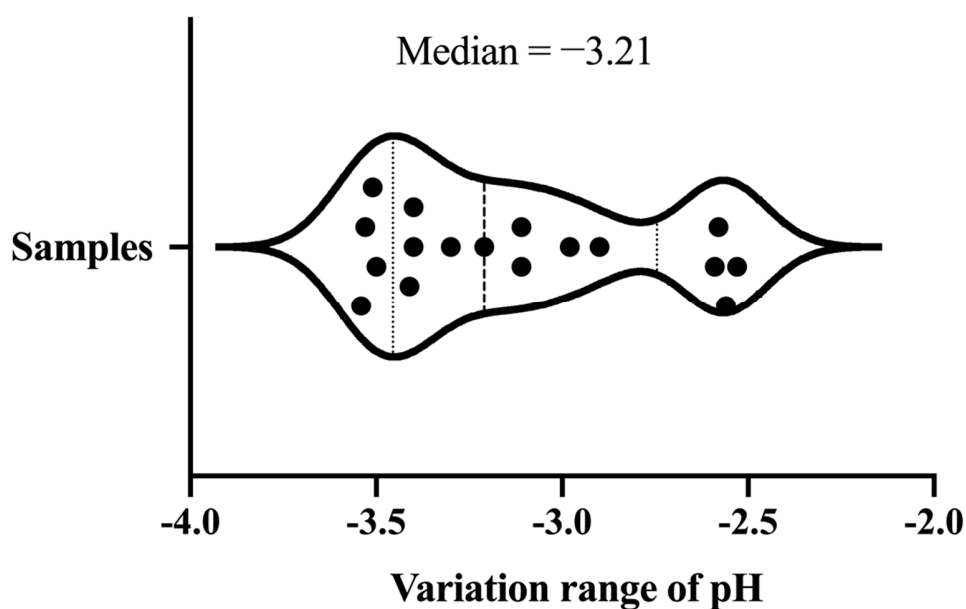


Figure S2. The effect of the maximum concentration of benzoic acid and its derivatives on the pH value of the reaction system before adjusting the concentration of the PBS buffer.

Table S1. CDOCKER Energy and CDOCKER Interaction Energy data for benzoic acid and its derivatives.

| Compound No. | Compound Name | CDOCKER Energy * (kcal·mol ⁻¹) | CDOCKER Interaction Energy * (kcal·mol ⁻¹) |
|--------------|-------------------------------------|---|---|
| 1 | Benzoic acid | -13.0580 | -15.5730 |
| 2 | 4-Hydroxybenzoic acid | -18.3349 | -19.0955 |
| 3 | 2,4-Dihydroxybenzoic acid | -16.5076 | -17.9185 |
| 4 | 3,4-Dihydroxybenzoic acid | -23.7652 | -19.9858 |
| 5 | 2,3,4-Trihydroxybenzoic acid | -17.7669 | -27.9624 |
| 6 | 2,4,6-Trihydroxybenzoic acid | -16.5577 | -18.5385 |
| 7 | 3,4,5-Trihydroxybenzoic acid | -22.1409 | -20.6498 |
| 8 | 4-Methylbenzoic acid | -16.1707 | -18.1230 |
| 9 | 4-Hydroxy-2-methylbenzoic acid | -20.5714 | -25.4675 |
| 10 | 4-Hydroxy-3-methylbenzoic acid | -19.0811 | -20.4046 |
| 11 | 4-Hydroxy-3,5-dimethylbenzoic acid | -21.6985 | -23.6935 |
| 12 | 2,4-Dihydroxy-6-methylbenzoic acid | -14.9262 | -18.8302 |
| 13 | 4-Methoxybenzoic acid | -15.0808 | -19.6385 |
| 14 | 4-Hydroxy-2-methoxybenzoic acid | -16.3666 | -24.9607 |
| 15 | 4-Hydroxy-3-methoxybenzoic acid | -19.6819 | -21.8122 |
| 16 | 3,4-Dihydroxy-5-methoxybenzoic acid | -24.6296 | -27.9799 |
| 17 | 4-Hydroxy-3,5-dimethoxybenzoic acid | -10.1005 | -25.4468 |

* The CDOCKER Energy and CDOCKER Interaction Energy for the top ranked binding poses of 17 phenolic acids obtained after conducting the molecular docking studies on the α -amylase (PDB ID: 4W93 using the CDOCKER algorithm in the software Discovery Studio 2019, BIOVIA Inc., San Diego, CA, USA).