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## Data Article

## Interactive effects of gallic/ferulic/caffeic acids and anthocyanins on pigment thermal stabilities

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## ABSTRACT

The data presented in this article are related to the research article entitled “The effects of gallic/ferulic/caffeic acids on colour intensification and anthocyanin stability” (Qian et al., 2017) [1]. This paper described preparation and isolation of anthocyanins from purple sweet potatoes (PSP) and the time-course of anthocyanin profiles treated with gallic, ferulic, or caffeic acids at 95 °C. The color appearance of PSP anthocyanins alone, or with gallic, ferulic, or caffeic acids was described after the 15 h of thermal treatment. The high resolution mass spectrographs of PSP anthocyanins were determined using UPLC-ESI-HRMS. The spatial interaction of peonidin 3-O-(2-O-β-D-glucopyranocyl-β-D-glucopyranoside)-5-O-β-D-glucopyranoside and gallic/ferulic/caffeic acids was illustrated by molecular dynamic simulation.

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## Specifications Table

Subject area	Chemistry
More specific subject area	Pigments and food colorants
Type of data	Figure

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E-mail address: [pjing@sjtu.edu.cn](mailto:pjing@sjtu.edu.cn) (P. Jing).<http://dx.doi.org/10.1016/j.dib.2017.04.036>2352-3409/© 2017 Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

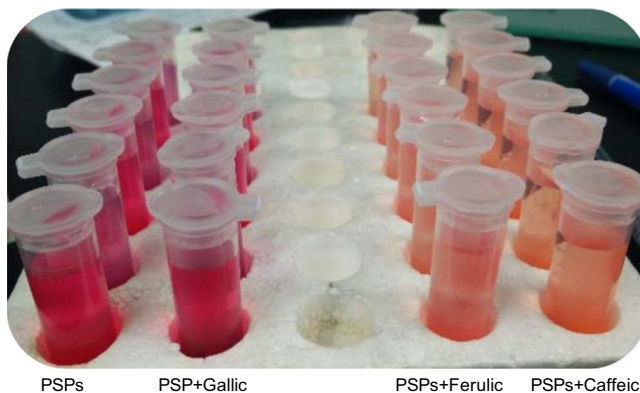
How data was acquired	HPLC, mass spectroscopy, computer simulation
Data format	Raw data collection and analysis
Experimental factors	Thermal treatment
Experimental features	Experimental and theoretical studies. 3 replicates were used in the experiment as complete randomized design. Computationally analyzed.
Data source location	Shanghai, China
Data accessibility	The data is with this article.

### Value of the data

- Data of anthocyanin profiles during thermal treatment can be valuable to further study for stability of individual anthocyanin complexes with gallic, ferulic, or caffeic acids.
- The data provide a theoretically understanding the interaction of peonidin 3-O-(2-O- $\beta$ -D-glucopyranocyl- $\beta$ -D-glucopyranoside)-5-O- $\beta$ -D-glucopyranoside with gallic, ferulic, or caffeic acids.
- Identification of the interaction of anthocyanins and other potential copigments serve as the paradigm for the researcher in further studies for pigments and food colorants.

### 1. Data

Anthocyanins in complexes with gallic/ferulic/caffeic acids were evaluated using an accelerated stability test at 95 °C, and sampled at regular intervals (0, 0.5, 1, 2, 5, 10, and 15 h). Fig. 1.1 shows the color appearance of anthocyanin complexes collected at 15 h. Fig. 1.2 shows the dynamic variation in anthocyanins added with gallic/ferulic/caffeic acids by HPLC profiles. Fig. 1.2 shows the remaining anthocyanins during thermal treatment at 95 °C. Fig. 1.2b–d shows the remaining anthocyanins with gallic, ferulic, or caffeic acids during thermal treatment at 95 °C. Anthocyanins in PSPs were identified *via* a high-resolution mass spectrometer in Figs. 1.3–1.18. Additionally, Fig. 1.19 shows molecular dynamics simulation for analysis of the copigmentation behavior of gallic (Fig. 1.19a), ferulic (Fig. 1.19b), and caffeic (Fig. 1.19c) acids over peonidin 3-O-(2-O- $\beta$ -D-glucopyranocyl- $\beta$ -D-glucopyranoside)-5-O- $\beta$ -D-glucopyranoside, which was predominant in PSPs.



**Fig.1.1.** Samples of complexes of PSP anthocyanins with gallic, ferulic, or caffeic acids at 95 °C for 15 h.

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