Data Article

Data for β-lactoglobulin conformational analysis after (-)-epigallocatechin gallate and metal ions binding

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\textbf{Article history:}
Received 2 December 2016
Received in revised form 7 December 2016
Accepted 12 December 2016
Available online 21 December 2016

\textbf{Abstract}
This data article contains complementary results related to the paper “Effect of metal ions on the binding reaction of (-)-epigallocatechin gallate to β-lactoglobulin” (Zhang et al., 2017) [1]. Data was obtained by circular dichroism (CD) spectroscopy to investigate potential β-lactoglobulin (β-Lg) conformational changes with different concentrations of EGCg and Cu\textsuperscript{2+} or Al\textsuperscript{3+} added to β-Lg. 500 μL of the 25 μM β-Lg solution containing EGCg (25 μM) or metal ions (0–500 μM) were measured, and the spectra were recorded. CD spectroscopy data present in this article indicated that the β-Lg-Cu, β-Lg-Al and β-Lg-EGCg interaction resulted in unfolding of the secondary structure of β-Lg.

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\section*{Specifications Table}

| Subject area         | Chemistry                      |
|----------------------|--------------------------------|
| More specific subject area | Polyphenol chemistry          |

DOI of original article: http://dx.doi.org/10.1016/j.foodchem.2016.11.158
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http://dx.doi.org/10.1016/j.dib.2016.12.021
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Type of data | Figure
---|---
How data was acquired | MOS-500 spectropolarimeter (Bio-Logic, France)
Data format | Analyzed
Experimental factors | CD spectroscopy was performed with the method of Li et al. [2].
Experimental features | All samples were prepared in 20 mM PBS buffer at pH 7.4. 500 µL of the 25 µM β-Lg solution containing EGCg (25 µM) or metal ions (0–500 µM) were measured, and the spectra were recorded.
Data source location | Nanjing, China
Data accessibility | Data is with this article

Value of the data

- The data provides some additional data on the effects of metal ions on the binding reaction of EGCg to β-Lg.
- The data indicated the conformational change of β-Lg after binding with EGCg or metal ions Cu, Al.
- The interaction between [β-Lg-Cu] and [β-Lg-Al] results in unfolding of the secondary structure of β-Lg.
- This data provide insights in understanding the effects of metal ions on the binding reaction of polyphenol compounds to β-Lg.

1. Data

Fig. 1 reports the CD spectra of β-Lg with different concentrations of EGCg or Cu²⁺ or Al³⁺. The negative bands at 222 nm could indicate the α-helix structure of the proteins [1,3].

2. Experimental design, materials and methods

2.1. Materials

EGCg (≥ 95%) and β-Lg (A variant, purity ≥ 90%) were purchased from Sigma-Aldrich Co. (St. Louis, MO, USA). Working solutions of EGCg (0.25 mM) were prepared by dissolving the EGCg in a 50% methanol solution. The working solution of β-Lg (25 µM) was prepared in 20 mM PBS buffer, pH 7.4 and stored in a refrigerator prior to use. The β-Lg and EGCg concentrations were determined spectrophotometrically by their extinction coefficients: \(\varepsilon_{280}(\beta-Lg) = 17600 \text{ M}^{-1} \text{ cm}^{-1}\) and \(\varepsilon_{280}(\text{EGCg}) = 9700 \text{ M}^{-1} \text{ cm}^{-1}\) at 280 nm [4,5]. For in vitro experiments, the working solutions of Cu²⁺ and Al³⁺ (1.0 mM) were prepared by dissolving CuCl₂·2H₂O and AlCl₃, respectively, in double-distilled water containing 0.1 M HCl to facilitate dissolution. All other reagents and solvents were of analytical reagent grade and used without further purification. All aqueous solutions were prepared using freshly double-distilled water.

2.2. Experimental design

CD spectroscopy was performed using a MOS-500 spectropolarimeter (Bio-Logic, France) with the modified method of Li et al. [2]. The CD spectra of the β-Lg, [β-Lg-EGCg] and [β-Lg-metal] systems were recorded between 190 and 250 nm by scanning the spectrum at 25 °C, with a scanning speed of 100 nm min⁻¹, 2 s response time, and 1.0 nm step size. All samples were prepared in 20 mM PBS buffer at pH 7.4. To investigate the effect of EGCg, Cu²⁺ and Al³⁺ on the secondary structure of β-Lg, 500 µL of the 25 µM β-Lg solution containing EGCg (25 µM) or metal ions (0–500 µM) were measured, and the spectra were recorded. The samples were loaded into a rectangular quartz cuvette with a path...
length of 1 mm. The spectra of three consecutive scans were averaged and corrected by subtracting the solvent/buffer spectra.

Acknowledgements

This work was supported by the Key Lab. of Biomass and Energy and Material Jiangsu Province (KLBE) (JSBEM-S-201707) and National Key Research and Development Plan (2016YFD0600806).

Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.12.021.

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