Data in Brief 10 (2017) 474–477

Contents lists available at ScienceDirect

Data in Brief

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Data Article

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

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ARTICLE INFO

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

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^{2+} or Al^{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.

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

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 Cu^{2+} or Al^{3+}. 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: ε_{280}(β-Lg) = 17600 M^{-1} cm^{-1} and ε_{280}(EGCg) = 9700 M^{-1} cm^{-1} at 280 nm [4,5]. For *in vitro* experiments, the working solutions of Cu^{2+} and Al^{3+} (1.0 mM) were prepared by dissolving $CuCl_2 \cdot 2H_2O$ and $AlCl_3$, 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, Cu^{2+} and Al^{3+} 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

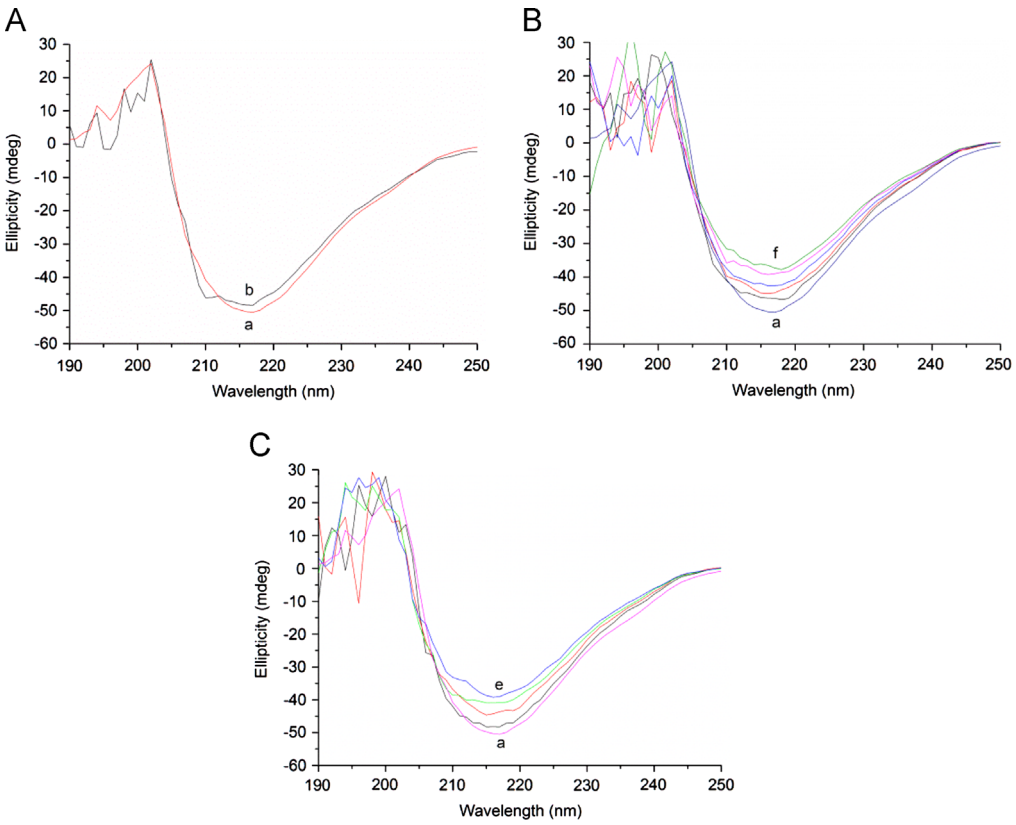

Fig. 1. (A) CD spectra of β-Lg-EGCg system. a, (25 μM β-Lg), b (25 μM EGCg); (B) CD spectra of β-Lg-Cu system. a, (25 μM β-Lg), $c(Cu^{2+})$: a (0), b (100 μM), c (200 μM), d (300 μM), e (400 μM), f (500 μM); (C) CD spectra of β-Lg-Al system. a (25 μM β-Lg), $c(Al^{3+})$: a (0), b (100 μM), c (200 μM), d (300 μM), e (400 μM).

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 (KLBEM) (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.

References

[1] L.L. Zhang, I.D. Sahu, M. Xu, Y.M. Wang, X.Y. Hu. Effect of metal ions on the binding reaction of (-)-epigallocatechin gallate to β-lactoglobulin, Food Chem. 221 (2017) 1923–1929.

[2] R.F. Li, Z.F. Lu, Y.N. Sun, S.H. Chen, Y.J. Yi, H.R. Zhang, S.Y. Yang, G.H. Yu, L. Huang, C.N. Li, Molecular design, structural analysis and antifungal activity of derivatives of peptide CGA-N46, Interdiscip. Sci. Comput. Life Sci. 8 (2016) 319–326.
[3] K. Shiraki, K. Nishikawa, Y. Goto, Trifluoroethanol-induced stabilization of the α-helical structure of β-lactoglobulin: implication for non-hierarchical protein folding, J. Mol. Biol. 245 (1995) 180–194.
[4] M. Li, A.E. Hagerman, Role of the flavan-3-ol and galloyl moieties in the interaction of (-)-epigallocatechin gallate with serum albumin, J. Agric. Food Chem. 62 (2014) 3768–3775.
[5] J. Yang, J.R. Powers, S. Clark, A.K. Dunker, B.G. Swanson, Hydrophobic probe binding of β-lactoglobulin in the native and molten globule state induced by high pressure as affected by pH, KIO_3 and N-ethylmaleimide, J. Agric. Food Chem. 50 (2002) 5207–5214.