Electronic Supplementary Information

Competitive interactions between glucose and lactose with BSA. Which sugar is better for children?

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1. The application of the infrared self-deconvolution with second derivative resolution enhancement and curve-fitting procedures to evaluate the secondary structure of BSA

The overall shape of the amide I band is determined by the various secondary structure components, such as α-helix (1650-1660 cm^{-1}), β-sheet (1610-1640 cm^{-1}), β-turn structure (1660-1680 cm^{-1}), β-antiparallel (1680-1690 cm^{-1}) and random coil (1641-1648 cm^{-1}) (J. A. Pierce, R. S. Jackson, K. W. Vanevery, P. R. Griffiths and H. J. Gao, *Anal. Chem.*, 1990, **62**, 477–484). A quantitative analysis of the protein secondary structure for the free BSA and its sweeters adducts has been carried out, and the result are showed in Figs. 1A-1C. The free protein was 45.16% α-helix (1652 cm^{-1}), 18.01% β-sheet (1602, 1612 and 1625 cm^{-1}), 10.32% β-turn structure (1664 and 1674 cm^{-1}), 3.23% β-antiparallel (1682 cm^{-1}), and 23.23% random coil (1640 cm^{-1}). The results are consistent with the spectroscopic studies of bovine serum albumin previously reported (P. Bourassa, C. D. Kanakis, P. Tarantilis, M. G. Pollissiou and H. A. Tajmir-Riahi, *J. Phys. Chem. B*, 2010, **114**, 3348–3354). Upon sweeters interaction, a major decrease of α-helix from 45.16% (free BSA) to 38.22% (glucose-BSA) and 42.49% (lactose-BSA) with a decrease in β-sheet from 18.01% (free BSA) to 13.22% (glucose), 17.28% (lactose) was observed. An increase was observed for the β-turn structure from 10.32% (free BSA) to 14.33% (glucose), 11.90% (lactose). Similarly, a similar increase was also observed for the β-anti and random coil for glucose-BSA and lactose-BSA. These results are consistent with the decrease in the intensity of the protein amide I band discussed above. The results show that the influence of glucose on the protein conformational change seems to be more prominent than that of lactose, which makes BSA unfold and adapt a more incompact conformational state.

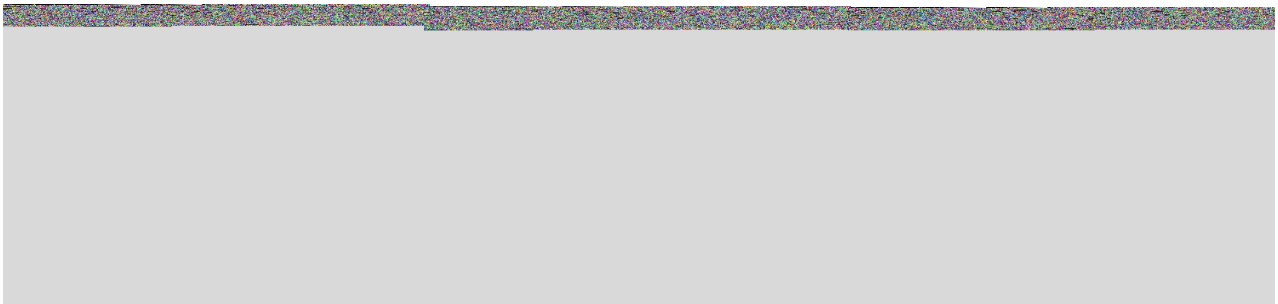

Fig. S 1A-C. Curve-fitted amide I region (1700-1600 cm^{-1}) of free BSA and its lactose-BSA/glucose-BSA complex.

2. The glucose-to-BSA ratio is about 7:1, which is higher than that found with the ratio obtained initially when BSA was involved with small molecules

Crystal structure of BSA is a heart–shaped helical monomer composed of three homologous domains named I, II, III and each domain includes two sub-domains called A and B to form a cylinder (Y. Z. Zhang, B. Zhou and B. Zhang, *J. Hazard. Mater.*, 2009, **163**, 1345–1352). The principal regions of ligand-binding sites on albumin are located in hydrophobic cavities in sub-domains IIA and IIIA, which exhibit similar chemical properties. The binding ratio of small molecules with BSA is different. Generally, the binding ratio of ligand-to-BSA is 1:1 or 2:1. However, there are some small molecules which have high binding ratio with BSA. The molar binding ratio of the tannic acid with BSA is about 10 (M. L. Liu, Y. Y. Zhang, Q. Yang, Q. J. Xie and S. Z. Yao, *J. Agric. Food Chem*., 2006, **54**, 4087–4094) and the Antithrombin with BSA is 6 (B. B. Minsky, B. Q. Zheng and P. L. Dubin, *Langmuir*, 2014, **30**, 278–287). The ligand-to-BSA ratio of about 7:1 is credible and the ratio is adjacent to the blood glucose level. Glucose, the most absorbable sugar, is frequently used for recovery of a patient, young or old; also, the intravenous infusion of glucose solution can be used for supplying electrolytes and vitamins. Thus, the consumption of sweets, cakes and cookies, i.e. the intake of the so-called simple carbohydrates, which are quickly digested, would lead to a rapid rise in blood sugar.