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Investigation on the interactions between glucomannans and bifidobacterium protein by using molecular dynamics simulations

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Abstract

Konjac glucomannan is a polysaccharide extracted from the Amorphophallus konjac K.Koch plant. It is often used as food additives due to their low toxicity, biodegradability and low calories. The unique properties of konjac glucomannan is its prebiotic activities. Konjac glucomannan which cannot be digested and absorbed in human stomachs and small intestines. Therefore, it is fermented in the large intestine and becomes food for the beneficial bacteria or probiotics especially bifidobacteria and lactobacilli in human colons. This study examined the effect of the size of konjac glucomannan on the prebiotic property. The interactions between the different degrees of polymerization of konjac glucomannan and Bifidobacterium protein were investigated in 0.15 M sodium chloride solution at 310 K by using molecular dynamics simulation. The results have shown that water molecules dramatically affect the alignment of konjac glucomannan in the system. The active site of Bifidobacterium protein that determined by the calculations are composed of ASP154, ARG49, ASN206, and ASN401. The lowest flexibility of GM5 structure shows strong interactions with Bifidobacterium protein. The most suitable size of konjac glucomannan that can bind with the protein has the degrees of polymerization no more than 8.

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Keywords: Konjac glucomannan ; Bifidobacterium ; Molecular dynamics simulations;

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