Revealing the compact structure of lactic acid bacterial hetero-exopolysaccharides by SAXS and DLS

Molecular structures of exopolysaccharides are required to understand their functions and the relationships between the structure and physical and rheological properties. Small-angle X-ray scattering and dynamic light scattering were used in conjunction with molecular modeling to characterize solution structures of three lactic acid bacterial hetero-exopolysaccharides (HePS-1, HePS-2 and HePS-3). Values of radius of gyration $R_G$, cross-sectional radius of gyration $R_X$, approximate length $L$ and hydrodynamic diameter were not directly proportional to the molar mass and indicated the HePSs adopted a compact coil-like rather than an extended conformation. Constrained molecular modeling of 15,000 randomised HePS-1 conformers resulted in five best-fit structures with R factor of 3.94.6% revealing random coil-like structure. $\phi$ and $\psi$ angle analysis of glycosidic linkages in HePS-1 structures suggests Galf residues significantly influence the conformation. Ab initio scattering modeling of HePS-2 and HePS-3 gave excellent curve fittings with $\chi^2$ of 0.43 and 0.34 for best-fit models, respectively, compatible with coil-like conformation. The findings disclose solution behaviour of HePS relevant for their interactions with biomacromolecules e.g. milk proteins.

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