THREE DIMENSIONAL STRUCTURE OF BACTERIAL FRUCTAN LEVAN: COMPUTATIONAL ANALYSIS

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An original biologically active bacterial fructan levan, synthesised by a special strain of *Zymomonas mobilis*, has been isolated and purified from proteins and toxins, and it meets the requirements of medicine [1]. Only limited studies have been made up to present on the structure of levan. We reported previously on the activation of macroorganism immune cell-mediated protective mechanisms by levan, and tied this to the levan monomeric unit D-fructofuranose ß-configuration [2]. Since the spatial structure of high molmass natural compounds, determines their biological activity, we initiated the systematical study of the structure of polyfructan levan. Computational analysis using the ''HyperChem'' program was chosen for investigation of levan molecule conformation. Firstly, the structure of levan homologous monomeric units was determined. It was found that ß-D-fructofuranose forms a five-membered ring with an inner angle C2-O-C5 of about 104°. Conditioned planarity was shown with one C or O atom projected forward out of the ring plane, in the next ring being the alternate atom. As a result of fructose unit polymerisation, the chain turns in space clockwise to form a full turn of a coil within 5-6 monomeric units.
It was shown by us that *Zymomonas mobilis* 113S synthesises a high molecular levan with branching every 9-12 monomeric units [3]. A schematic model was developed, with aggregated unbranched regions and solvated branched ones, explaining the weak rigidity of levan gel and its good solubility, important for its medicinal use. The computer-assisted analysis of the highly branched chain of levan showed an ellipsoid with plenty of non-reducing end-groups on the surface of the molecule. According to the common conception of the significant role of polysaccharide chain terminal residues in immunochemical reactions, there is an obvious structural basis for the high immunological activity of levan. The spatial dimensions of 1-5 terminal fructose residues of the nonreducing end were determined. It was found that the volume of free terminal fructose residues corresponds to the dimensions of the IgG antigen binding spot, equal to 34x12x7 Å. Some approaches for identification of bacterial fructan levan immunomodulating mechanisms will be discussed.

References

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