

Abstract Submitted
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Investigation of the structure of levan polysaccharide chains in water via molecular dynamics simulations¹ DENIZ TURGUT, Rensselaer Polytechnic Institute, BINNAZ COSKUNKAN, GULCIN CEM, Yeditepe University, DENIZ RENDE, Rensselaer Polytechnic Institute, K. YALCIN ARGAS, Marmara University, SEYDA BUCAK, Yeditepe University, NIHAT BAYSAL, Rensselaer Polytechnic Institute, EBRU TOKSOY-ONER, Marmara University, RAHMI OZISIK, Rensselaer Polytechnic Institute — Levan is a biopolymer consisting of β -D-fructofuranose units with β (2-6) linkages between fructose rings. Investigation of the structure and behavior of levan in aqueous environments is necessary to understand its biological activity and its potential use in various applications such as carbohydrate-derived drug release. The use of different *in vivo* and *in vitro* bioactivity assays fail to relate the chemical structure and conformation to the observed biological activity. Therefore, considerable research has been directed on elucidating the biological activity mechanisms of polysaccharides by structure-function analysis. To overcome the inherent difficulties of experiments, molecular dynamics (MD) simulations have been used to retrieve comprehensive information regarding the conformations of polysaccharides and their dynamic properties. In the current study, the structure of levan is investigated in aqueous medium and in saline solutions via fully atomistic MD simulations at 298 and 310 K, representing room temperature and physiological temperatures, respectively.

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