Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Sulfation effect on levan polysaccharide chains structure with molecular dynamics simulations[1] BINNAZ COSKUNKAN, Yeditepe University, DENIZ TURGUT, DENIZ RENDE, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute, EBRU TOKSOY-ONER, Marmara University — Diversity in conformations and structural heterogeneity make polysaccharides the most challenging biopolymer type for experimental and theoretical characterization studies. Levan is a biopolymer chain that consists of fructose rings with β(2-6) linkages. It is a glycan that has great potential as a functional biopolymer in foods, feeds, cosmetics, pharmaceutical and chemical industries. Sulfated polysaccharides are group of macromolecules with sulfated groups in their hydroxyl parts with a range of important biological properties. Sulfate groups and their positions have a major effect on anticoagulant activity. It is reported that sulfate modified levan has anticoagulant activity such as heparin. In the current study, the effect of sulfation on the structure and dynamics of unmodified and sulfate modified levan are investigated via fully atomistic Molecular Dynamics simulations in aqueous media and varying salt concentrations at 310 K.

[1]This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730.

Rahmi Ozisik
Rensselaer Polytechnic Institute

Date submitted: 06 Nov 2015 Electronic form version 1.4