World Academy of Science, Engineering and Technology
International Journal of Biotechnology and Bioengineering
Vol:17, No:07, 2023

Simulation of GAG-Analogue Biomimetics for Intervertebral Disc Repair

Authors : Dafna Knani, Sarit S. Sivan

Abstract : Aggrecan, one of the main components of the intervertebral disc (IVD), belongs to the family of proteoglycans (PGs) that are composed of glycosaminoglycan (GAG) chains covalently attached to a core protein. Its primary function is to maintain tissue hydration and hence disc height under the high loads imposed by muscle activity and body weight. Significant PG loss is one of the first indications of disc degeneration. A possible solution to recover disc functions is by injecting a synthetic hydrogel into the joint cavity, hence mimicking the role of PGs. One of the hydrogels proposed is GAG-analogues, based on sulfate-containing polymers, which are responsible for hydration in disc tissue. In the present work, we used molecular dynamics (MD) to study the effect of the hydrogel crosslinking (type and degree) on the swelling behavior of the suggested GAG-analogue biomimetics by calculation of cohesive energy density (CED), solubility parameter, enthalpy of mixing (ΔEmix) and the interactions between the molecules at the pure form and as a mixture with water. The simulation results showed that hydrophobicity plays an important role in the swelling of the hydrogel, as indicated by the linear correlation observed between solubility parameter values of the copolymers and crosslinker weight ratio (w/w); this correlation was found useful in predicting the amount of PEGDA needed for the desirable hydration behavior of $(CS)_4$-peptide. Enthalpy of mixing calculations showed that all the GAG analogs, $(CS)_4$ and $(CS)_4$-peptide are water-soluble; radial distribution function analysis revealed that they form interactions with water molecules, which is important for the hydration process. To conclude, our simulation results, beyond supporting the experimental data, can be used as a useful predictive tool in the future development of biomaterials, such as disc replacement.

Keywords : molecular dynamics, proteoglycans, enthalpy of mixing, swelling
Conference Title : ICSMCB 2023 : International Conference on Soft Materials Chemistry and Biopolymers
Conference Location : Copenhagen, Denmark
Conference Dates : July 10-11, 2023