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Capstan-like mechanism in hyaluronan-phospholipid systems

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Abstract

Functionality of articular cartilage results from complex interactions between its molecular components. Among many biomolecules, two are of prime importance for lubrication: hyaluronic acid (HA) and phospholipids (PL). The purpose of this study is to discuss a mechanism of interaction between these two components and how their synergies contribute to nanobiolubrication of articular cartilage. Preliminary molecular dynamics simulations have been performed to investigate these interactions by adopting a capstan-like mechanism of action. By applying a constant pulling force to both ends of a HA molecule, wrapped around a PL micelle, we viewed the rotation of the PL micelle. The simulations were performed upon two physicochemical constraints: force- and solvent-dependency. The results show the efficiency of rotation from intermolecular bond creation and annihilation. We found a direct relation between the available surface of the micelle and the magnitude of the force, which varies significantly through the unwinding. The movement of the attached molecules are characterized by a slide-to-roll relation, which is affected by the viscosity of the surrounding medium. As a

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