

## STRUCTURAL AND DYNAMICAL CHARACTERIZATION OF HYALURONAN OLIGOMERS

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Hyaluronan (HA), a linear polymer of exceptionally high molecular weight, is found in all tissues and body fluids of vertebrates as well as in some bacteria. It is a simple molecule of variable length that consists of repeating disaccharide units each containing glucuronic acid and N-acetylglucosamine linked by alternate beta 1-3 and beta 1-4 linkages [1].

The polymer in solution has interesting hydrodynamic properties such as viscosity, stiffness which seem to be influenced by the length of the hyaluronan [2]. Our work is motivated by the fact that certain HA degrading enzymes like Hyaluronate Lyase specifically degrade beta 1-4 linkage [3]. In this project we aim to study structural and dynamical properties of hyaluronan by Molecular dynamics (MD) simulations. The main focus is on the question to see the difference between the two glycosidic linkages and the factors that are responsible for it.

Long (~500 ns) MD simulations of HA oligomers in explicit water of various lengths of Hyaluronan (disaccharide, tetrasaccharide, hexasaccharide, octasaccharide and decasaccharide) are performed and analyzed for structural as well as dynamical properties. Glycosidic bond distribution over the evolution is compared with the available experimental data which shows a clear distinction between the beta 1-3 and beta 1-4 linkages. This may be implicated in the fact why certain HA degrading enzymes such as Hyaluronate lyases specifically degrade beta 1-4 linkage. Dynamical properties like intra-molecular hydrogen bonding and its influence on the structures as well as aggregation of Hyaluronan for different oligomer lengths is studied. Here we present our preliminary results on these studies.

### References:

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