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Interaction of albumin with chondroitin sulphate IV and VI, a molecular docking study

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Abstract: This work presents a study of the mechanism of physical interaction of albumin with chondroitin sulfate IV and albumin with chondroitin sulfate VI in a water environment. We use the molecular docking method. That gives information about supramolecular complexes, which statistical tools can study.

Keywords: albumin, chondroitin sulphate IV and chondroitin sulphate VI, molecular docking method

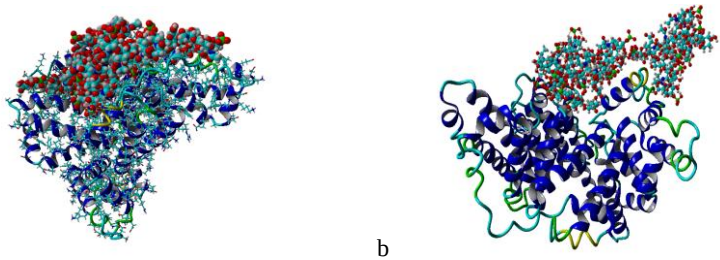
1. Introduction

We study the interaction between albumin and chondroitin sulfate IV and VI in an aqueous environment. Albumin is the most abundant component of synovial fluid. Interaction with other compounds of synovial fluid determines the appearance of a synergistic effect, the low friction between articulating cartilage surfaces [1]. Chondroitin sulfate IV and chondroitin sulfate VI are organic chemical compounds from the group of glycosaminoglycans, which are also an essential component of cartilage tissue.

Despite many theories and dynamical models that describe articulating cartilage lubrication phenomenon, there is still little information about the nanoscopic function of components of the synovial fluid under physiological conditions at the nanometer level [2]. This work is a step towards analysis processes between the components of the synovial fluid at the nanoscopic level under physiological conditions and is an extension of our previous study [3].

2. Results and Discussion

We perform a molecular docking procedure, a molecular modeling method that allows us to find the location (and conformation) of a ligand at the receptor-binding site. We perform numerical simulations by means of YASARA docking method VINA. The information from simulations enables the evaluation of the free energy of binding (free enthalpy) and the calculation of the chemical affinity. In the Fig.1 we present graphical result of the docking of chondroitin sulphate IV (CS-4) to the albumin and the docking of chondroitin sulphate VI (CS-6) to the albumin.



a b

Fig. 1. The panel a presents albumin and chondroitin sulphate IV as a results of docking algorithm and in the panel b presents a albumin and chondroitin sulphate VI.

	Affinity [kcal/mol]	
Complex no	CS-4	CS-6
1	4,432	2,643
2	4,429	2,5885
3	4,247	2,677
4	4,0435	2,5897
5	3,929	2,618
6	3,916	2,587
7	3,912	2,5295
8	3,886	2,571
9	3,878	2,5194
10	3,834	2,437

Fig. 2. Result of molecular docking, of albumin - CS complexes.

3. Concluding Remarks

Our results imply that binding chondroitin sulfate 4 has the highest affinity to albumin. As the ratio between CS4:CS6 changes with age in synovial fluid, this may result in frictional properties of lubricin. The current consensus among scientists studying the subject is that efficient lubrication results from synergy between SF components.

References

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