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Interaction of mucin with glycosaminoglycans in water environment

PIOTR WEBER[1*], PIOTR BEŁDOWSKI[2A], ADAM GADOMSKI[2B], KRZYSZTOF DOMINO[3], DAMIAN LEDZIŃSKI[4].

1. Gdańsk University of Technology, Faculty of Applied Physics and Mathematics, Institute of Physics and Computer Science, Department of Atomic, Molecular and Optical Physics, Gdańsk, Poland [0000-0002-9405-5461]
2. Institute of Mathematics and Physics, UTP University of Science and Technology, Bydgoszcz, Poland [A][0000-0002-7505-6063], [B] [0000-0002-8201-1736]
3. Institute of Theoretical and Applied Informatics, Polish Academy of Sciences, Poland [0000-0001-7386-5441]
4. Faculty of Telecommunications, Computer Science and Technology, UTP University of Science and Technology, Bydgoszcz, Poland [0000-0003-0796-4390]

* Presenting Author

Abstract: We present a study of the interaction between mucin and several glycosaminoglycans. These molecules are a compound of extracellular matrix in the articular cartilage and play a significant role in the lubrication phenomenon. We use molecular docking numerical experiments that allow to describe the interaction between one mucin molecule and one selected glycosaminoglycan molecule. As a result, we obtain binding energy, hydrogen bonds, and hydrophobic contacts between two molecules. For one pair of molecules we can generate several values of one above-mentioned property and use a statistical methods to compare this property between pairs.

Keywords: glycosaminoglycans, mucin, biolubrication, molecular docking method

1. Introduction

The joint organ surfaces are covered by articular cartilage (AC) and separated by a thin layer of synovial fluid (SF). The SF of the joints organ functions as a biological lubricant. It provides low-friction and low-wear properties to articulating cartilage surfaces. This property is due to the synergistic interaction between high molecular weight molecules in an aqueous solution which build SF and extracellular matrix of AC. These components are secreted by cells: chondrocytes in the AC and synoviocytes in the synovium. One of the components of the extracellular articular cartilage matrix is complexes of mucin with glycosaminoglycans (GAGs). GAGs are linear polysaccharides, which are highly polar and water-soluble. Mucin is a heavily glycosylated protein, which can form gels. In Fig.1, we present some GAGs.

Many theories and dynamical models are contributing to the lubrication phenomenon in AC due to SF. But there are not many studies that conclusively describe the nanoscopic function of components of SF and extracellular articular cartilage matrix [1]. This work, like our previous works [2], is a step towards analysis biolubrication processes at the nanoscopic level under physiological conditions.

2. Results and Discussion

Our calculation suggest that that there are some significant differences between chemical affinity in the pair of molecules: mucin and one GAG – Fig.1. In Fig. 2 graphical visualisation of interaction.

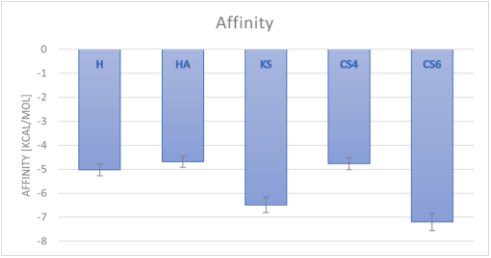

Fig. 1. Affinity between mucin and selected GAGs. Hyaluronic acid (HA), chondroitin sulfate-4 (CS4), chondroitin sulfate-6 (CS6), keratan sulphate (KS) and heparin (H).

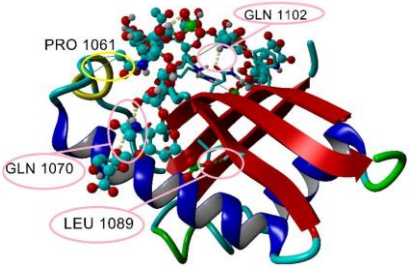

Fig. 2. Visualization of interactions between one selected GAG and mucin: a) hydrogen bonds (yellow dotted lines); b) hydrophobic contacts (green lines).

3. Concluding Remarks

Our results imply that binding between GAGs and mucin is more robust than those present in the synovial fluid (SF), i.e., all but heparin. SF is a natural lubricant that contributes to an extremely low friction coefficient. Main finding: chondroitin sulfate 6 has the highest affinity to mucin. As the ratio between CS4:CS6 changes with age in synovial fluid, this may result in frictional properties of lubricin. Namely, different hydration of the complex and hydration repulsion may not be as efficient. The current consensus among scientists studying the subject is that efficient lubrication results from synergy between SF components.

References

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