INTERACTION OF HYALURONIC ACID WITH DERMAL MEMBRANE: A MOLECULAR DYNAMICS SIMULATION STUDY

Bozdaganyan M.E.^{1, 2}, Orekhov P.S.^{1,3,4}

 ¹Department of Biology, Lomonosov Moscow State University, Moscow, Russia
²Federal Research and Clinical Center of Specialized Medical Care and Medical Technologies, Federal Medical and Biological Agency of Russia, Moscow, Russia
³ Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia
⁴ Sechenov University, Moscow, Russia

Hyaluronic acid (HA) is a naturally occurring polyanionic polysaccharide that consists of Nacetyl-d-glucosamine and β -glucoronic acid. It is present in the intercellular matrix of most vertebrate connective tissues especially skin where it has a protective, structure stabilizing and shock-absorbing role. The unique viscoelastic nature of HA along with its biocompatibility and non-immunogenicity has led to its use in a number of clinical applications. When applied to the skin HA provides beneficial effects such as skin hydration, elasticity regeneration, and improved wound healing [1].

The major limitation for active compounds penetration through the skin is overcoming the most outer layer of the non-viable epidermis – stratum corneum (SC). SC serves as a ratelimiting lipophilic barrier against the uptake of chemical and biological toxins as well transepidermal water loss. The structure of SC is organized as stacked bilayers of ceramides in a splayed chain conformation with cholesterol associated with the ceramide sphingoid moiety and free fatty acids associated with the ceramide fatty acid moiety [2].

The mechanisms of HA mediated skin penetration, however, are still poorly understood. In the present study we propose the mechanism by which HA can penetrate the SC barrier with and without (dimethyl sulfoxide) DMSO which is often used in cosmetics. We have carried out the coarse-grained molecular dynamics simulations of model SC together with: (1) DMSO; (2) DMSO with HA in different concentrations; (3) pure HA also in different concentrations. The work was partially supported by the RFBR grant No. 18-504-12045.

References

- 1. *Witting, M. et al.* Interactions of hyaluronic Acid with the skin and implications for the dermal delivery of biomacromolecules // Mol. Pharm. **12**, 2015. Pp. 1391–1401
- Gupta, R. & Rai, B. Molecular Dynamics Simulation Study of Skin Lipids: Effects of the Molar Ratio of Individual Components over a Wide Temperature Range // J. Phys. Chem. B 119, 2015. Pp. 11643–11655.