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ABSTRACT BOOK

STINTS9

MOLECULAR DYNAMICS APPROACH TO INVESTIGATE THE ROLE OF HYDRATION AND OTHER SURFACTANTS ON THE GEOMETRICAL AND BARRIER PROPERTIES OF STRATUM CORNEUM

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Introduction: Unravelling the mechanisms beneath the skin barrier and permeation properties is pivotal for a broad range of applications, ranging from skin hygiene to skin care products design. Of particular importance are changes in microclimate conditions such as temperature and hydration, which affect not only skin's barrier but also its mechanical properties and have been related to the risk of developing pressure ulcers1. Indeed, excessive hydration makes skin fragile, reducing its tolerance to mechanical loads including pressure and shear2.

Recently, molecular dynamics (MD) simulations have been reported to deliver valuable knowledge about the molecular and structural properties of inter-corneocytes lipid bilayers3. The aim of this Ph.D. is to use MD simulations to build microscopic in silico systems mimicking the SC lipid bilayers to achieve a better molecular understanding of skin health and barrier property.

Methods: The systems are being simulated via GROMACS with the CHARMM forcefield and barrier properties are predicted via MD and thermodynamical approaches. Different models are probed by changing both the lipids' ratio and their geometrical conformation. Hydration (surfactant) effects are modelled by varying the amount of water (surfactant) molecules simulated and quantified by measuring lipid structural parameters.

Results: The hydration level changes the geometrical properties of SC lipid bilayers and, consequently, the diffusive behaviour of water across them. Lipid bilayers are thinner and more disordered as the hydration level decreases, with water trapped in the polar regions of the lipids exhibiting strongly hindered diffusion. Predicted barrier properties for water compare well with experimental data, but surfactants' effects depend on the numerical implementation and the dimension of simulated system.

Conclusions: MD results compare well with experimental data for water diffusion, partition, and permeability across SC lipid bilayers. Further studies are needed to better assess the effect of surfactants and sample the mechanical properties of the SC lipid bilayers.

References:

1. *Holloway, S.; Jones, V., Br J Nurs 2005, 14 (22), 1172-6.*
2. *Gray, M.; Black, J. M.; Baharestani, M. M.; Bliss, D. Z.; Colwell, J. C.; Goldberg, M.; Kennedy-Evans, K. L.; Logan, S.; Ratliff, C. R., J Wound Ostomy Continence Nurs 2011, 38 (3), 233-41.*
3. *Lundborg, M.; Narangifard, A.; Wennberg, C. L.; Lindahl, E.; Daneholt, B.; Norlen, L., J Struct Biol 2018, 203 (2), 149-161.*