Effect of the ceramide composition on the structure of a stratum corneum model system - a molecular dynamics study

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The stratum corneum lipid matrix (SC) is essential for human survival, acting as a barrier that prevents rapid dehydration and at the same time keeping the body protected against viruses, bacteria and UV radiation. Many skin diseases such as psoriasis, atopic dermatitis and ichthyosis result from alterations in the concentration of ceramides in this extracellular matrix. The complex structure of the SC makes it challenging to determine the relation between its molecular organization and its physicochemical properties. In this work we use molecular dynamics simulations to study the effect of the concentrations of non-hydroxyphitosphingosine ceramide (CER[NP]) and α-hydroxyphitosphingosine ceramide (CER[AP]) on structural properties of a model lipid matrix that has been investigated experimentally recently [Langmuir. 34(4): 1742-1749 (2018)]. Two lipid bilayer models, composed of CER[NP], CER[AP], cholesterol and lignoceric acid, with CER[NP]/CER[AP] ratios of 1:2 and 2:1 are investigated. The relation between the structural properties and the solvation dynamics of each lipid matrix is analyzed. Our results show that: (i) the two models with CER[NP]/CER[AP] present characteristics of a fluid lipid bilayer, (ii) the acyl chains of CER[NP] and lignoceric acid of one monolayer overlap with those of the other monolayer and (iii) hydration of CER[AP] is larger than that of CER[NP], which increases the number of hydrogen bonds formed and the affinity with the solvent. Therefore, CER[NP] has greater mobility towards the laminar midplane.