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Disposition of small molecules in stacked bilayers of stratum corneum lipids by neutron diffraction and selective deuteration

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The stratum corneum (SC) is a thin layer of anucleated cells in a lipid matrix and forms the outermost layer of skin, often depicted with a brick-and-mortar structure.[1] Understanding the molecular basis of the barrier properties of skin has important implications for diseased states such as atopic dermatitis and for topical application of therapeutics. The self-assembly of the intercellular lipid matrix forms an important aspect of the barrier properties of the SC, and it is mainly composed of ceramides, cholesterol and free fatty acids. Together, these lipids form two lamellar structures with periodicities (d) of 6 nm (short periodicity phase - SPP) and 13 nm (long periodicity phase - LPP).[2] The ceramides dictate the formation of these lamellar phases and in particular the ceramide EOS is important due to its exceptionally long structure, having an unsaturated fatty acid esterified to an ω-hydroxy fatty acyl chain. Our lipid matrix model, consisting of a 1:1:1 molar ratio of cholesterol, free fatty acids and ceramides, has a ceramide mixture of ceramide NS and ceramide EOS. In this study we have used neutron diffraction (D16 –ILL), over range of scattering vectors which span classical diffraction measurements to the range usually associated with small angle scattering to probe the localization of a small molecule, salicylic acid, within oriented lipid stacks. We used contrast variation of sorbed water to solve the phasing problem of unit cell reconstruction and provide a reconstruction of the scattering length density (SLD) profile of the lamellar/1D unit cell. By modulation of the SLD contribution of the salicylic acid to the overall profile by deuteration we are able to provide an insight of the localization of salicylic acid within the profile.

References
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