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Increase in Area/Unit Cell of Alamethicin in DOPC Seen by XRD and MD Simulations

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A 1:20 Alamethicin(Alm)/DOPC mole ratio mixture was oriented onto silicon wafers from organic solvent and then fully hydrated through the vapor. Diffuse X-ray scattering data were collected at 30 °C at the CHESS synchrotron. The continuous relative form factor $F(q_z)$ for 0.2 $Å^{-1} < q_z < 0.6$ $Å^{-1}$ was obtained using the method of Liu and Nagle, Phys. Rev. E 69 (2004) 040901. The relative form factor in the range 0.1 $Å^{-1} < q_z < 0.4$ $Å^{-1}$ was obtained independently from large unilamellar vesicles (LUVs) and was put on the same relative scale as the oriented data using the overlapped q_z region. The composite relative form factor was fit to models. The model with the peptide fully inserted parallel to the bilayer normal fit the data better than surface models, either with the peptide outside the phosphate group or near the carbonyls. The area/unit cell increased to 81 $Å^2$ from 72 $Å^2$ for fully hydrated DOPC, but the head-head thickness and the area/DOPC remained nearly constant. The number of waters/unit cell increased by 10 consistent with the measured increase in D and also the need for water to fill the space between headgroups above Alm.

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