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Alamethicin Structure in Lipid Bilayers[1] STEPHANIE TRISTRAM-NAGLE, JIAN-JUN PAN, Biol. Phys. Group, Physics Dept., Carnegie Mellon University, Pittsburgh, PA, JOHN NAGLE, Dept. Biol. Sci. and Physics Dept., Carnegie Mellon University, Pittsburgh, PA — This investigation uses x-ray diffuse scattering and MD simulations to study alamethicin (Alm) in fully hydrated bilayers of DOPC and diC22:1PC. Comparison of the experimental and simulated form factors supports the standard conclusion that Alm helices are inserted transmembrane along the bilayer normal at high humidity and high concentrations. Little change in membrane thickness with inserted Alm helices occurs for DOPC up to 1/10 Alm/DOPC. By contrast, the x-ray data strongly indicate that the diC22:1PC membrane, which is thicker than DOPC by 7 Å, thins with added Alm. Fitting the data to models of the electron density gives a decrease in thickness of 4 Å at 1/10 Alm/diC22:1PC. Although Alm's helical length is close to the hydrophobic thickness of DOPC (27 Å), it is mismatched with the thicker diC22:1PC. Alm decreases the bending modulus (K_C) by a factor of ∼2 in DOPC and a factor ∼10 in diC22:1PC membranes at P/L ∼1/10. Determination of the B modulus reveals a large increase in Hamaker parameter when Alm is added to diC22:1PC, but not to DOPC.

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