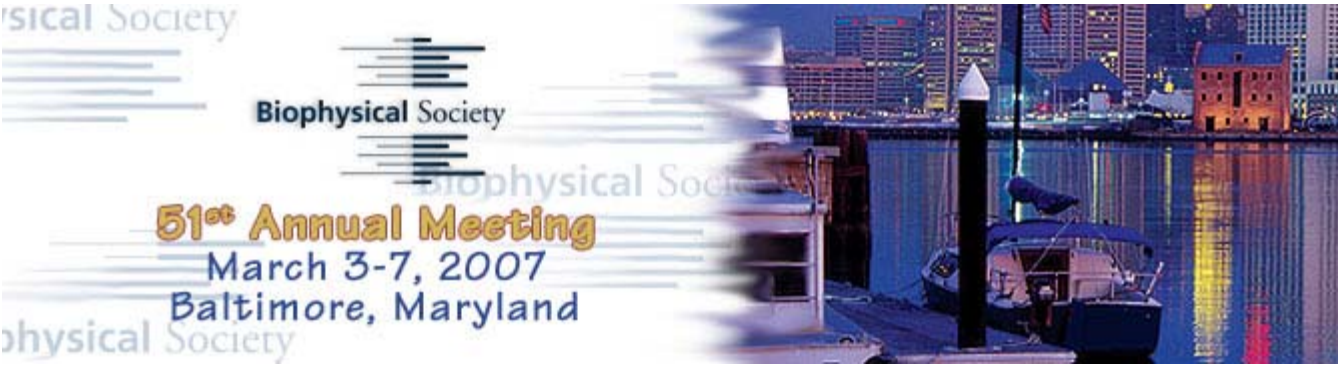

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Presentation Number:	2038-Pos
Abstract Title:	Strategy for Structure Determination of Lipid/Cholesterol Bilayers
Location:	Halls A/B/C/D
Topic:	3E Membrane Structure
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X-ray diffuse scattering data were collected from fully hydrated bilayers of DOPC with a series of cholesterol compositions. The samples consisted of oriented stacks for high q and of unilamellar vesicles for smaller q. Diffuse scattering theory (PRE, 2001) determines the bending modulus Kc and the compression modulus B from the oriented stacks. Surprisingly, diffuse scattering remained strong with addition of cholesterol, and this qualitative result is consistent with the results of the detailed analysis that show little increase in Kc even for cholesterol mole fraction 0.4, unlike the increase in Kc that occurs when cholesterol is added to lipids with one or more saturated hydrocarbon chains. We obtain the form factor consisting of the Fourier transform F(q) of the electron density of the bilayer. This reciprocal space F(q) must be matched by putative real space structures. Two methods are being used to obtain structure. The first method uses the H2 electron density model (Klauda et al., Biophys. J. 90 (2006) 2796-2807) with an extra Gaussian for the cholesterol. The second method employs a model free MD simulation method (op. cit.) that determines the area that gives best agreement with the F(q) data and also recent volumetric data (Greenwood et al., Chem. Phys. Lipids 143 (2006) 1-10). For two component bilayers the model free method is being extended by employing different initial configurations to overcome slow lateral diffusion on the MD time scale. Compared to single component lipid bilayers, the modeling method requires extra constraints and these constraints are being evaluated synergistically with the MD simulations. Research supported in part by NIH Grant GM44976.

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