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Session Title: Membrane Structure I

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Abstract Title: X-ray scattering and molecular dynamics simulations of cholesterol effects in

short- and long-chain mono-unsaturated lipid bilayers

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Topic: 3E Membrane Structure

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Issue:

High resolution structure determination for membranes composed of complex mixtures is a difficult task. Here, we build upon initial efforts to determine the effect of high cholesterol concentrations on the thickness of membranes composed of short- and long-chain mono-unsaturated lipids (Gallova et al, 2004). Those studies used SANS and analysis based upon the Kratky-Porod approximation to show a significant cholesterol-induced change (on the order of 5Å) in thickness for the short-chain di14:1PC, but were unable to resolve a significant change outside of experimental error for the long-chain di22:1PC. Here, we have used SAXS measurements on unilamellar vesicles in an attempt to supplement these previous data. Additionally, we employ all-atom molecular dynamics simulations in order to determine bilayer structural parameters not available from these types of experimental measurements. This study complements ongoing work in collaboration with the Nagle lab on di18:1PC presented elsewhere at this meeting.

Commercial Relationship: J.N. Sachs, None; J. Perlmutter, None; N. Kucerka, None.

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