

## **1818-Pos/B168. Modeling and evaluating SANS measurements of membrane thickness via molecular dynamics simulations**

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We investigate the influence of cholesterol on the thickness of di14:1 and di22:1 PC bilayers. We compare our results from MD simulations (using both the CHARMM and GROMOS force-fields) with a previously published study which used a Krotky-Porod treatment of SANS data to approximate thickness. This study suggested that 40 mol% cholesterol thickens di14:1 by 5 Angstroms, but has no effect on the thickness of di22:1. We compare results in Fourier space to draw the most meaningful conclusions regarding this experimental approach, while interrogating the real space results to gain insight into the underlying molecular behavior. Differences between the CHARMM and GROMOS results are highlighted.

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