

Joint Meeting of the Biophysical Society
52nd Annual Meeting
& 16th International Biophysics Congress

February 2 - 6, 2008
Long Beach, California



 [Print this Page for Your Records](#)

[Close Window](#)

Session Title: Membrane Structure I

Presentation Number: 1160-Pos

Abstract Title: Lipid Area Refinement Based On A Simultaneous Analysis Of Neutron And X-ray Scattering Data And All-atom Molecular Dynamics Simulations.

Location: Halls A/B/C

Topic: 3E Membrane Structure

Author Block: **Norbert Kučerka**¹, John Nagle², Jonathan Sachs³, Scott Feller⁴, Jeremy Pencer⁵, Andrew Jackson⁶, John Katsaras¹.

¹National Research Council, Chalk River, ON, Canada, ²Carnegie Mellon University, Pittsburgh, PA, USA, ³University of Minnesota, Minneapolis, MN, USA, ⁴Wabash College, Crawfordville, IN, USA, ⁵Atomic Energy of Canada Ltd., Chalk River, ON, Canada, ⁶NIST Center for Neutron Research, Gaithersburg, MD, USA.

Page Number in Print 236

Abstract Issue:

Quantitative structures were obtained for fully hydrated, fluid phase dioleoyl-phosphatidylcholine (DOPC at 30 °C) and dipalmitoyl-phosphatidylcholine (DPPC at 50 °C) bilayers. The structures were evaluated by the simultaneous analysis of x-ray and neutron scattering data using a new structural model for the bilayer scattering density profile (SDP). The model's design was guided by results from molecular dynamics simulations, and addresses features found in both electron and neutron scattering length density profiles of a lipid bilayer. After developing and testing the SDP model, using simulated data, it was applied to evaluating small-angle x-ray and neutron scattering data of DOPC collected under two different external contrast conditions. In the case of DPPC bilayers, additional contrast variation data were obtained through the use of specifically deuterated DPPC analogues (i.e. DPPC_d62, DPPC_d13 and DPPC_d9). Analysis of the data yielded the lateral areas for liquid crystalline DPPC and DOPC bilayers. Although, the obtained area/DPPC molecule was not so different from previously published reports, this was not the case for DOPC bilayers whose area/lipid was found to be ~ 10 % smaller. This newly developed area refinement method will reconcile long-standing inconsistencies in lipid areas.

Commercial Relationship: **N. Kučerka**, None; **J. Nagle**, None; **J. Sachs**, None; **S. Feller**, None; **J. Pencer**, None; **A. Jackson**, None; **J. Katsaras**, None.

[Biophysical Society](#)

9650 Rockville Pike

Bethesda, MD 20814

Phone: 301.634.7114

OASIS - Online Abstract Submission and Invitation System™ ©1996-2008, Coe-Truman Technologies, Inc.