

**Figure S1.** Normalized gel filtration chromatograms from the Superdex 200 HR 10/30 gel filtration column equilibrated in buffer (10 mM Tris/HCl, 100 mM NaCl pH 7.4). The mobile phase flow rate was 0.5 ml/min on a Waters Millennium system, with monitoring of protein absorbance at 280 nm, and one fraction collected per minute. Injection volume was 150 ml for Sample A, and 200 ml for Sample B. Sample A: POPC Nanodiscs before lyophilization. Fractions 29, 30 and 31 were pooled together and lyophilized. Sample B: POPC Nanodiscs after lyophilization, resuspended in water.

Table S1. Molecular Dynamics Ratio for Water-Protein and Lipid-Protein

## **Correlations for Crosspeaks Detected in the Water Plane Only**

Amino Acid MD Ratio<sup>a</sup>
Lys C $\beta$ -C $\gamma$  14.2
Glu C $\beta$ -C $\gamma$  15.5

Pro Cγ-Cδ NA

<sup>a</sup>Calculated as the ratio of CG carbons within 4.0 Å of water or lipid over the last 0.75 ns of a 4.5 ns MD simulation of MSP Nanodiscs.

NA – no proline CG carbons within 4.0  $\mbox{\normalfont\AA}$  of the lipid