

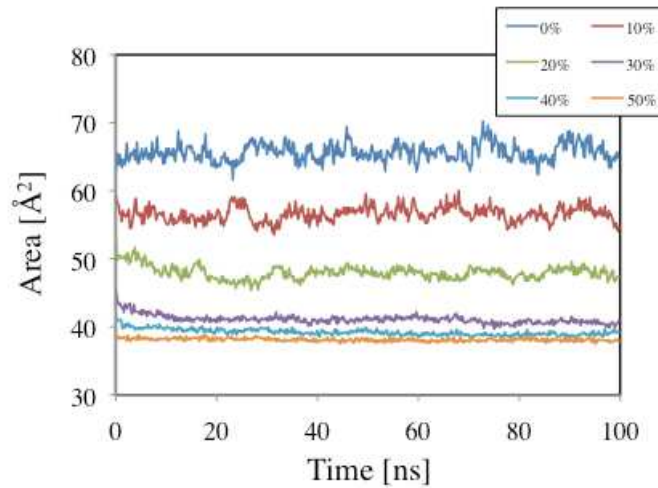
# Cholesterol Effect on Water Permeability Through DPPC and PSM Lipid Bilayer: A Molecular Dynamics Study

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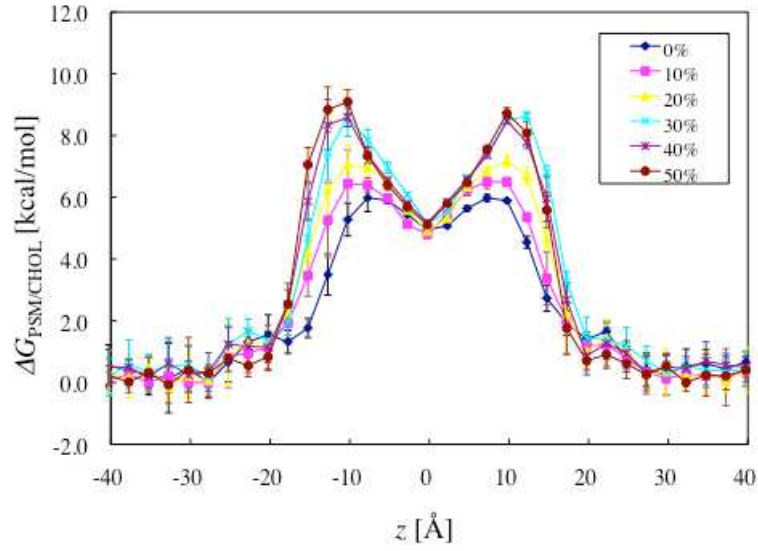
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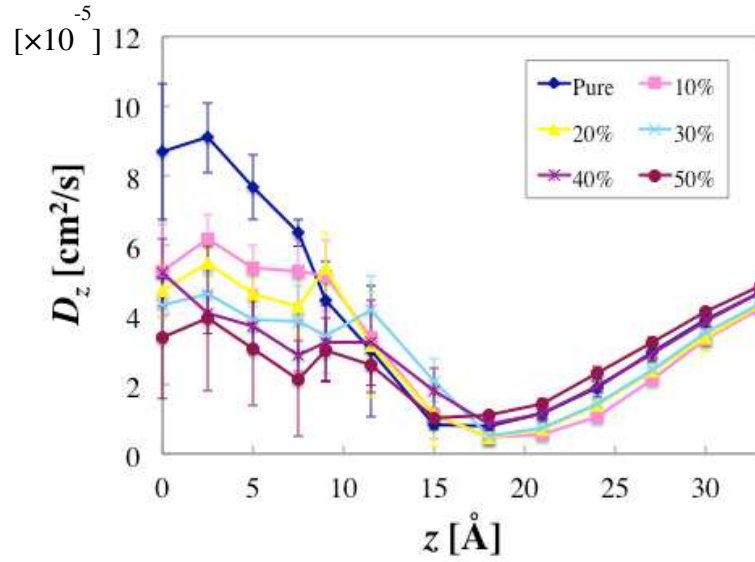
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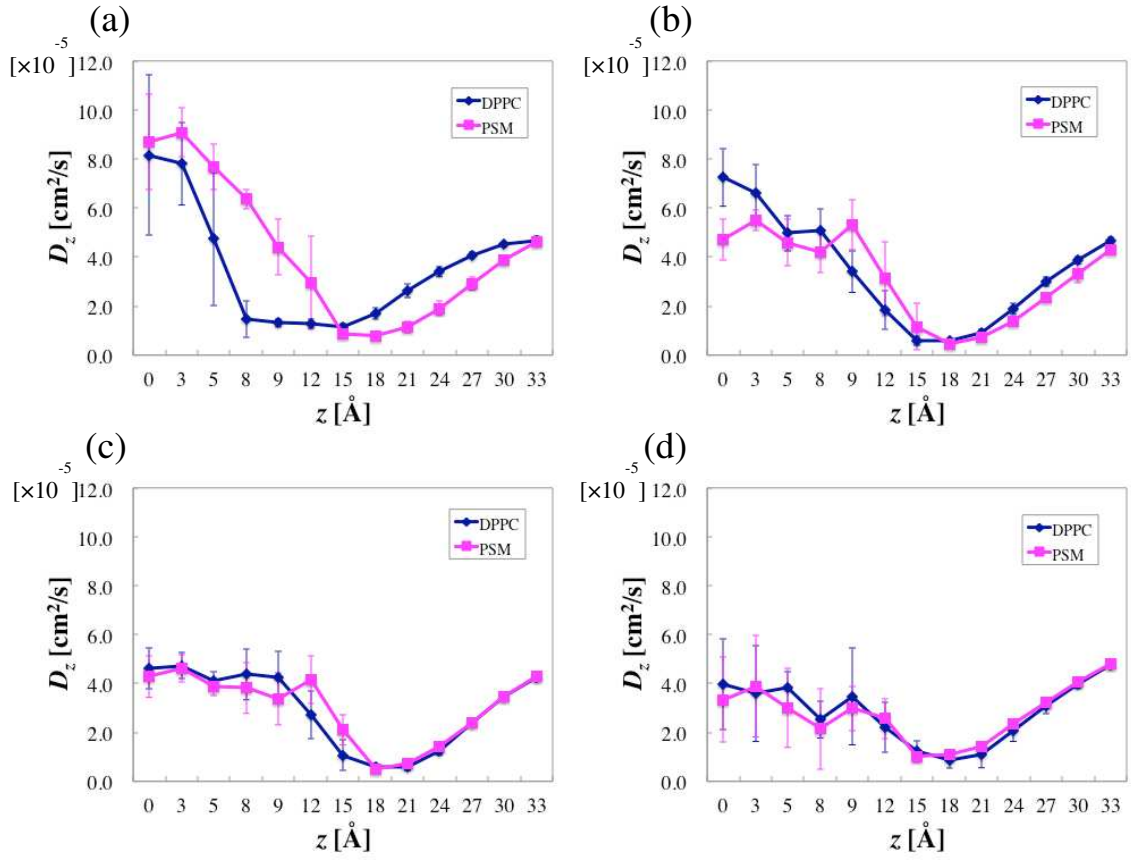
SI Figure 1. Time evolutions of molecular area of the DPPC/CHOL membrane at each cholesterol concentration.



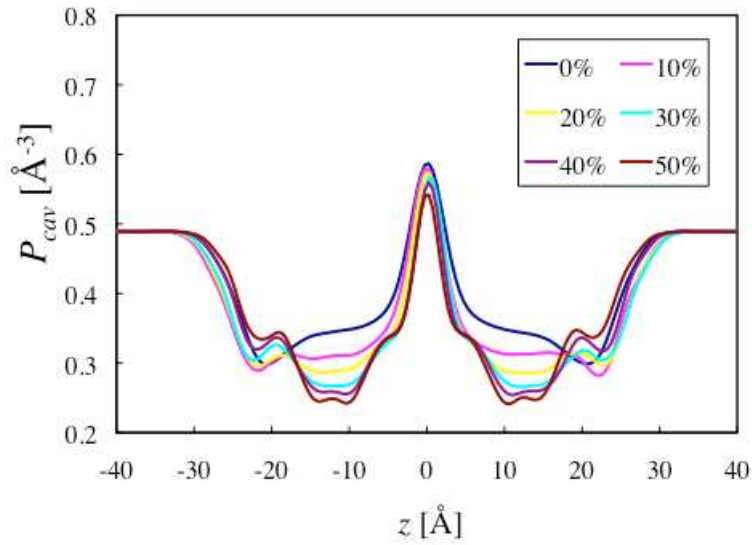
SI Figure 2. Variation of free energy profiles of water across the PSM/CHOL membrane at different cholesterol concentrations.



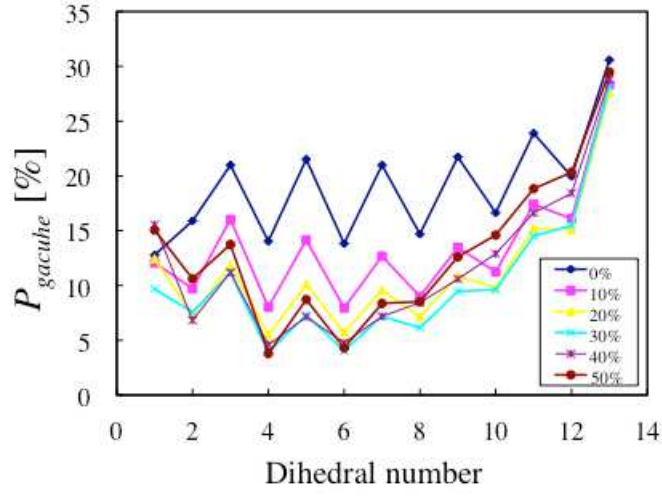
SI Figure 3. Local diffusion coefficients of a water molecule across the PSM/CHOL membrane at different cholesterol concentrations.



SI Figure 4. Comparison of local diffusion profiles of DPPC/CHOL and PSM/CHOL membranes at cholesterol concentrations of (a) 0 mol%, (b) 20 mol%, (c) 30 mol%, and (d) 50 mol%.



SI Figure 5. Variation of probability distribution of cavity  $P_{cav}$  of the PSM/CHOL membranes at different cholesterol concentrations.



SI Figure 6. Fractions of *gauche* conformation  $P_{gauche}$  of the PSM lipid chain (PA) at different cholesterol concentrations.

SI Table 1. Free energy barriers for the DPPC/CHOL ( $\Delta G_{DPPC/CHOL}$ ) and PSM/CHOL ( $\Delta G_{PSM/CHOL}$ ) membrane at different cholesterol concentrations in kcal/mol.

Cholesterol	0%	10%	20%	30%	40%	50%
$\Delta G_{DPPC/CHOL}$	5.1	5.4	5.5	7.3	8.7	9.0
$\Delta G_{PSM/CHOL}$	6.0	6.5	7.3	8.5	8.7	9.1