Electronic Supplementary Information (ESI)

Free Energetic Study of Cell-Penetrating HIV-1 TAT Peptide Translocation into DPPC/DPPS/CHOL Bilayers

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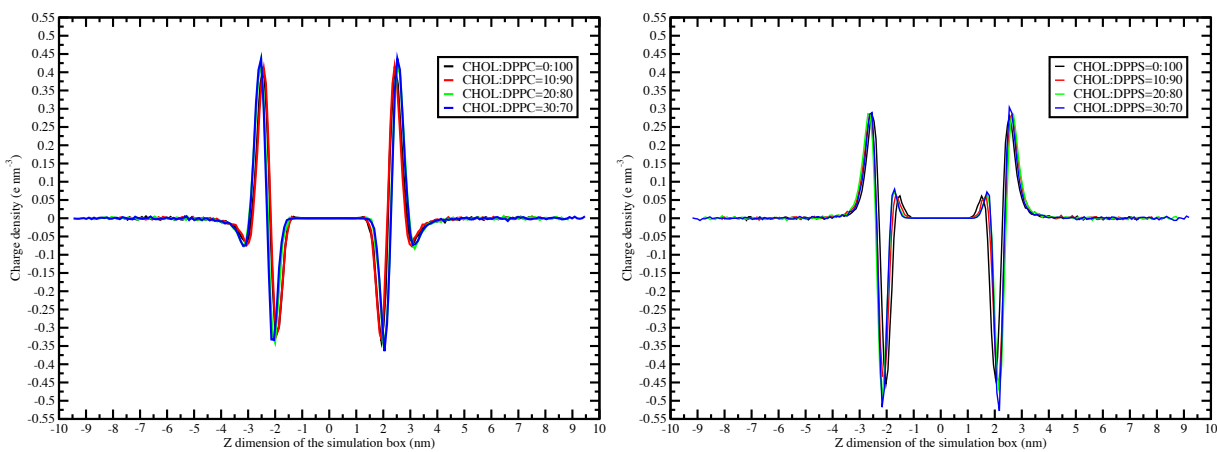
Charge Density Profile

Figure S1: Charge density profiles of (left panel) DPPC systems and (right panel) DPPS systems with 0-30 mol % cholesterol.
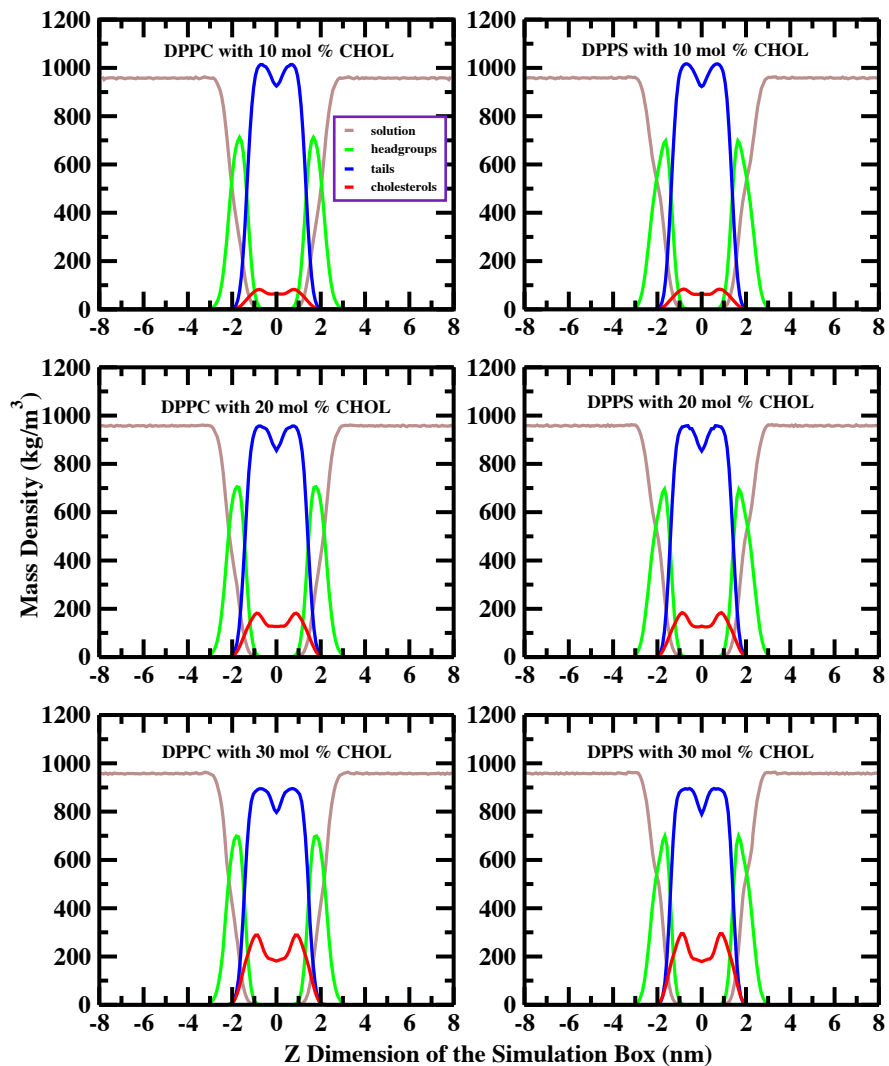
Mass Density Profile

Figure S2: Mass density profiles of (left panels) DPPC systems and (right panels) DPPS systems with 0-30 mol % cholesterol. The densities of water and ion solution, headgroups, tails and cholesterols are shown in each panel.
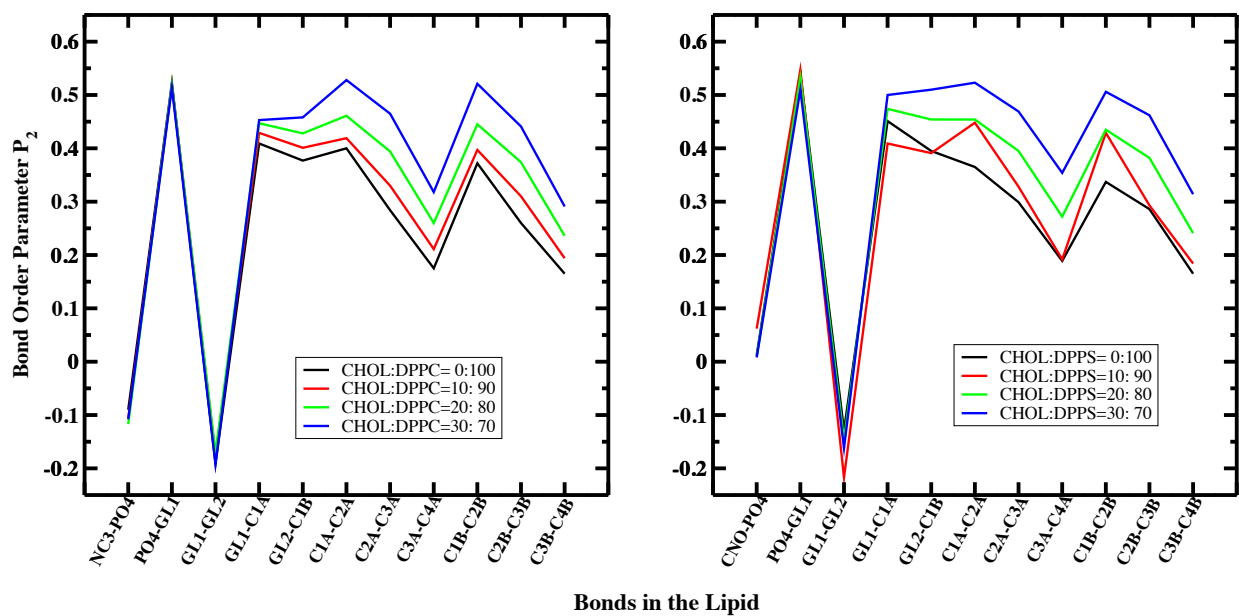
Lipid Bond Order Parameter

Figure S3: Lipid Bond Order Parameter P_2 of (left panel) DPPC lipid and (right panel) DPPS lipid with 0-30 mol % cholesterol
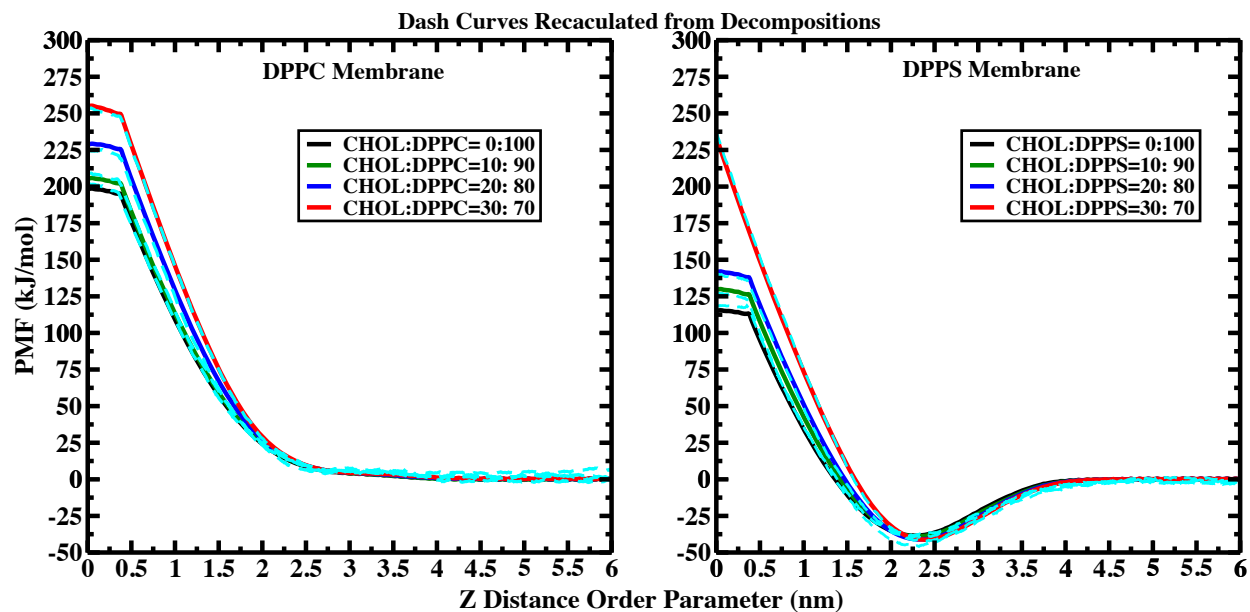
PMF Decomposition

Figure S4: Comparison of total free energy profiles from WHAM calculation (solid curves) and force integration (dash curves). (left panel) TAT penetration into model DPPC lipid bilayers with different percentage of CHOL.(right panel) TAT penetration into model DPPS lipid bilayers with different percentage of CHOL.
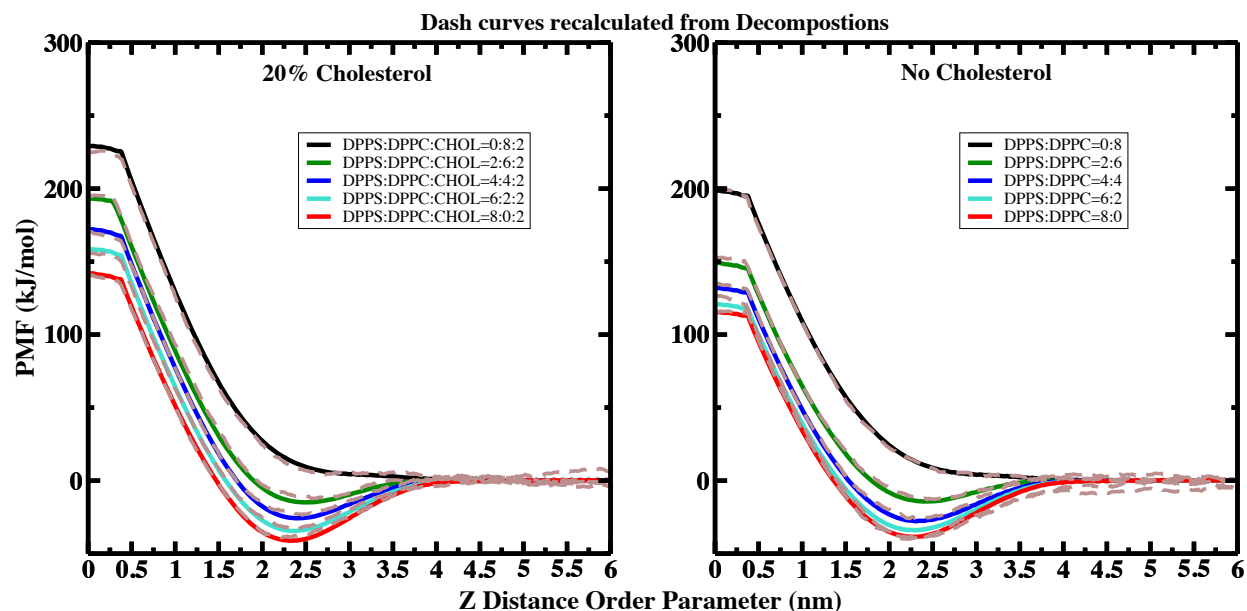
Figure S5: Comparison of total free energy profiles from WHAM calculation (solid curves) and force integration (dash curves). (left panel) 20% CHOL. TAT penetration into model DPPC/DPPS lipid bilayers with different percentage of DPPS.(right panel) NO CHOL. TAT penetration into model DPPC/DPPS lipid bilayers with different percentage of DPPS
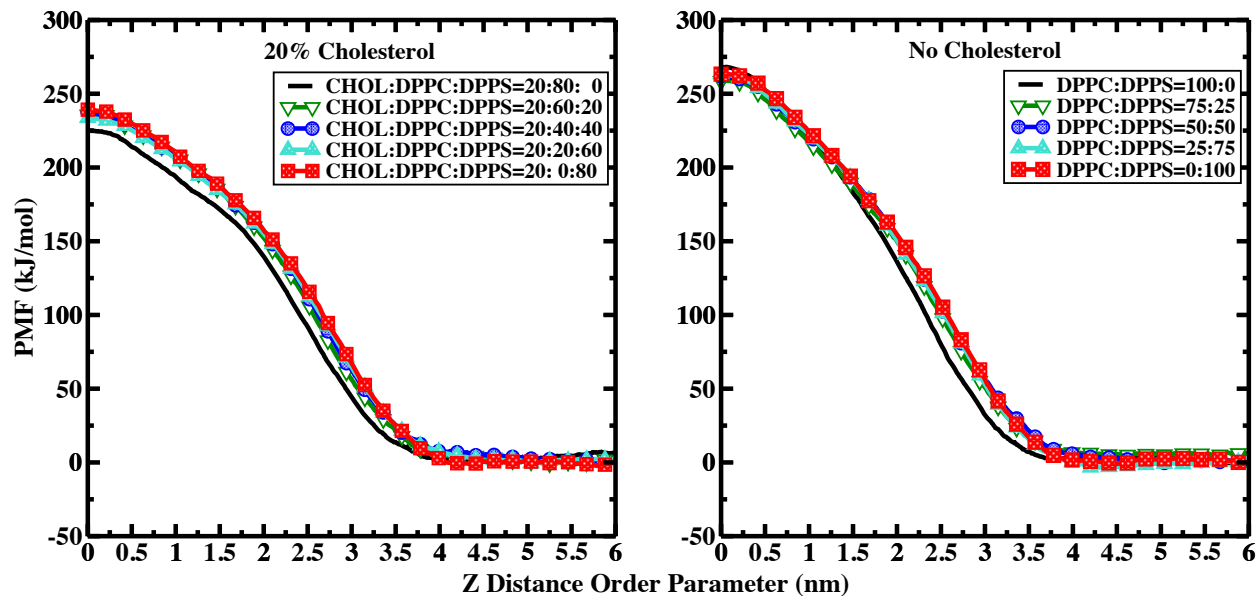

Figure S6: PMF Decomposition: contribution from water in 20% CHOL and no CHOL mixture systems.
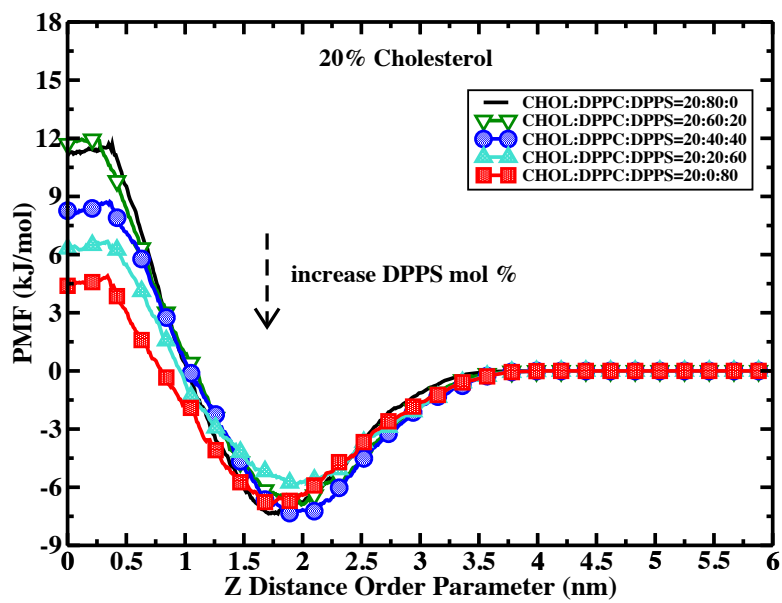
Figure S7: PMF Decomposition: contribution from cholesterol in 20% CHOL systems.