Investigating the effects of POPC-POPG Lipid Bilayer Composition on PAP248-286 Binding using CG Molecular Dynamics Simulations

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Supplementary Table 1: System size (x,y z coordinates) of PAP248-286 (HIS charged) with membranes.

System type	X	Y	Z
PAP248-286- 100% POPC	8.00363	8.00363	21.31466
PAP248-286- 70% POPC-30%	8.01917	8.01917	20.74326
PAP248-286- 50% POPC-50%	7.97891	7.97891	20.81991

Supplementary Table 2: System size (x,y z coordinates) of PAP248-286 (HIS neutral) with membranes.

System type	X	Y	Z
PAP248-286- 100% POPC	8.05836	8.05836	20.95987
PAP248-286- 70% POPC-30%	7.98507	7.98507	20.86382
PAP248-286- 50% POPC-50%	7.96629	7.96629	20.88478