# SUPPLEMENTARY MATERIAL

## Molecular Dynamics Simulation Strategies for Protein-Micelle Complexes

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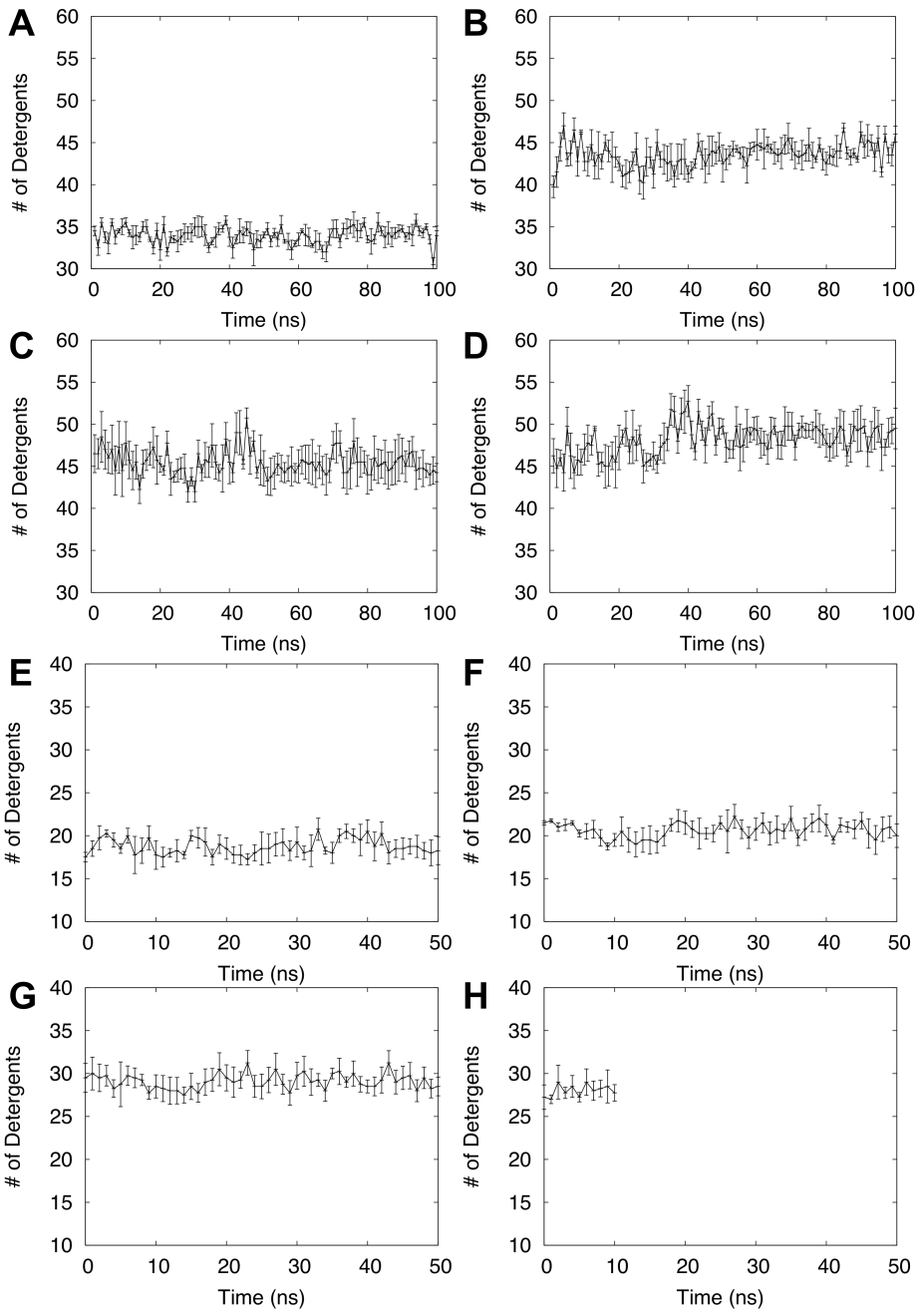


**Figure S1.** The average number of detergents in direct contact with (A-D) KvAP VSD and (E-D) papiliocin as a function of time in the micelle systems of (A) 40 DHPC, (B) 60 DHPC, (C) 80 DHPC, (D) 100 DHPC, (E) 60 DPC, (F) 100 DPC, (G) 200 DPC, and (H) 300 DPC. The number of detergents and the error bars are the average and the standard errors over five replicated simulations in each system.