

Supporting Information for Sphingomyelin Effects in Caveolin-1 Mediated Membrane Curvature

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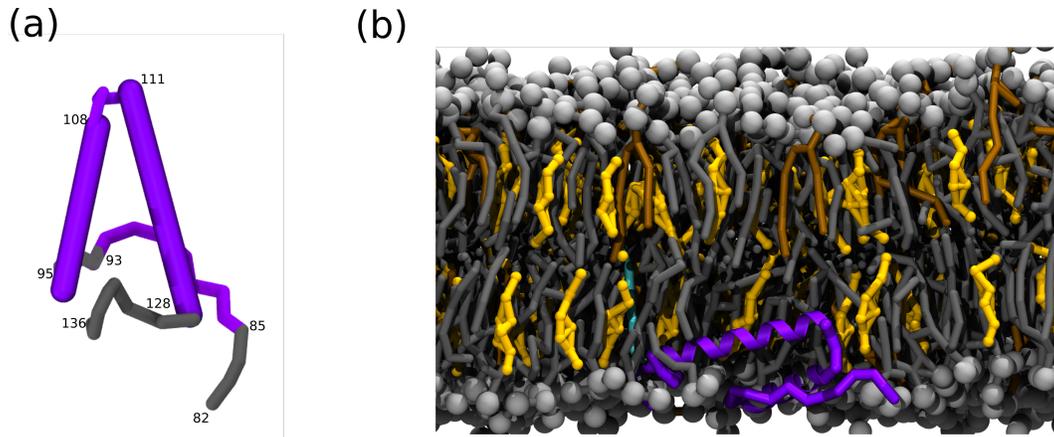


Figure S1: Representative snapshots of cav-1 construct considered in this study and zoom in to the bound state. The cav-1 protein is shown in a ribbon representation in purple and its palmitoyl tail in cyan. The cholesterol molecules are represented in yellow, DPPC lipids in gray and silver and sphingomyelin molecules are shown in ochre. The surrounding water is represented in dark blue.

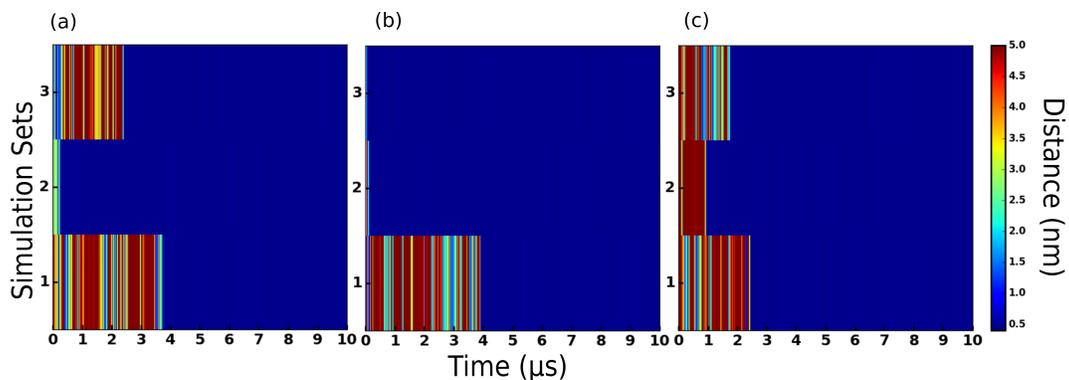


Figure S2: Time evolution of the interactions of cav-1 with DPPC/cholesterol membrane with varying sphingomyelin concentration. The minimum distance between cav-1 and the membrane is color coded and shown as a scale bar. The panels correspond to bilayers with (a) 5% (b) 10% and (c) 15% sphingomyelin. The membrane-bound regime of cav-1 is represented by distances less than 0.5 nm, indicated by the dark blue stretches in the plot. The simulation time is plotted along the abscissa whereas each independent replicate simulation set is numbered along the ordinate.

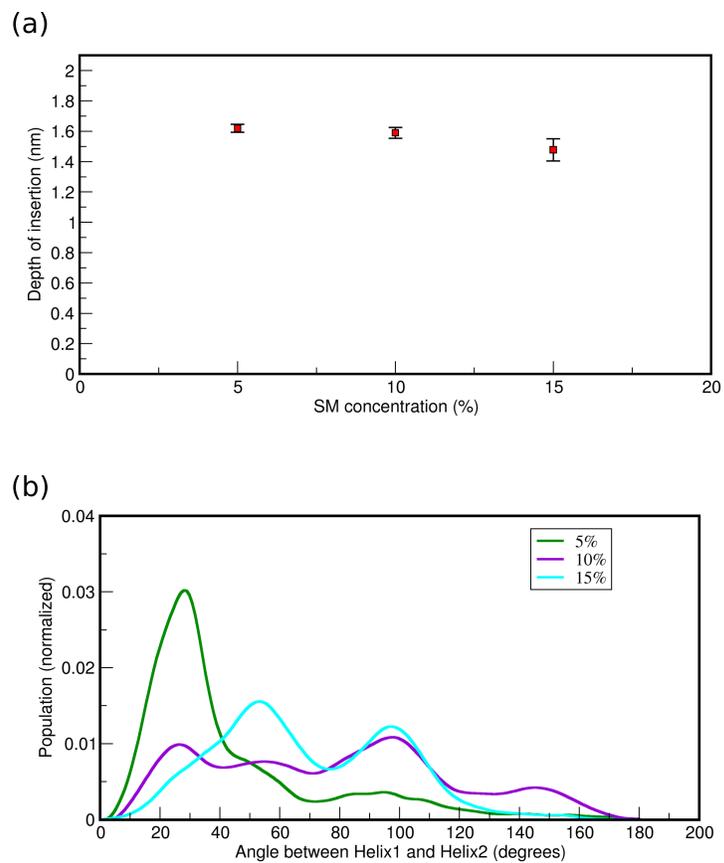


Figure S3: (a) Depth of insertion of cav-1 upon binding. The distance is measured for cav-1 (excluding palmitoyl tail) from the the bilayer center. (b) The inter-helical angle distributions for cav-1 sampled during the simulations.

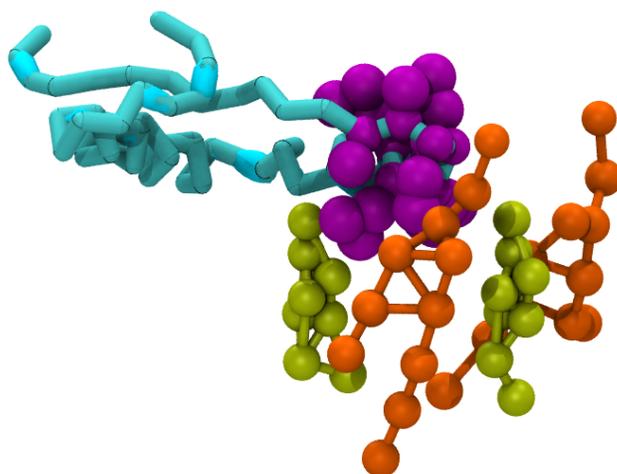


Figure S4: A schematic representative of the interaction of cav-1 with cholesterol and sphingomyelin. The protein backbone is shown in cyan and the CRAC domain is highlighted in purple. The cholesterol molecules are represented in yellow and sphingomyelin in ochre.

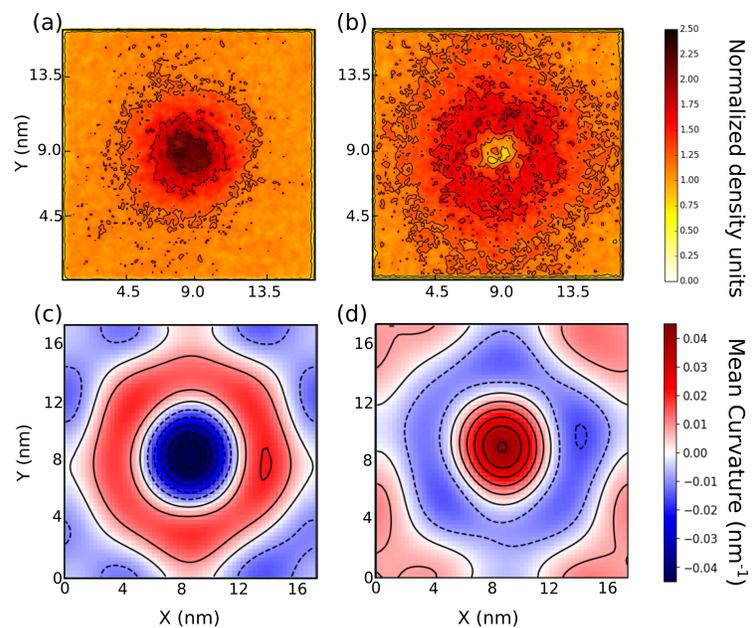


Figure S5: Cholesterol density and curvature in the absence of sphingomyelin (control simulations at 0% sphingomyelin). The cholesterol density (a,b) and curvature (c,d) for the extracellular (a,c) and intracellular (b,d) leaflets of DPPC/cholesterol bilayers.

Table S1: Simulations performed in this study

Protein	Bilayer	Sets	Simulation Time (μ s)	Total Time (μ s)
Palmitoylated cav-1	DPPC/cholesterol with 0% sphingomyelin	3	10	30
Palmitoylated cav-1	DPPC/cholesterol with 5% sphingomyelin	3	10	30
Palmitoylated cav-1	DPPC/cholesterol with 10% sphingomyelin	3	10	30
Palmitoylated cav-1	DPPC/cholesterol with 15% sphingomyelin	3	10	30