Supplemental Material: Interactions Between Fengycin and Model Bilayers Quantified by Coarse-grained Molecular Dynamics

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Bilayer	**Lipopeptides**	**Replicates**	**Temperature (K)**	**Duration(μs)**
DPPC	0	16	323	1.0
	1	16		2.0
	13	16		2.0
POPC	0	16	300	1.1
	1	16		2.2
	13	16		2.1
POPE/POPG	0	16	300	1
	1	16		2.3
	13	16		2.1

Table S1: Table of all simulations and compositions. "Duration" refers to the average length of the trajectories.

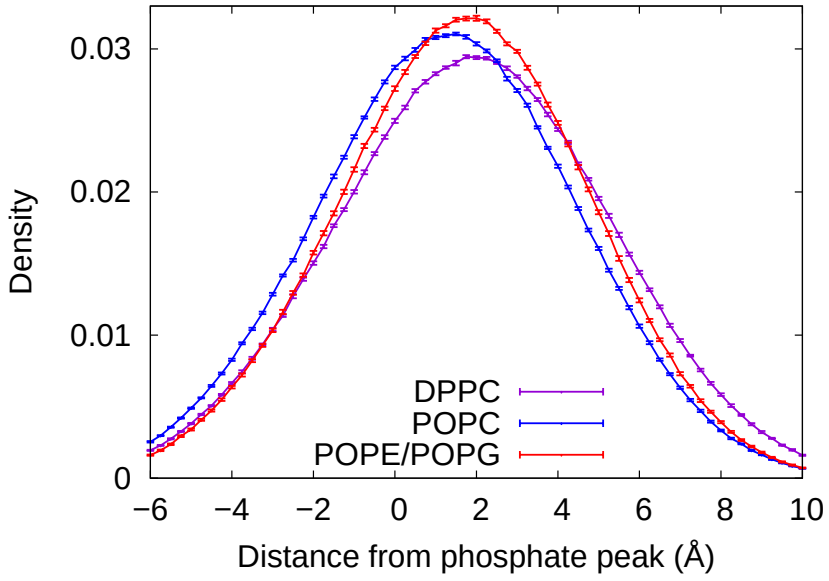

Figure S1: Average normalized density for fengycin relative to the peak of phosphate density for each of the bilayer systems with a single fengycin.

Fengycin Cluster Analysis and Curation

To quantify the curvature of the bilayer induced by fengycin, we created maps measuring the height of the lipid phosphate beads relative to the center of the lipid bilayer as a function of lateral distance from fengycin. We began by hand-curating a collection of clusters that persist for at least one hundred nanoseconds in the simulation. Clusters were gathered until we had more than 1.5 μs total of clusters for a given cluster size and for a given bilayer: 6 fengycins in DPPC (7 clusters, 1.6 μs), 9 fengycins in DPPC (7 clusters, 1.5 μs), 6 fengycins in POPC (7 clusters, 2.9 μs), and 9 fengycins in POPC (2 clusters, 1.8 μs). No persistent clusters of these sizes could be gathered in a POPE/POPG system.