Table 1. List of simulations of GV4

System	Time (per run)	Peptides	Water molecules	Octane molecules	Box size (nm)	Number of runs	Total peptides	Time (total)	Concentration (water)	Concentrat (slab)†
A	55.8 ns	2	1353!	75	3.59x3.59x5.5	8	16	446 ns	0.027 M	0.082 M
B1	10 ns	8	15948!	599	9.13x9.13x7.67	43	344	430 ns	0.042 M	0.090 M
B2	20 ns	8	5739!	599	9.27x9.27x4.06	43	344	860 ns	—	0.090 M
C1*	50 ns	40	7960	1000	8.30x8.30x8	1	40	82 ns	—	0.439 M
C2	136 ns	40	7960	1000	"	1	40	219 ns	—	0.439 M
D	20 ns	8	12643!**	0	9.13x9.13x4.81	5	40	100 ns	0.042 M	—

*Run C1 was generated by addition of 8 chains for 10 ns, then 16 for 10 ns, then another 16 for another 12 ns (until all peptides were on the slab).

†Concentration on the slab is calculated assuming that the Z dimension of the interface is about 1 nm—this is the general size of the range of Z values for the center of mass of adsorbed chains.

! varies depending on conformation of peptide and the amount of space it takes up

** Number is slightly smaller than B1 because of removal of overlapping waters between top and bottom halves of box.