Biophysical Journal, Volume *115*

Supplemental Information

Optimal Hydrophobicity and Reorientation of Amphiphilic Peptides Translocating through Membrane

Ivo Kabelka and Robert Vácha

SUPPLEMENTARY INFORMATION

Table S1: System compositions of coarse-grained simulations

	4, 6 nm	1, 2, 3, 8 nm
Peptide	1	1
Lipid	200	500

Table S2: System compositions of all-atom simulations

	Parallel				Perpendicular			
	5	8	11	21	5	8	11	21
Peptide	1	1	1	1	1	1	1	1
POPC	128	128	128	128	118	118	118	118
TIP3P	6827	6817	6817	6826	7358	7373	7373	7344
Na	37	37	37	37	37	37	37	37
Cl	37	37	37	37	37	37	37	37

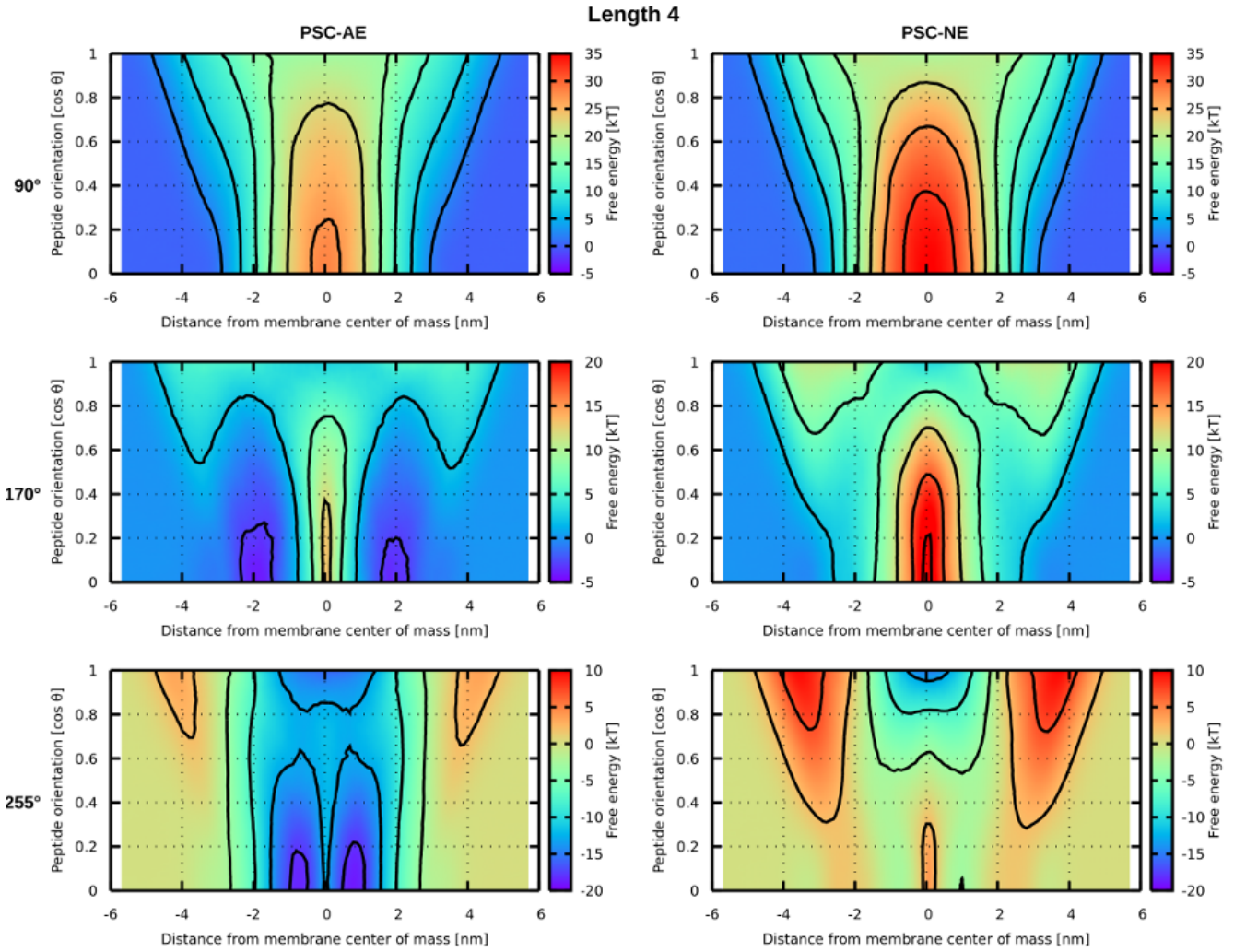

Figure S1: Calculated free energy surface of peptde translocation across lipid bilayer. Peptides of length 4 nm are shown. Peptides with attractive and non-attractive endcaps are shown in the left and right columns, respectively. Hydrophobic patch width is 90, 170, and 250°. Contours are drawn at every 10 kT.

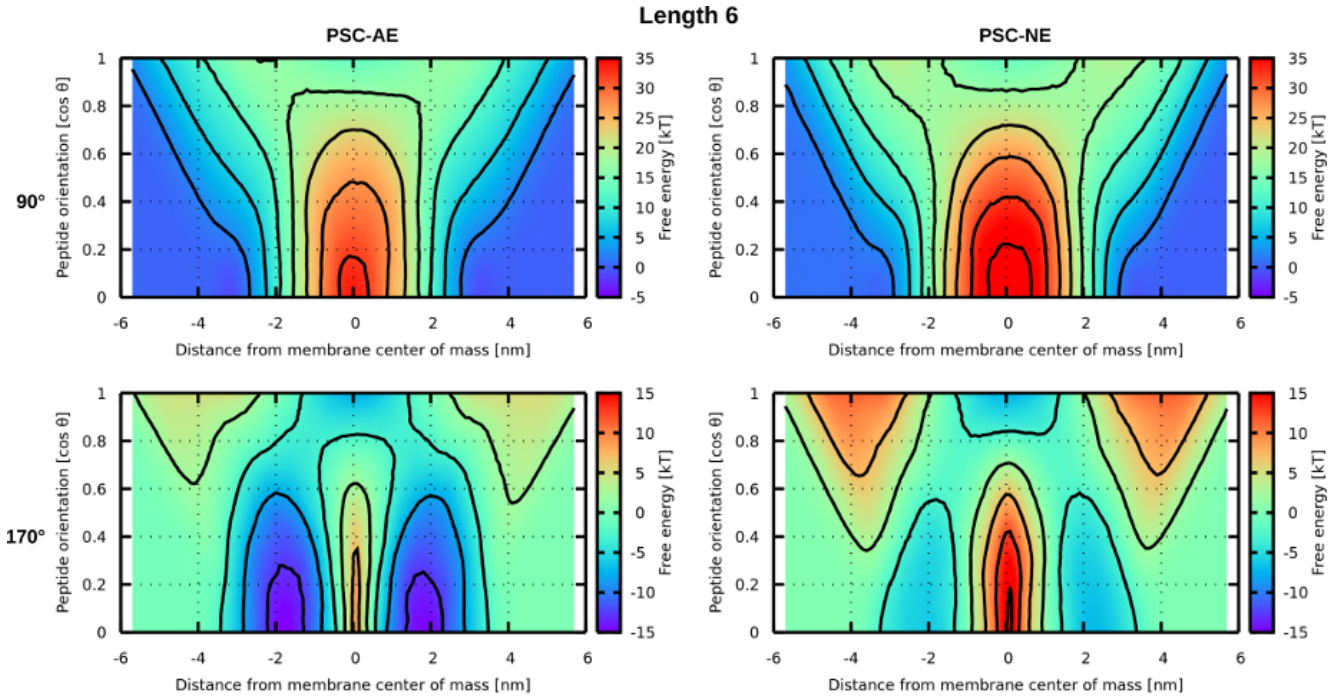

Figure S2: Calculated free energy surface of peptde translocation across lipid bilayer. Peptides of length 6 nm are shown. Peptides with attractive and non-attractive endcaps are shown in the left and right columns, respectively. Hydrophobic patch width is 90 and 170°. Contours are drawn at every 10 kT.

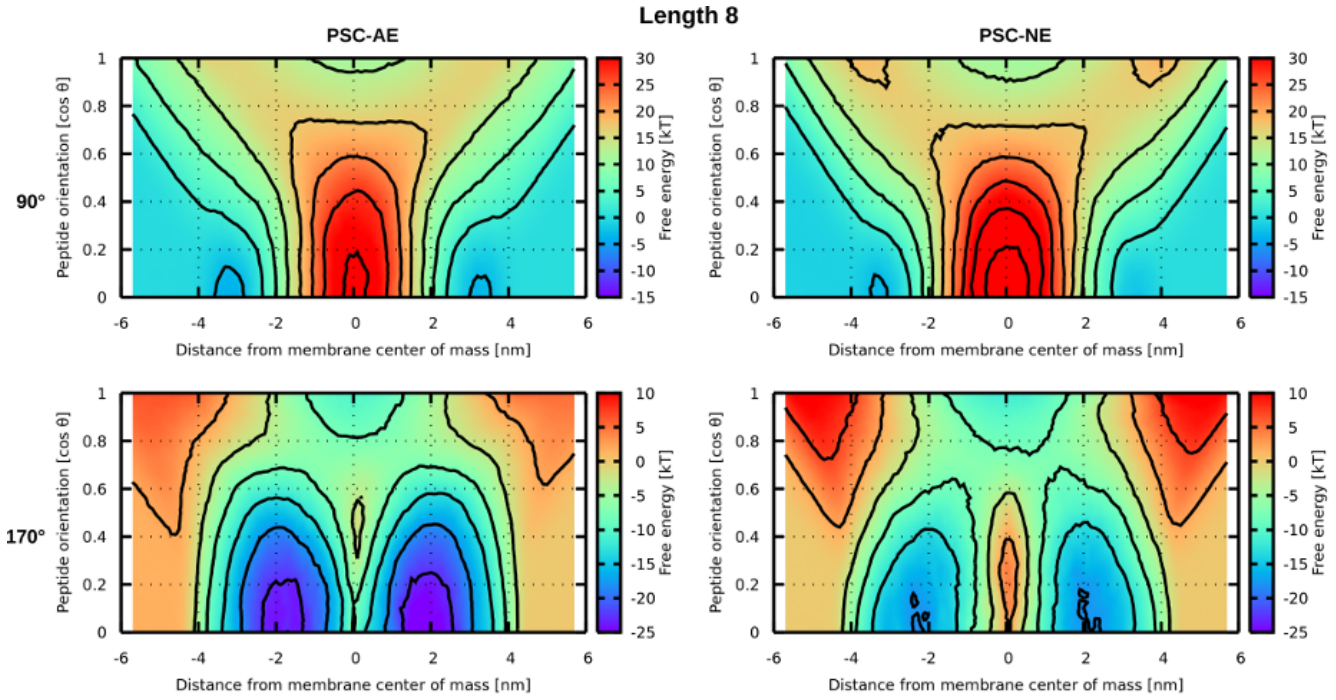

Figure S3: Calculated free energy surface of peptde translocation across lipid bilayer. Peptides of length 8 nm are shown. Peptides with attractive and non-attractive endcaps are shown in the left and right columns, respectively. Hydrophobic patch width is 90 and 170°. Contours are drawn at every 10 kT.

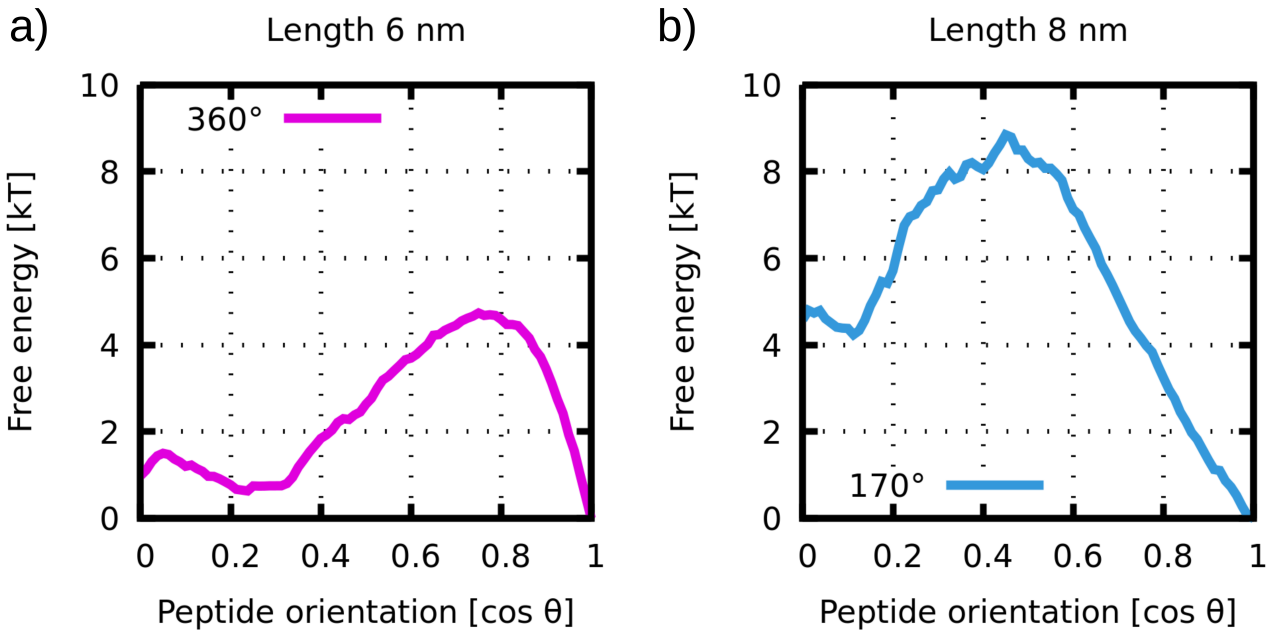

Figure S4: Free energy profile for the change of peptide orientation. The peptides are located in the membrane center. [IVO co je to PSC CPSC...? trochu se u toho popisu rozepis]

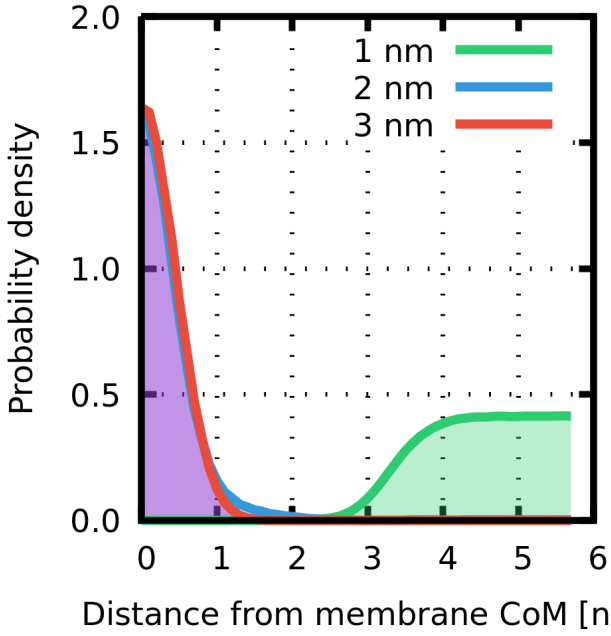

Figure S5: Distribution of short hydrophobic peptides (modeled by PSC particles) as a function of distance from membrane center of mass.

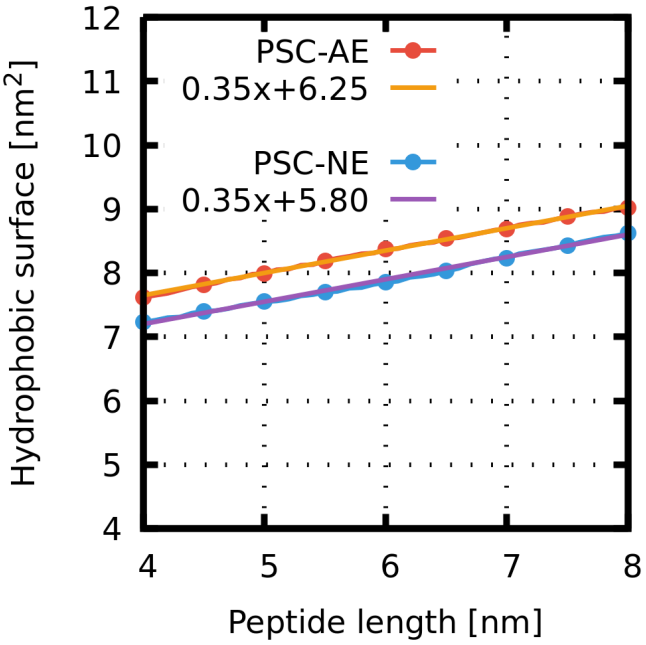

Figure S6: Optimal hydrophobic surface area for given peptide length. Lines with circles are calculated data points and smooth lines are linear fits.