SUPPLEMENRARY INFORMATION

Adsorption Characteristics of Peptides on the ω-Functionalized Self-assembled Monolayers: A Molecular Dynamics Study

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Table S1. Initial configuration parameters for SCA adsorption on different SAMs, where l_x and l_y are the simulation box lengths in x and y directions, respectively.

<i>l_x</i> (nm)	$l_y(nm)$	No. of SAM chains	No. of water molecules
3.500	3.464	56	1400 - 1600

Table S2. Initial configuration parameters for β -hairpin (HP7) peptide adsorption on different SAMs.

<i>l_x</i> (nm)	$l_y(nm)$	No. of SAM chains	No. of water molecules
5.500	5.196	132	4500 - 5000



Figure S1. (a) Umbrella histograms and (b) adsorption free energy, V_{PMF} , as a function of distance, z_{cm} , at different simulation lengths for the value (VAL) side chain on the PFA SAM, where z_{cm} denotes the z-distance between the centers of mass of PFA SAM and VAL side chain.







Figure S2. V_{PMFs} of SCAs as a function of z_{cm} -distance on (a) PHEA, (b) PMEA, (c) PBA, and (d) PFA SAM surfaces.



Figure S3. Adsorption free energy, V_{PMF}° , of SCAs at equilibrium pair separation as a function of SCAs. The data is arranged based on the increasing magnitude of V_{PMF}° on the PFA SAM surface.



Figure S4. Correlation of the adsorption free energy of SCAs, V_{PMF}° , on the PFA SAM surface with previous experimental hydrophobicity scales, λ , based on the (a) transmembrane tendency^{S1} and (b) transfer free energy of peptides at the membrane interfaces.^{S2} The SCAs are shown in the plots with their traditional one letter symbols.



Figure S5. V_{PMF} profile of the HP7 peptide on the four different ω -functionalized SAM surfaces.



Figure S6. Solvent accessible surface area (SASA) (left panels) and water coordination number, n_w , (right panels) of the (a) SAMs and (b) HP7 peptide.



Figure S7. Number of hydrogen bonds, n_{HB} , between the PHEA SAM surface and water (blue line), between the OH groups of PHEA (green line), and between the ester group of PHEA and water as a function of time



Figure S8. Z-density distribution, ρ , of SAM, HP7, and water along the surface normal, z.

REFERENCES

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