Electronic Supplementary Material (ESI) for Nanoscale.

Nanoscale *in-silico* classification of ligand functionalised surfaces for protein adsorption resistance

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Supplementary Figures

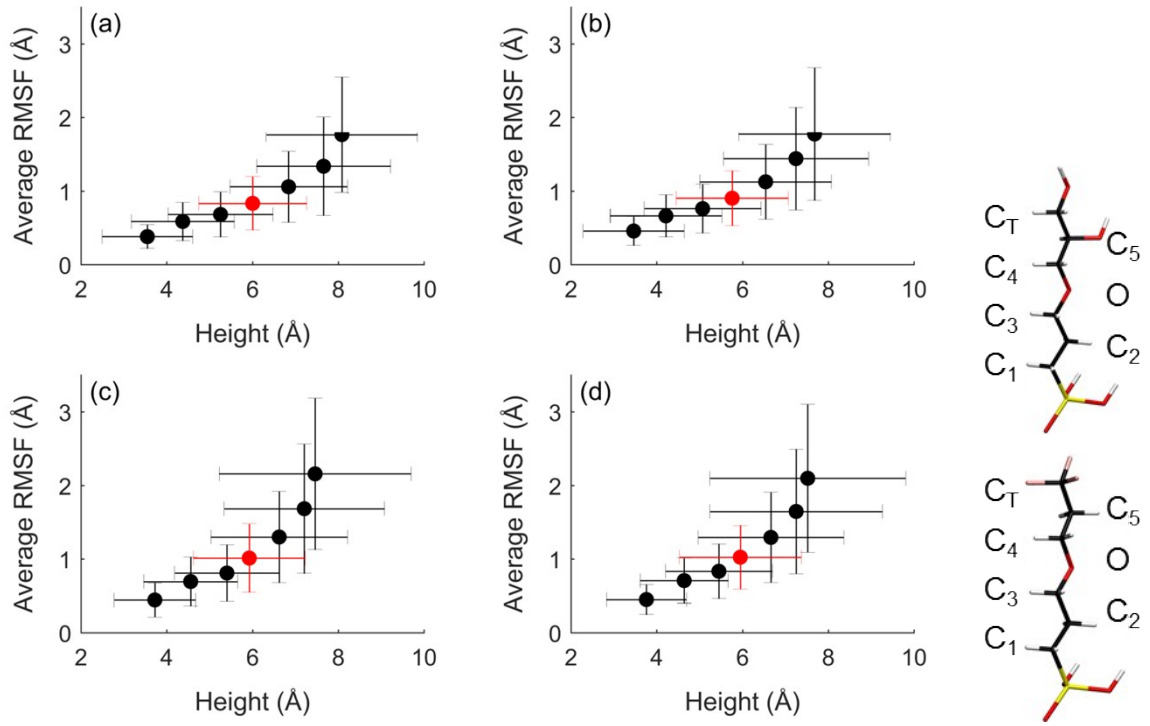

Fig. S1: Average RMSFs of heavy atoms along the ligand chain (from left to right C_1, C_2, C_3, O, C_4, C_5, C_T) against the height above the substrate for (a) GPS, (b) CF_3, (c) GPS:sNH_2, and (d) GPS:sCF_3 systems.

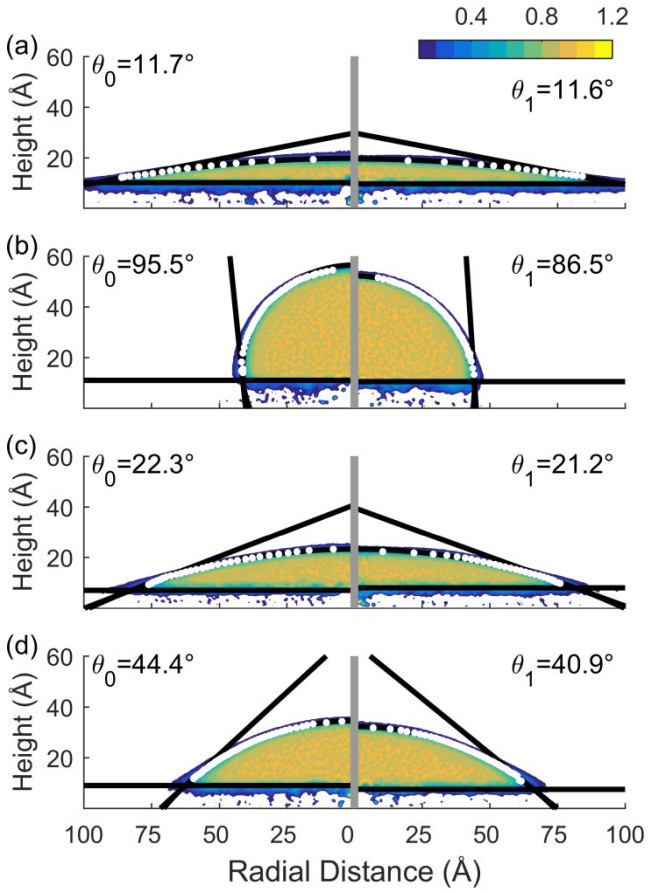

Fig. S2: Relative density maps for 2 equilibrated water droplets on the (a) GPS, (b) CF_3, (c) GPS:sNH_2, and (d) GPS:sCF_3 systems in-vacuum with colorbar showing relative atomic density compared to bulk TIP3P water and contact angle estimates shown.

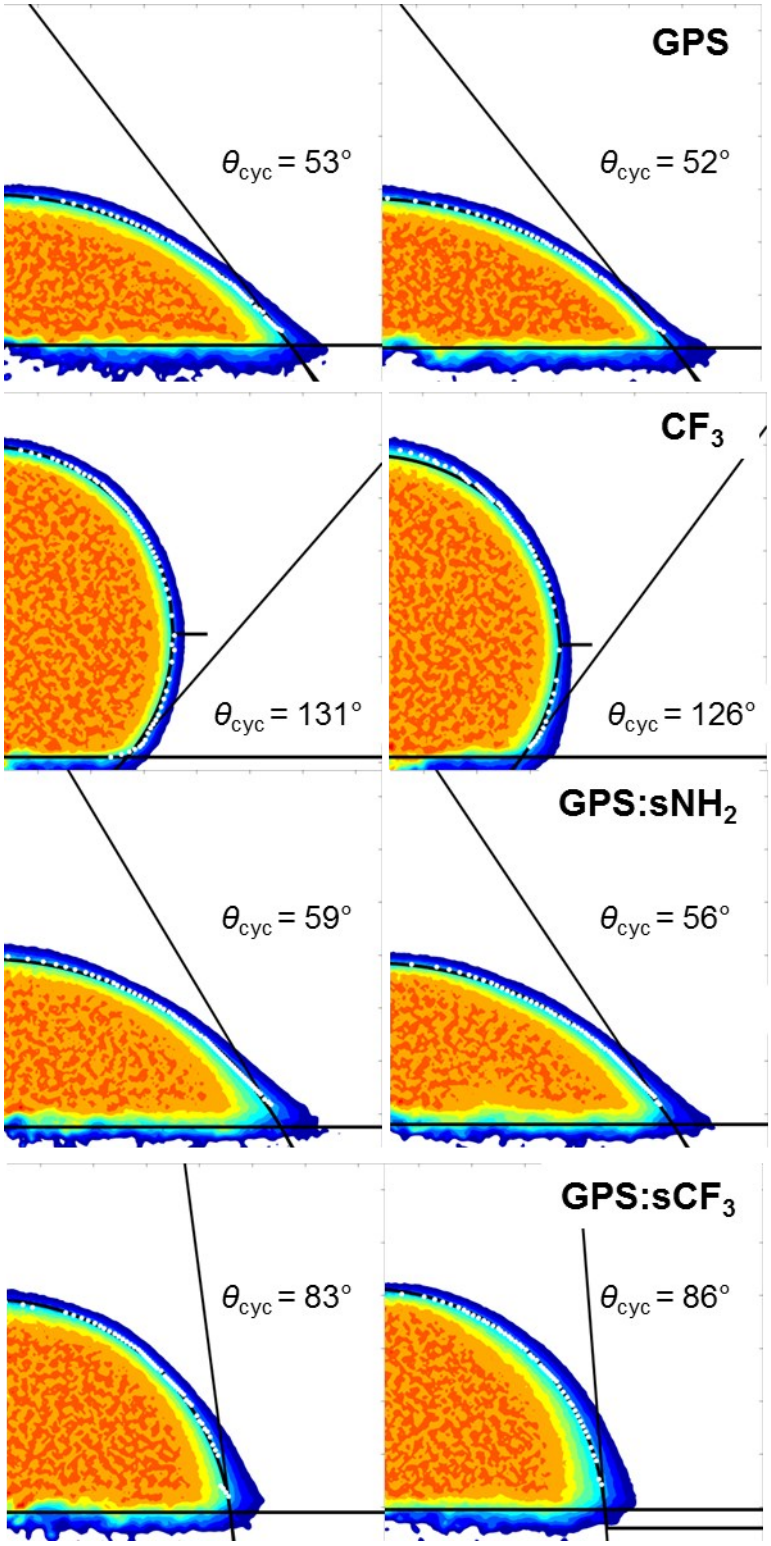

Fig. S3: Relative density maps of water droplet immersed in cyclooctane for the time from 10 to 5 ns before run termination; droplet fitted circle, droplet base height and tangent at the cross over point are shown in black, water contact angle estimates, θ_{co}, are shown for each system

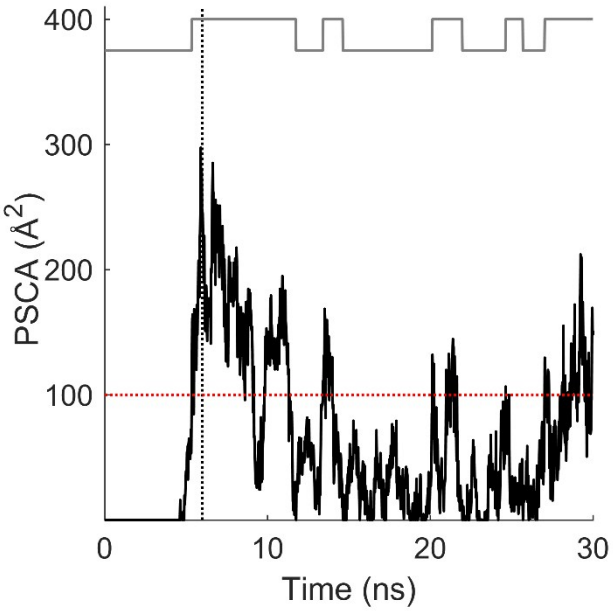

Fig. S4: Magnified PSCA data for exemplar trajectory.

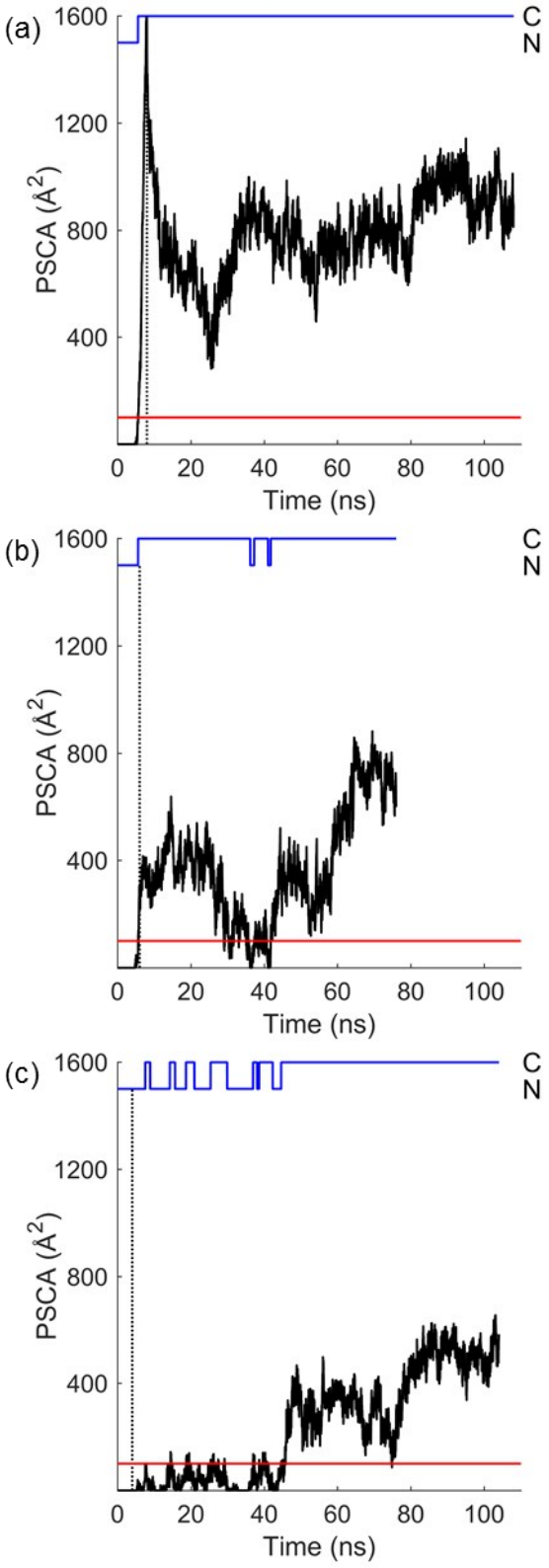

Fig. S5: Protein-surface contact area as a function of run time (black); time evolution of whether the protein is in contact (C) or not in contact (N) with the surface by the PAE definition (blue); PSCA for defining a PAE (horizontal red); force release point (vertical black dotted) for the protein at (a) GPS from the bound release point; (b) GPS from the transition release point; and (c) GPS from the association release point.

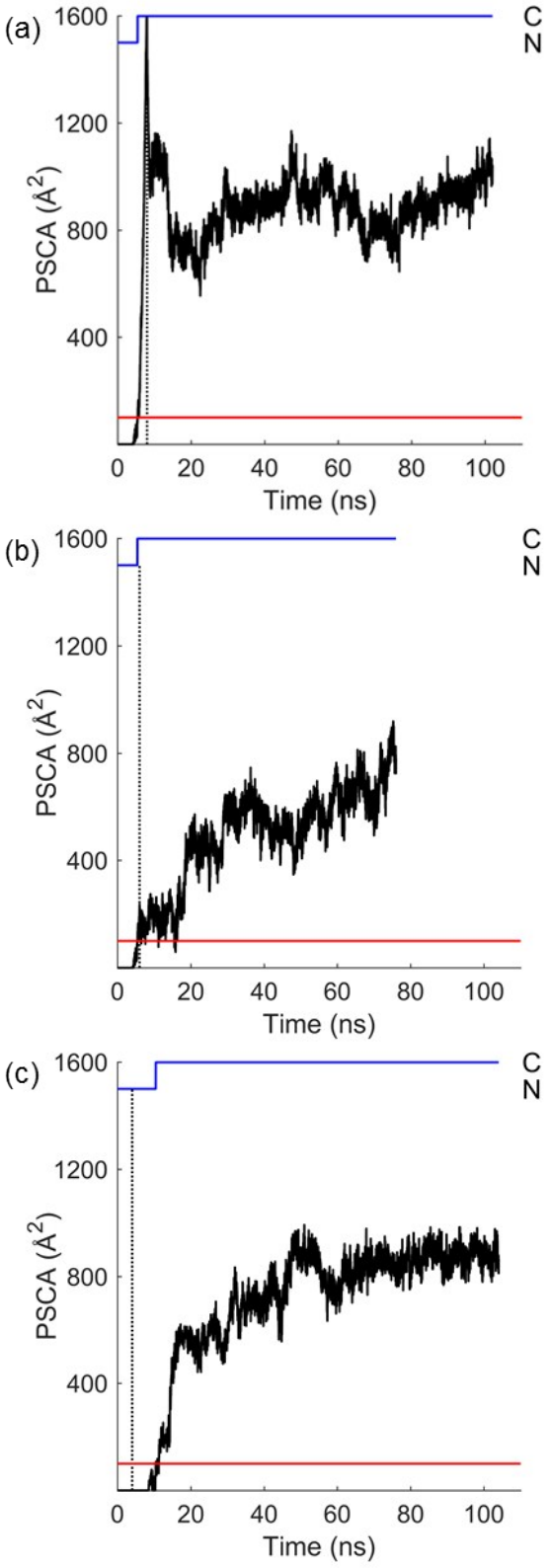

Fig. S6: Protein-surface contact area as a function of run time (black); time evolution of whether the protein is in contact (C) or not in contact (N) with the surface by the PAE definition (blue); PSCA for defining a PAE (horizontal red); force release point (vertical black dotted) for the protein at (a) CF_3 from the bound release point; (b) CF_3 from the transition release point; and (c) CF_3 from the association release point.

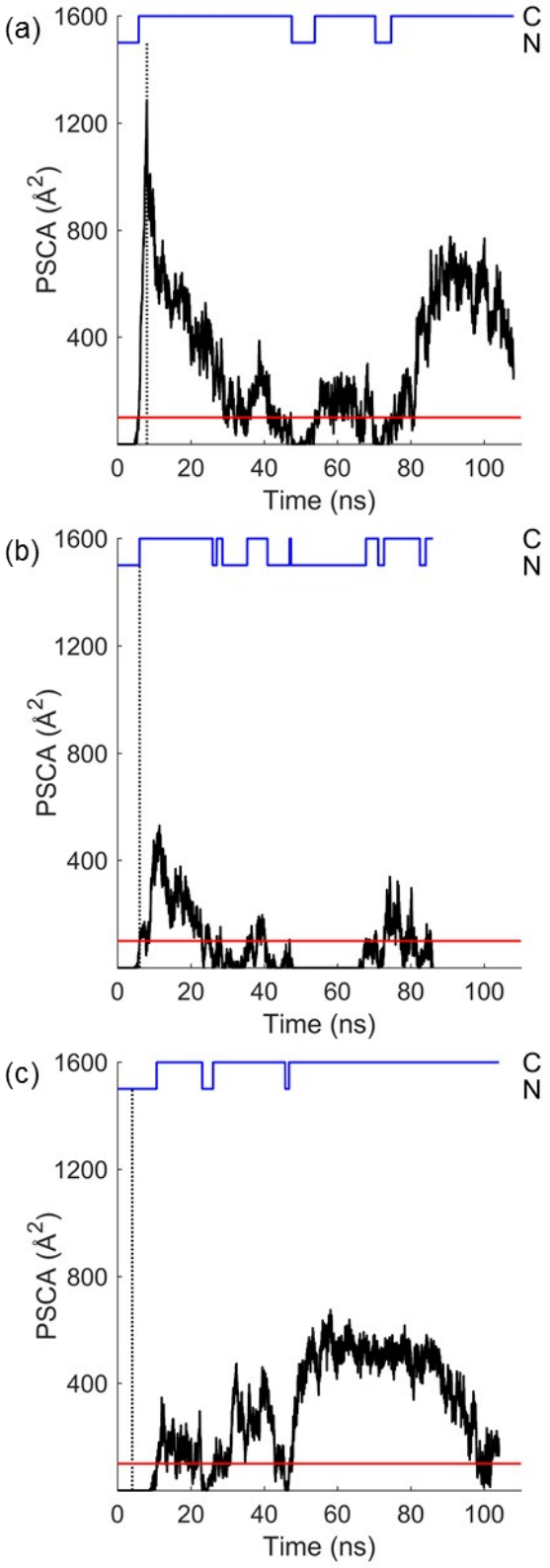

Fig. S7: Protein-surface contact area as a function of run time (black); time evolution of whether the protein is in contact (C) or not in contact (N) with the surface by the PAE definition (blue); PSCA for defining a PAE (horizontal red); force release point (vertical black dotted) for the protein at (a) GPS:sNH$_2$ from the bound release point; (b) GPS:sNH$_2$ from the transition release point; and (c) GPS:sNH$_2$ from the association release point.

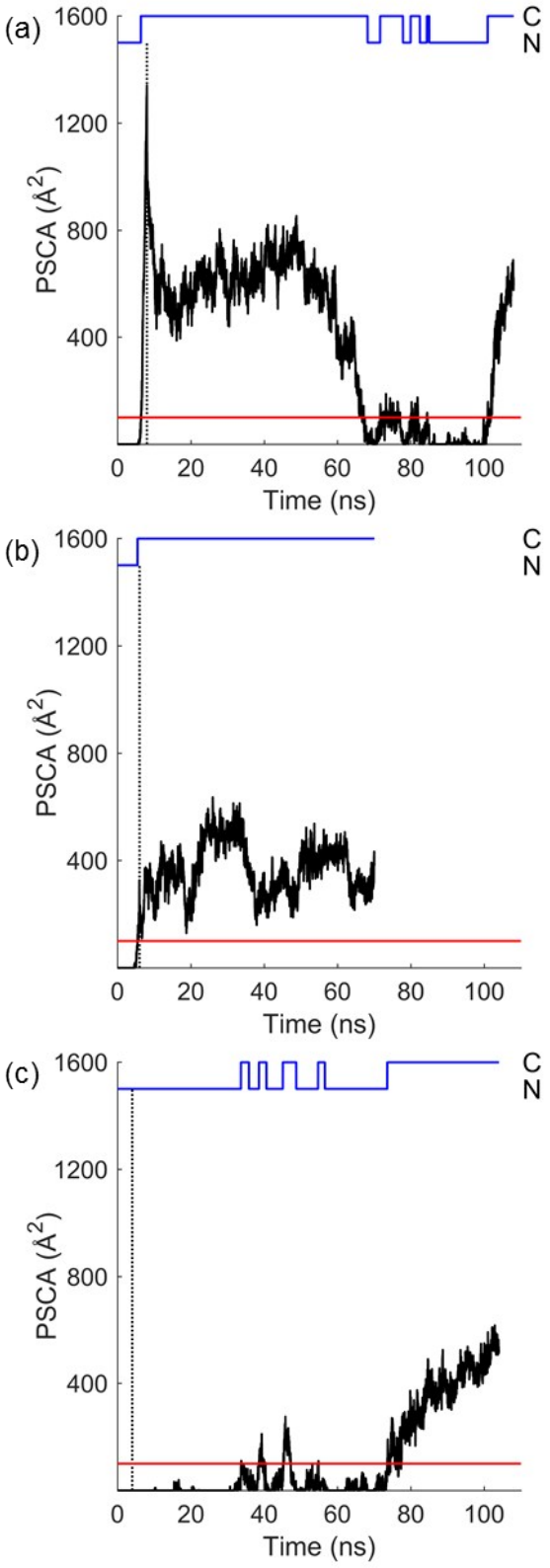

Fig. S8: Protein-surface contact area as a function of run time (black); time evolution of whether the protein is in contact (C) or not in contact (N) with the surface by the PAE definition (blue); PSCA for defining a PAE (horizontal red); force release point (vertical black dotted) for the protein at (a) GPS:sCF_3 from the bound release point; (b) GPS:sCF_3 from the transition release point; and (c) GPS:sCF_3 from the association release point.

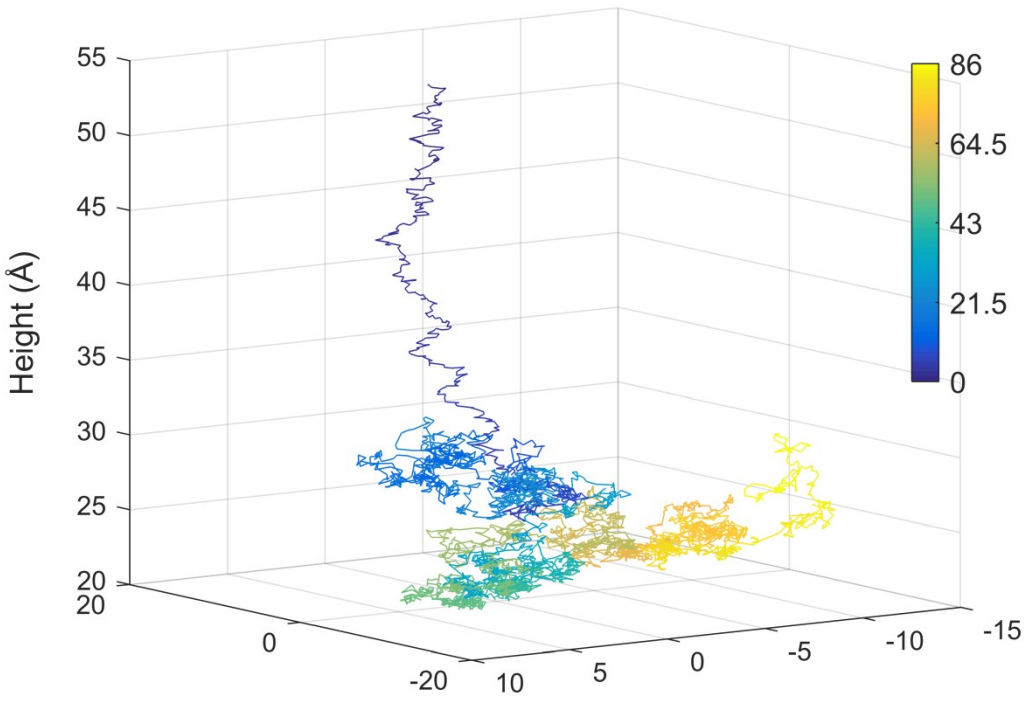

Fig. S9: Temporal evolution of the centre of mass of the protein from the exemplar trajectory presented in Fig 4, colorbar showing time in ns.

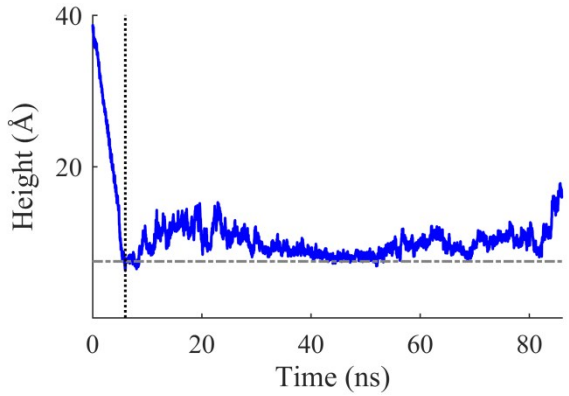

Fig. S10: Minimum height of protein from exemplar trajectory presented in Fig 4, average height of ligand C_T atoms (horizontal dot-dash), force release time (vertical dot line).

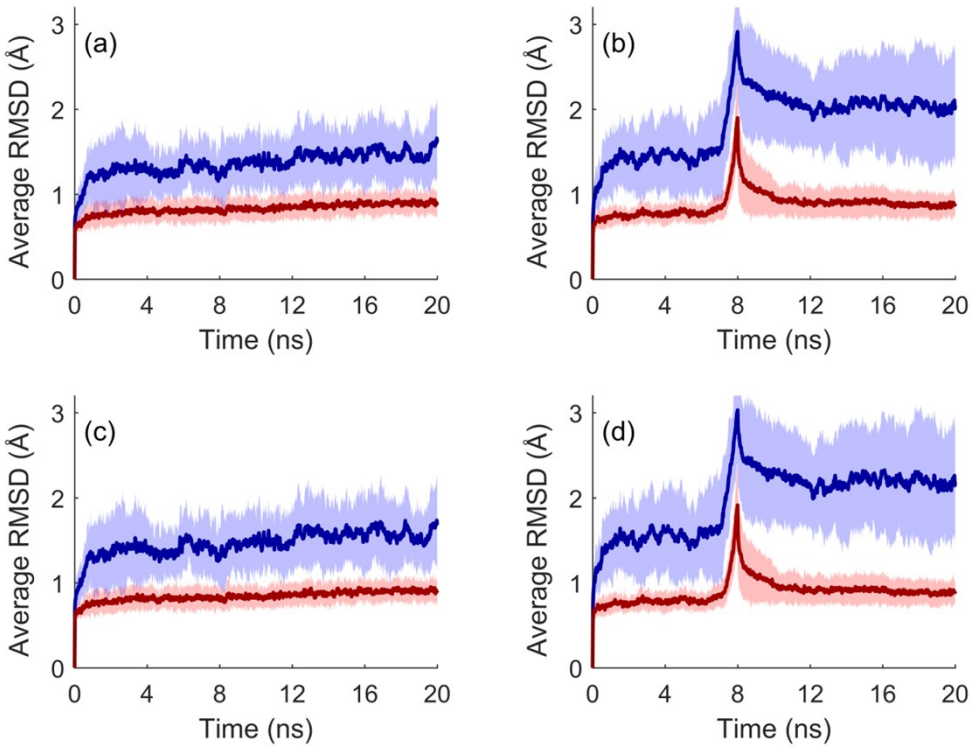

Fig. S11: Aligned RMSD trajectories for ubiquitin in (a and c) bulk water averaged from 20 x 20 ns blocks from the 400 ns bulk solvent simulation and (b and d) from bound release point runs for the GPS:sNH$_2$ system averaged from 20 runs performed. The shaded region shows 1 standard deviation for all systems. (a and b) RMSD based on C$_\alpha$ atoms, (c and d) RMSD based on all heavy backbone atoms calculated over all residues (blue) and excluding C-terminal residues 72-76 (red).

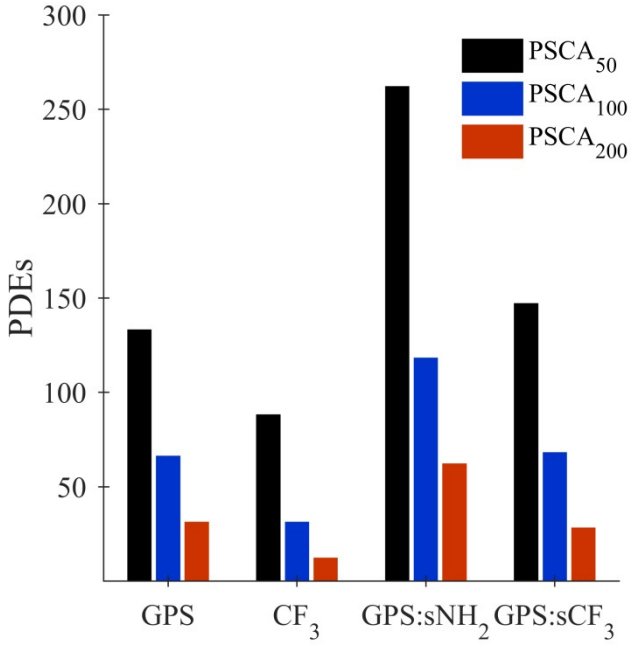

Fig. S12: Total number of PDEs with different threshold for defining contact.

Table S1: Interfacial hydration data; the count of interfacial water molecules, $I(H_2O)$; the count of embedded water molecules, $E(H_2O)$; the total number of ligand associated water molecules, $T(H_2O)$; and the maximum of the relative atomic density profile of embedded and interfacial water, $(\rho_I+\rho_E)_{max}$.

System	$I(H_2O)$ molecules per Å^2	$E(H_2O)$ molecules per Å^2	$T(H_2O)$ molecules per Å^2	$(\rho_I+\rho_E)_{max}$
GPS	0.096	0.034	0.130	0.67
CF3	0.093	0.026	0.119	0.69
GPS:sNH_2	0.102	0.032	0.133	0.59
GPS:sCF_3	0.098	0.030	0.128	0.64