

Supplementary Information

Proteins at air-water and oil-water interfaces in an all-atom model

Yani Zhao and Marek Cieplak*
*Institute of Physics, Polish Academy of Sciences,
Al. Lotników 32/46, 02-668 Warsaw,
Poland*

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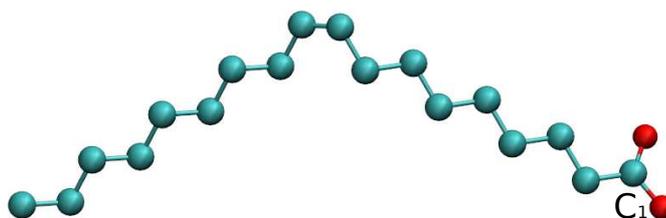


Fig. S 1: The schematic representation of a chain of the oleic acid. The oxygens and carbons are showed as red and cyan beads. The hydrogens are not displayed.

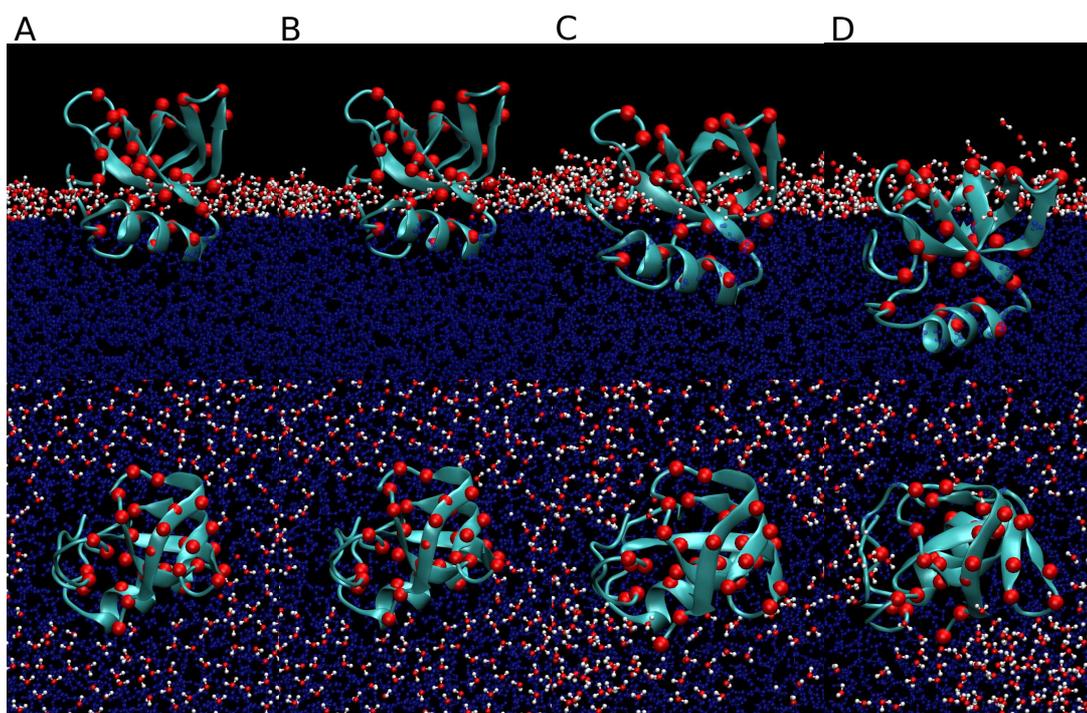


Fig. S 2: Protein 2FZ6 with $n_{SS} = 4$ in orientation I. A: The initial state of the system. B: The state after the energy minimization. C: The state after 2 ns equilibration at $T = 150$ K. D: The final state of the system after 10 ns equilibration at $T = 300$ K.

* Electronic address: mc@ifpan.edu.pl

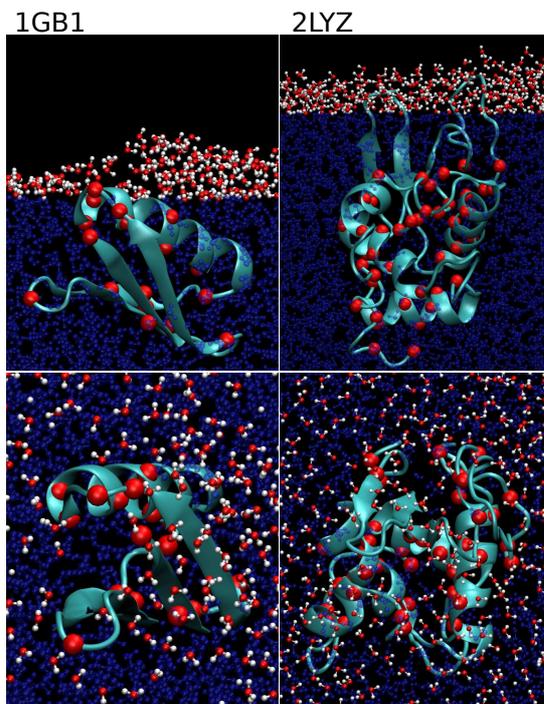


Fig. S 3: The side (top panel) and top (bottom panel) views of the optimal surface orientation of 1GB1 (left) and 2LYZ (right).

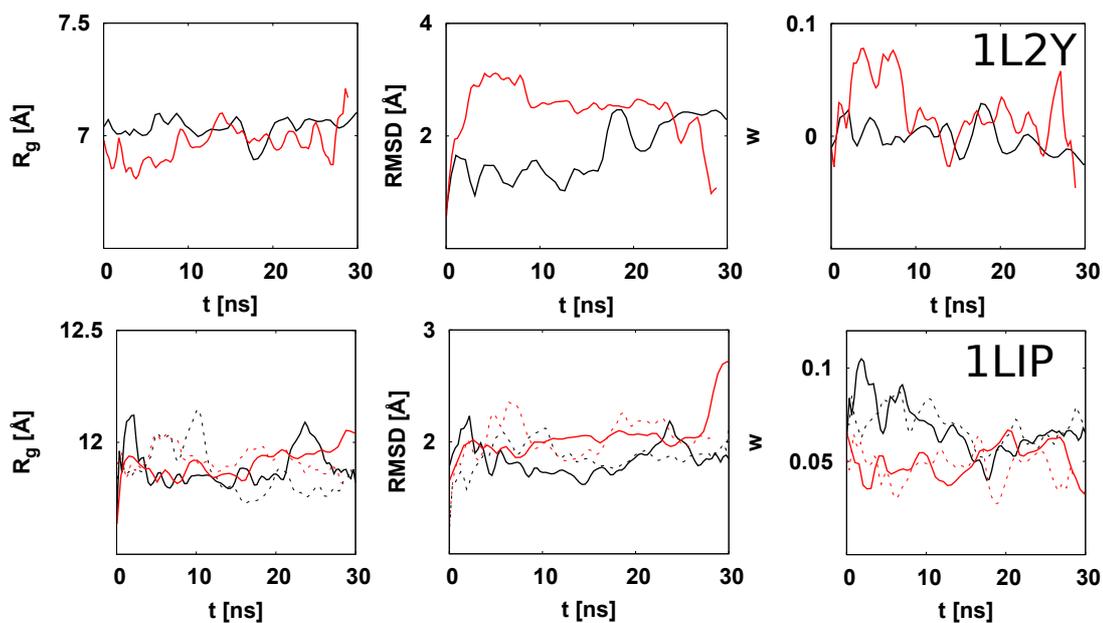


Fig. S 4: The shape-related parameters R_g , RMSD and w for 1L2Y (top) and 1LIP (bottom) at the air-water (black lines) and oil-water (red lines) interfaces. For 1LIP, the solid lines are for $n_{SS} = 4$ and the dashed lines are for $n_{SS} = 0$.