

Adsorption and Unfolding of Lysozyme at a Polarized Aqueous-Organic Liquid Interface

Supporting Information

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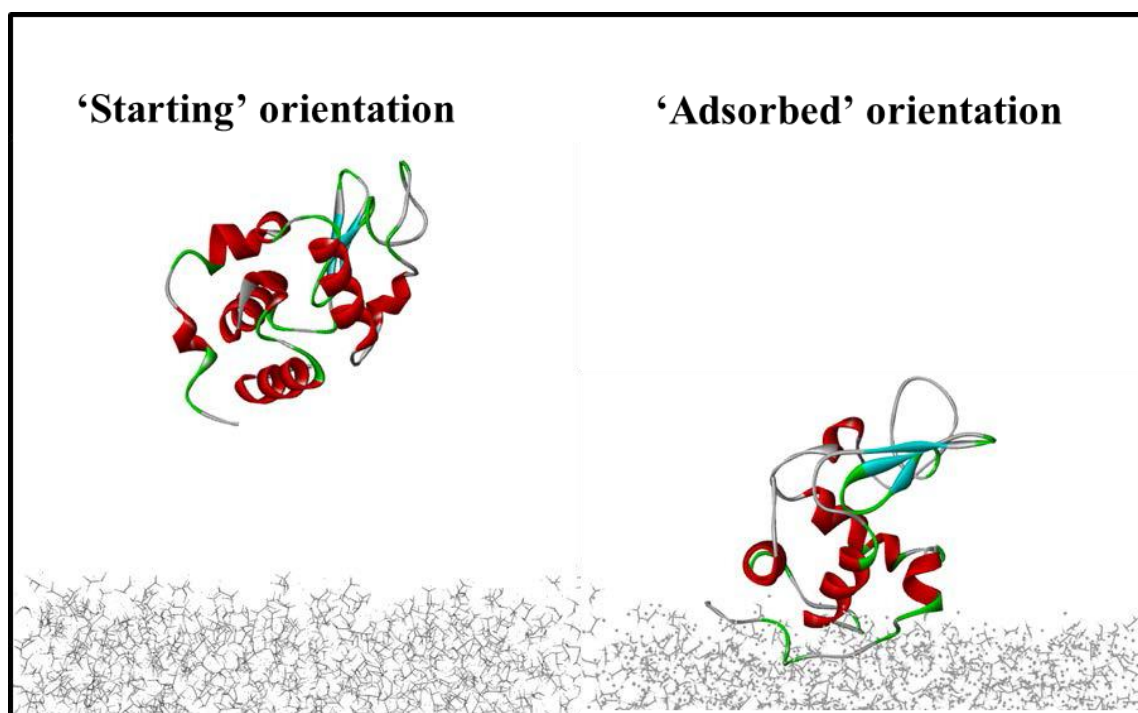


Figure S1: Orientation of HEWL at the start of the simulation and after adsorption at the water/DCE interface.

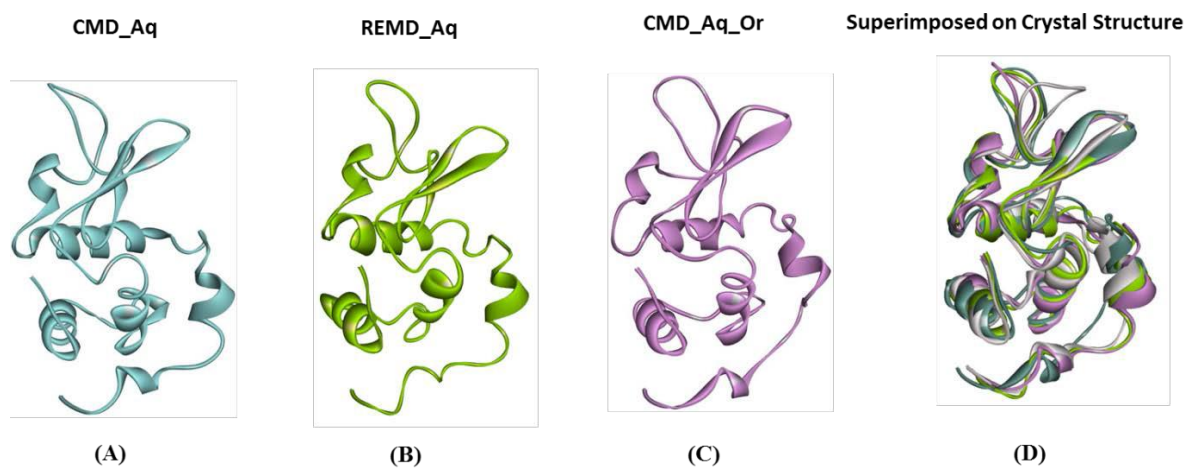


Figure S2: Representative structures of HEWL from cluster analysis of (A) CMD_Aq, (B) REMD_Aq, and (C) CMD_Aq_Org simulations. Superimposition of these representative structures onto the crystal structure of HEWL is shown in D.

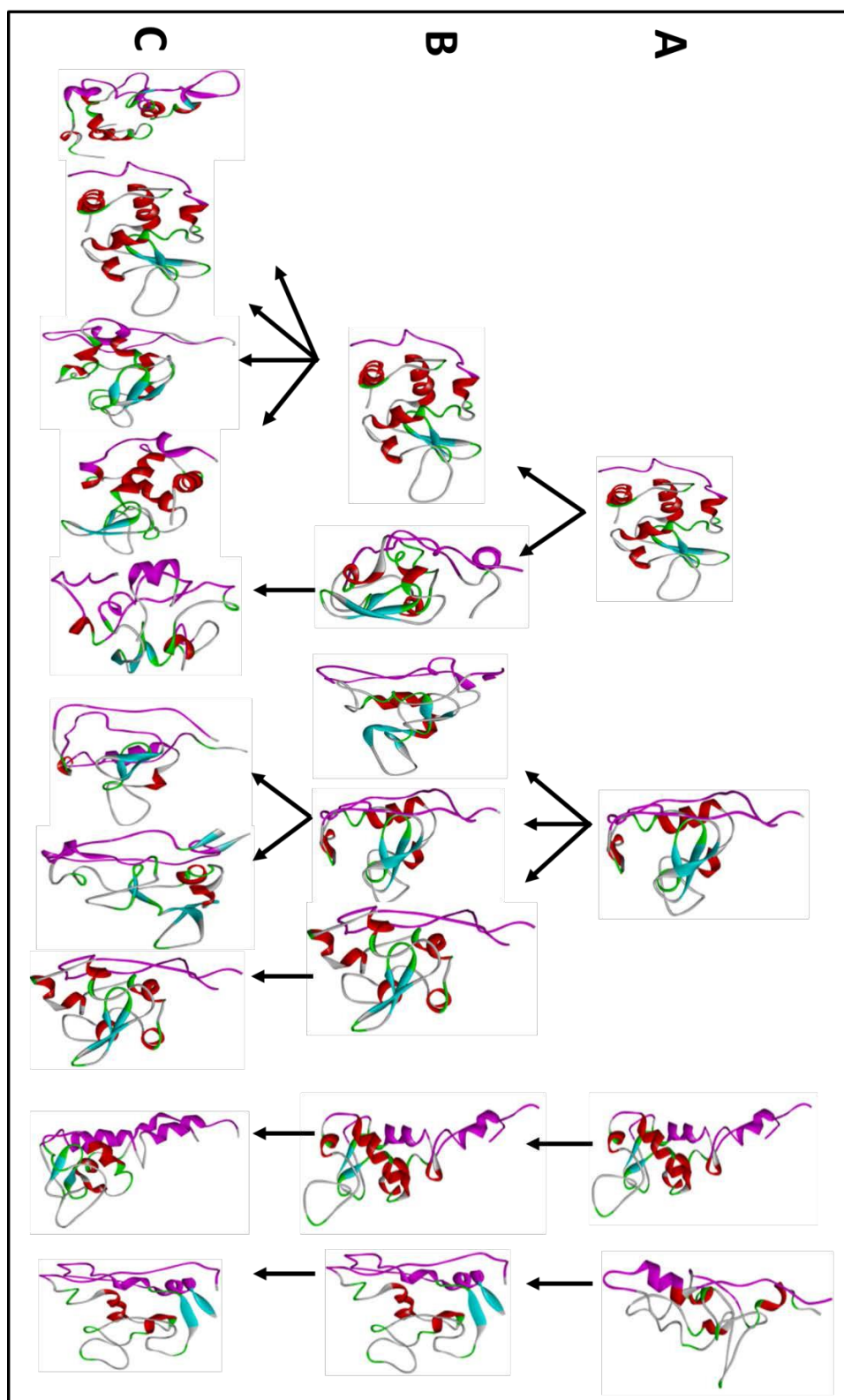


Figure S3: Representative structures of top clusters of HEWL adsorbed at the water/DCE interface (REMD_Aq_Org simulation) obtained with clustering cut-off values of 0.8 nm (**A**), 0.7 nm (**B**), and 0.6 nm (**C**).

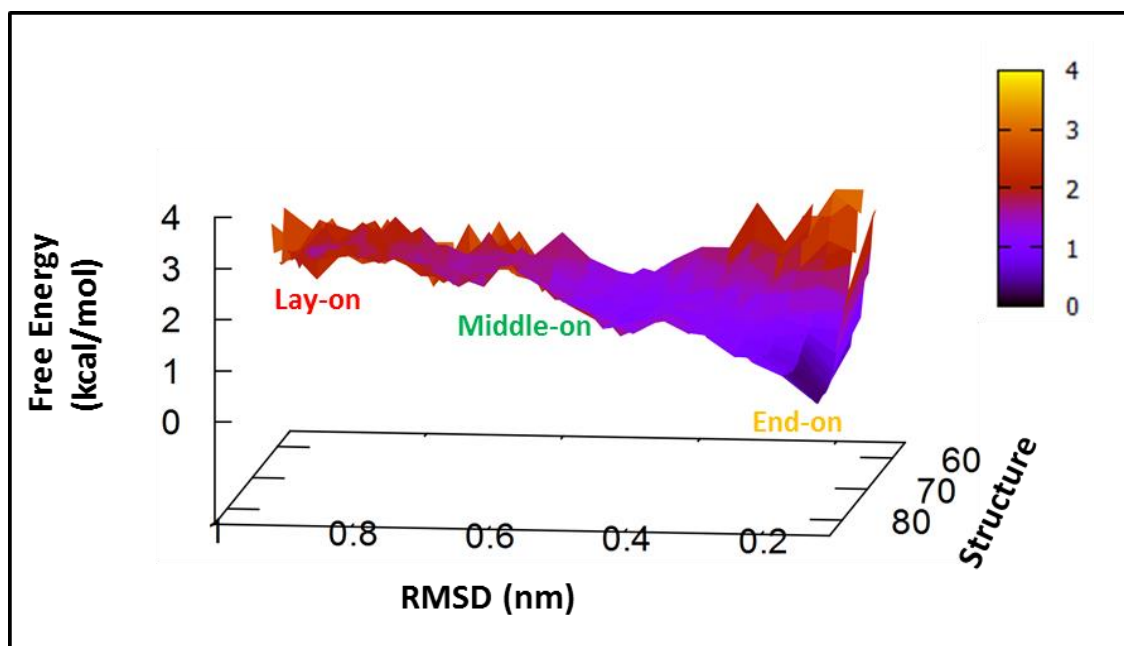


Figure S4: Free energy landscape for the unfolding of HEWL as a function of RMSD and secondary structure content for conformations belonging to the dominant three orientations of the protein at the water/DCE interface.