

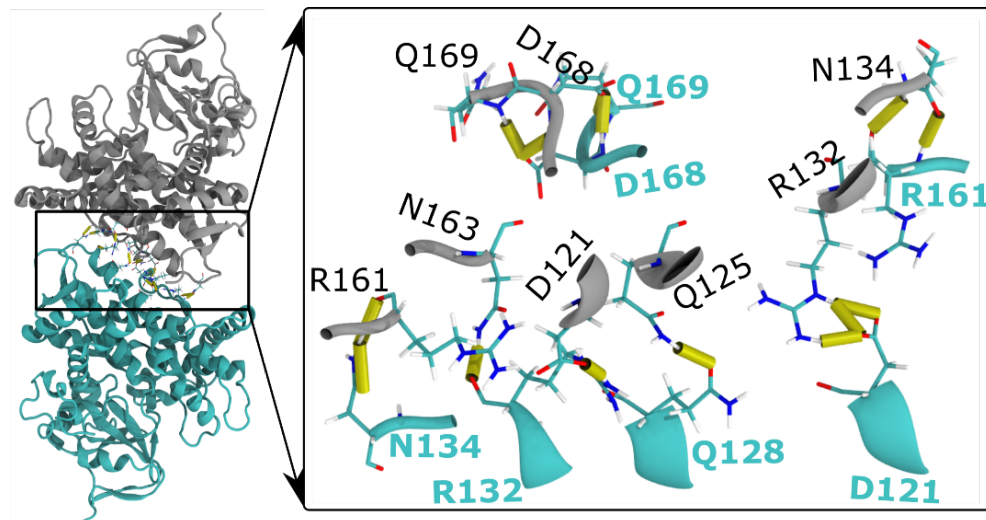
“Mirror”-like Protein Dimers Stabilized by Local Heterogeneity at Protein Surfaces

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Proteins are composed of amino acids which are positively charged, negative charged, polar charge-neutral and nonpolar. They coexist at protein surfaces, forming small surface domains of the length of few Å to few nm. These small protein domains are crucial in protein solubility, mutation, and recognition of molecules of protein, ligands, and DNA/RNA. Nevertheless, they are highly under-investigated.



By means of all-atom molecular dynamics (MD) simulations, umbrella sampling, and protein-protein docking calculations, we showed that the protein surface domains play a significant role in protein dimerization. Two industrially important enzymes, cytochrome P450 (P450) and organophosphorus hydrolase (OPH) were investigated. Analysis of the protein-protein contact regions reveal that the protein monomers are forming “mirror”-like orientations. The “mirror”-like structures are ascribed to the polar amino acid domains at protein surfaces. Our work will potentially aid the design of molecules that can deliver and protect native protein function in various environments.



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