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Computational analysis of odorant binding to OBPs BOMI KIM, JAMES PINO, MANUEL SANTIAGO, STEFANIE WHITSON, KRISTIN WHITSON, Departments of Chemistry and Physics, University of Tennessee of Chattanooga — Humans can detect countless odors but the mechanism by which much of the pathway occurs is not elucidated. Odorant binding proteins (OBPs) carry hydrophobic odorants across aqueous mucus to be deposited at olfactory receptors, triggering a neuronal response. The active site within the beta-barrel structure is conducive for hydrophobic odorants, where a lysine residue has been implicated as essential for binding of aldehyde moieties. The studies herein aim to determine the relative stability of various odorant/OBP combinations by energy minimization and computational modeling with ligand docked to active sites in wild-type OBP2A, mutant OBP2A, or OBP2B. The results demonstrate other specific interactions between odorants and protein, revealing wild-type OBP2A may have two binding sites, with initial binding occurring near the barrel opening. Energies indicate protein stability though two ligands are present in the active site. In addition, ligands with similar structures bind the same location on the protein, indicating directionality of the protein in ligand binding.

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