From molecular binding to conformational change, an extensive study on Olfactory Binding Protein (OBPs)

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OBP binding specificity, providing valuable information for future protein engineering attempts. Finally, we explored and proposed a rationale for the conformational change induced upon binding of molecules to rOBP3. Local conformational changes were observed in MD simulations and validated by circular dichroism. The integrated computational-experimental approach not only improves the efficiency of in vitro assays, but also offers a comprehensive understanding of protein behavior and binding dynamics.

[1] Moitrier, L., Belloir, C., Lalis, M., Hou, Y., Topin, J., & Briand, L. (2022). Ligand Binding Properties of Odorant-Binding Protein OBP5 from Mus musculus. Biology, 12(1), 2.