Analysis of Thiophene- and Pyrrole-Substituted Fatty Acids in FABP5 by Molecular Dynamics Simulations

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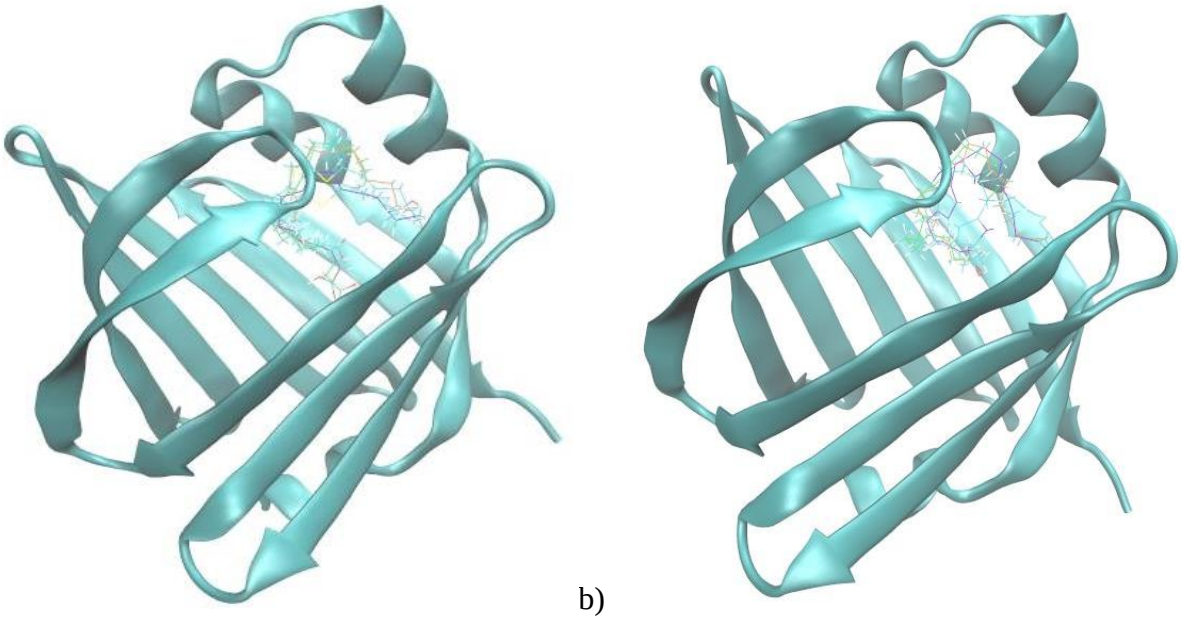
Fatty Acid Binding Protein 5 (FABP5), an intracellular lipid-binding protein, can be activated by long-chain fatty acids (LCFA) acting as binding ligands. Upon the activation by retinoic acid, a naturally occurring ligand, cell growth and proliferation are promoted. Potential applications in cancer therapy require finding an alternative binding ligand to inhibit retinoic acid induced FABP5 activity. Using molecular dynamics (MD) simulations, four different starting structures of both a thiophene-containing LCFA and a pyrrole-containing LCFA are analyzed, in addition to their binding interactions with FABP5 to better understand ligand binding in FABP5.



a) b)

Figure 1: Starting structures of a) thiophene (THP) and b) pyrrole (PYR) containing LCFAs in FABP5. (Orange = THP1 & PYR1, Blue = THP2 & PYR2, Purple = THP3 & PYR3, Green = THP4 & PYR4)