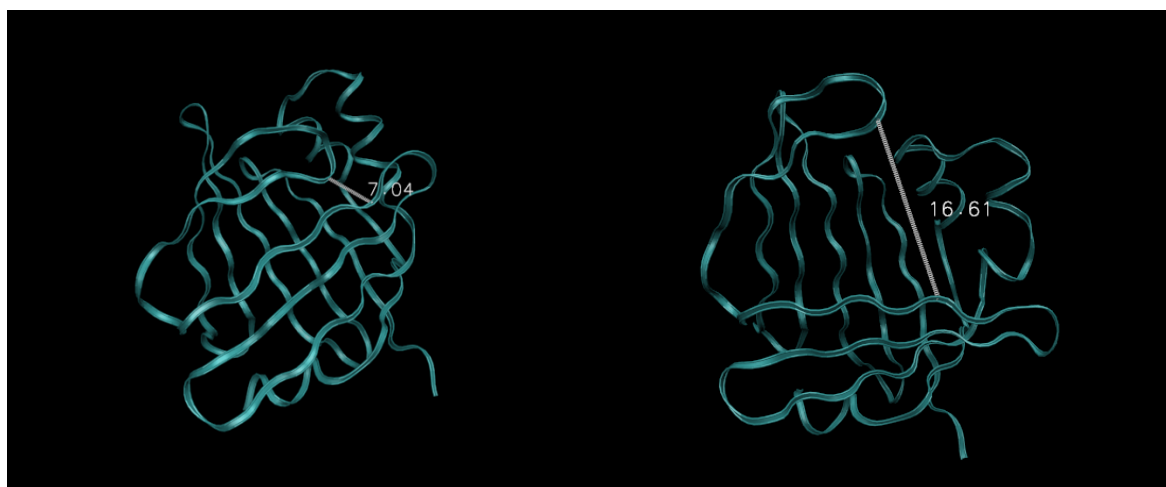


## Molecular Dynamics of Fatty Acid Binding Protein 5 Conformations and Ligand Binding

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When activated by a binding ligand, cellular retinoic acid binding protein II (CRABP-II) inhibits the cell cycle and promotes apoptosis, whereas fatty acid binding protein 5 (FABP5) stimulates cell growth and proliferation. Finding a ligand to inhibit FABP5's activity and promote cell cycle arrest can be a potential method for cancer therapy. In this project, two substituted fatty acids, one with a pyrrole moiety and one with a thiophene moiety, known to competitively bind to FABP5 are studied through MD simulations. Additionally, the conformations of FABP5 without a ligand, one in its "open" form and one in its "closed" form, have been studied for differences in its structure and activity. The MD simulation results and structural features will be presented. GPU accelerated AMBER14 was used to perform the simulation, and the AMBERTools15 package was used for analysis.



**Figure 1** FABP5 in its "closed" conformation (left) and "open" conformation (right). FABP5 in its "open" conformation (left) and "closed" conformation (right).