# The Significance of Hydrogen Bonding in Designing a Pharmacophore

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Recent research by Albany Medical Center hypothesized that a hydrogen bond between the terminal amino acids of a segment of Alpha-feto protein (AFP) is what caused the peptide to retain a cyclic conformation. The cyclic form is hypothesized to fit into an unknown receptor site and inhibit estrogen dependent breast cancer from forming. We used the molecular dynamics program, AMBER, and the visualization program VMD to investigate all of the possible hydrogen bonds that could exist within the peptide. Our research has shown that it is not a hydrogen bond between the terminal amino acids that causes the structure to cyclize, but a series of hydrogen bonds between the central amino acids. This research is significant because it enables us to better understand the structure of the peptide and how it interacts with the unknown receptor site. The ultimate goal of our research is to design a pharmacophore based off of the AFP peptide to treat breast cancer.

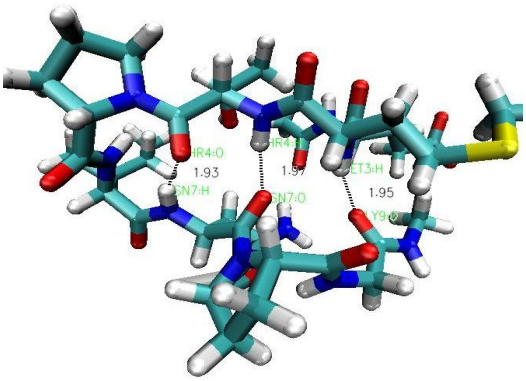


Figure 1: An analog of the active 8 peptide region of AFP. This analog shows three hydrogen bonds holding the structure into a cyclic conformation.