Generation of Novel Fatty Acid Binding Protein (FABP) Inhibitors with Analgesic and Anti-Cancer Properties

Ziadkhanpour, Kiana (School: Plainview-Old Bethpage John F. Kennedy High School)

Fatty acid binding proteins (FABPs) are a group of macromolecules that regulate lipid activity in cells and function as lipid transporters. Notably, the inhibition of certain FABPs, namely FABP5 and FABP7, produce analgesic and anti-cancer effects that can potentially mitigate the opioid epidemic as inhibiting these compounds elicits non-addictive pain relief sensations in the body. This study is one vital step in a novel initiative that is wholly focused on the synthesis of these inhibitors and their potential application in a clinical setting. Specifically, this study concentrates on the in silico creation of FABP5 and FABP7 ligands and the analysis of their ability to act as inhibitors. Building upon a chemical structure known to bind to FABP5 and FABP7, modifications to the compound were made in order to optimize molecular docking scores. These scores, produced through the AutoDock Vina algorithm, predict the optimal binding geometry (pose) of a ligand. In this case, the poses of the potential inhibitors were scored, offering unique predictions of binding affinity. As a result of this analysis and many others, a promising compound, Compound3, has been identified from over 150 compounds, screened as a potential FABP5 and FABP7 inhibitor, and prepared for synthesis and further evaluation.

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