INVESTIGATING THE REGENERATIVE CAPABILITIES OF HARMINE AND ITS DERIVATIVES ON HUMAN PANCREATIC BETA CELLS: AN *IN SILICO* EXPLORATION

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ABSTRACT

Controlling hyperglycaemia with possible drug target inhibitors is a promising approach since uncontrolled diabetes can result in hyperglycaemia and damage to the neurological system. This study aimed to discover an effective novel antidiabetic therapy based on beta cell proliferation, utilising the inhibitory action of harmine and its derivatives on DYRK1A. We selected harmine and its derivatives because various studies have shown that beta-cell proliferation can be activated by harmine. Modifications were introduced at the 1st, 7th, and 9th positions, alongside the addition of some ring substituents typically associated with oral hypoglycaemic agents. These modifications served as ligands, specifically targeting the protein 6EIQ of interest. Molecular docking was performed using Easy Dock Vina 2.2. The docking result indicated that 9-cyclohexyl-7-methoxy-1-methyl-9*H*-pyrido[3,4-b] indole showed a higher docking score than the standard harmine, and it may have the potential for being a good antidiabetic, beta-cell-regenerative-capable drug in future research.