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Computer-aided screening for potential GSK-3β inhibitors: a combination of pharmacophore modeling, molecular docking simulation approaches

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Alzheimer's disease (AD) is a progressive and irreversible neurodegenerative disorder that is a type of dementia that affects memory, thinking and behavior. Alzheimer's disease (AD) is primarily associated with the abnormal accumulation of tau protein, which forms the microtubules in neurons. Recent research has identified hyperphosphorylation of tau protein as a major contributor to this accumulation. In this process, GSK-3β is recognized as a key regulatory enzyme, making it the focus of significant attention as a therapeutic target. In this study, we utilized computer-based drug design methods to explore novel compound candidates effectively inhibiting GSK-3β. First, potential candidates were screened using pharmacophore modeling, which analyzes the structural characteristics of existing inhibitors of GSK-3β. At the last step, the final candidates were selected by molecular docking calculation. It was used to identify the molecular interaction between key residues of GSK-3β and screened inhibitors. Our finding provides deep insights into the discovery of novel GSK-3β inhibitors at the molecular level.