In silico docking studies and computational approach of *Dopamine Receptor D3* (DRD3) gene analyzing binding efficiency of Paliperidone palmitate and Ziprasidone drug

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ABSTRACT

Schizophrenia (SZ) is a complex psychiatric disorder which leads to abnormal behavior such as hallucinations and delusions. It affects nearly 5% of the population worldwide and regarded as a major public health problem ranked nine in the global disease burden of World Health Organization. The pathophysiology of SZ shows dysregulation of dopaminergic and glutamatergic neurotransmitter signaling. Recent studies have reported that DRD3, a dopaminergic receptor, as a potential therapeutic target for SZ. It regulates T-cells, macrophages through G-protein coupled receptors signaling pathways. Receptor-ligand binding determines the effective cellular response to external stimuli and it is used to determine efficacy of drug candidate. In this study, an attempt has been made through computational docking methods to evaluate the binding efficiency of dopamine receptors binding drugs. Molecular docking was implemented in AutoDock 4 software, receptor-ligand Docking was carried out for DRD3 receptor with Paliperidone palmitate and Ziprasidone (FDA approved therapeutic antagonist) along with its natural ligand (L-dopamine). Binding energy of both drugs was compared with L-dopamine.

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