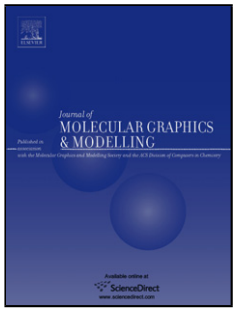

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Assessing the Binding of Cholinesterase Inhibitors by Docking and Molecular Dynamics Studies

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HIGHLIGHT

In this report we assessed by docking and molecular dynamics the binding mechanisms of three FDA-approved Alzheimer drugs, inhibitors of the enzyme acetylcholinesterase (AChE): donepezil, galantamine and rivastigmine. Dockings by the softwares Autodock-Vina, PatchDock and Plant reproduced the docked conformations of the inhibitor-enzyme complexes within 2 Å of RMSD of the X-ray structure. Free-energy scores show strong affinity of the inhibitors for the enzyme binding pocket. Three independent Molecular