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Computer Simulation of Angiotensin II Binding to Its Receptor for *de novo* Lead Search

Dooil Kim · Youngdo Won
Department of Chemistry, Hanyang University, Seoul 133-791

A working molecular model of the angiotensin II type 1 receptor is built based on the seven transmembrane helix structure of the recently refined bacteriorhodopsin atomic coordinates. A multiple copy simultaneous search (MCSS) method is used to search the pharmacophore of angiotensin on the surface of the receptor. Multiple copies of amino acid fragments and organic functional groups are scattered around the possible binding site and the time dependent Hartree approximation is empolyed in minimization and molecular dynamics simulations. The receptor modeling and MCSS method itself are at the development stage and their optimized application should shed lights upon *de novo* lead design of the target therapeutics.