Molecular modeling and docking the parathyroid hormone receptor

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G-protein coupled receptors (GPCRs) are considered to be one of the most important groups of drug targets because they are involved in communication between cell and its environment by passing chemical signals across the cell membrane. To date, over 30 % of the clinically marketed drugs are active at this receptor family. In structure-based drug design, information of the 3D structure of a target protein is of utmost importance. However, due to the technical difficulties, the 3D structure of GPCR must be inferred with the aid of computer models. Parathyroid hormone receptor (PTH receptor) plays a critical role in the cell-signaling process responsible for the regulation of calcium and phosphate homeostasis in blood. Development of improved therapeutics would be significantly enhanced with the availability of a structural model for the PTH receptor and of the binding site for agonists and antagonists. This model was constructed using a combination of computation and comparative-modeling techniques starting with the experimentally determined 3D structure of bovine rhodopsin (PDB: 1L9H) as a template. The docking models of PTH receptor and 20 PTH analogues were built for the feature analysis of the binding site.