New Structure and Function Predictions for the $\beta_1$ Adrenergic Receptor

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$\beta_1$-adrenergic receptors belong to the family of GPCRs that respond to epinephrine and norepinephrine and mediate the system-wide stress response. Many drugs, known as beta-blockers, target the $\beta_1$ receptor to regulate heart rate and blood pressure. Using established Membstruk software and the newly developed MSCDock procedures, an updated structure prediction for $\beta_1$ and a preliminary agonist binding site were obtained. This binding site includes several residues shown to be important in mutagenesis studies, and may provide insight into the transition between the active and inactive states of the receptor. The relative binding energies for a series of agonists correspond to experimental binding affinities. Comparison of this binding site to the previously predicted $\beta_2$ binding site may assist rational design of potent and selective drugs.

Predicted $\beta_1$ agonist binding site.