Computer modeling of human delta opioid receptor

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Motivations

The development of strong analgesics without potential for abuse and adverse side effects is connected to understanding of the differences in opioid receptor subtypes as well as the model of interaction of ligands whit these receptors. In the absence of crystal structures of opioid receptors, 3D homology models with different templates have been reported in the literature.

Methods

The aim of our study is to choose within recently published crystallographic structures templates for homology modeling of the human delta-opioid receptor. We generate several models using different templates and all they were evaluated by docking procedure. Ligands used in this study were already synthesized by our group and their biological activity was evaluated. They are analogues of the endogenous opioid peptides - enkephalins with substitutions in second position.

Results

The best model of the human delta-opioid receptor was chosen according to data obtained from docking and in vitro biological activity.

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