Computer Modeling of the Human Cannabinoid Receptors

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Cannabinoid receptors are cell membrane receptors from the G protein-coupled receptor superfamily. They are part of the endocannabinoid system (ECS) which is involved in a variety of physiological processes including appetite, pain-sensation, mood, and memory. Cannabinoid receptors are activated by cannabinoids, generated naturally inside the body (endocannabinoids) or introduced into the body as cannabis or a related synthetic compound. The ECS produces an endocannabinoid within the brain called anandamide.
This paper focuses on the crystal structure of the human cannabinoid receptors 1 (CB1), published in RCSB and several known cannabinoid ligands.
The aim of the presented study is to explore the interaction in the binding sites of the crystal structure of CB1 in order to determine the structure activity relationship using molecular docking.
We defined the crucial point in the binding sites of the receptor and designed several new structures which will have potentials as agonists, antagonists and inverse agonists.

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