

Cannabinoid CB1 Receptor Model Research Tool:

Invention:

The University of North Carolina at Greensboro is actively seeking parties interested in acquiring in silica model of Cannabinoid CB1 Receptor. The technology represents a computer model of transmembrane helix bundle of the cannabinoid CB1 Receptor. This model evolved from the commonly known rhodopsin structure, and at its final stage incorporates the unique conformations of CB1 individual helices. Designed uniquely to describe the CB1 receptor, the model is exquisitely detailed, and thus possesses absolute predictive power. It is targeted at computational chemists and pharmacists involved directly in compound generation.

Applications:

The immediate use of the model is the design of inverse agonists and cannabinoid agonists of the CB1 receptor. These compounds have potential clinical applications as appetite stimulants, analgesics, anti-emetics, anti-diarrheals, anti-spasmodics, tumor anti-proliferative agents, anti-glaucoma agents and as agents for the treatment of diseases associated with inappropriate retention of adverse memories such as post traumatic stress disorders and phobias.

Advantages:

- Precision of the model enables efficient docking of drug molecules in order to analyze exactness of fit.
- Flexibility of the in silica formulation makes it possible to design new drugs based on the shape requirements of the binding pocket and the identity of the amino acid residues surrounding this binding pocket.
- Its detailed specification allows examining the amino acids accessible to the G protein to which the receptor couples.
- The model is capable of aiding in the design of a wide spectrum of drugs that turn the CB1 Receptor both on and off.
- High predictive power of the model effectively decreases the time spent on laboratory testing, allowing to test multiple combinations and observe receptor response at timely fashion reserving extensive laboratory testing for most promising routes.

Technology:

The technology represents a computer model of transmembrane helix bundle of the cannabinoid CB1 Receptor. This modeled evolved from the commonly known rhodopsin structure, and at its final stage incorporates the unique conformations of CB1 individual helices. Designed uniquely to describe CB1 receptor, the model is exquisitely detailed, and thus possesses absolute predictive power. It is targeted at computational chemists and pharmacists involved directly in compound synthesis.