Identification of a Novel Chemical Probe for Cannabinoid Receptor Subtype 2(CB2): diazenyl-propanamide compound and its analogs

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Technology description

Background

The discovery of the cannabinoid (CB) receptors, their endogenous ligands, and enzymes for CB ligand metabolism has triggered intensive pharmacological research into the therapeutic potential of cannabinergic ligands. Clinical evaluation of the therapeutic potential of CB ligands for the treatment of nausea, glaucoma, cancer, stroke, pain, neuronal disorders, multiple sclerosis, and autoimmune disorders has generated active cannabinoid research. However, work to design novel CB2 ligands that do not confer psychotropic side effects has been limited due to a lack of information about 3D CB receptor structure and ligand binding sites.

Technology

The inventors have established novel methods to fill gaps in the knowledgebase of the 3D structure and conformation of CB2 ligands, and identified novel CB2 lead compounds that possess the appropriate novel chemical scaffolds and high CB2 biological selectivity. They have established the combined approaches of NMR conformations, pharmacophore models, efficient 3D pharmacophore database queries, and biovalidation of database searched (hits) and discovered new CB2 active ligand compounds for further drug development. The invention discloses a new biological active chemical probe for cannabinoid receptor CB2 subtype and its class of cannabinoid receptor CB2 ligands. Applicants have demonstrated that the compound has a new chemical scaffold and is a highly CB2-selective molecule that has never been reported. The new compound and its analogs can be used as novel chemical probe for further cannabinoid drug research, and also have a potential to be used as an active fluorescence dye compound for fluorometric binding assay and an anti-inflammatory agent.

Application area

1) The compound is a newly identified chemical probe with a high biological activity that binds or interacts strongly and selectively with the cannabinoid receptor subtype2 (CB2).

2) The compound as an active CB2 lead can be used for further chemistry modification to establish a novel class of potent CB2 ligands.

3) It can be used as an active fluorescence dye control for fluorometric binding assay and an anti-inflammatory agent.
4) The CB2 receptor is a known protein target that has an important role in the signal transduction processes of immune systems, and thus a potential drug target for immune therapy.

Advantages

1) This novel CB2 compound has new chemical scaffold and high CB2 selectivity that has never been reported before.

Institution

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