投稿 ▶原著

定量的構造活性相関（QSAR）によるTHC類縁体及びHHC類縁体のカンナビノイド受容体1（CB_1）親和性インシリコ予測

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（受付：令和6年9月10日，受理：令和7年7月7日）

In Silico Prediction of Cannabinoid Receptor 1（CB_1）Affinity of THC and HHC Analogues by Quantitative Structure-Activity Relationship（QSAR）Model

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Summary

In the present study, we used quantitative structure-activity relationship (QSAR) models to predict the binding affinities of tetrahydrocannabinol (THC) and hexahydrocannabinol (HHC) analogues for cannabinoid receptor 1 (CB_1). In the THC analogues study, the QSAR model was constructed based on 10 THC analogues with known CB_1 affinity (as K_i values). Using this QSAR model, we predicted the CB_1 binding affinity of four Δ^9-THC analogues and one Δ^8-THC analogue. In the subsequent study of HHC analogues, a QSAR model was constructed using 14 THC analogues with known CB_1 affinity, and then the activity of six HHC analogues was predicted. These results were used for comprehensive regulation of THC and HHC analogues in 2023.

Key words

New psychoactive substance, Quantitative structure-activity relationship, Bioactivity prediction, THC analogues, HHC analogues