Abstract

G protein coupled receptor 119 (GPR119) is promising and exciting target for the treatment of type 2 diabetes mellitus (T2DM). In this study, three dimensional quantitative structure activity relationships (3D-QSAR), molecular docking and virtual screening have been carried out on a novel series of GPR 119 agonists. The results show the more prediction power and reliability of the models. A quality pharmacophore model was built by Hip-Hop algorithm. The quality of this model is satisfactory and it is utilized to search the ZINC database for a virtual screening task. Virtual screening was performed by pharmacophore model and molecular docking. Furthermore, *in silico* ADME and toxicity risk assessment analysis was carried out on the 7 hits with highest gold score fitness and compared with standard ranges. Six of the new hits from virtual screening have diverse structures and are reported as new scaffold candidates for GPR 119 agonists.

Keywords: G protein coupled receptor 119; pharmacophore; molecular docking; virtual screening; ADME; toxicity risk assessment; Gold algorithm.

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Ligand and structure based virtual screening and 3D-QSAR study for identification of novel GPR 119 agonists

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