

Search PPAR- γ agonist or antagonist from traditional Chinese medicine
by *in silico* analysis

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Peroxisome proliferator-activated receptor γ (PPAR γ) is a ligand-activated nuclear transcription factor that expressed in liver, muscle and adipose tissue, macrophages and inflammatory cells. Activated or suppressed PPAR γ would regulated glucose and fatty acid homeostasis, and reduce production of inflammatory cytokines. Therefore, we set up a 3D structure database of phytochemicals from the traditional Chinese medicine (TCM) to search the PPAR- γ agonists or antagonist by *in silico* analysis- docking. 600 phytochemicals, which belong to 12 different kinds of structures (including monoterpenes, sesquiterpenes, iridoids, diterpenes, triterpenoids, alkaloids, quinones, flavonoids, tannins, phenylpropanoids, sterols, and others), were constructed and the interactions between phytochemicals and PPAR γ were evaluated by docking analysis. Our data showed those 21 iridoids, 23 monoterpenes, 23 diterpenes, 25 triterpenes, 15 sterols, 60 flavonoids, 10 tannins, 15 quinones, and 22 other types of phytochemicals could dock into the active sites of PPAR γ . Flavonoids were the most active type phytochemicals and its average binding energy score was -9.89 ± 1.19 kcal/mol. Amentoflavone exhibited the lowest binding energy score among the flavonoids and its binding energy score was -13.19 kcal/mol.