Latin American Journal of Pharmacy
(formerly *Acta Farmacéutica Bonaerense)*
Lat. Am. J. Pharm. **30** (8): 1608-13 (2011)

Regular Article
Received: July 16, 2011
Revised version: August 6, 2011
Accepted: August 13, 2011

Molecular Research on a Hypotensive Herb Formula and PPARα Activation

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***SUMMARY*. Surflex-dock method was explored to study interactions between Qingxuanjiangya decoction (QXJYD in abbreviation, a famous hypotensive herb formula from Traditional Chinese Medicine prescription) and Peroxisome proliferators activated receptor-alpha (PPARα) for detecting its pharmacological effects as well as to screen out PPARα agonists. First, 28 compounds with values of PPARα EC_{50} from reported were introduced as a test set to evaluate the docking accuracy according to the good validation between experimental values and surflex-dock scores (correlation coefficient R = 0.866, RMSD = 1.169 Å, similarity = 0.804). And then, 739 molecules from QXJYD were docked to PPARα by the validated way. The result showed 200 compounds from QXJYD had activity with PPARα and discovered that a flavones compound (moralbanone, extracted from folium mori) with an excellent docking score might be considered as a guide to design a new scaffold of PPARα agonists in the further study.**

KEY WORDS: PPARα Agonists, Qingxuanjiangya decoction, Surflex-dock.

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ISSN 0326-2383