

عنوان مقاله:

Evaluation of medicinal plants' effects for inhibition of H₁ receptor to control and treatment of allergic diseases using the bioinformatics approach

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خلاصه مقاله:

Allergic diseases are caused by the immune system's extreme reaction to harmless substances. The H₁ receptor is one of histamine receptors that play a significant role in causing allergy symptoms. Herbal active ingredients have been introduced to reduce allergy symptoms with fewer side effects. First, herbal active ingredients effective in reducing allergy symptoms were found from articles; the structures of these substances were collected from the PubChem database. The best H₁R structure was also obtained using PDB and SWISS-MODEL databases, next, they were docked with H₁R by vina AutoDock software. Furthermore, the structures of available antihistamines were docked with the H₁R. Finally, the properties of the active ingredients having the highest affinity to H₁R were collected from different servers. The results showed that Beta-carotene, an active ingredient of *Daucus carota* L, *Cordia myxa*, *Asparagus officinalis*, *Ilex guayusa*, *Plantago major* L, *Hibiscus sabdariffa*, *Crocus sativus*, and *Allium sativum*, had a greater affinity than other active ingredients and antihistamines except Doxepin. Using the Lazar Toxicity Predictions and way2drug databases, it was found that the active ingredients with the highest affinity have many beneficial medicinal properties and relatively few side effects and can probably be considered as anti-allergic agents. Beta-carotene, 2- [4-Methyl-6- (2,6,6-trimethylcyclohex-1-enyl) hexa-1,3,5-trienyl] cyclohex-1-en-1-carboxaldehyde Alpha-carotene, Antheraxanthin, Luteolin 4'-O-Glucoside, Licoisoflavone B and 1,7-Bis (4-hydroxyphenyl) -1-heptene-3,5-dione had a high affinity to H₁R compared to existing antihistamines, these substances can be introduced as anti-allergic substances with fewer side effects. However, in-vivo and in-vitro studies to confirm the results of this study .need to be performed to prove their characteristics

کلمات کلیدی:

Allergy, active ingredients, molecular docking, inflammation, antihistamine, H₁ receptor

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