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Network pharmacology and molecular docking investigation of *Curcuma xanthorrhiza* Roxb. rhizome with the mechanisms underlying as the potential drug of eczema treatment

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Abstract

A chronic inflammatory dermatosis, eczema, affects more than 12% of the pediatric population and 7.2% of adults. Clinically, it presents with erythematous, scaly, and intensely pruritic lesions. Severe forms of the disease frequently exhibit poor responsiveness to treatments aimed at a single inflammatory pathway. *Curcuma xanthorrhiza* Roxb. rhizomes possess antioxidant, anti-inflammatory, and anti-

allergic activities through a multi-target mechanism. This study aimed to evaluate the secondary metabolites of *C. xanthorrhiza* Roxb. rhizomes that can be developed into eczema drugs using virtual screening in silico. Secondary metabolite compounds from *C. xanthorrhiza* rhizomes were evaluated for their drug-likeness properties. Subsequently, the similarity of their physicochemical properties was assessed using the principal component analysis. A target search of drug candidates was performed using the Swiss Target Prediction and Gene Expression Omnibus (GEO) Omnibus. Docking was performed using Molegro by comparing the rerank scores of the drug candidates with those of the original ligands. Absorption, distribution, metabolism, excretion, and toxicity (ADMET) prediction was performed using the pkCSM. Carbonic anhydrase II, epidermal growth factor receptor, and the mammalian target of rapamycin came as the protein target for eczema disease. For the docking result, demethoxycurcumin (C00037023), 1,5-dihydroxy-1,7-bis (4-hydroxy-3-methoxyphenyl)-4,6-heptadien-3-one (C00055412), 1,7-bis (4-hydroxy-3-methoxyphenyl)-3,5-heptanediol (C00055175), and 3'-demethoxycyclocurcumin (C00054761) had both better rerank score than the native ligand and good ADMET profiles. Four compounds derived from *C. xanthorrhiza* Roxb. rhizomes can be developed as an eczema potential treatment. © 2025 Journal of Advanced Pharmaceutical Technology & Research.

Author keywords

Absorption; and toxicity; atopic dermatitis; distribution; excretion; metabolism; neglected tropical disease; network analysis; virtual screening

Indexed keywords

EMTREE drug terms

1,5 dihydroxy 1,7 bis (4 hydroxy 3 methoxyphenyl) 4,6 heptadien 3 one; 1,7 bis (4 hydroxy 3 methoxyphenyl) 3,5 heptanediol; 3' demethoxycyclocurcumin; alpha terpinolene; antieczema agent; beta atlantone; c 00000136; c 00000819; c 00000823; c 00000853; c 00000861; c 000029335; c 00011646; c 00011728; c 00012443; c 00012483; c 00029674; c 00037023; c 00054761; c 00055175; c 00055412; camphor; carbonate dehydratase II; caryophyllene oxide; cineole; Curcuma xanthorrhiza rhizome extract; demethoxycurcumin; epidermal growth factor receptor; germacrone; humulene; humulene epoxide; ligand; limonene; mammalian target of rapamycin; myrcene; ocimene; plant extract; terpeneol; terpinolene; unclassified drug

EMTREE medical terms

adipocyte; Article; carbon metabolism; chemical fingerprinting; computer model; Curcuma xanthorrhiza; drug absorption; drug distribution; drug excretion; drug isolation; drug mechanism; drug metabolism; drug receptor binding; drug screening; drug targeting; eczema; lipolysis; molecular docking; nitrogen metabolism; pathway enrichment analysis; physical chemistry;