عنوان مقاله:

Investigating the Antipruritic Effects of Lemongrass BiochemicalComponents Using Molecular Docking Study

محل انتشار:

پنجمین کنگره ملی شیمی و نانوشیمی از پژوهش تا فناوری (سال: 1401)

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خلاصه مقاله:

Lemongrass oil (LGO) has been reported for anti-inflammatory, anti-microbial, antifungal, and analgesic properties. In this study, we aimed to investigate the antipruritic efficacy of LGO. From the GC-MS analysis, lemongrass oil contains several biochemical components. The major components of LGO, ۴-tert-butylcalix, panaquinquecol ۷, and diethyl-, ۳, ۴-dihydro-۱-naphthalenyl ester, besides some other components, having anti-inflammatory or analgesic properties, are selected as the ligands. Kappa-opioid receptors are chosen as the target proteins since the neuronal pathways involved in transmitting pain and inflammation are the same as pruritus. A molecular docking study revealed that all the selected components docked to the receptors via good bonding scores. The best results were obtained for luteolin and quercetin against all the KOR receptors. The ligands were more efficient than the antipruritic-approved drug, gabapentin.

کلمات کلیدی:

Antipruritic, Herbal medicine, Lemongrass oil, Molecular docking