

## عنوان مقاله:

In vitro and in silico investigation of garlic's (*Allium sativum*) bioactivity against 15-lipoxygenase mediated inflammopathies

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## خلاصه مقاله:

Introduction: Garlic (*Allium sativum*) is widely used as a flavor-enhancing dietary ingredient and exhibits a wide spectrum of pharmacological effects. This study aimed to investigate the therapeutic effects of aqueous garlic extract to explore the bioactivity against 15-lipoxygenase (15-LOX) mediated inflammopathies. Methods: In this study, the antioxidant (DPPH free radical scavenging assay and reducing power assay), anti-inflammatory (hypotonicity-induced hemolysis assay and 15-LOX inhibition assay) and anticoagulation (serine protease inhibition assay and prothrombin time assay) effects of the aqueous garlic extract were investigated. Furthermore, in silico molecular docking and dynamic simulation analysis of reported small compounds of garlic against 15-LOX<sub>1</sub> and 15-LOX<sub>2</sub> were performed to figure out the most efficient phytochemical ligands and validate the anti-inflammatory potential. Results: The DPPH scavenging effect and the reducing power of the extract were found with the IC<sub>50</sub> of  $213.87 \pm 1.49 \mu\text{g mL}^{-1}$  and EC<sub>50</sub> of  $124.78 \pm 3.39 \mu\text{g mL}^{-1}$ , respectively. In the hypotonicity-induced hemolysis and 15-LOX inhibition assay, the IC<sub>50</sub> values were observed as  $147.59 \pm 2.98 \mu\text{g mL}^{-1}$  and  $250.05 \pm 8.48 \mu\text{g mL}^{-1}$ , respectively. The extract inhibited serine protease activity with an IC<sub>50</sub> of  $301.33 \pm 1.31 \mu\text{g mL}^{-1}$  and prevented blood coagulation for  $10.05 \pm 0.35$  minutes in prothrombin time assay. The in silico study identified Rhamnetin as a potential 15-LOX<sub>1</sub> and 15-LOX<sub>2</sub> inhibitor, and it exhibited a stable interaction with the targets throughout the 100 ns dynamic simulation. Conclusion: The findings of this study provide molecular insights into garlic's medicinal properties as well as its bioactive compounds, which can be potential therapeutic interventions for 15-LOX mediated inflammations.

## کلمات کلیدی:

Antioxidant, Anti-inflammatory agents Anticoagulant, Inflammation, Phenolic compounds

## لینک ثابت مقاله در پایگاه سیویلیکا:

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