عنوان مقاله:

Study the Antipyretic Activity of Bioactive Compounds of Avena Sativa (Oats) Using Molecular Docking

محل انتشار:

چهارمین کنگره ملی شیمی و نانوشیمی از پژوهش تا فناوری (سال: 1400)

تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

Oats (Avena Sativa) have known and used commonly as foods. Besides, they offer numerous health benefits, such as reduced inflammation and improved brain function and mood. The purpose of this study is to investigate the antipyretic potential of four bioactive compounds of Avena Sativa. An in-silico molecular docking approach is carried out as a means of evaluating the probable effect. Since prostaglandin E۲ (PGE۲) is the key component in the fever mechanism, the isoforms of the cyclooxygenase enzyme (COX-۱ and COX-۲) which are reported to inhibit PGE۲, are selected as receptors. Ascorbic acid, Caffeic acid, Quercetin, and Salicylate are docked to the target proteins, and the best binding modes are analyzed. Only Quercetin showed good binding affinity against the receptors, COX-۱ and COX-۲, with a docking score of -۶.۲۹ and -۵.۴۴, respectively

کلمات کلیدی:

Antipyretic, Fever, Herbal medicine, Molecular docking, Oats