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# Comparison of the Antiitch Activity of Avenanthramides in Oats Using Molecular Docking Study

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Ancient literature describes the anti-inflammatory and antiitch properties of oat extracts. Medical texts by Pliny and other notables promoted the topical application of oatmeal flour for a variety of dermatologic conditions [1]. Avenanthramides (AVAs) are a group of unique, low-molecular-weight hydroxycinnamoyl anthranilate alkaloids uniquely present in oats. AVAs, besides affecting the flavor of oat products, have been reported to improve health parameters in animal and human studies. They have antiproliferative, antioxidant, anti-inflammatory, and anti-atherogenic properties [2]. While 25 distinct Avns have been identified in oats, the most plenteous forms are N-(3′,4′-dihydroxy-(E)-cinnamoyl)-5-hydroxy anthranilic acid (2c; AvnC), N-(4′-hydroxy-3′-methoxy-(E)-cinnamoyl)-5-hydroxy anthranilic acid (2f; AvnB), and N-(4′-hydroxy-(E)-cinnamoyl)-5-hydroxy anthranilic acid (2p; AvnA), which differ by a single moiety on the hydroxycinnamic acid ring. It is widely believed that AvnA, AvnB, and AvnC are mainly responsible for the antioxidant functions of oats [3].

In this work, a molecular docking study was performed to investigate the antiitch activity of avenanthramides (AvnA, AvnB, and AvnC). Also, the results were compared with gabapentin, an effective antiitch-approved drug. Since one of the most important treatments for itching is κ-opioid antagonists [4], three κ-opioid receptors are selected for the study. Ligands are docked to the target proteins, and the best binding modes are analyzed. Among the results, AvnC showed better binding affinity against the receptors, with docking scores ranging from -7.72 to -8.40 kcal/mol. Besides, the number of hydrogen bindings created by AvanC is remarkably higher than other AVAs and also gabapentin.

***Keywords:*** Antiitch, Avenanthramides, Molecular docking, Oat

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