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Abstract

Enlarging the NSAIDs Family: Molecular Docking of Designed Pyrazole and Oxadiazole Derivatives as Novel Anti-Inflammatory Agents †

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Abstract: The development of the NSAID family has represented a excitingapproach in the treatment of inflammatory disorders, such as arthritis, and for the management of acute pain, in relation to the well-known traditional Non-Steroidal Anti-Inflammatory Drugs (t-NSAIDs). Over the years, research has shown that essential mediators such as arachidonic acid metabolites are important in inflammation. The cyclooxygenase (COX) and lipoxygenase (LOX) pathways take primary roles in inflammation and are responsible for many human diseases, such as cancer, arthritis, psoriasis, and neurological disorders. Prompted by the pursuit for new cyclooxygenase-2 (COX-2) inhibitors, we have identified novel classes of pyrazole and oxadiazole derivatives as potentially powerful anti-inflammatory molecules. This virtual screening aims to predict the binding affinity of newly designed pyrazole and oxadiazole derivatives against potential molecular targets related to the inflammatory process through the molecular docking approach. Results showed very good anti-inflammatory activity against cyclooxygenase-2 (COX-2) binding protein 1CX2. Additionally, based on the molecular docking results, it was observed that two molecules have good binding affinity with a targeted protein. The issues gained with these classes of compounds represent, currently, a potent stimulus for the further enlargement of the NSAIDs family.

Keywords: COX-2; in silico; inflammation; molecular docking; NSAIDs

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