ORIGINAL RESEARCH ARTICLES

IN SILICO STUDY OF NSAIDs CONJUGATED WITH COUMARINS AS NEW ANTI-INFLAMMATORY COMPOUNDS

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ABSTRACT

The serious GIT side effects of NSAIDs, due to their carboxylic acid groups, aroused the attention of researchers to manipulate such drugs. Conjugates with NSAIDs are a strategic, way for both augmenting the anti-inflammatory activities and reducing side effects. Natural or synthetic coumarins are interesting motifs for anti-inflammatory activity. The scope of this work was to conjugate NSAIDs (ibuprofen, diclofenac, mefenamic acid, ketorolac and indomethacin) with various substituted coumarins through an ester or amide linkages using a virtual screening molecular docking study to investigate their anti-inflammatory activities. COX-1, COX-2, phospholipase A2, and carbonic anhydrase were selected to study the anti-inflammatory activities. Results showed that 20 compounds (out of 75) could be considered as having such effects with scores more than those of the standard inhibitors. These compounds display talented docking connections with the active site in each enzyme with different anti-inflammatory mechanisms. The estimation of the kinetic-pharmacological performance and the drugs similarity (drug-likeness) for the tested compound according to the ADME study were encouraging with respect to gastrointestinal (GI) absorption, circulation bioavailability and overall drugs similarity, so there is a good chance for these compounds to be established as real drugs.