Research in Pharmaceutical Sciences, 2012;7(5)
School of Pharmacy and Pharmaceutical Sciences
Isfahan University of Medical Sciences

Synthesis of new 2,3-diphenyl-3-oxo-propanamide derivatives as selective COX-2 inhibitors

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Background and Aims:NASAIDs are among the most frequently prescribed pharmaceutical categories as analgesic and anti-inflammatory agents. Since the classic groups of these drugs that inhibit both COX-1 and COX-2 isoenzymes, cause a number of adverse effects, efforts for discovery of new selective COX-2 inhibitors with fewer side effects continue. In this research, based on docking studies, we designed and synthesized a numberof new2,3–Diphenyl-3-oxo-propanamide derivatives as selective COX-2 inhibitors.
Methods: Methyl 3-(4-(methylsulfonyl) phenyl)-3-oxo-2-phenylpropanoate was synthesized from 1-(4-(methylsulfonyl) benzoate and methyl 2-phenylacetate through Claisen condensation. new amide derivatives were synthesized from the reaction of above ester with corresponding amines in xylene.
Results: Some new molecules were designed based on the SAR of the selective COX-2 inhibitors. They were docked in COX-2 and COX-1 and showed favorable selectivity for COX-2. The designed compounds were synthesized and their structures were approved using instrumental methods including IR, NMR and Mass spectrometry.
Conclusions: In this research, new 2,3–Diphenyl-3-oxo-propanamide derivatives as selective COX-2 Inhibitors were designed, synthesized and approved by IR, NMR and Mass spectra. The docking studies showed that the designed compounds had good selectivity for COX-2 isoenzyme.

Keywords: Synthesis; 2,3-diphenyl-3-oxo-propanamide derivatives; COX-2 inhibitors