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Synthesis of new 2,5-diaryl 1,3,4-oxadiazole derivatives as selective COX-2 inhibitors

S. Tabatabaia, E. Rezaee, T. Vahedpour*,

Department of Medicinal Chemistry, School of Pharmacy, Shahid Beheshti University of Medical Sciences, Tehran, Iran.

Background and Aims: Non-steroidal anti-inflammatory drugs (NSAIDs) are among the most widely used therapeutics. they represent a choice treatment in various inflammatory diseases such as arthritis, rheumatisms as well as relieving the pains . 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 number of new 2,5-diaryl 1,3,4-oxadiazole derivatives as selective COX-2 inhibitors.
Methods: 4-(methylsulfonyl)benzoic acid was synthesized from oxidation of 4-(methylthio) benzaldehyde. After the resulting acid esterified and subsequently reacted with hydrazine hydrate to give corresponding hydrazide which treated with benzoyl chloride derivatives Followed by reacting with P2O5 in Toluene to close the 1,3,4 - oxadiazole ring.
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 2,5-diaryl 1,3,4-oxadiazole 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; New 2,5-diaryl 1,3,4-oxadiazole derivatives; COX-2 inhibitors