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

Synthesis of (1-benzyl-2-(methylsulfonyl)-1h-imidazol-5-yl) methanol as a selective COX-2 inhibitor

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Background and Aims: Nonsteroidal anti-inflammatory drugs (NSAIDs) are the most commonly prescribed analgesic and anti-inflammatory agents. The major limitation of NSAIDs is gastrointestinal (GI) adverse effects (perforation, ulceration, and bleeding).A new class of NSAIDs, the COX-2 selective inhibitors, have been developed with the aim of reducing the GI adverse effects of traditional NSAIDs that inhibit both COX-1 and COX-2 isoenzymes, while maintaining their effective anti-inflammatory and analgesic properties. In this research, based on docking studies, 1-benzyl-2-(methylsulfonyl)-1H-imidazol-5-yl)methanol was designed and synthesized as a selective COX-2 inhibitor.

Methods: (1-benzyl-2-mercapto-1H-imidazol-5-yl)methanol was synthesized from phenylmethamine and potassium thiocyanate and dihydroxyacetone through nucleophilic substitution reaction then Dehydrative Cyclization.The product was S-methylated and oxidated to give of (1-benzyl-2-(methylsulfonyl)-1H-imidazol-5-yl) methanol.

Results: The designed molecule was synthesized and structurally elucidated by IR, NMR and Mass spectra. It was designed based on the SAR of the selective COX-2 inhibitor and docked in COX-2 and COX-1 and showed favorable selectivity for COX-2 isoenzyme.

Conclusions: In this research (1-benzyl-2-(methylsulfonyl)-1H-imidazol-5-yl)methanol as a selective COX-2 Inhibitor was designed, synthesized and approved by IR, NMR and Mass spectra. The docking studies showed that the designed compound has good selectivity for COX-2 isoenzyme.

Keywords: Synthesis; (1-benzyl-2-(methylsulfonyl)-1H-imidazol-5-yl) methanol; COX-2 inhibitors