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## Designed, synthesized and molecular modeling studies of a novel group of 5-substituted (1-benzyl-2-(methylsulfonyl)-1-H-imidazole) as selective cyclooxygenase-2 inhibitors

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Inflammation is a process involving many inflammatory cells and mediators, in respond to traumatic, infectious, post-ischemic, toxic or autoimmune injury that mostly leads to healing, however, if assisted repair and target destruction are not properly phased, it can lead to tissue damage. Non-steroidal anti-inflammatory drugs (NSAIDs) are the first choice therapeutic agents for the treatment of inflammation, by inhibition of cyclooxygenase enzymes (COX-1 and COX-2). COX-1 is constitutively expressed for regulation of platelet aggregation, gastric mucosa, renal blood flow and to maintain homeostasis in most cells but COX-2 is significantly up regulated in inflammatory conditions. Due to non-selective COX-1 and COX-2 inhibition of NAIDs, ulceration, kidney failure and gastrointestinal hemorrhage have been identified as their major side effects. Therefore selective cyclooxygenase-2 inhibitors are considered to have less adverse effects in compare to classic NSAIDs. Although recent studies report cardiovascular side effects for the selective cyclooxygenase-2 inhibitors, regarding to their clinical value, researches in this area still continue. Herein, based on structure and activity relationship of selective cyclooxygenase-2 inhibitors, a novel group of 5-substituted (1-benzyl-2-(methylsulfonyl)-1-H-imidazole) are synthesized in 5 steps of imidazole cyclyzation, nucleophilic substitution, oxidation and nucleophilic substitution with a strong leaving group, and characterized by IR, Mass and 1HNMR. Molecular modeling of the designed structures revealed the role of methylsulfonile as the pharmacophore group and interactions of imidazole nitrogens, NH and phenyl groups with essential amino acids in secondary internal pocket of cyclooxygenase 2. Biological evaluation would be investigated in future studies.



#### Biography

Azin Kiani has received her PharmD in 2012 at the age of 25 from Shahid Beheshti University of Medical Sciences, Iran. She has a 2-year experience as a member of medicinal chemistry researchteam in the laboratory and has one poster and two accepted papers. Currently, she is the Chief Pharmacist of the northern branch of Iranian professional chain pharmacies. She serves not only as a part of the medical team but also responsible for extemporaneous combinations of her branch.

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