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Design and synthesis of new isoquinoline derivatives as selective cyclooxygenase-2 (COX-2) inhibitors and their molecular modeling studies

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Background and Aims: Nonsteroidal anti-inflammatory drugs are known as an important class used in the treatment of inflammation, pain and fever . Their adverse effect reactions mostly affect the gastrointestinal tract. Regarding to the point that the selective COX-2 inhibitors have less GI adverse effects than the non-selective ones, in this study based on the structure activity relationship of selective COX-2 inhibitors, new Isoquinoline derivatives have been designed and synthesized in order to specify the effects of these drugs and to decrease the adverse reactions.
Methods: New Isoquinoline derivatives was synthesized through multi-step reactions.
Results: The new Isoquinoline derivatives were docked in COX-2 and COX-1 and showed favorable results. Some of them were synthesized and their molecular structures were confirmed by IR, 1HNMR spectroscopy and Mass spectrometry.
Conclusions: In this research, new Isoquinoline derivatives as selective COX-2 Inhibitors were docked, synthesized and confirmed by IR, NMR and Mass spectrometry.

Keywords: Cyclooxygenase-2; Synthesis; Design; Isoquinoline