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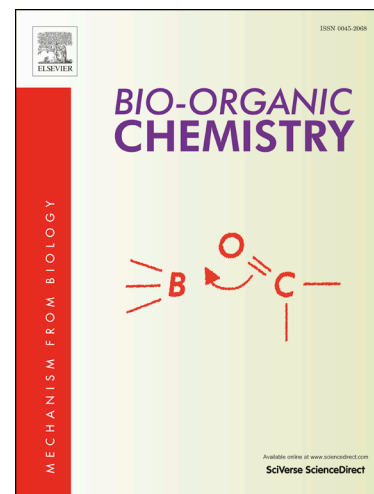
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Synthesis, anti-inflammatory, p38 α MAP kinase inhibitory activities and molecular docking studies of quinoxaline derivatives containing triazole moiety

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Abstract: A new series of 3-[2-(5-mercapto-4-phenyl-4*H*-1,2,4-triazol-3-yl)ethyl]quinoxalin-2(1*H*)-one (**5a-v**) derivatives was synthesized and subjected to *in vitro* evaluation for anti-inflammatory activity (BSA anti-denaturation assay) and p38 α MAPK inhibition. Few selected compounds (**5a**, **5e**, **5f**, **5g**, **5h**, **5l**, **5q** and **5u**) were studied for their *in vivo* anti-inflammatory activity, ulcerogenicity and lipid peroxidation potential. Compounds **5e** and **5f** were found to be the most active in the series showing 83.45% and 84.15% anti-inflammatory activity respectively when compared to diclofenac sodium (83.22%). They were also found to have low ulcerogenic potential and lipid peroxidation. The p38 α MAP kinase inhibition of the compounds **5e** and **5f** was also found to be slightly better than the standard SB 203580. The compounds were also docked against p38 α MAP kinase enzyme in order to predict their binding mode. Compounds **5e** and **5f** showed stronger binding with an additional hydrogen bond interaction with ASP-168 which was not observed in SB 203580.

Keywords Quinoxaline • p38 α MAP kinase • Docking • Anti-inflammatory • Ulcerogenicity

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