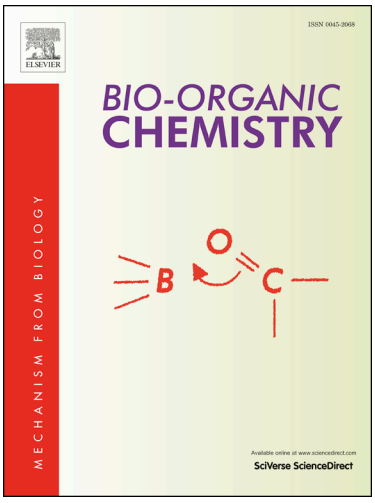

Synthesis, anti-inflammatory, p38α MAP kinase inhibitory activities and molecular docking studies of quinoxaline derivatives containing triazole moiety

Sana Tariq, Ozair Alam, Mohd. Amir

PII: S0045-2068(17)30610-7
DOI: https://doi.org/10.1016/j.bioorg.2017.12.003
Reference: YBIOO 2184

To appear in: *Bioorganic Chemistry*

Received Date: 8 August 2017
Revised Date: 17 November 2017
Accepted Date: 1 December 2017

Please cite this article as: S. Tariq, O. Alam, Mohd. Amir, Synthesis, anti-inflammatory, p38α MAP kinase inhibitory activities and molecular docking studies of quinoxaline derivatives containing triazole moiety, *Bioorganic Chemistry* (2017), doi: https://doi.org/10.1016/j.bioorg.2017.12.003

Synthesis, anti-inflammatory, p38α MAP kinase inhibitory activities and molecular docking studies of quinoxaline derivatives containing triazole moiety

Sana Tariq, Ozair Alam, Mohd. Amir*

Department of Pharmaceutical Chemistry, School of Pharmaceutical Education and Research, Hamdard University, New Delhi-110062, India.

Abstract: A new series of 3-[2-(5-mercapto-4-phenyl-4*H*-1,2,4-traiazol-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 p38α 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 p38α 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 p38α 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 ● p38α MAP kinase ● Docking ● Anti-inflammatory ● Ulcerogenicity

*Corresponding author, Department of Pharmaceutical Chemistry, School of Pharmaceutical Education and Research, Hamdard University, New Delhi-110062, India
Email address: mamir_s2003@yahoo.co.in, mamir@jamiahamdard.ac.in