Selective Inhibition of p38 MAPK Isoforms using Bipyrazole Derivatives: An in Silico Approach

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Abstract

The p38 MAPK family of proteins comprised of four members; p38α, p38β, p38γ, and p38δ. All p38 MAPKs are strongly activated by environmental stresses and inflammatory cytokines. MAPKs have been shown to play a pivotal role in diverse diseases, including cancer. Majority of studies have focussed on targeting p38 MAPK isoform alpha. However, the report computational in silico molecular docking analysis of 34 bipyrazole analogs as possible p38 MAPK inhibitors. Results obtained are compared and it was observed that the top hit in all cases was found to be compound 26 with dock scores more than 200 kcal/mol whereas reported inhibitors in literature SB203580, SB202190, PD169316 resulted in dock scores between 164-189 kcal/mol. Hence, it is worthwhile to study these bipyrazole analogs as a new class of p38 MAPK inhibitors.

References

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Index Terms

Computer Science Circuits and Systems

Keywords

Docking, p38 MAPK Isoforms, Bipyrazoles