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Computational Chemistryaided Study Of Pyrazolopyrimidines As Thymidylate Synthase Inhibitors

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ABSTRACT:

Molecular modelling docking is very useful tool that predict the preferred orientation of one molecule to another when bound to each other to form a stable complex. Knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules using, for example, gliding score functions. Herein we focused the pyrazolopyrimidineshaving potential in the field of medicinal chemistry because of their structural relevance of biogenic purine class moiety with wide spectrum of biological activities. Many well-known active pharmaceutical ingredients such as Allopurinol, Zaleplon, etc.that are based on pyrazolopyrimidine moiety.A number of pharmacological activities such as mitotic, CNS stimulant, analgesic, antipyretic, antiinflammatory, antifungal, antibacterial and anticancer activity have been reported for pyrazolopyrimidines. Considering all these facts pyrazolopyrimidines received special attention for lead compound identification. Synthesis, computational study and antibacterial activity has been undertaken for pyrazolopyrimidines. Thymidylate synthase of Escherichia coliorganism was taken as a case study which is common for Mycobacterim tuberculosis organism.