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Synthesis, biological evaluation and molecular dynamics studies of 1,2,4triazole clubbed Mannich bases

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Graphical Abstract:

A series of newer analogous of triazole were synthesized by introduction of N-Mannich reaction using conventional as well as microwave synthetic route and assessed for their antimicrobial, antituberculosis and antiprotozoal activity. The computational studies revealed for that Mannich derivative showed a high affinity toward the active site of enzyme which provides a strong platform for new structure-based design efforts.



Polar → H-bond (sidechain) ○ Solvent exposure Polar → Pi-Pi stacking Download English Version:

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