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Computational drug designing of newly synthesized triazoles against potential targets of methicillin resistant *Staphylococcus aureus*

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Today methicillin resistant *Staphylococcus aureus* (MRSA) is resistant to many commonly used antibiotics and has become a great challenge for healthcare professionals, therefore new molecules are needed to cope with this situation. In this study, we synthesized new lead molecules 4-Amino-5-(2-Hydroxyphenyl)-1,2,4-Triazol-3-Thione (U1) and 4-(2-hydroxybenzalidine) amine-5-(2-hydroxy) phenyl-1,2,4-triazole-3-thiol (U1A Schiff base) by fusion method (refluxed at 160°C) that showed promising antibacterial activity against MRSA. These compounds were structurally characterized by FTIR and NMR and their drug likeness properties were evaluated by applying Lipinski's rule of 5. We identified new alternative potential drug targets of this bacterium by comparative and subtraction genomics analysis. The quality of these protein targets were evaluated by Qualitative Model Energy Analysis (QMEAN) Z-score and Ramachandran plot. In particular, we used octanoyl-[GcvH] protein N-octanoyltransferase and phosphomevalonate kinase as alternative potential targets in Auto Dock Vina wizard drug-target interactive study. This study can provide a framework to find potential drug targets for other pathogenic microorganisms that can successfully be docked with compound U1 and U1A.

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