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Binding Conformation Analysis of Topoisomerse-I Bound DNA in *Staphylococcus aureus* and Screening of Novel Compounds to Block DNA-protein Interactions†

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Abstract: *Staphylococcus aureus (S. aureus*) is major human pathogenic bacteria and causes an array of communicable human diseases. Virulence factors in this bacterium are organized and coordinated by a network of multiple DNA binding proteins. Bacterial DNA topoisomerase 1 are ubiquitous enzymes that organize the position of DNA topology and also plan an important responsibility in many biological processes, such as replication, transcription, and recombination, so it considers as a potential target. To have structural insight on this protein, a three-dimensional structure was build using homology modeling, and the structure was validated using various validation servers. The stability of the model was checked using molecular dynamics simulation. Protein-DNA interactions are the main physical foundation of gene expression and DNA modification. Structural models of this protein-DNA expose these interactions are for their understanding. Only a few numbers of protein-DNA complexes were identified by experimental methods;computational methods are available to fill up the need. Here we performed the docking studies in order to identify the interaction between DNA - DNA topoisomerase 1.

Keywords: *S.aureus;* homology modeling; molecular docking; dynamics.

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Conflicts of Interest

The authors declare no conflict of interest.