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Homology Modeling, Virtual Screening and ADME Prediction Studies on LukS Subunit Protein from *Staphylococcus aureus* †

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Abstract: (1) Background: *Staphylococcus aureus*, a gram-positive coccal bacterium, is responsible for many diseases ranging from minor skin infection to life-threatening diseases such as pneumonia, meningitis, and septicemia. Luks, a major protein of *Staphylococcus aureus* is responsible for pore formation in the transmembrane of macrophages and polymorphnuclearleuckocytes. To date, the crystal structure is unavailable for this LukS protein. (2) Methods: To elucidate the three-dimensional structure of this protein, homology modeling has been performed using MODELLER 9.10 software. In order to make out a potent inhibitor, virtual screening has been performed using the Binding database. (3) Results: We found that compound ids 7694, 7695, 8285, 6817, and 7696 have abetter docking score, docking energy, and drug-like properties. (4) Conclusion: Experimental validation of these compounds could emerge as a potent inhibitor against LukS subunit protein in *Staphylococcus aureus.*

Keywords: *Staphylococcus aureus*; LukS subunit; homology modeling; secondary structure prediction; virtual screening; ADME properties.

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Conflicts of Interest

The authors declare no conflict of interest.