In Silico drug design represents a new approach for drug discovery and industry. Structure based computer aided drug design (CADD) was used in this study to find an antibiofilm agents to suppress Staphylococcus epidermidis biofilm production which is considered the main virulence factor of this bacterium. The sarA protein was chosen as the target for this process as it stimulates icaADBC operon which is responsible for biofilm production. The first step was constructing a 3D structure of the protein which was obtained using the RaptorX homology modelling.

Pharmacophore generation was performed using the Hip Hop generator from Discovery Studio package. One hundred seventy seven molecules were chosen by ligand based virtual screening using ZincPharmer. Thirty seven molecules were found suitable as having negative binding free energies with sarA protein in EADock engine from the Swissdock Website. Seven of them were tested in lab and four of which gave antibiofilm activity (acetaminophen, acetylsalicylic acid, ibuprofen and acetic acid).

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