

A Novel Terpenoid from *Elephantopus Scaber* - Antibacterial Activity on *Staphylococcus Aureus*: A Substantiate Computational Approach

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Staphylococcus aureus has gained much attention in the last decade as it is a major cause of the Urinary Tract Infection in Diabetic patients. The Extended Spectrum β -Lactamases (ES β L) producers are highly resistant to several conventional antibiotics. This limits the therapeutic options. Hence efforts are now taken to screen few medicinal plants, which are both economic and less toxic. Among the several plants screened, we have chosen the acetone extract of *Elephantopus scaber* from which we purified a new terpenoid for our study. Its structure was generated using CHEMSKETCH software and the activity prediction was done using PASS PREDICTION software. We have confirmed the mechanism of anti-bacterial effect of terpenoid using Computer –Aided Drug Design (CADD) with computational methods to simulate drug – receptor interactions. The Protein-Ligand interaction plays a significant role in the structural based drug designing. In this present study we have taken the Autolysin, the bacteriolytic enzyme, that digest the cell wall peptidoglycon. The autolysin and terpenoid were docked using HEX docking software and the docking score with minimum energy value of -209.54 was calculated. It infers that the terpenoid can inhibit the activity of autolysin by forming a strong atomic interaction with the active site residues. Hence the terpenoid can act as a drug for bacterial infections. Further investigations can be carried out to predict the activity of terpenoid on other targets.

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