



Category: Bioinformatics

# Homology modeling of *FtsZ* protein from virulent bacterial strains and its interaction with *Eucalyptol*: An In silico approach for therapeutics

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## Abstract

The spread of virulent factors by hgt (Horizontal gene transfer) among bacterial strains causes community acquired infections in tertiary care hospital leading to emergence of PDR (Pan Drug Resistant) strains. This phenomenon is matter of great concern worldwide, now-a-days. Therefore, it is a high time to find alternative chemotherapeutic agents to combat these antibiotic-resistant microorganisms. Plants are said to be reservoirs of natural resources that are been used for the betterment of mankind. Higher plants may serve as the resource for new antimicrobials to replace or augment current therapeutic options [1]. In the current investigation we have selected *Eucalyptol* syn. 1,8 Cineole, an active constituent of Eucalyptus (23.2%), Peppermint (5.9%) and Kewda (0.405%) essential oils for the molecular docking studies with *FtsZ* protein, a drug target molecule. The template pdb files for homology modelling of *FtsZ* protein was retrieved from RSCB protein data bank. The 3D structure of *FtsZ* protein was predicted by modeller tool followed by structure refinement and loop modelling using various tool and online servers. *Eucalyptol* molecule was screened for “Lipinski's rule of five or Pfizer's rule of five, where the drug likeness of *Eucalyptol* was predicted. Both the receptor (*FtsZ*) and ligand molecule (*Eucalyptol*) were optimized for docking using Auto dock tool. It was observed that *eucalyptol* was docked inside the crevices of *FtsZ* molecule. The interacting pocket comprising specific amino acids of *FtsZ* molecule were found to be ala-345, met-224, tyr-222, thr-162, lys-133 and thr-348. But, the Hydrogen-bonding interaction was observed between Threonine-348 and the C2 of *Eucalyptol* molecule. The outcome of this study was well corroborated with In vitro studies carried out by presenting author [2]. The current investigation unzips the chemotherapeutic nature of *Eucalyptol* against various bacterial strains which could be formulated as a potential drug after confirmation of the efficacy and potency.

## References

- [1] Snow Setzer, M., Sharifi-Rad, J. and Setzer, W.N. (2016) The Search for Herbal Antibiotics: An In-Silico Investigation of Antibacterial Phytochemicals. *Antibiotics (Basel)* 5: 30. <https://doi.org/10.3390/antibiotics5030030>
- [2] Pattnaik, S., Subramanyam, V.R., Bapaji, M. and Kole, C.R. (1997) Antibacterial and antifungal activity of aromatic constituents of essential oils. *Microbios* 89: 39-46.

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