Combating Superbugs: Using Natural Compounds as Down-Regulators of Biofilms Formation in ESKAPE Pathogens (An in silico Study)

Gupta, Jai (School: Seminole High School)
Gupta, Avi (School: Seminole High School)

Biofilm is the consortia of sessile groups of microbial colonies that adhere on biotic and abiotic surfaces with the help of extracellular polymeric substances (EPS) and glycocalyx. ESKAPE bacteria are the most common types of nosocomial disease-causing organisms and are considered to be the model biofilm-forming organisms. The biofilm formed by ESKAPE pathogens prevents penetration of conventional antibiotics due to the presence of extracellular polymeric substances (EPS) thereby creating multi-drug or antibiotic resistance. Natural therapeutics have been chosen due to their potential to disrupt biofilms. The in silico studies performed on biofilm-forming bacterial proteins of ESKAPE pathogens revealed the role of various known bioactive compounds. This study investigates twenty-three natural compounds for their drug-like properties for fighting against antibiotic-resistant biofilms. The overall safety and efficiency of oral drug reception are maintained, emphasizing their potential for further drug development. Molecular docking analysis employing SwissDock was used to evaluate the binding affinities of these ligands to key biofilm-forming genes and membrane proteins in ESKAPE pathogens. The results show specific ligands, such as Baicalin, Curcumin, etc., demonstrating high binding affinities against biofilm-associated proteins that we studied. The selected ligands were thoroughly observed for their molecular electrostatic properties and protein-ligand interactions. It was further observed that the newly designed compounds shared all drug-like properties and showed maximum interaction with the biofilm-forming protein. Thus, this study provides a new dimension of antibiofilm compound (drug) which possesses a maximum potency of eradicating biofilms and AMR bacteria.