In vitro assessment on designing novel antibiofilms of pseudomonas aeruginosa using a computational approach

ABSTRACT

An anti-biofilm that can inhibit the matrix of biofilm formation is necessary to prevent recurrent and chronic Pseudomonas aeruginosa infection. This study aimed to design compounds with a new mechanism through competitive inhibitory activity against phosphomannomutase/phosphoglucomutase (PMM/PGM), using in vitro assessment and a computational (in silico) approach. The active site of PMM/PGM was assessed through molecular redocking using L-tartaric acid as the native ligand and other small molecules, such as glucaric acid, D-sorbitol, and ascorbic acid. The docking program set the small molecules to the active site, showing a stable complex formation. Analysis of structural similarity, bioavailability, absorption, distribution, metabolism, excretion, and toxicity properties proved the potential application of ligands as an anti-biofilm. In vitro assessment with crystal violet showed that the ligands could reach up to 95.87% inhibition at different concentrations. The nitrocellulose membrane and scanning electron microscopic visualization showed that the untreated P. aeruginosa biofilm was denser than the ligand-treated biofilm.