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In silico disrupting quorum sensing of porphyromonas gingivalis via essential oils and coumarin derivatives

The emergence of Porphyromonas gingivalis biofilm is a hallmark of risky burden diseases including Alzheimer's disease and atherosclerosis. The current study aims to screen some natural essential oil compounds and coumarin derivatives to interfere with quorum sensing of the bacterium and thus biofilm formation. A total of 20 ligands (10 essential oil molecules and 10 coumarin derivatives) were docked to P.gingivalis heme-binding protein HmuY using UCSF Chimera built-in AutoDock interface. Alongside, ADMET properties were also predicted via ADMETsar 2.0 and ProTox-II webservers. All of the selected ligands had higher free energy values than the reference inhibitor MES and native coumarin as well. Moreover, ADME parameters are in good agreement with Lipinski's rule of five. Nevertheless, the best molecules with top binding energy exhibited slight immunogenicity as well as carcinogenicity issues requiring in vitro confirmation. In conclusion, the tested ligands had better efficacy against P.gingivalis quorum sensing and biofilm.