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Computational Identification of Inhibitors Against Porphyromonas gingivalis Virulence Factors in Oral Squamous Cell Carcinoma

Nandini
M.Sc Student, Centre of Biotechnology (Bioinformatics)
Maharshi Dayanand University, Rohtak
dr.nandni2k1@gmail.com

Abstract: *Oral squamous cell carcinoma (OSCC) is a major global malignancy, accounting for about 90% of oral cancer cases and ranking eighth in cancer incidence worldwide. While tobacco, alcohol, nicotine, and HPV are established risk factors, nearly 15% of OSCC cases occur without these, suggesting other contributors. Recent studies implicate bacterial infections, particularly Porphyromonas gingivalis, a periodontal pathogen, as an oncogenic factor in OSCC. P. gingivalis influences multiple cancer hallmarks, disrupting tumor suppression and apoptosis pathways while activating oncogenic signaling. Its virulence factors—Fimbriae (FimA), nucleoside diphosphate kinase (NDK), Lysine gingipain (Kgp), and Arginine gingipain (RgpB)—play crucial roles in OSCC pathogenesis. FimA promotes uncontrolled cell proliferation, NDK inhibits apoptosis and enables immune evasion, and gingipains (Kgp, RgpB) enhance metastasis. This in-silico study employed molecular modeling, high-throughput virtual screening, molecular docking, 3D-QSAR pharmacophore modeling, and molecular dynamics simulations to identify potential inhibitors of these virulence factors. Homology modeling was used to predict the 3D structure of NDK. For targets lacking known inhibitors (FimA and NDK), structure-based drug design was applied, while both structure- and ligand-based approaches were used for Kgp and RgpB. Natural and anticancer compound libraries were screened to identify potential leads. Docking scores, binding energies, and ADMET analyses guided the selection of top compounds with favorable pharmacokinetic properties. Molecular dynamics simulations provided insights into the stability and interactions of receptor-ligand complexes. Protocatechuic acid, Grossamide K, and shogasulfonic acid C emerged as promising inhibitors with potential therapeutic applications.*

Keywords: Oral squamous cell carcinoma (OSCC); *Porphyromonas gingivalis*; Virulence factors; Molecular docking; 3D-QSAR modelling

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