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Mining the Proteome of Fusobacterium nucleatum for Potential Therapeutics Discovery

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Abstract : The plethora of genome sequence information of bacteria in recent times has ushered in many novel strategies for antibacterial drug discovery and facilitated medical science to take up the challenge of the increasing resistance of pathogenic bacteria to current antibiotics. In this study, we adopted subtractive genomics approach to analyze the whole genome sequence of the Fusobacterium nucleatum, a human oral pathogen having association with colorectal cancer. Our study divulged 1499 proteins of Fusobacterium nucleatum, which has no homolog in human genome. These proteins were subjected to screening further by using the Database of Essential Genes (DEG) that resulted in the identification of 32 vitally important proteins for the bacterium. Subsequent analysis of the identified pivotal proteins, using the KEGG Automated Annotation Server (KAAS) resulted in sorting 3 key enzymes of F. nucleatum that may be good candidates as potential drug targets, since they are unique for the bacterium and absent in humans. In addition, we have demonstrated the 3-D structure of these three proteins. Finally, determination of ligand binding sites of the key proteins as well as screening for functional inhibitors that best fitted with the ligands sites were conducted to discover effective novel therapeutic compounds against Fusobacterium nucleatum.

Keywords : colorectal cancer, drug target, Fusobacterium nucleatum, homology modeling, ligands
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