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Unraveling Colorectal Cancer: Computational Insights into Phytochemical Targeting and Therapeutic Potential

Abstract

Colorectal cancer, a major global health concern, necessitates early detection, screenings, and improved treatment strategies to enhance patient outcomes and decrease mortality rates. The intricate molecular mechanisms of colorectal cancer can be effectively understood through computational analysis, which could provide valuable therapeutic insights. This study used a computational approach to analyze gene expression data collected from GEO (Gene expression omnibus). This data set (GSE 62322) consisted of colon tumor samples from 21 advanced colorectal cancer patients. We used GEO2R and Microsoft Excel to identify differentially expressed genes, selected genes that were common among all the differentially expressed genes linked to colorectal cancer. Further, ShinyGO 0.77 was used to perform functional enrichment analysis, and explore protein-protein interaction networks of the genes involved in colorectal cancer. SwissTarget prediction was used to recognize potential targets for 10 phytochemicals found in Phyllanthus emblica (Indian gooseberry) that maybe linked to colorectal cancer-related differentially expressed genes. We performed molecular docking to study binding and interactions between the 10 phytochemicals and 6 target proteins which were 2SRC, 5FED, 4AG8, IGFR1, ESR1 and AURKA. Querecetin among all 10 phytochemicals showed best binding affinity for the protein targets. Following that, an ADME analysis using SwissADME was performed on Querecetin, comparing its drug-like properties and ADME parameters to control group. Physicochemical descriptors, pharmacokinetic properties, and drug-like qualities, as well as synthetic accessibility and bioavailability were evaluated. This integrated computational methodology investigated differential gene expression, potential compound-target interactions, and drug-like properties of natural compounds holistically. The systematic approach sheds light on potential therapeutic targets and provides insights into the suitability of natural compounds as colorectal carcinoma treatment alternatives, thereby contributing to oncology drug discovery efforts.