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Computational Drug Developmental Approach with the Help of Biomarkers

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DESCRIPTION

Onco-informatics algorithms were used to assess the expression and prognostic value of the MDM2 gene in brain Lower-Grade Glioma (LGG) cancer. To assess the designated MDM2 gene's differential expression and look for alterations and copy number variants, several transcriptome platforms were employed. The mortality rate of LGG cancer patients was calculated using GENT2. The Gene-MANIA programme was used to create the protein-protein interaction networks between the MDM2 gene and its co-expressed genes. Schrödinger Suite software was used to molecularly associate identified bioactive plants with the MDM2 target for evaluation. With regard to important macromolecular target sites, protein-ligand interactions were seen. The targeted protein was used in a molecular dynamics modelling of the new bioactive substances. Taxifolin and Epicatechin, two phytochemicals that target the MDM2 protein, have demonstrated results that are significantly more stable than those of the control drug, leading researchers to draw the conclusion that other therapeutic options for the treatment of LGG patients may include phytochemicals with bioactive potential. Our formerly informatics-based developed workflow has shown that the MDM2 gene may function as a predictive biomarker for LGG cancer, and after using *in silico* methods, a few phytochemicals had excellent interaction findings within the macromolecular target's active region. It is advised to conduct *in vitro* and *in vivo* studies to verify these findings. The P53 protein is a transcription factor that controls the production of a large number of genes involved in DNA repair, differentiation, cell cycle control, and death. In reaction to intracellular stresses, it is crucial in kicking off a programme for cell defence. As a result, numerous signal transmission networks activated by p53 participated in the cell's anti-cancer defence. Notably, the p53-directed pathway or pathways may be activated by internal and extrinsic stress cues that impact cellular homeostatic processes. On the other hand, p53 can promote transcription-independent DNA repair, apoptosis, or a DNA duplication process. In reality, P53 expression is minimal under typical circumstances, but damage to a cell's DNA can increase the P53 protein's expression pattern. Through interactions with MDM2, a protein translation negative modulator of the p53 protein, the p53 protein loses its functionality. Two closely similar proteins called MDM2 (also called HDM2 for its human homolog) and MDMX (also called MDM4) carefully watch p53 in higher eukaryotes. MDM2 and MDMX work together to suppress p53's transcriptional activity, mainly by adversely regulating the stability and activity of the p53 protein in a feedback loop. MDM2 has a shape resembling a hydrophobic groove composed of two helices and a loop. Two sheet layers make up the groove's bottom. Compared to synthetic goods, medicinal plants have less of a harmful impact on human health. Clinical study employs a number of plant-derived compounds as cancer therapeutics, including Vinblastine, Taxol, and Topotecan, among others. Finding the target probable phyto-compounds has demonstrated successful anticancer potential in multiple clinical cancer research trials as a result of recent developments in genomics and proteomics. However, due to an increase in the drug's tolerance to cancer cells, the development of novel anticancer medications is now urgently needed. Bioactive phytochemicals or compounds produced from plants, on the other hand, have considerably better results in numerous clinical studies. It has been found that a number of well-known compounds have anticancer properties in colon, prostate, breast, and glioblastomas.

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CONFLICT OF INTEREST

There are no conflicts of interest.

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