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Targeting Cancer Pathways: Licoagrodin as a Potent Bcl-2 Inhibitor

Abstract

The study sought to identify pivotal genes influencing cancer-related processes such as EMT, autophagy, anoikis, and metastasis, as well as to identify common genes across these pathways and assess their expression in various cancer types. Bcl-2 has emerged as a frequently overexpressed gene, particularly in cancers such as Acute Myeloid Leukemia, Diffuse Large B Cell Lymphoma, and Thymoma. Among 102 natural compounds, molecular docking identified licoagrodin as the highest-scoring molecule, which was confirmed by molecular dynamics simulation over 100 ns. GEO2R gene expression analysis revealed licoagrodin's impact, demonstrating its ability to suppress Bcl-2, BIRC3, and CHUK while increasing the pro-apoptotic protein Bax. The binding of licoagrodin at the Bcl-2 site was found to have a robust docking score and relevant interactions, as evidenced by calculated binding free energies of -52.21 kcal/mol (MM/GBSA) and -9.18 kcal/mol (MM/PBSA). A p-value of 0.05 was used to determine significance. The findings suggested that licoagrodin has the potential to be a protein inhibitor, owing to its high binding energy and interactions with the Bcl-2 binding site. By targeting multiple cancer pathways, this natural compound holds promise as an alternative for combating anoikis resistance across a wide range of tumors.