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Docking and Molecular Dynamics Simulation Revealed the Potential Inhibitory Activity of Amygdalin in Triple-Negative Breast Cancer Therapeutics Targeting the BRCT Domain of BARD1 Receptor

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Abstract

Triple-negative breast cancer (TNBC), is diagnosed as the most lethal molecular subtype of breast cancer (BC) preceded by an extremely poor prognosis. For enabling effective TNBC therapy, the identification of novel druggable biomarkers is an earnest need. Multigene paneling and genomewide association studies identify multiple genes with high-to-moderate penetrance in TNBC. Modern computer-aided drug designing techniques, thus aim to design more cost-effective natural small molecule inhibitors for TNBC prevention and diagnosis. Here Amygdalin, a natural glycosidic inhibitor is docked and simulated against three such high-to-moderate penetrance genes identified in TNBC, BARD1, RAD51, and PALB2. The preliminary result of the analysis, reports a highest, intermediate, and least binding energy score of - 6.69 kcal/mol, - 5.09 kcal/mol, and - 4.89 kcal/mol in BARD1, RAD51, and PALB2, respectively. The best-docked protein-ligand complex (BARD1-Amygdalin) was then simulated and compared with an approved drug for TNBC treatment, Olaparib. A comparable binding energy score of - 8.53 kcal/mol was obtained by docking olaparib with BARD1. A 100 ns MD simulation revealed, Amygdalin forms more H-bonds, providing more stable and compact protein-ligand complex with BARD1 than compared to Olaparib. The result was also supported by calculation of solvent accessible surface area and analysis of radius of gyration. Thus, our findings suggest that role of Amygdalin can further be studied in details for TNBC therapeutics, which was found to target the BRCT domain of the BARD1 receptor in stable manner. Please check and confirm that the authors and their respective affiliations have been correctly identified and amend if necessary. Name and affiliations are correctly identified.

Keywords: Amygdalin; Molecular docking; Molecular dynamic; Simulation; Triple-negative breast cancer.

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