

Target Identification and Screening of BRCA1 Gene Involved In Breast Cancer

Praveena P^{1*}

¹PG and Research and Department of Microbiology, Mohamed Sathak College of Arts And Science, Sholinganallur Chennai.

*Corresponding author e.mail:praveenaloy@gmail.com

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ABSTRACT

Certain variations of the BRCA1 gene lead to an increased risk for breast cancer. Researchers have identified hundreds of mutations in the BRCA1 gene, many of which are associated with an increased risk of Breast cancer. The 3D structure of protein brca1 is retrieved from PDB. Then the new drug is designed by obtaining similar features from the cyclophosphamide and then that structure is chemically modified using ChemsKetch. The various biochemical parameters are checked by Log p, Molsoft, Lipinski, ADMET properties etc. Finally the newly designed drug was allowed to dock with the protein and the energy score was calculated. Finally the tabular column was drawn to compare the Energy score. The lowest free Energy Binding has high Energy score. Thereby From the tabulation, the newly designed structure can also be used in the treatment of Breast cancer. Further modification of ligand molecule can increase the property of active site binding.