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Abstract

Cancer known medically as a malignant neoplasm, is a large group of different diseases, all involving unregulated cell growth. In cancer, cells divide and grow uncontrollably, forming malignant tumors, and invade nearby parts of the body. Homology modeling and flexible docking of Bcl2L10 has been studied in *silico* approach. Blast result was found to have similarity with Bcl2L10 of 48% identity with 2KUA. With the aid of Molecular dynamics and Molecular simulations studies it was identified that the generated structure was reliable. Active site of Bcl2L10 was identified by CASTP. Large potential drugs were designed for identifying molecules that can likely bind to protein target of interest. This structure was used to identify better inhibitor using docking studies. The drug derivatives were docked to the Bcl2L10 structure into the active site. The different drug derivatives designed were used for docking with the generated structure, among the 100 derivatives designed, fifth derivative showed highest docking result. The drug derivatives were docked to the protein by hydrogen bonding interactions and these interactions play an important role in the binding studies. Our investigations may be helpful for further studies.

Key words: BCL2L10, Cancer, Drug Designing, Modelling, Molecular dynamics.

Aim and Objectives

The main objective of this study is to help in treating cancer disease cause by Bcl2L10 by exploiting drug that docking with Bcl2L10. This study investigated in *silico* approach for identification inhibitor design with protein caused cancer. The project work is carried out on the following objectives:

- Prediction 3 D structure of protein
- Designing inhibitor drugs that may bind with protein
- Active-site identification
- screening the inhibitor drugs that docking with protein