J. Indian Chem. Soc.,
Vol. 96, January 2019, pp. 142-146

Studies on structural basis of epidermal growth factor receptor target using Tunicamycin on human cancer cell line

S. Sivaranjani and C. Arulvasu*

Department of Zoology, University of Madras, Guindy Campus, Chennai-600 025, India

E-mail: carulvasu@gmail.com

Manuscript received online 02 September 2018, accepted 10 October 2018

Cancer is the leading cause of death in both economically developed and developing countries. It is a fatal disease caused by an uncontrolled division of abnormal cells in the body. These abnormal cells called malignant cells which can invade nearby tissues can spread through bloodstream and lymphatic system to other parts of the body. Tunicamycin is an antibiotic isolated from *Streptomyces lysosuperificus* that inhibits the synthesis dolichyl-N-acetylglucosamine diphosphatase essential for the assembly of oligosaccharide chains and their subsequent transfer to aspargine residues in proteins. The epidermal growth factor receptor (EGFR) is the cell-surface receptor, it's over expression or over activity has been associated with a number of cancers, including breast, lung, ovarian, and anal cancers. EGFR, an N-glycosylated transmembrane protein used to study whether inhibition of N-glycosylation and stimulation of endoplasmic reticulum (ER) stress by Tunicamycin enhances growth inhibition in cancer cell line. The protein-ligand (EGFR and Tunicamycin) and the inhibitor is Aldose reductase. The structure prediction was done using 3D pymol and maestro analysis. The structure of the ligand is elucidated and it was docked with EGFR active pocket site. The docking score was –9.87 kcal/mol and gliding energy was –69.17 kcal/mol. In conclusion the structural details and docking interaction predicts that this model can be used for drug target delivery in cancer. It also anticipated that the findings may provide useful information or clue for designing effective drugs for the therapeutic treatment of EGFR-related cancer.

Keywords: EGFR, tunicamycin, aldose reductase, docking, drug target.