ISSN (ONLINE) : 2395-695X
ISSN (PRINT) : 2395-695X
Available online at www.ijarbest.com

International Journal of Advanced Research in Biology, Engineering, Science and Technology (IJARBEST)
Vol. 2, Special Issue 8, February 2016 in association with
KAMARAJ COLLEGE OF ENGINEERING AND TECHNOLOGY, VIRUDHUNAGAR
DEPARTMENT OF BIOTECHNOLOGY
ORGANIZES
DBT, NEW DELHI SPONSORED NATIONAL LEVEL CONFERENCE ON CONTEMPORARY TRENDS IN BIOENERGY AND GREEN TECHNOLOGY: CHALLENGES AND OPPORTUNITIES [ORA-2016]
(25-26TH FEBRUARY 2016)

IDENTIFICATION AND VIRTUAL SCREENING OF LEAD COMPOUNDS FOR CARCINOMA

Dr.V.Stephen Rapheal , T.Nithya
Depatment of Biotechnology,Kumaraguru College of Technology,Coimbatore
E-mail: tnithya93@yahoo.com **Ph:** +91 98422 26155;

Abstract :

The wnt pathway is a promising therapeutic and preventive target in various human cancers. In canonical wnt signaling plays a key role in tumor cell proliferation, which correlates with the accumulation of β-catenin in cell due to inactivation of glyciogen synthetase kinase-3 β. The transcriptional complex of β-catenin-T-cell factor(Tcf), a key mediator of canonical wnt signalling, has been implicated in human cancer development. Current treatment of cancer depends on traditional cytotoxic agents with limited effects. Elucidation of the binding mode of inhibitors to β-catenin, reporting more potent inhibitors for the disease causing protein based on naturally occurring compounds , curcumin (turmeric)and diallyl sulfide (garlic). A crystal structure of a human β_catenin 3D structure (PDB ID:1JDH, 1.9 E resolution) was downloaded from PDB bank. water, metals and HTcf-4 were stripped from the structure using schrodinger suit for virtual screening . curcumin compound were download from pubchem database of compounds and 3D coordinates were generated using Ligprep module of schrodinger . Two pockets were generated respectively within a 30$Å^3$. grid box length and size are based on the binding site of Tcf-4 with β-catenin. After formation of receptor grid file, docking of flexible ligands with rigid receptor was performed by using SP(standard precision) . virtual screening was performed using schrodinger suit .The results showed that, the binding energy of known inhibitors (curcumin and diallyl sulfide) pubchem ID:CID-969516 and CID-11617 was observed in the range of -2.126 and -0.51 kcal/mol, while novel inhibitors(pubchem ID : CID-90657988, CID-46926318 , and CID-46926100 for curcumin, pubchem ID: CID-90768403 and CID-21573815for diallyl sulfide) exhibited -6.035, -5.643 and -5.221kcal/mol (curcumin) and -2.602 and -2.248 kcal/mol. Moreover curcumin and their similar compounds , diallyl sulfide compounds and T cell factors 4(TCF4) compete for β-catenin binding site.

Key words: wnt pathway; β-catenin; virtual screening ; curcumin ; diallyl sulfide