

Application of Computational Chemistry for Searching Novel Anticancer Derivatives of 2-Phenazinamines as Bcr-Abl Tyrosine Kinase Inhibitors

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The computational studies on 2-phenazinamines with their protein targets have been carried out to design compounds with potential anticancer activity. This strategy of designing compounds possessing selectivity over specific tyrosine kinase has been achieved through G-QSAR and molecular docking studies. The objective of this research has been to design newer 2-phenazinamine derivatives as Bcr-Abl tyrosine kinase inhibitors by G-QSAR, molecular docking studies followed by wet lab studies along with evaluation of their anticancer potential. Computational chemistry was done by using VLife MDS 4.3 and Autodock 4.2 followed by wet lab experiments for synthesizing 2-phenazinamine derivatives. The chemical structures of ligands in 2D were drawn by employing Chemdraw 2D Ultra 8.0 and were converted into 3D. These were optimised by using semi-empirical method called MOPAC. The protein structure was retrieved from RCSC protein data bank as PDB file. The binding interactions of protein and ligands was done by using PYMOL. The molecular properties of the designed compounds were predicted in silico by using Osiris property explorer. The parent compound 2-phenazinamine was synthesized by reduction of 2,4-dinitro-N-phenyl-benzenamine in the presence of tin chloride followed by cyclization in presence of nitrobenzene and magnesium sulfate. The derivatization at amino function of 2-phenazinamine was performed by treating parent compound with various aldehydes in the presence of dicyclohexylcarbodiimide (DCC) and urea to afford 2-(2-chlorophenyl)-3-(phenazin-2-yl)thiazolidin-4-one.

Biography:

Gajanan Sonwane has submitted his PhD at the age of 28 years from Dr. Babasaheb Ambedkar Marathwada university, Aurangabad, India and working as lecturer in Governement College of pharmacy, Auranagabad. He has published more than 6 papers in reputed journals and has been serving as an editorial board member of repute.