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Application of computer-aided drug design strategies for optimization of Anticancer activity of Phenazinamine derivatives

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We have carried out efficient Group based quantitative structure–activity relationships (GQSAR) exploring the relationship between the structures of a new promising family of 2-phenazinamine derivatives and their anticancer activities. We have developed residential evocative model, in order to aid in further optimization and expansion of newer anticancer agents containing novel pharmacophore. G-QSAR was performed on VLife molecular design suite (MDS) 4.2 version software. The extrapolative authority of the G-QSAR was checked through the cross-validation method and also by separating some compounds as fraction for external test set. The synthesis of five novel 2-phenazinamine derivatives was carried out successfully by chemical modifications suggested by the GQSAR model developed and by making use of its molecular descriptors. The screening of *in vitro* anticancer activity on K562 cell line was done in Tata Memorial Cancer Research Center Mumbai, India. The results display an improvement in anti-cancer activity. Phenazinamine and the analogues have better binding interactions with Oxidoreductase (PDB: 1YYD.) The binding energies of the protein-ligand interactions also confirm that the ligands fit into the active pockets of receptor tightly. The docking scores of PDB cavity (most hydrophobic area) and ligand suggests efficient binding interactions. These studies have been performed by using Autodock 4.2 version software. Thus, the synthesized phenazinamine derivatives can be used as a lead for further preparing promising future anticancer drug candidates.

Biography

Gajanan M Sonwane has registered for his PhD from Dr. Babasaheb Marathwada University, India. He has completed his Master's degree and training in Drug Design from VLIFE Sciences, India. He has published more than 3 papers in reputed journals and attended many national and international conferences and presented posters.

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