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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 efficient group based quantitative structure-activity relationships (G-QSAR) for exploring the relationship between the structures of a new promising family of 2-Phenazinamine derivatives and their anticancer activities. We have residential evocative model, in order to aid in further optimization and expansion of newer anticancer agents containing 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 separation of some compounds as fraction of external test set. Synthesis of 5 novel derivatives and 2-phenazinamine derivative by using GQSAR and screening of *in vitro* anticancer activity on K562 cell line was done in Tata Memorial Cancer Research Center Mumbai, India, with improved anticancer activity. Phenazinamine and the analogues have showed better binding interactions with Oxidoreductase (PDB: 1YYD.) The binding energies of the protein-ligand interactions also confirmed that the ligands can fit into the active pockets of receptor tightly. Docking was performed in Autodock 4.2 version software.

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