Application of computer aided drug design strategies for optimization of anticancer activity of phenazinamine derivatives

Gajanan Sonwane and **Mayura Kale**
Government College of Pharmacy, India

We have efficient group based quantitative structure–activity relationships (G-QSAR). Exploring the relationship between the structures of a new promising family of 2- phenazinamine derivatives and their anticancer activities. We have residential evocative model, 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 by separation some compounds as fraction of external test set. Synthesis of 5 novel derivatives 2- phenazinamine derivative by using result of GQSAR and screening of *in vitro* anticancer activity on K562 cell line was done in Tata Memorial Cancer Research Center Mumbai, India, showing improve anticancer 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 are fit into the active pockets of receptor tightly. Docking perform in Autodock 4.2 version software.

e: sonwane.gajanan@rediffmail.com