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Pharmacophore modeling and 3d-qsar studies of acridones as chemosensitizing agents in cancer

V.V.S. Rajendra Prasad
Vishnu Institute of Pharmaceutical Education and Research, India

In the present study we have identified an efficient pharmacophore from a set of 38 acridones which reverts HL-60/DX cell line. Identified pharmacophoric features such as one hydrogen bond acceptor, one hydrophobic region, a positive ion group and three aromatic rings i.e, AHPRRR. Ligand based 3D-QSAR was performed by employing partial least square regression analysis which gave a regression coefficient R2 of 0.98 and Q2 of 0.86, and Pearson-R of 0.95. Another pharmacophore model of same compounds with same set of pharmacophoric features with different 3D spatial arrangement showed that 0.95 (R2), 0.87 (Q2) and 0.94 (Pearson-R). Molecular docking study was performed for fluoro acridones against calmodulin dependent cAMP phosphodiesterase (PDE1c) in order to identify the possible protein ligand interactions and results thus obtained were compared with in-vitro data, good correlations were found between in-silico and in-vitro results.

Biography

Dr. V.V.S. Rajendra Prasad has completed his Ph.D in the year 2009 from Rajiv Gandhi University of Health Sciences. He has published more than 15 papers in reputed journals.

drvvsrp@sips.ac.in