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Development of in-silico QSAR models of 1,2,4 oxadiazole derivatives as potential apoptosis inducer and anticancer agents

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The quest for the novel structural scaffolds to treat cancer is always at the heart of pharmaceutical industry. Novel caspase-3 activator 1,2,4-oxadiazole derivatives have for a long time enthused the curiosity of research workers. In order to explore the potential caspapse-3-activators class of compounds for anti-cancer activity, we have carried out computational studies on cell-lines DLD1 and T47. The studies involved 2D, 3D and group QSAR analysis which have been carried out to establish the relationship between physicochemical descriptors and the biological activity. In addition, group QSAR also helped to investigate structure activity relationships based on molecular fragments of set of molecules. The regression analysis was done by partial least square analysis (PLS) and kNN (k-nearest neighbor) method. The descriptors which were found to influence the activity involve T_C_C_5, T_S_Cl_3, T_C_S_3 and Sdss count on cell line DLD1 and descriptors such as T_N_N_6, T_N_Cl_4, T_C_S_3 and T_N_Br_7 influenced the activity on cell line T47. The studies were further extended to the pharmacophore analysis which involves the identification of the basic pharmacophore and the key features essential for the activity. Based on the survival scores, the best four featured pharmacophore hypothesis AAHR.9 was generated by PLS method which showed that the presence of two acceptor group, one hydrophobic group and one aromatic ring is essential for anticancer activity. The information provided by the present studies may be used to design novel potential compounds against cancer.

Biography

Sushil K Kashaw has completed his PhD in 2009 from Dr. Harisingh Gour University, (A Central University; 'A' Grade by UGC-NAAC), India. Currently, he has joined the Department of Pharmaceutical Sciences, Wayne State University, Detroit under the mentorship of Dr. Arun K Iyer as Post-doctoral Fellow under the visitor exchange program. To his credit, he has completed three research projects and two research projects are ongoing which are sponsored by State and Indian Government. Currently, he is guiding four PhD scholars and 34 MPharm students. He has published 58 research papers in the journals of great repute along with one book entitled "*Text book of organic name reactions*".

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