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A comparative 2D QSAR analysis of levetiracetam & its analogs: The inhibitor of glioblastoma, by different statistical techniques: MLR, PLS, SVM, ANN

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Levetiracetam is a class of antiepileptic drugs (AEDs) that inhibits glioblastoma by modulating O(6)-methylguanine-DNA methyltransferase (MGMT) resulting tumour cell resistance to alkylating agents. Levetiracetam (LEV) is the most potent MGMT inhibitor among other available AEDs with diversed MGMT regulatory actions. To know the main factors that are responsible for the activity A QSAR study was performed with 64 analogs of levetiracetam. For the study 3 classes of descriptors were calculated i.e., chemical feature distance matrix (CFDM), 2D constitutional & 2D geometrical descriptors using Molegro Data Modeller V2.5.0 tool. For the study Andrews coefficient was considered as the dependent variable. Then multiple regression analysis was performed by minitab 16 tool. From this calculation R-square value 0.93 was obtained for CFDM descriptors, which is higher than other two types (2D constitutional & 2D geometrical descriptors). To check the efficiency of the predicted values the results were further verified by PLS (partial least square), SVM (support vector machines) and ANN (artificial neural networks) based calculation. The obtained remained consistent with ANN statistics and shown R-sq value 0.93 for CFDM descriptor which also satisfied the above result with higher score. From this result it is suggested that CFDM descriptors modulates strong activity than 2D constitutional & geometrical descriptor in case of levetiracetam.

Biography

Rajesh Kumar Guru completed his M.Tech in Biotechnology from M.I.T.S. Rayagada, Odisha, India in the year 2012-13. From 2010-2012 he worked at MITS Innovation and research center in bioinformatics research group under the guidance of Raghunath Satpathy. The research group was involved in computational biology research, particularly in molecular dynamics & simulation using HPC, drug designing, biological database development and maintaince.

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