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Qsar Studies of Certain Novel Heterocycles Derived From bis-1, 2, 4 Triazoles as Anti-Tumor Agents

Authors : Madhusudan Purohit, Stephen Philip, Bharathkumar Inturi

Abstract : In this paper we report the quantitative structure activity relationship of novel bis-triazole derivatives for predicting the activity profile. The full model encompassed a dataset of 46 Bis- triazoles. Tripos Sybyl X 2.0 program was used to conduct CoMSIA QSAR modeling. The Partial Least-Squares (PLS) analysis method was used to conduct statistical analysis and to derive a QSAR model based on the field values of CoMSIA descriptor. The compounds were divided into test and training set. The compounds were evaluated by various CoMSIA parameters to predict the best QSAR model. An optimum numbers of components were first determined separately by cross-validation regression for CoMSIA model, which were then applied in the final analysis. A series of parameters were used for the study and the best fit model was obtained using donor, partition coefficient and steric parameters. The CoMSIA models demonstrated good statistical results with regression coefficient (r2) and the cross-validated coefficient (q2) of 0.575 and 0.830 respectively. The standard error for the predicted model was 0.16322. In the CoMSIA model, the steric descriptors make a marginally larger contribution than the electrostatic descriptors. The finding that the steric descriptor is the largest contributor for the CoMSIA QSAR models is consistent with the observation that more than half of the binding site area is occupied by steric regions.

Keywords : 3D QSAR, CoMSIA, triazoles, novel heterocycles
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