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QSAR Studies on Aminopyrazoles for the Prediction of Inhibition of CDK2/Cyclin A as Antitumor Agents

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***SUMMARY*. Cylin dependent kinases (CDKs) have emerged as novel mechanistic target due to their direct involvement in underlying genetic changes during the cancerous state. In order to identify the essential physiochemical parameters for CDK2 inhibitory activity in some 3-aminopyrazole derivatives, Quantitative Structure-Activity Relationship (QSAR) studies have been carried out on a series of total 35 compounds (taking 24 and 11 molecules in trainings set and test set respectively) using the multiple linear regression MLR) method. Among the generated models, the best QSAR model with good correlation coefficient (r^2 = 0.643) along high statistical significance (> 99.9 %) well explained variance in activity for both training and test set molecules (Pred. r^2 = 0.632). The two dimensional QSAR studies revealed that the activity is positively controlled by the indicator parameter (I), electronic parameter (field effect, F) and hydrophobic fragmentation constant (Fr) of substituents. Apart from that one of the interesting finding is that this model well discriminates between the Molar refractivity (MR) and hydrophobic fragmentation constant (Fr) in prediction of inhibitory activities based on the regression coefficient and associated error. Further the calculation of important descriptors like log P, hydrogen bond donor and acceptors etc. indicates the potential of these molecules in clinical trial as an anticancer drug.**

KEY WORDS: Cyclin dependent kinases, QSAR, Hansch Analysis, 3-aminopyrazole derivatives, Lipinski's rule.

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