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Atom Based QSAR Approach for the Design of Novel Purine Analogues for the Inhibition of Serine Threonine Kinases: an Approach Towards Design of Novel Antiproliferative Agents

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***SUMMARY*. A robust and reliable 3D QSAR model which is pharmacophore based has been developed in the present study, based on reported sequence of purine analogues for the inhibition of serine threonine class of cancer drug target. The present model showed statistical significance with regression coefficient value of $r^2 = 0.98$ and cross validation coefficient values of $q^2 = 0.7725$. The model was validated by allocating the compounds under two sets, namely, test and training set. The latter was made use to build model of QSAR whereas, the test was to endorse the QSAR model that was developed. Also the model showed a huge F value 654.7 and Pearson coefficient value of 0.8812, suggesting the accuracy of the model. The developed model could be utilized to develop selective inhibitors which are also novel, for serine threonine class of cancer drug targets.**

RESUMEN. En el presente estudio se ha desarrollado un modelo QSAR 3D robusto y confiable basado en farmacóforos, en base a la secuencia informada de análogos de purinas para la inhibición de la clase de serina y treonina del objetivo del fármaco contra el cáncer. El presente modelo mostró significación estadística con un valor del coeficiente de regresión de $r^2 = 0.98$ y valores del coeficiente de validación cruzada de $q^2 = 0,7725$. El modelo se validó asignando los compuestos en dos conjuntos, a saber, conjunto de prueba y entrenamiento. Este último se usó para construir el modelo de QSAR, mientras que la prueba fue para respaldar el modelo QSAR que se desarrolló. Además, el modelo mostró un gran valor de F 654.7 y un coeficiente de Pearson de 0.8812, lo que sugiere la precisión del modelo, el que podría ser utilizado para desarrollar inhibidores selectivos que también son novedosos, para la clase de medicamentos serina treonina contra el cáncer.

KEY WORDS: CDK, pharmacophore, QSAR, serine.

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