



Pharmacophore and Atom Based 3D QSAR Approach for the Development Of Novel Kinase Specific Antitumour Agents

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SUMMARY. The present study envisages a fast and reliable 3D QSAR approach utilising pharmacophore mapping for the identification of specific inhibitors for the CDK2 inhibitors belonging to the kinase class. The model generated resulted in a statistically significant 3D QSAR equation with regression coefficient value of ($r^2 = 0.8131$) and cross validation coefficient value of ($q^2 = 0.8991$). The generated QSAR equation was validated by leave one out method. The present model could be used in the design of novel and specific inhibitors of CDK2.

RESUMEN. El presente estudio prevé un enfoque de QSAR 3D rápido y confiable que utiliza el mapeo de farmacóforos para la identificación de inhibidores específicos para los inhibidores de CDK2 que pertenecen a la clase de quinasas. El modelo generado dio como resultado una ecuación QSAR 3D estadísticamente significativa con el valor del coeficiente de regresión de ($r^2 = 0,8131$) y el valor del coeficiente de validación cruzada de ($q^2 = 0,8991$). La ecuación QSAR generada fue validada por el método de dejar salir uno. El presente modelo podría usarse en el diseño de inhibidores novedosos y específicos de CDK2.

KEY WORDS: flavones, pharmacophore, QSAR, tankyrase.

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