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

Richard LOBO [1] & Aravinda PAI [2] *

[1] *Department of Pharmacognosy, Manipal College of Pharmaceutical Sciences (MCOPS), Manipal Academy of Higher Education, Manipal (576104), Karnataka, India.*

[2] *Department of Pharmaceutical Chemistry, Manipal College of Pharmaceutical Sciences (MCOPS), Manipal Academy of Higher Education, Manipal (576104), Karnataka, India.*

***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.

* Author to whom correspondence should be addressed. *E-mail:* pai.aravind@gmail.com

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