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Molecular Modeling Studies of Trisubstituted Thiazoles as Cdc7 Kinase Inhibitors through 3D π - π Stacking, QSAR and Molecular Docking Simulation

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Abstract

The cell division cycle 7 (Cdc7) is a serine/threonine protein kinase which plays an essential role in replication and initiation of DNA synthesis. Overexpression of the Cdc7 in various tumor growths and in cell proliferation makes it a novel target for cancer therapy. In the present study, we have performed 3D quantitative structure/activity relationship (3D-QSAR) studies on a series of trisubstituted thiazole derivatives targeting Cdc7 kinase. Reasonable CoMFA ($q^2 = 0.838$, $\text{NOCA } r^2 = 0.984$) and CoMSIA ($q^2 = 0.875$, $\text{NOCA } r^2 = 0.979$) models were developed. All the developed models were validated using an external validation test set, leave-five-out, bootstrapping, progressive samplings, and rm^2 metrics. Both the models exhibited acceptable values on all validation techniques and hence were considered to be robust and predictive. Molecular docking study revealed the crucial interaction of the most active compound (compound **49**) with the conserved active site residues. Our results are in line with the previous studies. Contour map analysis revealed the important insights that would help in increasing the potency of the compounds. From these results, we could suggest that bulky positive substitutions are favored in the R^2 position of the phenyl ring. Hydrogen bond acceptor groups in the R^1 position could increase the activity. Hydrogen bond donor groups are favored near the amino group of R^3 position. Long substitution in the R^3 position will reduce the activity and must be avoided. Our results could be used to design more potent trisubstituted thiazole derivative of Cdc7 kinase inhibitors in future.

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- Pavithra K. Balasubramanian, Anand Balupuri, Hee-Young Kang and Seung Joo Cho, Receptor-guided 3D-QSAR studies, molecular dynamics simulation and free energy calculations of Btk kinase inhibitors, *BMC Systems Biology*, 10.1186/s12918-017-0385-5, **11**, S2, (2017).
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```