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QSAR Analysis and Pharmacophore Mapping of Catecholic Flavonoids for Telomerase Inhibitory Activity

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***SUMMARY*. A quantitative structure-activity relationship (QSAR) analysis has been performed with the objective of understanding the interaction between nineteen catecholic flavonoids and the active site of telomerase. The lack of thorough structural information on this enzyme renders the present QSAR analysis a valuable tool in the current anti-cancer drug discovery research. A good correlation (r = 0.831) was found between telomerase inhibitory activity and a 2-dimensional descriptor namely topological polar surface area (TPSA). The positive coefficient of TPSA in our linear regression equation indicates the importance of molecular interactions among the polar functions like O and N centered fragments of catecholic flavanoids with active site of telomerase enzyme. We extended our QSAR analysis to a pharmacophore mapping study to explore possible bioactive conformations. A 3D-QSAR pharmacophore, which consists of four hydrogen-bond acceptors, one hydrogen-bond donor, and one aromatic ring, were generated using the PHASE program. This 3D-QSAR model might be useful for the design and optimization of new telomerase inhibitors.**

KEY WORDS: Catecholic flavonoids, Pharmacophore, QSAR, Telomerase, TPSA.

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