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Three dimensional QSAR analysis of Quinazolinone derivatives as EGFR Inhibitors

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Abstract : In the present investigation, a 3D QSAR studies had been employed for a series of quinazolinone derivatives which were acts as an EGFR inhibitors. CoMFA and CoMSIA, PLS fit methods were extensively used to predict the steric and electrostatic molecular field interactions for the better activity. The CoMFA and CoMSIA studies were achieved using a training set of 14 compounds. The 3D QSAR models of title compounds demonstrated that steric and hydrophobic interactions are dominant however, that substitution patterns are an important factor in determining activity. The actual assessed 3D-QSAR model has demonstrated a very good result, having r^2 value regarding 0.983 and also cross-validated coefficient q^2 value as 0.873. Molecular docking studies were useful in distinguishing a bioactive conformer and in addition a conceivable binding energies. The evaluation of CoMFA and CoMSIA contour maps furnished insight into the viable amendment of the molecules for higher activity.

Keywords: Protein tyrosine kinase (EGFR), 3D-QSAR, CoMFA, CoMSIA, 4-benzothiazole amino quinazoline dasatinib derivatives.

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