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QSAR STUDIES INVOLVING 2D, 3D QSAR AND PHARMACOPHORE MAPPING STUDIES ON ARYLSULFONYL IMIDAZOLIDINONE DERIVATIVES AS ANTICANCER AGENTS

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QSAR analysis including 2D QSAR, 3D QSAR and pharmacophore mapping studies have been performed on a series of arylsulfonylimidazolidinone derivatives to explore the physicochemical properties and basic pharmacophore responsible for anti-cancer activity. The 2D-QSAR studies were carried out using the partial least squares (PLS) method coupled with stepwise variable selection, with r^2 = 0.7106 and q^2 = 0.5176; the 3D-QSAR studies were performed using stepwise variable selection k-nearest-neighbor molecular field analysis (kNNMF) approach; with cross-validated correlation coefficient (q^2) of 0.5909. Pharmacophore mapping resulted in highly predictive pharmacophore based 3D-QSAR model with five point hypotheses (AADHR.18) with two acceptor atom, one donor group, one hydrophobic group and one aromatic ring as pharmacophore features. This is denoted as A2A3D5R10H7. Research indicated that alignment-independent descriptors, steric field and electrostatic field descriptors were significantly correlating with anticancer activity of arylsulfonylimidazolidinone derivatives.

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