Proceedings
International Journal of Nanomaterials, Nanotechnology and Nanomedicine

Special Issue: NCNN-2014
(National Conference on Nanoscience and Nanotechnology - 2014)

QSAR and Pharmacophore Studies on Thiazolidinone Derivatives as Potential Epidermal Growth Factor Receptor Inhibitors

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The epidermal growth factor receptor (EGFR) inhibitory activity of some thiazolidinone analogues was subjected to 2D and 3D quantitative structure activity relationship analysis and pharmacophore studies using Molecular Design Suite (VLife MDS) software and web server Pharmagist respectively. 2D QSAR analysis was performed using partial least squares regression (PLSR) while 3D QSAR models were generated using k-nearest neighbour (kNN) methodology. The variable selection method applied for both strategies was stepwise forward backward. The QSAR models generated by both the methods were subjected to internal and external validation. The best 2D QSAR model had r^2, q^2 and pred_r^2 values of 0.8758, 0.8002 and 0.9141 respectively. This model indicates that the descriptors T_N_O_4 and RadiusOfGyration contribute (positively) 43% and 34.11% respectively and descriptor T_T_C_4 contributes (inversely) 22.46% to the biological activity. The best 3D QSAR model exhibited q^2 and pred_r^2 values of 0.8032 and 0.7843 respectively. In this 3D QSAR model, the steric field points S_374 and S_209 with their negative values indicate the need of less bulky group in these positions. The identified pharmacophoric features are aromatic, hydrogen bond donors (2) and hydrogen bond acceptor (3). The present work may be of help in providing guidance for further lead optimization and designing of potent anticancer agents.

Citation: *Ghode P, Tripathi R, Jain SK (2015) QSAR and Pharmacophore Studies on Thiazolidinone Derivatives as Potential Epidermal Growth Factor Receptor Inhibitors. Int J Nanomater Nanotechnol Nanomed S: 160.*