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QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP (QSAR) ANALYSIS ON IMIDAZO [2,1-*b*] [1,3,4] THIADIAZOLE DERIVATIVES AS MURINE LEUKEMIA CELL (L1210) INHIBITORS : A FREE-WILSON APPROACH

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In search of newer and potent anticancer agents, a series of imidazothiadiazole derivatives was subjected to quantitative structure activity relationship using Free Wilson approach. Multiple linear regression (MLR) analysis was performed to derive QSAR models for better activity. The most significant model exhibited correlation co-efficient (r), cross validated correlation coefficient (q^2) and predictive correlation co-efficient (r^2 pred) 0.835, 0.523 and 0.598 respectively. The generated QSAR models indicate that substituents like coumarin-3-yl at R_2 position and CHO group at R_1 position of imidazothiadiazole have a positive coefficient value suggesting that their presence has an important role for murine leukemia cell (L1210) inhibitory activity whereas 4-$NO_2C_6H_4$ group at R_2 position has a negative coefficient value indicating that its absence may be favourable for the biological activity.