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Conventional-QSAR analysis on 1-H,indole,2,3-dione derivatives as selective carboxylesterase inhibitor

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A quantitative structure activity relationship study was performed on a series of 1-H Indole2-3, dione derivatives possessing selective carboxylesterases inhibitory activity for establishing quantitative relationship between biological activity and their physicochemical / structural properties. The statistical regression expressions were obtained using partial least squares regression (PLSR) analysis. Two statistical significant models were generated ($r^2=0.9450$, $r^2=0.8755$) indicating that biological activity is influenced by the descriptors, T_N_Cl_6, T_2_Cl_6, T_2_Cl_6, T_2_O_7, SdssCE-index, slogp etc.

Key words: 2D-QSAR, Selective carboxylesterases inhibitors, 1-H,indole,2-3 dione derivative.

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