

Prediction of Anticancer Potential of Curcumin Nanoparticles by Means of Quasi-Qsar Analysis Using Monte Carlo Method

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Abstract : The experimental data for anticancer potential of curcumin nanoparticles was calculated by means of eclectic data. The optimal descriptors were examined using Monte Carlo method based CORAL SEA software. The statistical quality of the model is following: $n = 14$, $R^2 = 0.6809$, $Q^2 = 0.5943$, $s = 0.175$, $MAE = 0.114$, $F = 26$ (sub-training set), $n = 5$, $R^2 = 0.9529$, $Q^2 = 0.7982$, $s = 0.086$, $MAE = 0.068$, $F = 61$, $Av Rm^2 = 0.7601$, $\Delta R^2m = 0.0840$, $k = 0.9856$ and $kk = 1.0146$ (test set) and $n = 5$, $R^2 = 0.6075$ (validation set). This data can be used to build predictive QSAR models for anticancer activity.

Keywords : anticancer potential, curcumin, model, nanoparticles, optimal descriptors, QSAR

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