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Quantitative Structure-Activity Relationship Study of Some Quinoline Derivatives as Antimalarial Agents

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Abstract : A series of quinoline derivatives with antimalarial activity were subjected to two-dimensional quantitative structure-activity relationship (2D-QSAR) studies. Three models were implemented using multiple regression linear MLR, a regression partial least squares (PLS), nonlinear regression (MNLR), to see which descriptors are closely related to the activity biologic. We relied on a principal component analysis (PCA). Based on our results, a comparison of the quality of, MLR, PLS, and MNLR models shows that the MNLR (R = 0.914 and R^2 = 0.835, RCV= 0.853) models have substantially better predictive capability because the MNLR approach gives better results than MLR (R = 0.835 and R^2 = 0,752, RCV=0.601)), PLS (R = 0.742 and R^2 = 0.552, RCV=0.550) The model of MNLR gave statistically significant results and showed good stability to data variation in leave-one-out cross-validation. The obtained results suggested that our proposed model MNLR may be useful to predict the biological activity of derivatives of quinoline.

Keywords : antimalarial, quinoline, QSAR, PCA, MLR ,MNLR, MLR
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