

A Pharmacovigilance Study on Linear and Non – Linear Quantitative Structure (Chromatographic) Retention Relationships (QSRR) Models for the Prediction of Retention Time of Anti – Cancer Nano Drugs under Synchrotron Radiations

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Editorial

Linear and non-linear Quantitative Structure (Chromatographic) Retention Relationships (QSRR) models for the prediction of retention time of anti-cancer Nano drugs under synchrotron radiations (Figures 1 and 2) were developed based on a diverse dataset with anti-cancer Nano drugs using Multiple Linear Regression (MLR) analysis and feed-forward Artificial Neural Networks (ANN) model [1–21]. Then, the suitable set of the molecular descriptors was calculated and the important descriptors were selected using stepwise regression method and synchrotron radiations. Stepwise Multiple Linear Regression (MLR) analysis and non-linear Artificial Neural Network (ANN) model were performed to build the models. The statistical and computational parameters by multiple linear model indicated satisfactory stability and predictive ability, while the predictive ability of Artificial Neural Networks (ANN) model is somewhat superior. Comparison the results of these two methods reveals that those obtained by the Artificial Neural Networks (ANN) model are much better under synchrotron radiations.

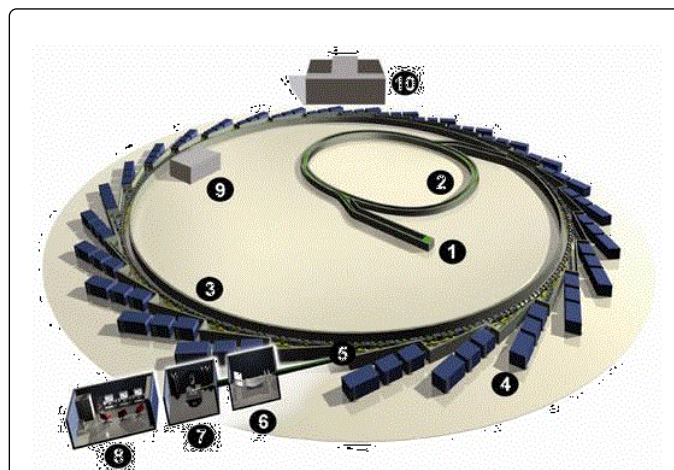


Figure 2: Schematic of non-linear Quantitative Structure (Chromatographic) Retention Relationships (QSRR) models for the prediction of retention time of anti-cancer Nano drugs under synchrotron radiations [1–21].

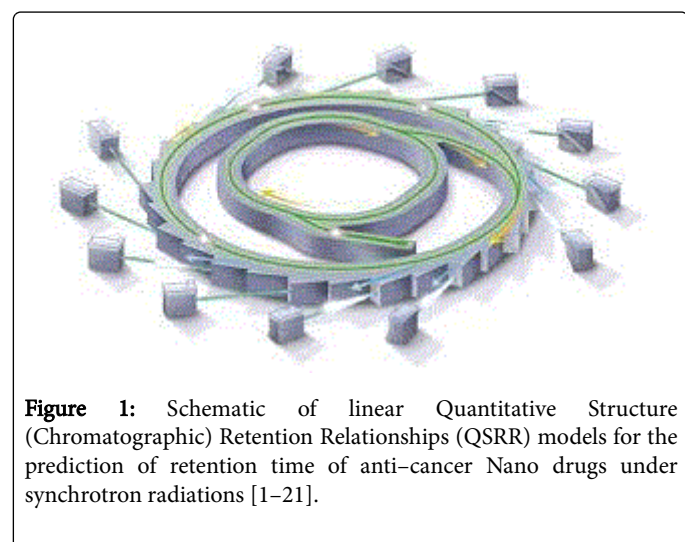


Figure 1: Schematic of linear Quantitative Structure (Chromatographic) Retention Relationships (QSRR) models for the prediction of retention time of anti-cancer Nano drugs under synchrotron radiations [1–21].

In this editorial, descriptors that appeared in the selected Multiple Linear Regression (MLR) analysis were used as inputs for the generated Artificial Neural Networks (ANN) model under synchrotron radiations. The stepwise Multiple Linear Regression (MLR) analysis led to the derivation of one model, with three variables and acceptable and reasonable statistical and computational parameters. Then, descriptors that appeared in the selected Multiple Linear Regression (MLR) analysis were used as inputs for the generated Artificial Neural Networks (ANN) model under synchrotron radiations. Artificial Neural Networks (ANN) model resulted in the generation of one model with acceptable and reasonable statistical and computational parameters for the training set and prediction set. After the comparison of the stepwise Multiple Linear Regression (MLR) analysis and Artificial Neural Networks (ANN) model under synchrotron radiations, it could be observed that the Artificial Neural Networks (ANN) model was superior to the Multiple Linear Regression (MLR) analysis under synchrotron radiations.

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