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Quantitative Structure–Activity Relationship (QSAR) Approximation for Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) Nanoparticles as Anti-Cancer Drugs for the Catalytic Formation of Proviral DNA from Viral RNA Using Multiple Linear and Non-Linear Correlation Approach

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Editorial

Human cancer cells are one of the main medical, clinical, biochemical, pharmaceutical, physiochemical, photodynamical and social issues in our era. Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) nanoparticles are potent inhibitor of cancer Reverse Transcriptase (RT) which is necessary for the catalytic formation of proviral DNA from viral RNA [1-29,57, 58]. In the current editorial, the three-dimensional (3D) autocorrelation pool was used for encoding structural information of Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) nanoparticles analogous and development of linear and non-linear models for prognostication of anti-cancer properties of these nanoparticles [27-60].

Quantitative structure-activity relationship (QSAR) models study has been applied in a series of Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) nanoparticles analogous acting as non-nucleoside reverse transcriptase (NNRT) and non-nucleoside reverse transcriptase inhibitors (NNRTIs). The molecular information has been encoded in three-dimensional (3D) autocorrelation descriptors, obtained from different weighting designs. Analysis of the linear and non-linear quantitative structure-activity relationship (QSAR) models revealed a correlation coefficient and root mean square error of 0.974 and 0.637, respectively. The predictive ability of the model indicates that this model can be used for virtual library screening of databases for novel potent anti-cancer drugs.

Three spatial autocorrelation vectors were employed for modelling the inhibitory activities: Broto-Moreau's autocorrelation coefficients (ATS), Moran's indices (MATS) and Geary's coefficients (GATS). Autocorrelation vectors were calculated at spatial lags ranging from 1 up to 10. The biochemical, medical, clinical, pharmaceutical, photodynamical and physiochemical properties considered in the twenty different weighting plans.

A data set containing 200 Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) nanoparticles analogous were used in this editorial. The biological evaluation of these nanoparticles was made by scanning electron microscope (SEM), x-ray diffraction (XRD), attenuated total reflectance fourier transform infrared spectroscopy (ATR-FTIR), transmission electron microscope (TEM), differential thermal analysis-thermal gravim analysis (DTA-TGA), energy-dispersive x-ray spectroscopy (EDX), mass spectroscopy (MS), UV-Vis spectroscopy, FT-Raman spectroscopy, ^{1}HNMR spectroscopy, ^{13}CNMR spectroscopy and ^{31}PNMR spectroscopy, positive logarithm of molar concentration of a drug required to achieve 75% protection of cancer cells against the cytopathic effect of cancer. ESI MS, PM5 and DFT studies were used to optimize the three-dimensional (3D) geometry of the molecules.

Using the stepwise multiple regression method, the models were developed for 200 Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) nanoparticles analogous. The correlations performed for the whole set provided the optimal equations for different numbers of descriptions in the range of 1 to 10. The robustness of the model and their prediction ability for the anti-cancer activity, were evaluated by leave-one-out cross-validation (LOO-CV) and external validation (EV) procedures. In order to identify novel potent nanoparticles, the developed model considered as good tools for a virtual library screening when the descriptor values, calculated for the molecules belonging to virtual libraries. Virtual screening identified some attractive nanoparticles that have high-quality activities and these deserve further study.

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In the present editorial, a quantitative structure-activity relationship (QSAR) approximation using multiple linear and non-linear correlation approach was developed to predict reverse transcriptase inhibition (RTI) of Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh2O3) nanoparticles analogues acting as non-nucleoside reverse transcriptase inhibitors (NNRTIs). The employment of three–dimensional (3D) autocorrelation descriptors is extremely useful in modelling the biological activities. We expect this model to be useful in conjunction with computational and experimental methods for filtering likely Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh_2O_3) nanoparticles analogous from chemical and physical libraries and virtual chemical databases for identify new potential and selective nanoparticles.

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