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Linear and Non–Linear Quantitative Structure–Anti–Cancer–Activity Relationship (QSACAR) Study of Hydrous Ruthenium (IV) Oxide (RuO_2) Nanoparticles as Non–Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) and Anti–Cancer Nano Drugs

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Editorial

A Quantitative Structure–Anti–Cancer–Activity Relationship (QSACAR) study has been applied in a series of hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles as Non–Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) and also anti–cancer Nano drugs. The molecular simulation and modeling has been investigated in three dimensions (3D) autocorrelation descriptors, obtained from different weighting schemes. Analysis of the linear and non–linear Quantitative Structure–Anti–Cancer–Activity Relationship (QSACAR) simulations and models revealed a correlation coefficient and root mean square errors. The predictive ability of the simulations and models indicates that these simulations and models can be used for virtual library screening of databases for novel potent anti–cancer Nano drugs such as hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles. It should be noted that hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles as novel potent anti–cancer Nano drugs were characterized by ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR–FTIR), FT–Raman, HR Mass and UV–Vis spectroscopies and also by Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Differential Thermal Analysis–Thermal Gravim Analysis (DTA–TGA), Energy–Dispersive X–Ray Spectroscopy (EDX) and X–Ray Diffraction (XRD) analysis and crystallography. *Ab initio* and Density Functional Theory (DFT) calculations have been carried out for the hydrous Ruthenium (IV) Oxide (RuO_2) anti–cancer Nano drugs by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6–31G*, 6–31+G*, 6–31G(3df, 3pd), 6–311G, 6–311G* and 6–311+G* basis sets of the Gaussian 09.

On the other hand, human immunodeficiency is the primary cause of cancer which is one of the main medical, medicinal, clinical, biological, physiological, pharmaceutical, biochemical and social problems in our epoch. Hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles as novel potent anti–cancer Nano drugs are potent inhibitors of cancer Reverse Transcriptase (RT) which is necessary for the catalytic formation of proviral DNA from viral RNA and vice versa [1-33]. Moreover, in the present editorial, the three dimensions (3D) autocorrelation pool was used for investigation of structural simulation and modeling of hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles as novel potent anti–cancer Nano drugs development of linear and non–linear simulations and models for prediction of anti–cancer activities of these anti–cancer Nano drugs.

In addition, it can be concluded that in order to identify novel potent anti–cancer Nano drugs, the developed simulations and models considered as reasonable and acceptable tools for a vital library screening when the descriptor values computed for the molecules belonging to virtual libraries. Virtual screening identified some attractive anti–cancer Nano drugs such as hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles that have high–quality activities and these deserve further and future studies. Furthermore, in the present editorial, a quantitative structure–property–anti–cancer–activity relationship approximation using a multiple linear and non–linear correlation approach was developed to predict Reverse Transcriptase Inhibition (RTI) of hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles as Non–Nucleoside Reverse Transcriptase Inhibitors (NNRTIs). The employment of three dimensions (3D) autocorrelation descriptors is extremely useful in simulation and modeling the medical, medicinal, clinical, biological, physiological, pharmaceutical and biochemical activities. We expect these simulations and models to be useful in conjunction with experimental, computational and theoretical methods and techniques for filtering likely hydrous Ruthenium (IV) Oxide (RuO_2) nanoparticles from chemical libraries and virtual chemical databases for identify new potential and selective anti– cancer Nano drugs.

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