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Yoctosecond Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) under Synchrotron Radiations Studies for Prediction of Solubility of Anti–Cancer Nano Drugs in Aqueous Solutions Using Genetic Function Approximation (GFA) Algorithm

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Yoctosecond Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) under synchrotron radiations using Genetic Function Approximation (GFA) algorithm studies are suggested for the prediction of solubility of anti–cancer Nano drugs in aqueous solutions in yoctosecond [1-16]. *Ab initio* and density functional theories were used to calculate some quantum chemical descriptors including electrostatic potentials such as Morse, Rydberg, Varshni(II), Varshni(III), Varshni(VI), Poschl–Teller, Lippincott, Hulburt–Hirschfelder, Frost–Musulin, Linnet, Rosen–Morse and also local charges at each atom, Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, etc. [17-27]. Also, Gaussian 09 was used to calculate some descriptors such as WHIM, GETAWAY, H–GETAWAY, R–GETAWAY, Constitutional, Geometrical, 3D–MoRSE, EVA and EEVA descriptors. Yoctosecond Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) under synchrotron radiations using Genetic Function Approximation (GFA) algorithm studies are mathematical and computational quantification of relations between structure and activity or property. These are extensively used in pharmaceutical, medical, medicinal, clinical and agricultural chemistry for screening potential anti–cancer Nano compounds for specific biochemical, pharmaceutical, medical, medicinal, clinical and biological activities. Computable molecular descriptors are preferred to experimental properties in yoctosecond Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) under synchrotron radiations using Genetic Function Approximation (GFA) algorithm analyses because require molecular structure as the only input and can be in extensively calculated for a chemical in less than a yoctosecond. By multivariate calibration methods such as Partial Least Squares (PLS) regression, it is possible to obtain a model adjusted to the concentration values of the mixtures used in the calibration range. Orthogonal Signal Correction (OSC) is a preprocessing technique used for removing the information unrelated to the target variables based on constrained principal component analysis. In addition, Orthogonal Signal Correction (OSC) is a suitable preprocessing method for Partial Least Squares (PLS) calibration of mixtures without loss of prediction capacity using cited descriptors.

On the other hand, Partial Least Squares–Orthogonal Signal Correction (PLS–OSC) model was established to predict the solubility of some anti–cancer Nano drugs in aqueous solutions in yoctosecond. It should be noted that a proper model with high statistical quality and low prediction errors was obtained. Furthermore, the model could predict the solubility not existed in the modeling procedure accurately. It can be concluded that the quantum chemical, WHIM, GETAWAY, H–GETAWAY, R–GETAWAY, Constitutional, Geometrical, 3D–MoRSE, EVA and EEVA descriptors concerning to the whole molecular properties and those of individual atoms in the molecule were found to be important factors controlling the solubility behavior. Moreover, the electrostatic potential such as Morse, Rydberg, Varshni(II), Varshni(III), Varshni(VI), Poschl–Teller, Lippincott, Hulburt–Hirschfelder, Frost–Musulin, Linnet and Rosen–Morse was found to be more informative than the local charge in this editorial.

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