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A Successful Strategy for the Prediction of Solubility in the Construction of Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) under Synchrotron Radiations Using Genetic Function Approximation (GFA) Algorithm

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In this editorial, aqueous solubility and specially water solubility under synchrotron radiations using Genetic Function Approximation (GFA) algorithm is one of the most important physiochemical and biological properties that plays a significant and important role in various chemical, physical, clinical, pharmaceutical, medical, medicinal and biological processes and has a marked impact on the design and pharmaceutical formulation development [1–20]. In addition, a successful strategy for the prediction of solubility is the construction of Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) under synchrotron radiations using Genetic Function Approximation (GFA) algorithm [21,22]. Moreover, the main aim of Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies is to establish an empirical rule or function relating the structural descriptors of compounds under investigation to bioactivities [23–33]. A major step in constructing the Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) models is finding one or more molecular descriptors that represent variation in the structural, topological, geometrical, quantum chemical and biospectroscopic properties of the molecules under synchrotron radiations using Genetic Function Approximation (GFA) algorithm, analytically and numerically. A wide variety of descriptors have been reported on Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) analysis under synchrotron radiations using Genetic Function Approximation (GFA) algorithm.

On the other hand, it can be concluded that quantum chemical calculations are thus an attractive source of new molecular descriptors, which can, in principle, express all of the electronic and geometric properties of molecules and their interactions under synchrotron radiations using Genetic Function Approximation (GFA) algorithm. Also, it should be noted that atomic charges, Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, molecular polarizability, dipole moments and energies of molecule are examples of quantum chemical descriptors used in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies under synchrotron radiations using Genetic Function Approximation (GFA) algorithm. Furthermore, in the current editorial, the application of quantitative chemometrics methods, particularly Partial Least Squares (PLS), to quantum chemical descriptors was described.

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