

# Quantum Chemical Descriptors in Computational Medicinal Chemistry for Chemoinformatics

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During the practice of chemoinformatics, it has been realized that molecular diversity is essential feature to characterize the reactivity of the molecules. In addition, it is of utmost importance to enrich potential libraries with those molecules which could be converted to suitable drug candidates or omitted as toxins. In addition, a paradigm shift in structure activity relationship has resulted in the integration of various descriptors and quantum chemical descriptors based drug development activities into early stages of lead discovery. In particular, various descriptors are being developed and used to help identify and screen out compounds that are unlikely to become drugs/toxins. This presentation highlights development of recent DFT based chemical reactivity descriptors and the applications of these descriptors approaches towards the prediction of chemical reactivity nature, in particular, the prediction of toxicity, biological activities and other chemical informatic properties in a more general sense as well as reactive site and group identification and recent developments towards recognition of potentially toxic molecules. Bridging experimental knowledge with effective computational information, management and prediction of various aspects of molecular reactivities thus facilitates the rapid and cost-effective process and helps focus attention on interesting molecules. The success of DFT based global and local quantum chemical descriptors in predicting the chemical reactivity and selectivity profiles of several systems selected by our group are highlighted here. The simple calculation procedure and the usefulness of all DFT descriptors in the QSAR and QSPR parlance have also been probed in detail. In this study, the applications of global and local descriptors in the development of QSAR and QSPR have been presented for prediction of physical properties of series of alkanes, biological activity of testosterone and estrogen derivatives and toxicity of polychlorinated biphenyls/ polychlorinated dibenzofurans. It is seen that the global descriptors such as electrophilicity and ionization potential are capable of predicting the biological activity of the selected molecules and local descriptors such as philicity and group philicity in the light of philicity are capable of identifying the activity of a particular site in the molecule which contribute to the toxicity of the molecule.