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Polarizability: A Promising Descriptor to Study Chemical-Biological Interactions

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Abstract

Recently, we have defined atomic polarizability, a Conceptual Density Functional Theory (CDFT)-based reactivity descriptor, through an empirical method. Though the method is empirical, it is competent enough to meet the criteria of periodic descriptors and exhibit relativistic effect. Since the atomic data are very accurate, we have applied them to determine molecular polarizability. Molecular polarizability is an electronic parameter and has an impact on chemical–biological interactions. Thus, it plays a pivotal role in explaining such interactions through Structure Activity Relationships (SAR). In the present work, we have explored the application of polarizability in the real field through investigation of chemical–biological interactions in terms of molecular polarizability. A Quantitative Structure–Activity Relationship (QSAR) model is constructed to account for electronic effects owing to polarizability in ligand–substrate interactions. The study involves the prediction of various biological activities in terms of minimum block concentration, relative biological response, inhibitory growth concentration or binding affinity. Superior results are presented for the predicted and observed activities which support the accuracy of the proposed polarizability-QSAR model. Further, the results are considered from a biological viewpoint in order to understand the mechanism of interactions. The study is performed to explore the efficacy of the computational model based on newly proposed polarizability and not to establish the finest QSAR. For future studies, it is suggested that the descriptor polarizability should be contrasted with the use of other drug-like descriptors.

Keywords:

Polarizability, Conceptual density functional theory (CDFT), Chemical reactivity descriptor, Quantitative, structure–activity relationship (QSAR), Chemical–biological interactions, Depolarization

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