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QSAR with ETA indices: Insecticidal activity of plant derived compounds against zika virus vector *Aedes aegypti*

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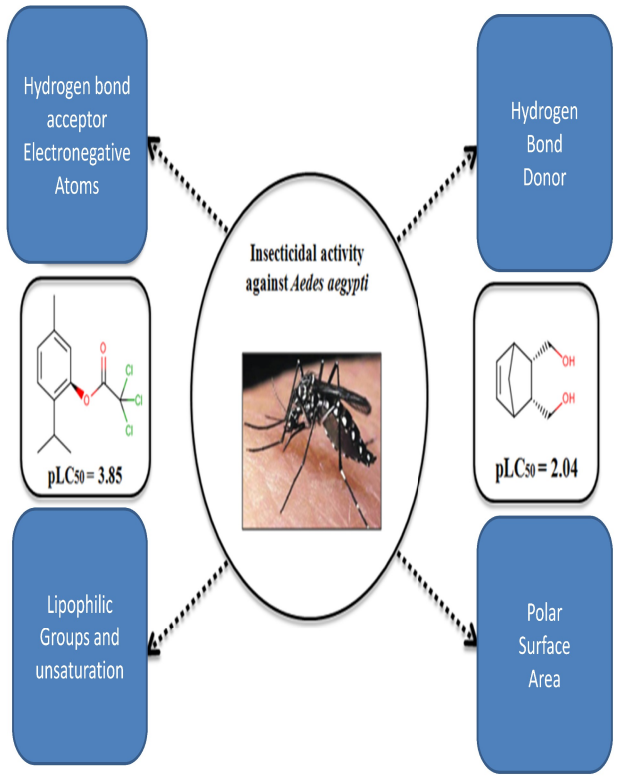
Graphical Abstract



Abstract

Dengue, zika and chikungunya have severe public health concerns in several countries. Human modification of the natural environment continues to create habitats in which mosquitoes, vectors of a wide variety of human and animal pathogens, thrive which can bring about enormous negative impact on public health if not controlled properly. Quantitative Structure–Activity Relationship (QSAR) modeling was applied in this work with the aim to explore features contributing to promising larvicidal and insecticidal property against the vector *Aedes aegypti* (Diptera:Culicidae). A dataset of 62 plant derived compounds obtained from the previous literatures was used in this present study where Genetic Algorithm (GA) was used for model development employing Double Cross Validation (DCV) tool. Simple topological descriptors like Extended Topochemical Atom (ETA) indices developed by the present authors' group were used for model development. A number of models were generated by the GA method and the descriptors obtained were pooled for Best Subset Selection method (BSS). Further, the best model obtained from BSS was used for Partial Least Square (PLS) regression to

obtain the final model. The model was validated extensively using different validation metrics to check the robustness and predictivity of the model for regulatory acceptance and enhancing confidence in QSAR predictions. Based on the insights obtained from the PLS model, we can conclude that presence of hydrogen bond acceptor atoms, presence of multiple bonds as well as sufficient lipophilicity and limited polar surface area play crucial roles in regulating the activity of the compounds.

Keywords: QSAR, Zika, Insecticidal activity, Double cross-validation

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