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Multiple Linear Regression to predict larvicidal activity against *Aedes aegypti* mosquito.

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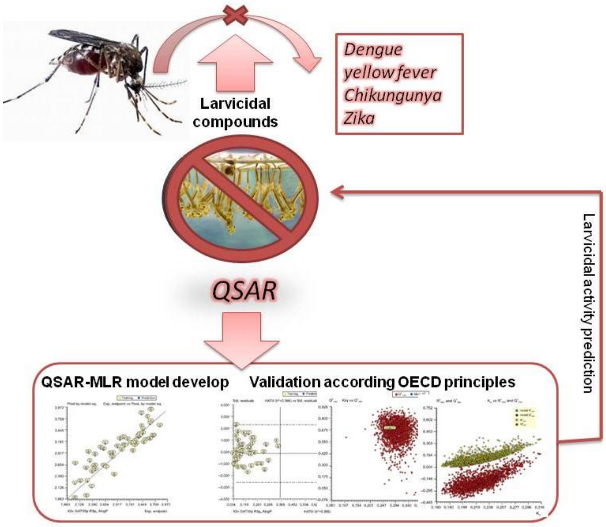
Graphical Abstract



Abstract.
Vector-borne diseases are one of the important health problems in most tropical countries. *Aedes aegypti* is an important vector for transmission of dengue, yellow fever, chikungunya, arthritis, and Zika fever. According to the World Health Organization, it is estimated that *Ae. aegypti* causes 50 million infections and 25,000 deaths per year. The emerging scenario highlights that the eco-friendly and effective control measures for mosquito vectors is of crucial importance. One of the most effective vector control measures has been the use of larvicidal compounds however; this success was short lived due to development of resistance against them in many mosquito strains, ecological imbalance and undesirable effects on non-target organisms. For this reason, the aim of present study was to deduce a mathematical model to predict the larvicidal action of chemical compounds, based on their structure. A series of different compounds with experimental evidence of larvicidal activity were selected to develop a predictive model, using Multiple Linear Regression and a Genetic Algorithm for the selection of variables, implemented in the QSARINS software. The model was assessed and validated using the

	OECDs principles. The best model showed good value for the determination coefficient (R^2=0.752), and others parameters were appropriate for fitting (*s*=0.278 and $RMSE_{tr}$=0.261). The validation results confirmed that the model has good robustness (Q^2_{LOO}=0.682) and stability (R^2–Q^2_{LOO}=0.070) with low correlation between the descriptors (K_{XX}=0.241), an excellent predictive power (R^2_{ext}=0.834) and was product of a non-random correlation (R^2_{Yscr}=0.100). The present model shows better parameters than the models reported earlier in the literature, using the same dataset, indicating that the proposed computational tools are more efficient in identifying novel larvicidal compounds against *Ae. aegypti*.

Full content of this work can be seen in reference 10.

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