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Application of molecular topology to the prediction and optimization of mosquito repellent activity of N-acyl-piperidine derivatives

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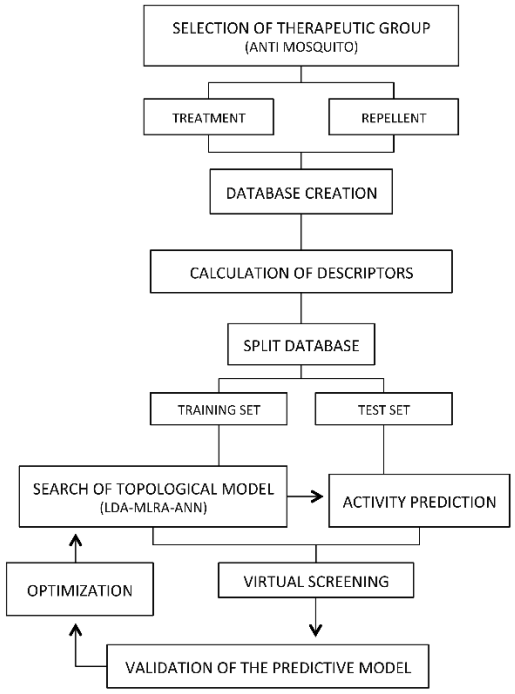
Graphical Abstract



Steps to follow in the search of QSAR prediction models by molecular topology

Abstract.

A topological-mathematical model has been developed based on Multilinear Regression Analysis in order to search new active molecules with mosquito repellent activity. The molecular characterization was performed using topological indexes and a 5-variable model was chosen for prediction of protection times (R^2 = 0.8457 and Q^2 = 0.7486). The model was validated by an internal leave-one-out type cross-validation and a randomization test. The results confirmed the predictive power for the property under study. Finally, after carrying out a virtual screening, new compounds have been proposed with expected higher potency as mosquito repellents.

References

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