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Application of molecular topology to the research of analogues to the E-β-Farnesene for plant louse pest control

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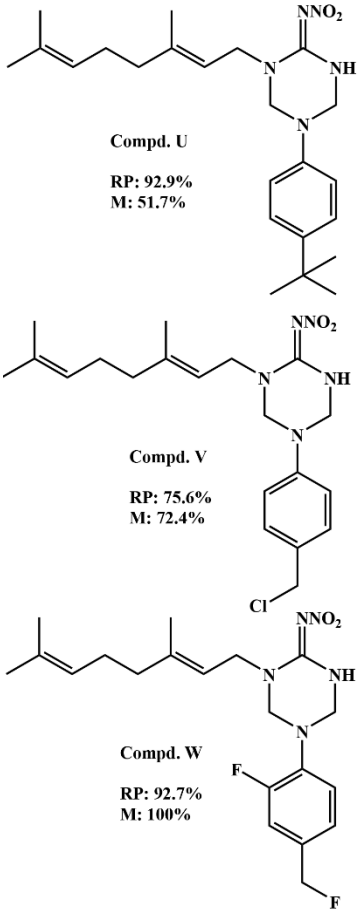
Graphical Abstract



New biocidal and repellent compounds potentially actives against aphids

Abstract.

The control of plant louse pests is very important for agriculture due to the great economic impact of its colonizing action. Currently, more sustainable pesticides with less impact are being sought and, therefore, we have developed here QSAR models based on molceular topology, to predict the activity of E-β-Farnesene (EβF) analogs. By means of multilinear regression analysis we predict both the biocidal (logM) and the repellent (logRP) activities of said EβF analogues. These two values were used as dependent variables and the topological descriptors as independent variables. An equation was obtained with 4 variables and determination coefficients of R^2=0.929, Q^2 = 0.886 respectively, for log RP and R^2 = 0.803, Q^2= 0.670 for logM. The model was validated by an internal validation and a randomness test, which showed satisfactory results. It was found a high predictive capability for the repellent activity and a pretty good but lower predictivity for the biocidal activity. Finally, the selected models were applied to search for new compounds with theoretical biocide and repellent activities.

References

Y. Qin, J. Zhang, D. Song, H. Duan, W. Li, X. Yang, Novel (E)-β-Farnesene Analogues Containing 2-Nitroiminohexahydro-1,3,5-triazine: Synthesis and Biological Activity Evaluation, *Molecules*. 21(7) (2016) 825.

R. García-Domenech, J. Aguilera, A. El Moncef, S. Pocovi and Jorge Gálvez, Application of molecular topology to the prediction of mosquito repellents of a group of terpenoid compounds, *Molecular Diversity* 14(2) (2010) 321-329.

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