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Abstract

A method for the prediction of retention indices of pesticides using the Monte Carlo method and with optimal molecular descriptors based on local graph invariants and the SMILES notation of studied compounds has been presented. Quite satisfactory results were obtained with the proposed method, since a robust model with good statistical quality was developed. The predictive potential of the applied approach was tested and the robustness of the model was proven with different methods. The best calculated QSPR model had following statistical parameters: r^2 = 0.9182 for the training set and r^2 = 0.8939 for the test set. Structural indicators