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Prediction of Gas Chromatographic Retention Indices Based on Monte Carlo Method

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Abstract

A new method for the prediction of retention indices using Monte Carlo method and based on local graph invariants and SMILES notation of studied compounds has been presented. Very satisfactory results were obtained with the proposed method, since 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: $r^2 = 0.8097$ for the training set and $r^2 = 0.9372$ for the test set. Structural indicators defined responsible for the increases and decreases of gas chromatographic retention indices activity have been calculated.

Keywords: QSPR; Molecular graph; SMILES; Monte Carlo; Gas Chromatographic Retention Indices

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