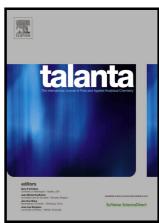
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ACCEPTED MANUSCRIPT

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

1

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