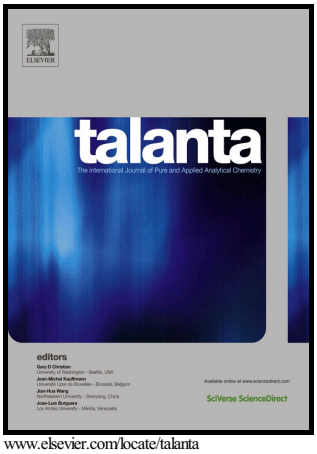

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PII: S0039-9140(17)30310-7
DOI: http://dx.doi.org/10.1016/j.talanta.2017.03.024
Reference: TAL17369

To appear in: *Talanta*

Received date: 13 January 2017
Revised date: 5 March 2017
Accepted date: 8 March 2017

Cite this article as: Aleksandar M. Veselinović, Dragan Velimorović, Biljana Kaličanin, Alla Toropova, Andrey Toropov and Jovana Veselinović, Prediction of Gas Chromatographic Retention Indices Based on Monte Carlo Method *Talanta,* http://dx.doi.org/10.1016/j.talanta.2017.03.024

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