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Artificial Neural Network Regression Modelling of GC/MS Retention of Terpenes Present in Satureja montana Extracts Obtained by Supercritical Carbon Dioxide

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Abstract : Supercritical extracts of highly valuated medicinal plant Satureja montana were prepared by application of supercritical carbon dioxide extraction in the carbon dioxide pressure range from 125 to 350 bar and temperature range from 40 to 60°C. Using GC/MS method of analysis chemical profiles (aromatic constituents) of S. montana extracts were obtained. Self-training artificial neural networks were applied to predict the retention time of the analyzed terpenes in GC/MS system. The best ANN model obtained was multilayer perceptron (MLP 11-11-1). Hidden activation was tanh and output activation was identity with Broyden–Fletcher–Goldfarb–Shanno training algorithm. Correlation measures of the obtained network were the following: R(training) = 0.9975, R(test) = 0.9971 and R(validation) = 0.9999. The comparison of the experimental and predicted retention times of the analyzed compounds showed very high correlation (R = 0.9913) and significant predictive power of the established neural network.

Keywords : ANN regression, GC/MS, Satureja montana, terpenes
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