Application of topological descriptors in quantitative structure–retention index relationship study

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Abstract In this project, quantitative structure-retention relationship (QSRR) studies were used for simultaneous modeling and prediction of retention indices of a group of saturated alcohols on gas chromatography columns of different polarities. The data set included 141 retention index values on six chromatographic columns of SE-30, OV-3, OV-7, OV-11, OV-17 and OV-25. QSRR modeling was performed by the multiple linear regression technique based on the stepwise variable ion method and only by combining the topological descriptors and McReynolds polarity parameter as a measure of polarity of the chromatographic columns. The best generated regression model consisted of four descriptors for which the statistics of R2, standard error, and Fisher-ratio were 0.994, 9.831, and 5468.4, respectively. The variables entered in the model included the atom-type-based topological descriptors of AI (>C

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