A new method of Structure-Activity Relationships methodology has been recently defined. It uses the so called Molecular Descriptors Family, a set of molecular descriptors obtained purely from molecular structure, by using tools of molecular topology and 3D geometry.

The experiments made on three sets of compounds on which retention time was measured in same experimental conditions on every set showed the good ability of the method to predict the retention time.

The method can serve as a tool for unknown samples on which a given compound is suspected to be present. The method can provide the expected retention time, and the confidence band where this compound is expected to be found, if it is present. Note that the method can produce reliable results only when experimental conditions of known compounds determinations are the same with the conditions for unknown compounds, in the same sample.

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References