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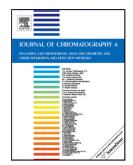
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ACCEPTED MANUSCRIPT

QSPR Analysis for the Retention Index of Fragrance-Like

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distance matrix has a high relevance for this purpose.

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Abstract - A quantitative structure-property relationship (QSPR) was developed for modeling the 18 19 retention index of 1184 flavor and fragrance compounds measured using a Carbowax 20M glass 20 capillary gas chromatography column. The 4885 molecular descriptors were calculated using 21 Dragon software, and then were simultaneously analyzed through multivariable linear regression 22 analysis using the replacement method (RM) variable subset selection technique. We proceeded in 23 three steps, the first one by considering all descriptor blocks, the second one by excluding 24 conformational descriptor blocks, and the last one by analyzing only 3D-descriptor families. The 25 models were validated through an external test set of compounds. Cross-validation methods such as 26 leave-one-out and leave-many-out were applied, together with Y-randomization and applicability 27 domain analysis. The developed model was used for estimate the I of a set of 22 molecules. The 28 results clearly suggest that 3D-descriptors did not offer relevant information for modeling the

retention index, while a topological index such as the Randić-like index from reciprocal squared

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