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QSPR Analysis for the Retention Index of Fragrance-Like Compounds on a Polar Stationary Phase

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Abstract - A quantitative structure-property relationship (QSPR) was developed for modeling the retention index of 1184 flavor and fragrance compounds measured using a Carbowax 20M glass capillary gas chromatography column. The 4885 molecular descriptors were calculated using Dragon software, and then were simultaneously analyzed through multivariable linear regression analysis using the replacement method (RM) variable subset selection technique. We proceeded in three steps, the first one by considering all descriptor blocks, the second one by excluding conformational descriptor blocks, and the last one by analyzing only 3D-descriptor families. The models were validated through an external test set of compounds. Cross-validation methods such as leave-one-out and leave-many-out were applied, together with Y-randomization and applicability domain analysis. The developed model was used for estimate the *I* of a set of 22 molecules. The 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 distance matrix has a high relevance for this purpose.

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