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QSRR Study of Substituted Phenol Compounds: Proposed Models for Inter-Column Comparison

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Abstract

In gas chromatography, the comparison of experimental results obtained from different columns is a complex problem. In this sense, the QSRR methodology could determine, with high quality of description and prediction, the chromatographic retention index, allowing to use this methodology for comparison of data obtained from different column polarities and even obtained from different laboratories. A set of phenolic compounds was studied by several QSRR models; however, the prediction of such models' descriptors is complicated, to understand, thus limiting its application. In the present work, three QSRR models from inter-column combinations are studied by quantum chemical descriptors, such as electronic energy (and its logarithm) and the corrected electronic energy (and its logarithm), zero point energy (ZPE), dipole moment in x-, y-, and z-axes, the total dipole moment, the HOMO and LUMO energies, hardness (η), electronegativity (χ), and electrophilicity (ω). These QSRR models allow the comparison of experimental chromatographic retention index with different column polarities for phenolic compounds.

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