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A DFT-Based QSARs Study of Kovats Retention Indices of Adamantane Derivatives

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Abstract : A quantitative structure–property relationship (QSPR) study was performed to develop models those relate the structures of 65 Kovats retention index (RI) of adamantane derivatives. Molecular descriptors derived solely from 3D structures of the molecular compounds. The usefulness of the quantum chemical descriptors, calculated at the level of the DFT theories using 6-311+G** basis set for QSAR study of adamantane derivatives was examined. The use of descriptors calculated only from molecular structure eliminates the need to experimental determination of properties for use in the correlation and allows for the estimation of RI for molecules not yet synthesized. The prediction results are in good agreement with the experimental value. A multi-parametric equation containing maximum Four descriptors at B3LYP/6-31+G** method with good statistical qualities (R2train=0.913, Ftrain=97.67, R2test=0.770, Ftest=3.21, Q2LOO=0.895, R2adj=0.904, Q2LGO=0.844) was obtained by Multiple Linear Regression using stepwise method.

Keywords : DFT, adamantane, QSAR, Kovat
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