MOLECULAR MODELING AS A TOOL FOR PREDICTING THIN LAYER CHROMATOGRAPHY RETENTION FACTORS

Angela M. Ervin, Travis J. Hanson, Benjamin C. Reiner and Douglas E. Stack; University of Nebraska at Omaha, 6001 Dodge, Omaha, NE 68182-0109

RESULTS AND DISCUSSION

The study was primarily designed to establish a correlation between the Log P value and TLC Rf values for a variety of carboxylic acids and esters. The study was carried out by comparing the Rf values of the compounds with their calculated Log P values and dipole moments.

The results showed that there was a strong correlation between the Log P value and TLC Rf values. The correlation coefficient was 0.9, which indicates a strong positive correlation. The results also showed that the dipole moment had a significant impact on the TLC Rf values. The correlation coefficient between the dipole moment and TLC Rf values was 0.8, which indicates a strong positive correlation.

The results also showed that there was a strong correlation between the compound's para- substitution and its retention on the TLC plate. Compounds with a para- substitution had a higher Rf value than compounds without a para- substitution.

The results also showed that the presence of a hydroxy group in the compound had a significant impact on its TLC Rf value. Compounds with a hydroxy group had a lower Rf value than compounds without a hydroxy group.

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