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Quantitative Structure--Retention Study of Some 2,4-dioksotetrahydro- 1,3--thiazole Derivatives Using the Partial Least Squares Method

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Abstract: Thin-layer chromatography on rice starch support and aqueous ammonia--organic modifier (methanol, dioxane, and acetone) mobile phases was used to study the effect on retention of the chromatographic system and the physicochemical properties of twelve 2,4-dioxotetrahydro-1,3-thiazoles. A multivariate approach to the retention behaviour of the investigated compounds with 3 quite different organic solvents was used to explain the interactions between the 1,3-thiazoles and the mobile phases. Partial least-squares (PLS) regression was used to quantify differences between the observed data and recognize the molecular properties with the greatest effect on retention for each modifier. Good correlation was obtained between experimental and calculated retention data.

Key Words: 2,4-dioksotetrahydro-1,3-thiazoles, Quantitative Structure-Retention Relationships (QSRR), Molecular descriptors, Partial Least Squares Regression (PLS)

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