Abstract

Chromatographic Retention Factor Obtained on Immobilized Keratin Stationary Phase—What Molecular Properties Does It Encode? [†]

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Abstract: Chromatographic retention factors (log k_{KERATIN}) of 33 molecules were obtained on an immobilized keratin stationary phase by Turowski and Kaliszan (J. Pharm. Biomed. Anal. 15, 1997, 1325–1333). Their objective was to develop a novel stationary phase that could be used to investigate the skin permeability coefficient of solutes (log K_p) *in vitro*. However, log k_{KERATIN} is not a sufficiently good predictor of skin permeability coefficient to be used as a sole descriptor in log K_p models. Turowski and Kaliszan reported that this descriptor can be used in combination with the chromatographic retention factor obtained by Immobilized Artificial Membrane Chromatography (log k_{IAM}) and the results of log K_p predictions using multiple linear regression (MLR) models are moderately satisfying. In this study, the values of log k_{KERATIN} obtained by Turowski and Kaliszan were correlated with a set of descriptors calculated using SwissADME software. It was discovered that log k_{KERATIN} encodes primarily lipophilicity, solubility, and molecular size descriptors, which are important factors governing the ability of compounds to cross the skin barrier. On the other hand, log k_{KERATIN} does not correlate with polar surface area (*PSA*) and the molecule's ability to form hydrogen bonds—which are important properties in the context of solutes' skin permeability. It was concluded that log k_{KERATIN} could be used as a descriptor in MLR models of log k_p in combination with other parameters, such as PSA or H-bond descriptors.

Keywords: immobilized keratin stationary phase; HPLC; QSAR models; skin permeability coefficient; calculated descriptors

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