



Abstract

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

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- † Presented at the 8th International Electronic Conference on Medicinal Chemistry, 1–30 November 2022; Available online: https://ecmc2022.sciforum.net/.

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_n 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 $k_{\rm IAM}$) 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 $\log k_{\text{KERATIN}}$ 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 $\log k_{\text{KERATIN}}$ 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

Supplementary Materials: The following are available online at https://www.mdpi.com/article/10 .3390/ECMC2022-13242/s1.

Author Contributions: Conceptualization, A.W.S.; methodology, A.W.S. and E.B.; investigation, A.W.S.; writing—original draft preparation, A.W.S. All authors have read and agreed to the published version of the manuscript.

Funding: This research study was supported by an internal grant of the Medical University of Lodz, no. 503/3-016-03/503-31-001.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data generated in this study can be found in the poster at https://ecmc2022.sciforum.net.

Conflicts of Interest: The authors declare no conflict of interest.



Citation: Sobanska, A.W.; Brzezińska, E. Chromatographic Retention Factor Obtained on Immobilized Keratin Stationary Phase—What Molecular Properties Does It Encode? *Med. Sci. Forum* 2022, 14, 67. https://doi.org/10.3390/FCMC2022-13242

Academic Editor: Alfredo Berzal-Herranz

Published: 1 November 2022

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