

Abstract

Application of topological indices to prediction the lipophilicity parameters of selected antimicrobial and immunosuppressive compounds

Dawid Wardecki ^{1,*}, Małgorzata Dołowy ², Katarzyna Bober-Majnuż ²

¹ Doctoral School of the Medical University of Silesia in Katowice, Faculty of Pharmaceutical Sciences in Sosnowiec, 41-200 Sosnowiec, Poland; d201072@365.sum.edu.pl (D.W.)

² Department of Analytical Chemistry, Faculty of Pharmaceutical Sciences in Sosnowiec, Medical University of Silesia in Katowice, Jagiellońska 4, 41-200 Sosnowiec, Poland; mdolowy@sum.edu.pl (M.D.); bober@sum.edu.pl (K.B.M.)

* Correspondence: d201072@365.sum.edu.pl (D.W.);

Abstract: Current technological advances are resulting in an increased interest in computational methods for predicting the physicochemical properties of biological active compounds, such as lipophilicity, for example. There is a strong need to develop new and accurate *in silico* models that can be based on structural descriptors such as topological indices, which are sets of numerical descriptors that describe the molecule under study. The arrangement of atoms in a molecule is closely related to its topology and geometry, which correlates with the pharmacokinetic properties of the substance, such as ADME/T. In this study, Wiener (W), Randić (${}^0\chi$, ${}^1\chi$, ${}^0\chi^v$, ${}^1\chi^v$), Gutman (M, M^v), Pyka (A, 0B , 1B) and Rouvray-Crafford (R) topological indices were calculated for selected antimicrobial compounds such as delafloxacin, linezolid, sutezolid, ceftazidime and selected immunosuppressive compounds like everolimus and zotarolimus. Linear regression analysis was used to create linear correlations between the calculated topological indices and the values of lipophilicity parameters previously obtained by TLC technique and calculated by computer algorithms. Our work indicates that structural descriptors like topological indices can be a useful tool for predicting selected important ADME/T properties of drugs, such as lipophilicity. The best predictive power ($r>0.9$) indicate the linear models based on the following topological indices: R,W,A. The proposed method is fast, easy to use, and economical because it avoids expensive laboratory experiments to study ADME/T properties by experimental methods.

Keywords: topological indices; ADME/T properties; antimicrobial drugs; immunosuppressive drugs

Citation: Lastname, F.; Lastname, F.; Lastname, F. Title. *Med. Sci. Forum* **2023**, *2*, x.

<https://doi.org/10.3390/xxxxx>

Academic Editor: Firstname Lastname

Published: date

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2023 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

Supplementary Materials:

Author Contributions: Conceptualization, D.W. and M.D.; methodology, D.W.; K.B.-M. and M.D.; software, D.W. and M.D.; investigation, D.W. and M.D.; data analysis, D.W. and M.D.; writing—review and editing, D.W. and M.D.; supervision, D.W. and M.D.; project administration, M.D. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Medical University of Silesia in Katowice, grant number-PCN-1-009/N/2/F

Institutional Review Board Statement: Not applicable.	1
Informed Consent Statement: Not applicable.	2
Data Availability Statement: Not applicable.	3
	4
Conflicts of Interest: The authors declare no conflict of interest.	5
	6