IN SILICO EVALUATION OF PHYSICOCHEMICAL PROPERTIES AND ADME PROFILE OF THE (E)-1-(2-((2-(1-(2-AMINO-4-METHYLTHIAZOL-5-YL) ETHYLIDENE)HYDRAZINYL)METHYL)-4-METHYLTHIAZOL-5-YL)ETHANONE

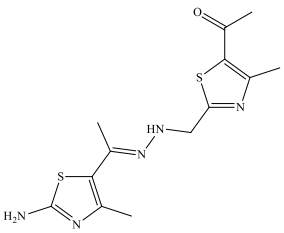
Abdullayeva F. M.[1,2], Safarova A. S.[3], Huseyinov E. Z.[3], Naghiyev F. N.[3]
[1]Azerbaijan State Oil and Industry University, Baku, Azerbaijan
[2]Ministry of Science and Education of the Republic of Azerbaijan, Institute of Petrochemical Processes named after academician Y. G. Mamedaliyev
[3]Baku State University, Baku, Azerbaijan
faxriye85@mail.ru

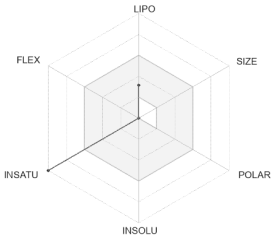
Modern approaches to drug design rely heavily on in silico methods that allow early-stage evaluation of the physicochemical properties and pharmacokinetic parameters of potential bioac-tive compounds. Prediction of absorption, distribution, metabolism, and excretion (ADME) para-meters plays a key role in identifying promising candidates and reducing the risk of failure at later stages of research.

Compounds containing thiazole fragments are widely represented among substances with antimicrobial, antitumor, and anti-inflammatory activities, which underlies their high medical and biological significance. In this context, of interest is (E)-1-(2-((2-(1-(2-amino-4-methylthiazol-5-yl)ethylidene)hydrazinyl)methyl)-4-methylthiazol-5-yl)ethanone – a molecule combining thiazo-le and hydrazone structural elements, potentially capable of effective interaction with biological targets.

The aim of the present work is a comprehensive in silico evaluation of the physicochemical properties and ADME profile of this compound for preliminary determination of its drug potential and the advisability of further pharmacological studies.

The physicochemical and ADME properties of the compound were predicted using the SwissADME web tool. Key descriptors included molecular formula, molecular weight, hydrogen bond donors and acceptors, rotatable bonds, Fraction Csp^3, molar refractivity, and TPSA. Lipophi-licity was evaluated using multiple models to obtain a consensus logP, while water solubi-lity was estimated by ESOL, Ali, and SILICOS-IT methods. Pharmacokinetic parameters such as GI absorption, BBB permeability, P-gp interaction, CYP450 inhibition, and skin permeability were also assessed. Drug-likeness was analyzed according to Lipinski, Ghose, Veber, Egan, and Muegge rules, together with bioavailability score, PAINS/Brenk alerts, lead-likeness, and synthetic accessibility.





The predicted parameters fall within ranges typical for orally active drug candidates. The compound demonstrates balanced lipophilicity, acceptable solubility, favorable gastrointestinal absorption, and a suitable metabolic profile, without critical structural alerts. Overall, the in silico evaluation indicates promising physicochemical and pharmacokinetic characteristics, supporting its potential for further biological investigation and drug development.