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INVESTIGATION OF A DRUGABILITY OF PYRAZOLO[1, 5-A] -1,3,5-TRIAZINE DERIVATIVES BY QUANTUM CHEMICAL PARAMETERS

Nizhenkovska Iryna
MD, Professor,
Head of the department of medicinal chemistry and toxicology
Bogomolets National Medical University

Matskevych Kateryna
Ph.D., Associate Professor
of the department of medicinal chemistry and toxicology
Bogomolets National Medical University

Alonge Halimat Shadiat,
student
Bogomolets National Medical University,

Pyrazolo[1, 5-a] -1,3,5-triazine derivatives are a prospective range of compounds with lots of pharmacological activities. The range consists of 4 compounds with laboratory codes PPT-1, PPT-2, PPT-3, PPT-4 [1]. However, the investigation of their quantum chemical parameters as future medicines was not done.

The Lipinski rule or rule of five is used for defining drugability. It is also known as a Pfizer filter. In the drug discovery, it helps to predict a poor absorption or permeation is more likely when there are more than 5 H-bond donors, 10 H-bond acceptors, the molecular weight is greater than 500, and the calculated Log P (C Log P) is greater than 5 [2].

The results of applying the rule to the investigated compounds are mentioned in Table 1.

Table 1 Correspondense of pyrazolo[1, 5-a] -1,3,5-triazine derivatives to the rule of 5

Parameter	Standard for drug	PPT-1	PPT-2	PPT-3	PPT-4
Molecular mass, g/mol	Less than 500	293.15	311.14	355.22	387.24
High lipophilicity, Log	Less than 5	2.97	3.09	3.47	3.79
Hydrogen bond donors	Less than 5	0	0	0	0
Hydrogen bond accepto	Less than 10	3	4	3	4
Molar refractivity	40-130	75.74	75.70	96.21	101.14

The results from Table 1 demonstrate us that meaning of all 5 key parameters of investigated compounds correspond to Lipinski rule.

Consequently, pyrazolo[1, 5-a] -1,3,5-triazine derivatives are highly probable to have a druglikeness, that is significant for their further preclinical investigation as medicines.

References:

1. Velihina YeS, Pil'o SG, Zyabrev VS, Brovarets VS, et al. Synthesis of 4-Hetaryl-2-(dichloromethyl)pyrazolo[1,5-a][1,3,5] triazines. *Ukranian Chemistry Journal*. 2020. 86(5): 53-62.

2. Electronic source: http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp

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