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INNOVATIVE TRENDS OF SCIENCE AND PRACTICE, TASKS AND WAYS TO SOLVE THEM

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

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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 Correspondence 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 acceptors | 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, Zybrev 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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