Since the corrosion rate depends on the contact area of steel with the corrosion medium, the degree of protection of the inhibitors is the higher, the more dispersion component of the free surface energy. Thus hydrophobization of the surface has a positive effect on the inhibition efficiency, as evidenced by the growth of the dispersion component of SFE.

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COMPUTATIONAL STUDY OF LUPININ AND ITS DERIVATIVES FOR DIHYDROFOLATE REDUCTASE INHIBITION

Pustolaikina I.A.[1],Fazylov S.D.[2], Nurmaganbetov Z.S.[2],
Normatov S.Sh. [1], KimV.V. [1]

[1]Karagandy University named after E.A.Buketov, Karaganda, 100024, Kazakhstan
[2]Institute of Organic Synthesis and Coal Chemistry, Karaganda, 100008, Kazakhstan

The quinolizidine alkaloid lupinine (Figure 1) was chemically modified at theInstitute of Organic Synthesis and Coal Chemistry (Karaganda, Kazakhstan). As a result, more than 25 of lupinine new derivatives were obtained [1-3].Antibacterial properties were established for the synthesized substances by the *in vitro* method. The aim of this study was to evaluate *in silico* the dihydrofolate reductase (Figure 2) inhibitory potential for the 7 most promising lupinine derivatives using the molecular docking method.

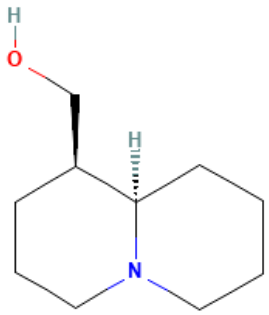


Figure 1 Lupinine structural formula

Figure 2 Ribbon diagram of human dihydrofolate reductase(PDB ID: 4KM2)

Dihydrofolate reductase (DHFR) is one of the key enzymes in the intracellular metabolism of folate, which is necessary to restore dihydrofolic acid to the active form of the vitamin. DHFR is a validated drug target in the treatment of cancer, bacterial infections, and anthrax.

Molecular docking was performed using the Lamarckian genetic algorithm (LGA)with the help ofAutoDock 4.2.6 software [4]. The binding energy of a low molecular weight ligand with a protein was used as an evaluation function, Binding energy includes electrostatic, hydrophobic, and solvation effects, as well as the entropy of the configuration.Semi-flexible docking method was used for calculations when the protein is considered as a solid body, and the ligand rotates and moves in a given cubic area. Produced by *Mycobacterium tuberculosis* dihydrofolate reductase (PDB ID: 4KM2) bacterial enzyme was used as a target for molecular docking

Table 1 presents the results of the computational evaluation of the inhibitory potential of the alkaloid lupinine and its 7 derivatives toowards the dihydrofolate reductase bacterial enzyme.

Table 1 – Inhibition constant and binding energy for the alkaloid lupinine and its derivatives complexes with the dihydrofolate reductase

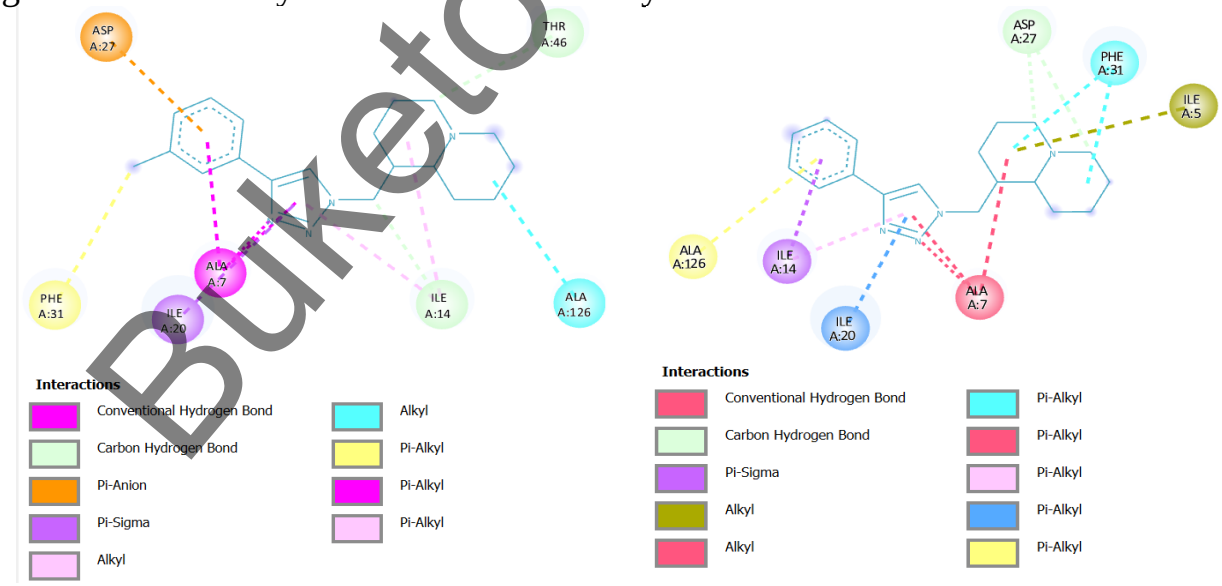
Compound		Inhibition constant Ki (T = 298.15°K)	Binding energy, kcal/mol
Abbreviation	IUPAC name		
Lup	((1R,9aR)-octahydro-1H-quinolizin-1-yl)methanol (Lupinine)	80.32 μM	-5.59
Lup-14	Octahydro-2H-quinolizin-1-yl)methylmethanesulfonate	6.71 μM	-7.06
Lup-15	(1S,9aR)-1-(azidomethyl)octahydro-2H-quinolizine	6.38 μM	-7.09
Lup-16	(1S,9aR)-1-((4-(4-methoxyphenyl)-	1.45 μM	-7.97

	1H-1,2,3-triazol-1-yl)methyl)octahydro-1H-quinolizine		
Lup-17	(1S,9aR)-1-((4-(m-tolyl)-1H-1,2,3-triazol-1-yl)methyl)octahydro-1H-quinolizine	1.15 μM	**-8.10**
Lup-18	(1S,9aR)-1-((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)octahydro-1H-quinolizine	250.73 nM	**-9.01**
Lup-22	(1-(((1S,9aR)-octahydro-1H-quinolizin-1-yl)methyl)-1H-1,2,3-triazol-4-yl)methanol	5.23 μM	-7.20
Lup-23	2-(1-(((1S,9aR)-octahydro-1H-quinolizin-1-yl)methyl)-1H-1,2,3-triazol-4-yl)propan-2-ol	547.81 nM	**-8.54**

In this case, if the value of the binding energy is negative and less than -5 kcal/mol, then this indicates the effective interaction of the studied ligand with the target protein. At the same time, a more stable ligand-protein complex corresponds to the smallest value of the inhibition constant.

As can be seen from the Table 1, compounds Lup-17, Lup-18 and Lup-23 (binding energy -8.10, -9.01, -8.54, respectively) demonstrated the most effective binding with the dihydrofolate reductase.In addition, compounds Lup-17 and Lup-18 have also been *in vitro* demonstrated the highestantimicrobial activity against *Staphylococcus aureus* bacteria.

It was interesting to evaluate the contribution of various types of interactions to the formation of complexes between the studied compounds and the dihydrofolate reductase enzyme.Figure 2 shows the active interactions of the Lup-17 and Lup-18 ligands with the dihydrofolate reductase enzyme.



a) Lup-17; b) Lup-18;

Figure 2 Active interactions of top compounds with the dihydrofolate reductase

The largest contribution of conventional hydrogen bonds, as well as carbon-hydrogen and π-alkyl bonding, was shown by analyzing the interactions of the studied compounds with the binding site of the dihydrofolate reductase enzyme.

Overall, Lup-17 and Lup-18 ligands were selected as the most promising dihydrofolate reductase inhibitors by molecular docking.These compounds can be recommended for further study of their pharmacological potential and toxicity.

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СОРБЦИОННОЕ РАЗДЕЛЕНИЕ ВОЛЬФРАМА И МОЛИБДЕНА

Рашит Д.Р., Исмаилова А.Г.
Казахский Национальный Университет имени аль-Фараби
Rashit.dilyara@gmail.com

Молибден и вольфрам используются как легирующая добавка в жаропрочных сплавах, контактный элемент в высокоточных приборах, чувствительный элемент в датчиках. Наноразмерные частицы оксида молибдена пользуются большим спросом в медицине: как носитель лекарственных средств, в составе препаратов при дефиците сульфат-оксидазы, он также является составной частью антибактериальных покрытий, обладающих высокой активностью. Покрытия, полученные из оксида молибдена (VI), необходимы для изготовления фильтров, в качестве газовых датчиков двойного оксида азота, для создания электрохромных и фотохрамных