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BOOK OF ABSTRACTS

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POLYPHARMACOLOGICAL DRUG-LIKE MOLECULES FROM THE 2,5-DIMETHYL-4-OXO-3,4-DIHYDROTHIENO[2,3-d]PYRIMIDINE-6-CARBOXAMIDE SERIES

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A considerable number of biologically active molecules are capable of binding to several targets in the body. Therefore, there is a question modern drug discovery is about modifications of privileged scaffolds, which are characterized by a wide spectrum of pharmacological activity.

Thieno[2,3-d]pyrimidine heterocyclic system, which is a fragment of the molecules of a large number of antimicrobial agents, with the potential to interact with bacterial TrmD, is among those scaffolds. On the other hand, this heterocyclic system is close in structure to purine and may be attractive from the point of view of interaction with adenosine receptors. In order to broaden the range of potential biologically active compounds, we conducted the synthesis of 2,5-dimethyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-6-carboxamides. The key stage was the preparation of ethyl 2,5-dimethyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-6-carboxylate within the one-reactor procedure using 1,1-dimethoxy-N,N-dimethylmethanamine with futher cyclization of the resulting amidine with ammonium acetate. Subsequently, the corresponding amides were synthesized from the acid obtained on the basis of hydrolysis of the ester.

The best parameters of antimicrobial activity were found for unsubstituted benzylamide. At the same time, the slightly less active at *in vitro* screening 4-methylbenzylamide showed better placement parameters in the active site of TrmD isolated from *Pseudomonas aeruginosa*. It is interesting that this particular amide also turned out to be the best ligand for the A_{2A} adenosine receptor active site in comparison to Istradefylline as a reference ligand.

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