

IN SILICO SEARCH FOR BIOLOGICALLY ACTIVE SUBSTANCES AMONG ASYMMETRIC THIOUREA DERIVATIVES CONTAINING N-METHYLPYPERAZINE FRAGMENT

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Introduction. The biological activity spectrum is an intrinsic property of a compound that is representative of different pharmacological effects, physiological and biochemical mechanisms of action and specific toxicity. The activity is largely dependent on the structural nature of a compound. Biologically active substances have therapeutic and supplementary actions, the latter manifesting as side effects. PASS web tool has the ability to predict 3678 pharmacological effects; mechanisms and special toxicities of the molecule. The web tool can freely display the predicted activity of a molecule at various threshold levels. The PASS training set which has been compiled from various sources including publications, patents, chemical databases, and “gray” literatures consists of over 26000 biological compounds and includes drugs, lead compounds, drug-candidates, and toxic substances. GUSAR web tool has the ability to predict of LD₅₀ values for rats with four types of administration (oral, intravenous, intraperitoneal, subcutaneous, inhalation). The training sets were created on the basis of data from SYMYX MDL Toxicity Database. They include the information about ~10000 chemical structures with data on acute rat’s toxicity represented on the LD₅₀ values (log₁₀ (mmol/kg)).

These pre-experimental studies *in silico* successfully used at various stages of the search and optimization of the structures of biologically active compounds.

Aim. Purpose of the present work is *in silico* studies of biological activity, adverse effects and acute toxicity of nine asymmetric thiourea derivatives containing N-methylpiperazine fragment.

Materials and methods. The *in silico* studies of biological activity, adverse effects using PASS-online programme and *in silico* studies of acute rat toxicity using GUSAR-online programme were carried out.

Results and discussion. According to the results of PASS-online prognosis, test compounds probably have antimycobacterial, antituberculosic and antiviral activity, have such adverse effects as twitching and inflammation. Results of GUSAR-prognosis demonstrated that the compounds probably belong to low-toxic substances.

Conclusions. So, three tested asymmetric thiourea derivatives have minimum adverse effects and can be recommended for synthesis and pharmacological screening for antimycobacterial activity.

SYNTHESIS OF DRUGS BASED ON COORDINATING COMPOUNDS OF Zn (II) WITH GLUTARIC ACID AND VITAMIN B₅

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Introduction. Microelements and pharmacologically active substances of organic nature play an extremely important role in the life of the human body. This is due to the fact that trace