ALGORITHM FOR SEARCH NEW BIOLOGICALLY ACTIVE COMPOUNDS AMONG N-CONTAINING HETEROCYCLES

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N-heterocycles are frequently found in natural products and pharmaceuticals and they have been recognized as privileged structural components for investigation in various scientific disciplines. These N-heterocycles are arguably among the most significant targets for drug discovery as more than half of the small-molecule drugs are N-heterocyclic compounds. In addition, the development of efficient methods and strategies for the construction of N-heterocycles is an important research topic in organic chemistry, as evident by the many classical and named reactions.

Among N-containing heterocycles – derivatives of thiazole and piperazine – was found new compounds that exhibit diverse pharmacological activities (antioxidant, antimicrobial, anti-inflammatory, neuroleptic, antidepressant, antitumor etc.). These heterocycles is also a part of a number of therapeutic agents. For example, the piperazine fragment is present in the structure of anthelmintic drugs (ditrazin quotes), antibiotics (cefaperazone), fluoroquinolones (pefloxacin), and anti-tuberculosis medicine (rifampicin). The thiazole fragment is present in the structure of beta-lactam antibiotics (ampicillin sodium, ceftriaxone), sulfonamides (phthalazol, sulfathiazole), antiviral medicines (nitazoxanide) etc.

Today an important problem is the search for new antimicrobial drugs. The introduction of antibiotics into clinical practice represented one of the most important interventions for the control of infectious diseases. Antibiotics have saved millions of lives and have also brought a revolution in medicine. However, an increasing threat has deteriorated the effectiveness of these drugs, that of bacterial resistance to antibiotics. Antibiotic resistance is rising to dangerously high levels in all parts of the world. New resistance mechanisms are emerging and spreading globally, threatening our ability to treat common infectious diseases. A growing list of infections – such as pneumonia, tuberculosis, blood poisoning, gonorrhoea, foodborne diseases – are becoming harder, and sometimes impossible, to treat as antibiotics become less effective.

For the purposeful synthesis of drugs with desired antimicrobial properties, it is important to establish the relationship between the structure of chemicals and their activity. When planning pharmacological studies, it is always necessary to take into account that this procedure is quite expensive, therefore it is very difficult to test a large number of compounds simultaneously and check acute toxicity under these conditions. One of the ways to solve this problem is the use of computer programs that make it possible to predict activity and toxicity. A computer prediction can serve as the initial stage in the selection of the most promising substances. Currently, many mathematical models have been developed that describe the relationship between the structure of organic compounds and pharmacological activity and toxicity.

Thus, an important step before the synthesis and pharmacological screening is the computer screening of the virtual library of the selected series of compounds.