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The relevance of the software development for anticonvulsant potential study of herbs and herbal remedies

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Implementation of the modern technologies from related fields of science and the use of computer modeling in new remedies development is a promising direction for drug design in future. The analysis of the obtained results of pharmacological and phytochemical study has shown, that the existing computer modeling methods are not objective in the case of herbal substances research due to they rely on individual compounds activity and don't consider their synergism.

Recently, the search strategy concerning determination of pharmacological activity of substances predominantly consists in the fact that three-dimensional structures of the molecule of the ligands and the target receptor are known. Thus, the structure of ligand-receptor complex with the evaluation of conformations and mutual affinity, or complementarity of the known structures with the given active center, is reproduced and evaluated [1]. It should be mentioned, that nowadays there are extensive databases of the known compounds.

The aim of our work was to systematize results of our research in area of the study of anticonvulsant potential of certain herbs and then to use them for software development devoted to the search for promising herbal substances, which provide anticonvulsant effect.

Materials and methods. The algorithm and the general sequence of actions for the software development were determined. The software was developed using Windows platform. During the process of the software development, the modularity principle was used, which allows applying the same algorithm for different types of pharmacological activity of compounds.

As a result of the study, the project of the software was developed. The given software tool correlates the data about the content of different groups of biologically active compounds and calculates the anticonvulsant potential of herbal sample.

Conclusions. Development of the software that takes into account the features of pharmacological activity of herbs is rather promising for the scientific studies.

References:

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