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Murad Mousa

STUDY IN SILICO: CARDIAC GLYCOSIDES AS WOUND HEALING ACTIVITY AGENTS

Scientific supervisor: Ph.D in chem., assoc. prof. Todar T. Lakhvich
Department of Bioorganic Chemistry
Belarusian State Medical University, Minsk

Relevance. Diseases associated with impaired tissue integrity (wounds, ulcers of various etiologies and localization, etc.) are one of the main causes of temporary disability. In many cases they complicate and slow down the rehabilitation process, and in some cases can lead to death of patients. Traditional treatment for these pathologies has a number of limitations and is not always effective. The search for new medications from the new classes of compounds in many cases costs a lot and requires additional investments. An alternative is Rational Drug Design technology, which includes *in silico* research. Based on the mechanism of cardiac glycoside action, we proposed the study of glycosides as a potential wound healing activity.

Purpose of the research: rational drug design of the new class of wound-healing agents based on cardiac glycoside structure.

Methods and procedures. Structures have been designed with the aid of ChemOffice chemical programs. Protein receptor proteins were selected from the Protein Data Bank 3D Protein and Nucleic Acid Data Bank. *In silico* study was performed using the Dockingserver resourse using the semi-empirical PM6 quantum chemistry calculation method, MMFF94 geometric optimization method, and Gasteiger charge calculation method at pH 7.0.

Results and discussion. The effect of cardiac convallotoxin glycoside on the proton pump has been studied previously. We hypothesized that these glycosides may affect tissue regeneration. From the Protein Data Bank (PDB) 3-D structure database of protein and nucleic acid structures, we selected a receptor substrate for analysis of its interaction *in silico* with digitoxygenin and its derivatives. To study the SAR (Structure activity relationship) we variated structures focusing on changes of the functional groups, the number and types of the cycle fusion, and the relative configuration of all chiral centers. It was shown the strong relationship between the structure and biological activity of cardiac glycoside.

Results. *In silico* study shows that digitoxygenin actively binds to the proposed substrate. The design of new digitoxygenin based derivatives potentially gives rise to a new class of wound-healing and anti-ulcer drugs.

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