Abstract

Synthesis, spectroscopic analysis and *in silico* biological studies of new steroid conjugates containing triazole systems

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The doctoral thesis focuses on the design, synthesis, isolation, purification, spectroscopic characterisation and prediction of biological activity of new steroid bioconjugates. The developed compounds constitute a combination of fragments of bile acids and pyrimidine bases using 1,2,3-triazole rings obtained by a „click" reaction in the context of searching for new compounds with pharmacological potential. The dissertation includes both a literature review and original experimental and theoretical studies.

The literature section discusses the importance of steroid bioconjugates in pharmacological therapies, such as squalamine and its derivatives. Special attention was paid to the use of „click" chemistry in the modification of bile acids and sterols. This approach allows the creation of stable and bioactive supramolecular structures. The contemporary achievements in steroid-triazole conjugates as enzyme inhibitors and potential anti-infective drugs were meticulously analysed.

In the research part, three groups of new compounds were developed: (1) bile acid and sterol conjugates with 1,2,3-triazole rings exhibit predicted antifungal and antibacterial activity; (2) quasi-podands with triazole systems structurally resemble supramolecular systems susceptible to forming host-guest complexes, which opens up opportunities in nanotechnology and drug delivery systems, especially in treating hypercholesterolemia; (3) steroid-pyrimidine hybrids (with uracil and 2-thiouracil) are characterized by the ability to interact with lipid metabolism enzymes and potential use in anticancer, antimicrobial and dermatological therapies.

The results of spectroscopy analyses (^{1}H and ^{13}C NMR, FT-IR), spectrometry analyses (ESI-MS, EI-MS) and theoretical calculations (PM5, GIAO) confirmed the correctness of the molecular structures and chemical stability. *In silico* studies using PASS and molecular docking methods have shown their broad spectrum of potential biological activity, including anticancer, antimicrobial, cytoprotective and anti-inflammatory effects.

The work contributes to the development of bioorganic chemistry, offering new perspectives in designing therapeutic compounds with multidirectional biological activity.