# Abstract

The theoretical part of the dissertation proves that among the vast number of chemical compounds, those based on the s-triazine (1,3,5-triazine) structure play an important role. In organic chemistry, the heterocyclic s-triazine ring, which is usually the core of the molecule, has found extensive use in crosslinking polymeric materials and combining the properties of various substituents. The spectrum of biological properties of s-triazine derivatives is broad and includes anti-microbial, anti-cancer, or anti-neurodegenerative activities, among others. Accepted and marketed drugs include Altretamine, Decitabine or Almitrine. However, there are many more s-triazine derivatives in the basic research phase, as well as clinical trials with promising results. Multi-target compounds are being sought as more effective therapeutic formulations. The s-triazine molecule, because of its ability to substitute three substituents, offers many opportunities to obtain compounds with hybrid properties.

In the experimental part, screening studies based on the synthesized group of eight s-triazine derivatives containing dipeptide, 2-ethylpiperazine and methoxyl group as substituents are presented. The developed compounds were obtained in high yields, and their structures were analysed by 1H and 13C NMR and MS methods. The compounds were subjected to biological tests in three fields: on bacteria and fungi, on cancer cells and on proteins involved in neurodegeneration.

An in vitro study was conducted on pathogenic bacteria (*E. coli, S. Aureus, B. subtilis and M. luteus*), yeasts (*C. albicans*) and filamentous fungi (*A. fumigatus, A. flavus, F. solani, P. citrinum*) by microdilution in broth and compared with antibacterial (Streptomycin) and antifungal (Ketoconazole and Nystatin) antibiotics. Several s-triazine analogues have minimal inhibitory concentrations lower than the standard used. To investigate the molecular targets of the most active compounds, a bacterial gyrase inhibition assay was performed. To gain a better insight into the interactions of the most active DNA gyrase inhibitors, a molecular docking study was performed with the two gyrases *E. coli* and *S. aureus*. Which confirmed the inhibitory potential of all selected compounds against *S. aureus* gyrase. On the other hand, with regard to *E. coli* gyrase, the most active were s-triazine derivatives with the Trp(Boc)AlaOMe and Asp(OtBu)AlaOMe groups.

The evaluation of the tumor capacity was performed on two cell lines MCF-7 and MDA-MB-231. Cells were derivatized at various concentrations (1, 5, 10, 50 and 100 µM) and this was related to the reference compound - Chlormabucil. The number of healthy, apoptotic and necrotic cells was observed. Based on these data, the IC50 was determined. All tested compounds showed antiproliferative activity against both lines of tumor cells. The derivative containing the Lys(Boc)AlaOMe dipeptide was shown to perform particularly well against MCF-7. The derivative with the Asp(OtBu)AlaOMe group showed a lower value than Chlorambucil relative to the MDA-MB-231 line.

The group of s-triazine derivatives was also tested for the ability to inhibit the enzymes AChE and BACE1. The study of the inhibitory potential against AChE was carried out using the Ellman colorimetric method, the BACE1 study was carried out using FRET. All derivatives showed an inhibitory effect. The derivative with the Lys(Boc)AlaOMe group showed the greatest inhibitory capacity.

The performed and presented studies confirm that s-triazine derivatives have great potential in the field of synthesis and biological research as new potential multifunctional.