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DNA/BSA binding study of *N*-benzylthiabendazole and its mononuclear silver(I) complex

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INTRODUCTION & AIM

The antimicrobial properties of silver(I) ions have been recognized since ancient times. In recent decades, silver(I) complexes have been extensively studied for their antimicrobial activity. The ligand plays a crucial role not only in stabilizing the complex but also in modulating its physicochemical properties, such as solubility, lipophilicity, and the ability to release silver(I) ions under biological conditions. In addition to their broad spectrum of applications, silver(I) complexes are noted for their low toxicity to human cells and the remarkably low tendency of microorganisms to develop resistance. These characteristics make silver(I) complexes promising candidates for the development of novel antimicrobial agents, particularly in the fight against bacterial resistance to clinically used antibiotics. The possible mechanism of the antimicrobial activity of silver(I) complexes can be attributed to their interactions with biological molecules, including DNA and proteins [1]. Thiabendazole is a benzimidazole derivative widely used as a pesticide, known for its potent antifungal and anthelmintic activities [2]. Due to its favorable pharmacological profile, thiabendazole has attracted attention as a structural scaffold for the development of metal complexes with potential biological activity. In this study, we employed a benzyl-substituted derivative of thiabendazole, *N*-benzylthiabendazole (*N*-BzTBZ), as a ligand to synthesize a novel mononuclear silver(I) complex, $[Ag(N\text{-BzTBZ})_2]CF_3SO_3$, exhibiting a distorted trigonal planar geometry. The binding affinity of both the free ligand and the synthesized complex with biologically relevant targets, bovine serum albumin (BSA, Figure 1 and Table 1) and calf thymus DNA (ct-DNA), were investigated using fluorescence emission spectroscopy.

METHOD

Fluorescence emission spectroscopy was used to study BSA in a phosphate buffer solution (PBS; pH 7.4). Fluorescence spectra of a BSA solution at a constant concentration (3.5 μM), in the absence and presence of increasing concentrations of the investigated compounds (up to 3.5 μM), were recorded in the range of 285–500 nm with excitation at 280 nm.

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RESULTS & DISCUSSION

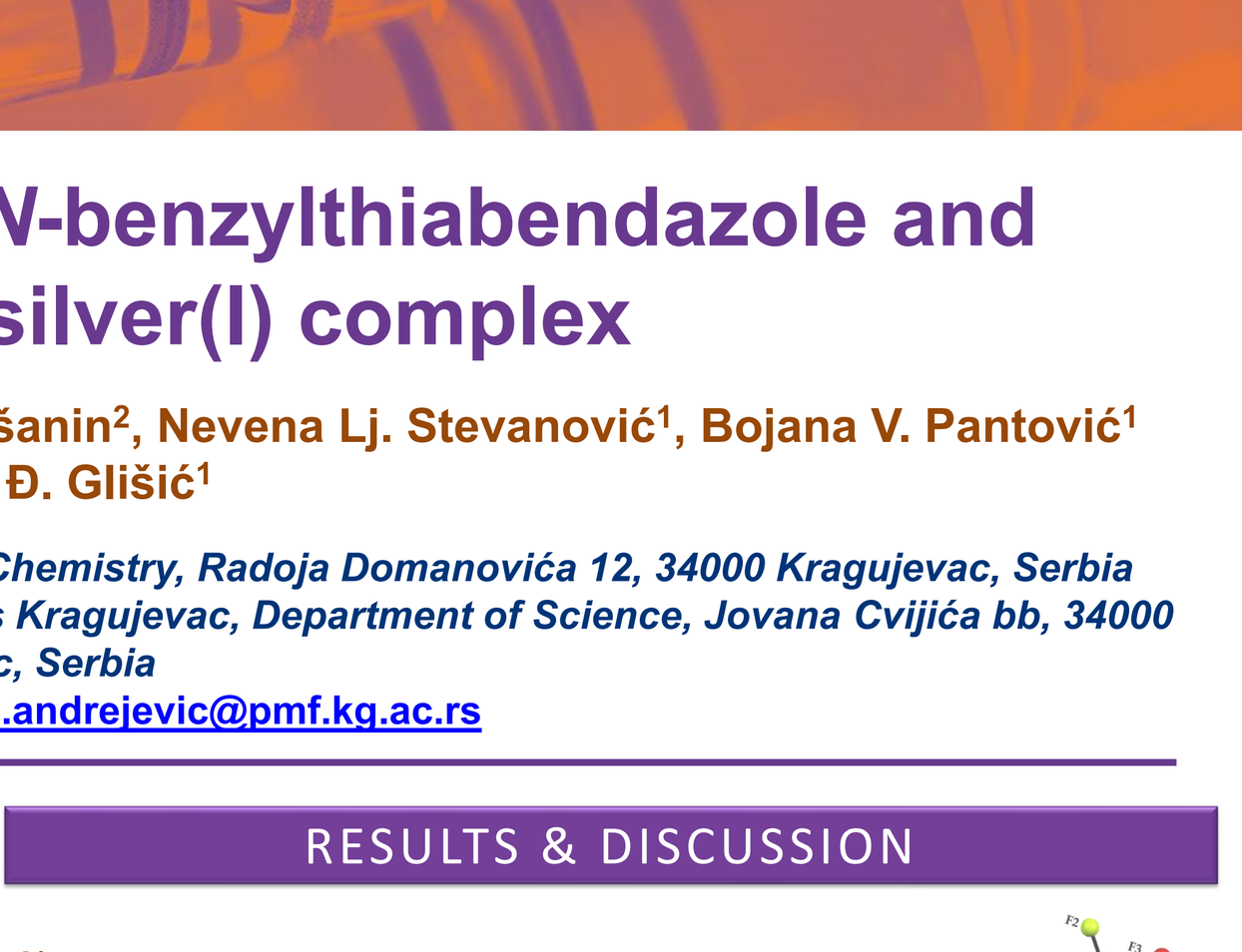

Figure 1. Fluorescence emission spectra of BSA in the presence of an increasing amount of silver(I) complex (A). Inserted graph: Stern-Volmer plot of F_0/F *vs.* [complex] (B). Plot of $\log(F_0\text{-}F)/F$ *vs.* log[complex] (C).

Table 1. Values of the binding constants of compounds with BSA

Compound	K_{sv} (M^{-1})	K_q ($M^{-1}s^{-1}$)	K_A (M^{-1})	*n*
N-BzTBZ	$(2.56 \pm 0.01) \times 10^6$	2.56×10^{12}	1.17×10^5	1.10
$[Ag(N\text{-BzTBZ})_2]CF_3SO_3$	$(4.11 \pm 0.01) \times 10^4$	4.11×10^{12}	1.67×10^3	0.73

CONCLUSION

- ✓ Both investigated compounds exhibited binding affinity toward BSA, suggesting their potential for transport to target cells
- ✓ The lower binding constant of the silver(I) complex suggests a weaker interaction with BSA, facilitating its easier release and potential biological activity at the target site
- ✓ Binding of both compounds to BSA occurs *via* a static quenching mechanism
- ✓ The observed red shift in the emission spectrum of the silver(I) complex indicates exposure of amino acid residues to a polar environment

FUTURE WORK

- Further work will focus on studying the interactions of these compounds with DNA using viscosity measurements, as no significant changes were observed in the emission spectra

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