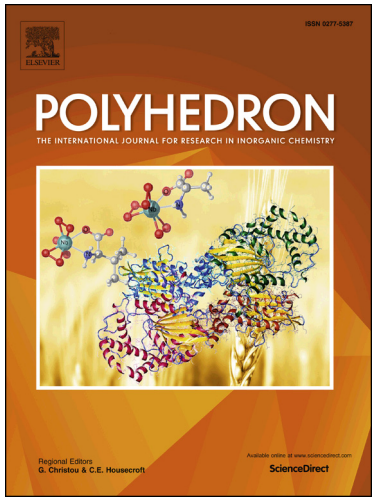

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Benzotriazole functionalized *N*-heterocyclic carbene-silver(I) complexes: Synthesis, cytotoxicity, antimicrobial, DNA binding, and molecular docking studies

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ABSTRACT

In this study, six $[Ag(NHC)_2]^+[AgCl_2]^-$ type silver complexes were synthesized by the reaction of corresponding carbene precursor and Ag_2O. One $[Ag(NHC)_2]^+NO_3^-$ type complex was synthesized by the anion exchange reaction of corresponding silver-NHC and $NaNO_3$. The synthesized complexes were characterized by ^{1}H NMR, ^{13}C NMR and IR spectroscopic methods, and elemental analysis. X-ray crystal structure of **5a** was also reported. Cytotoxicities of all compounds were evaluated against human breast (MCF-7) and colorectal (Caco-2) cancer cell lines and non-cancer mouse fibroblast (L-929) cell lines. All complexes performed stronger activity against both cancer cell lines than standard compound cisplatin while complex **3b** performed nearly equal cytotoxicity to cisplatin against non-cancer L-929. Antimicrobial effects of all compounds were evaluated against *Escherichia coli*, *Bacillus subtilis* and *Candida albicans* and good activities were observed. The docking results indicated that complex **3b** might be classified as druggable molecule in drug design. DNA binding study also demonstrates that **3b** complex has an interaction ability to DNA. Combination of experimental and molecular docking results revealed that reported complexes are promising structures and deserve further research as anticancer drugs.

Keywords: Silver(I), *N*-heterocyclic carbene, benzotriazole, cytotoxicity, antimicrobial.