

## **$\alpha$ -Substituted Phthalocyanines Based on Metal-Induced H- or J-Type Aggregation for Silver and Palladium Ions: Synthesis, Fluorescence, Antimicrobial and Antioxidant Properties**

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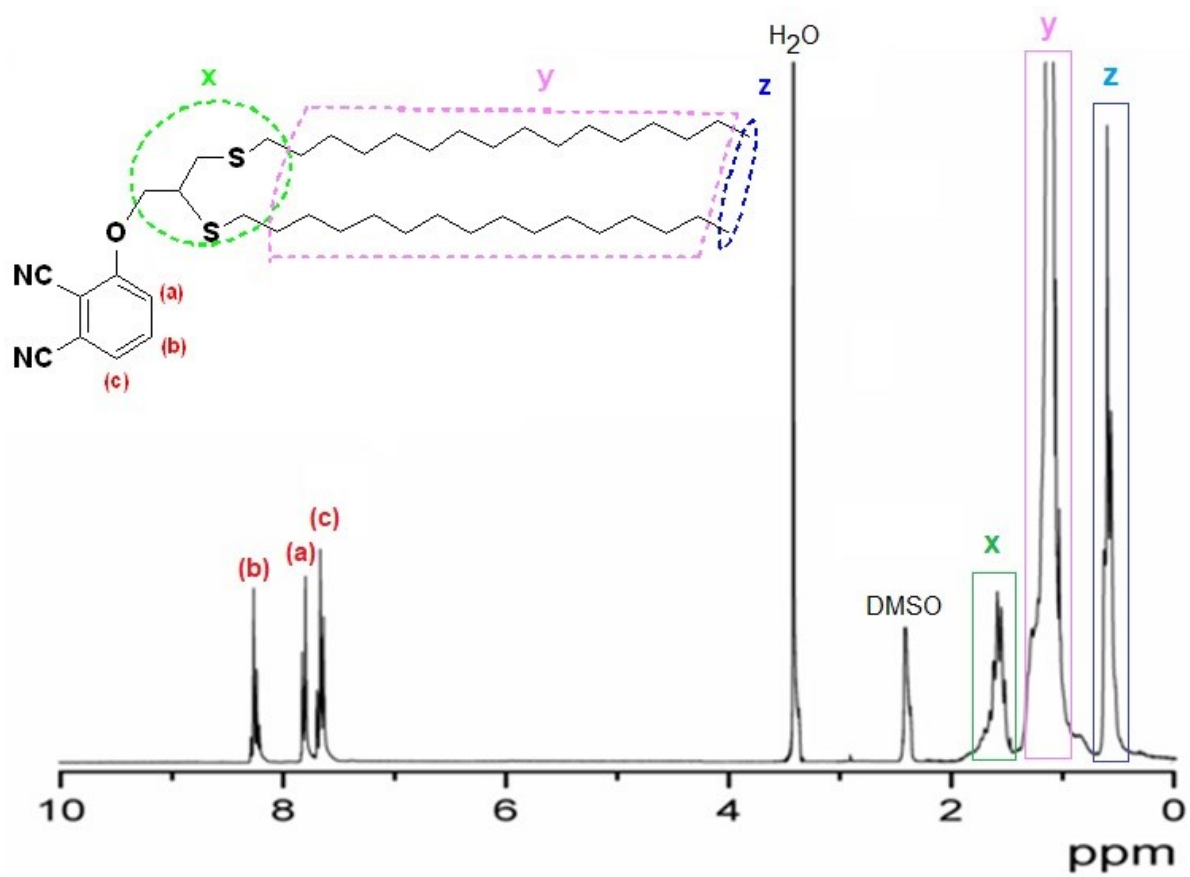
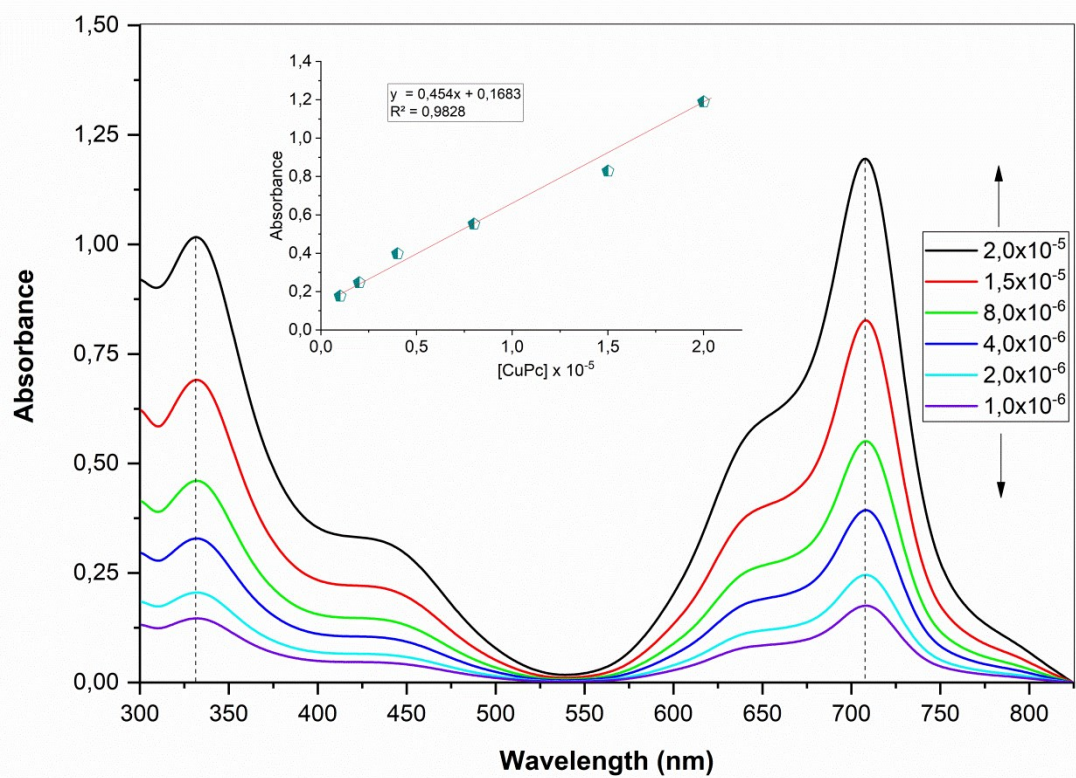
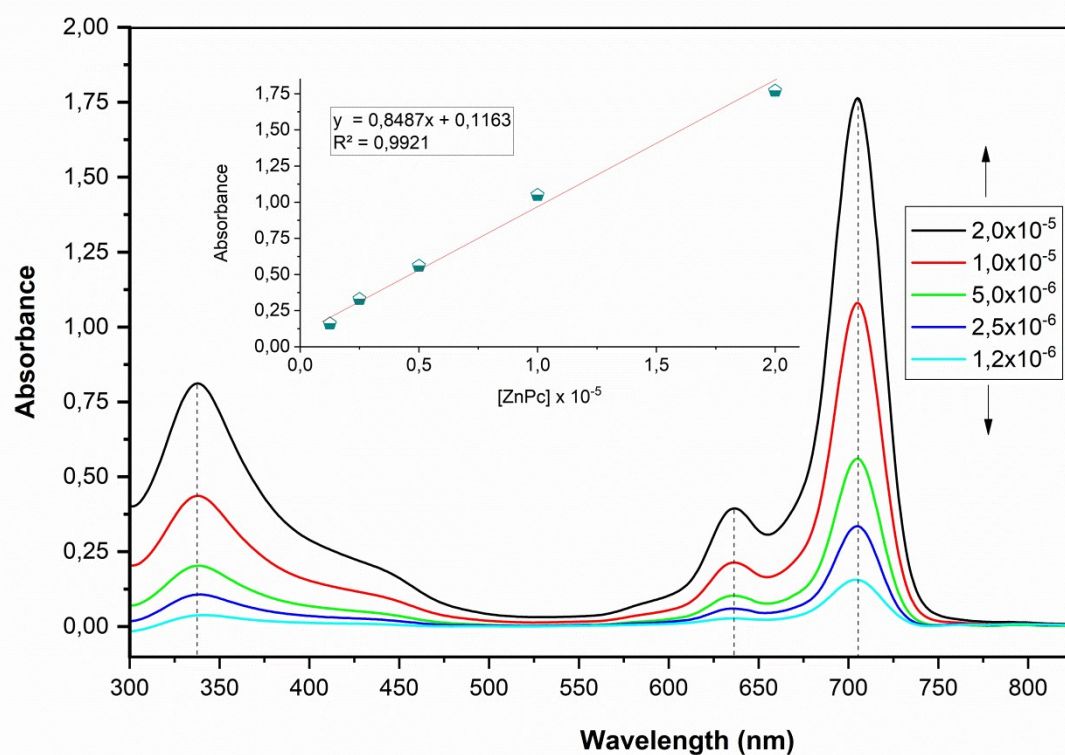


Fig S1. <sup>1</sup>H-NMR spectrum of compound (2)

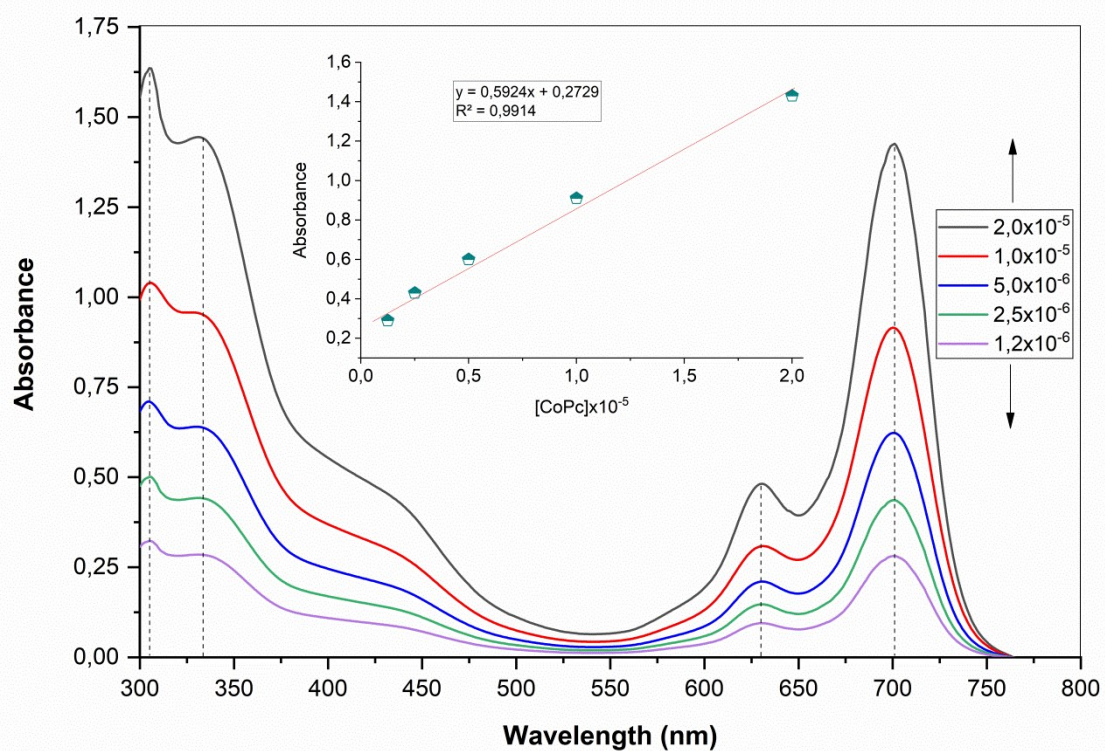


**Fig. S2** Electronic spectra of CuPc (**3**) in THF at different concentrations (inset: plot of Q band absorbance versus concentration)

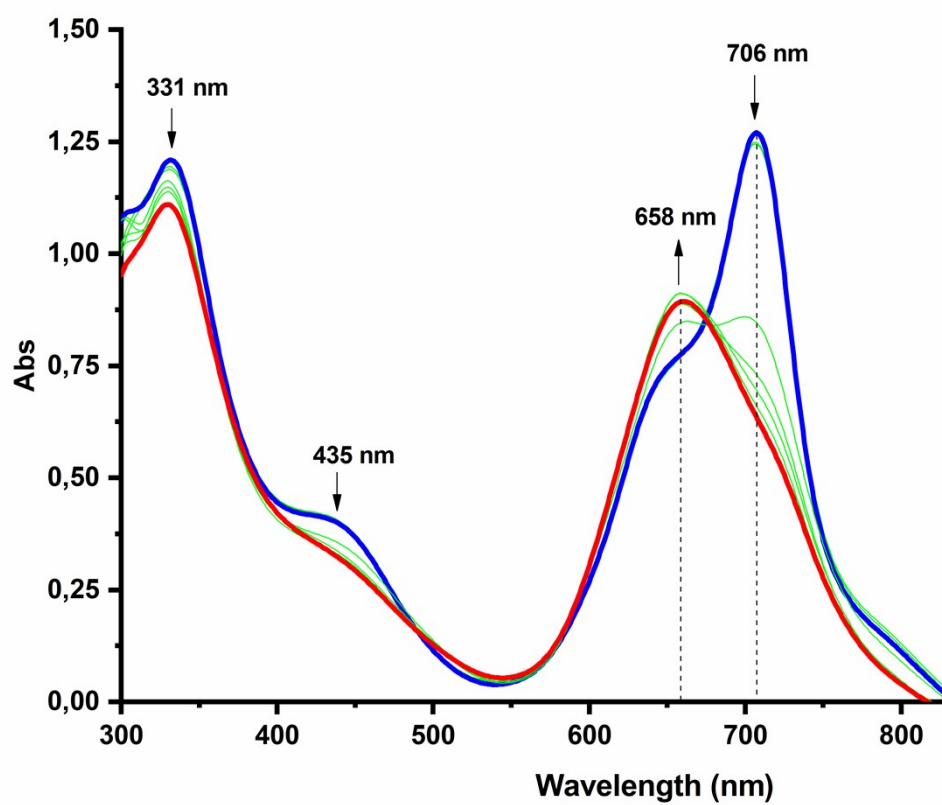




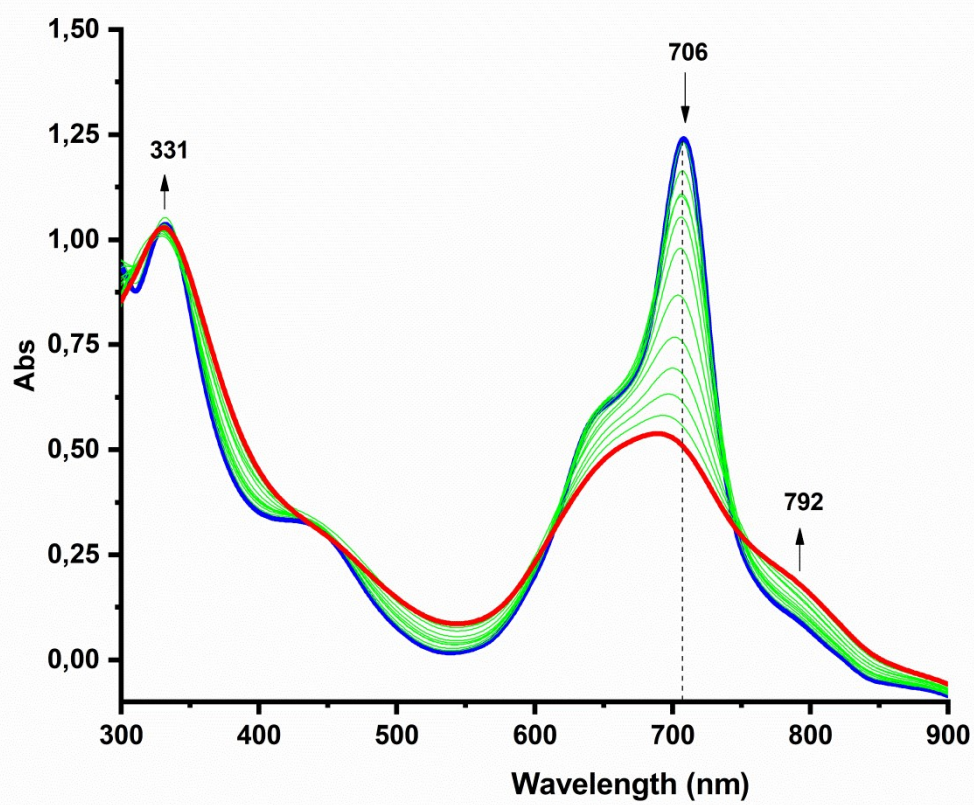
**Fig. S3** Electronic spectra of ZnPc (**4**) in THF at different concentrations (inset: plot of Q band absorbance versus concentration).



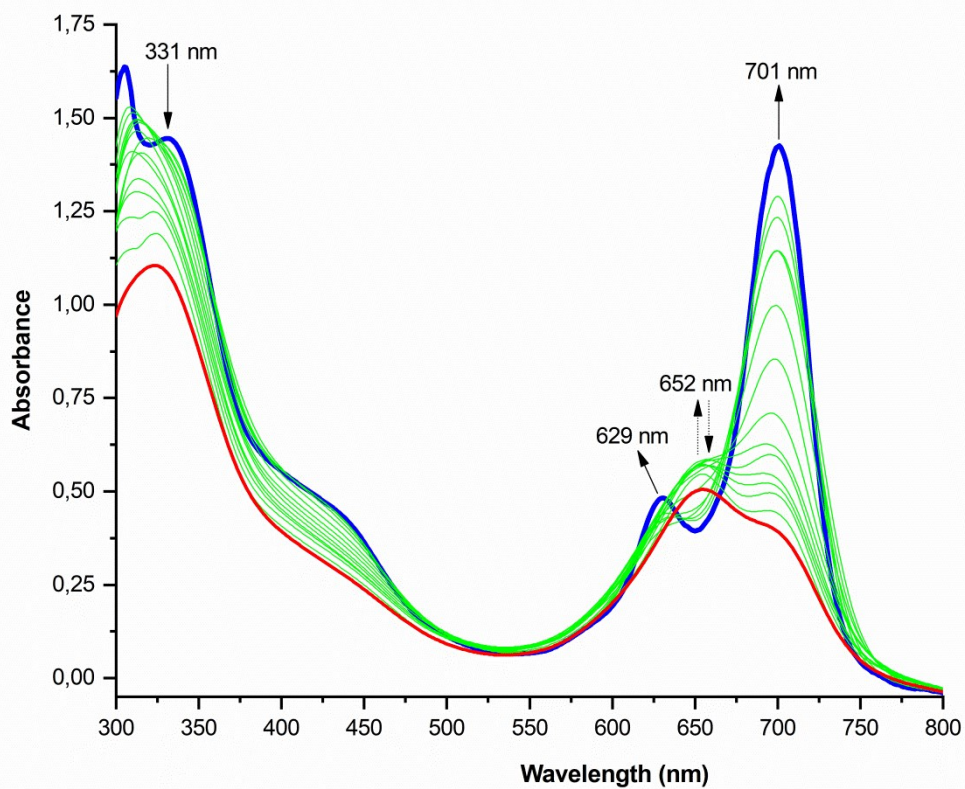
**Fig. S4** Electronic spectra of CpPc (**5**) in THF at different concentrations (inset: plot of Q band absorbance versus concentration).



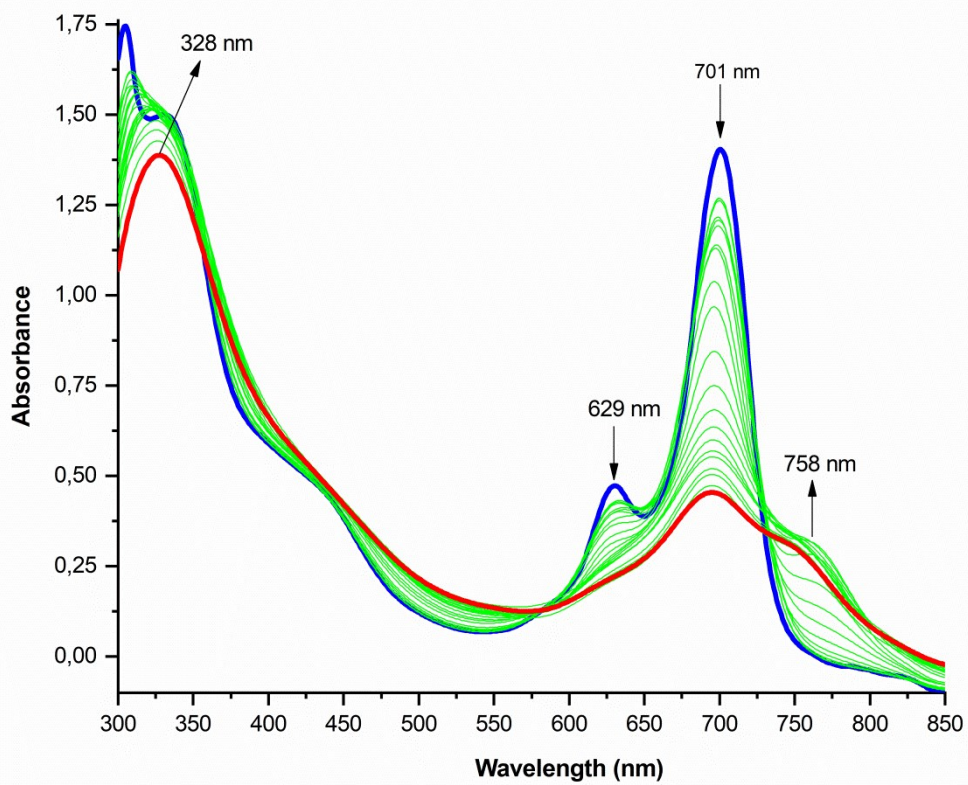
**Fig. S5** Electronic spectra of CuPc (**3**) during the titration with Ag(I) ions.



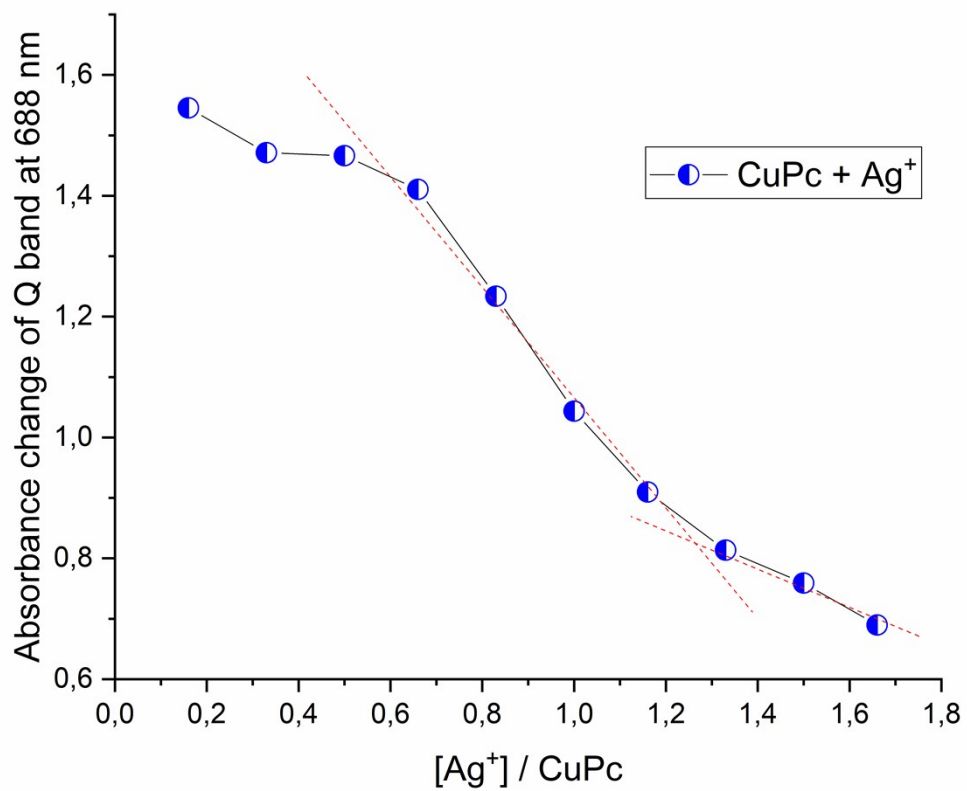
**Fig. S6** Electronic spectra of CuPc (**3**) during the titration with Pd(II) ions.



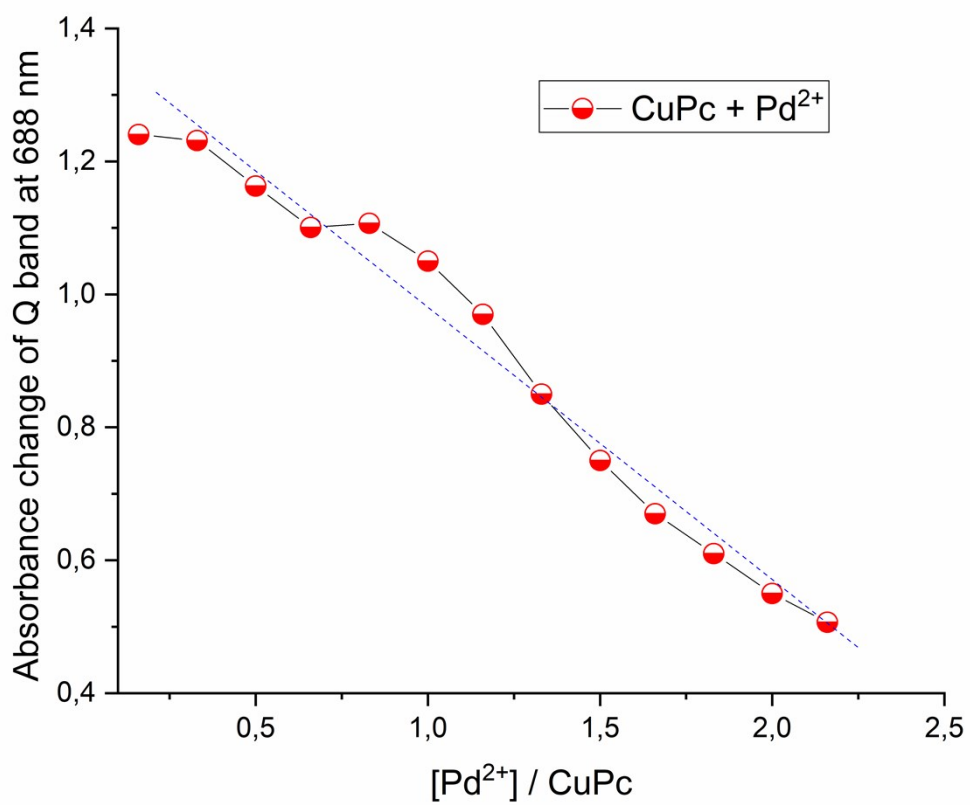
**Fig. S7** Electronic spectra of CoPc (**4**) during the titration with Ag(I) ions.



**Fig. S8** Electronic spectra of CoPc (**5**) during the titration with Pd(II) ions.

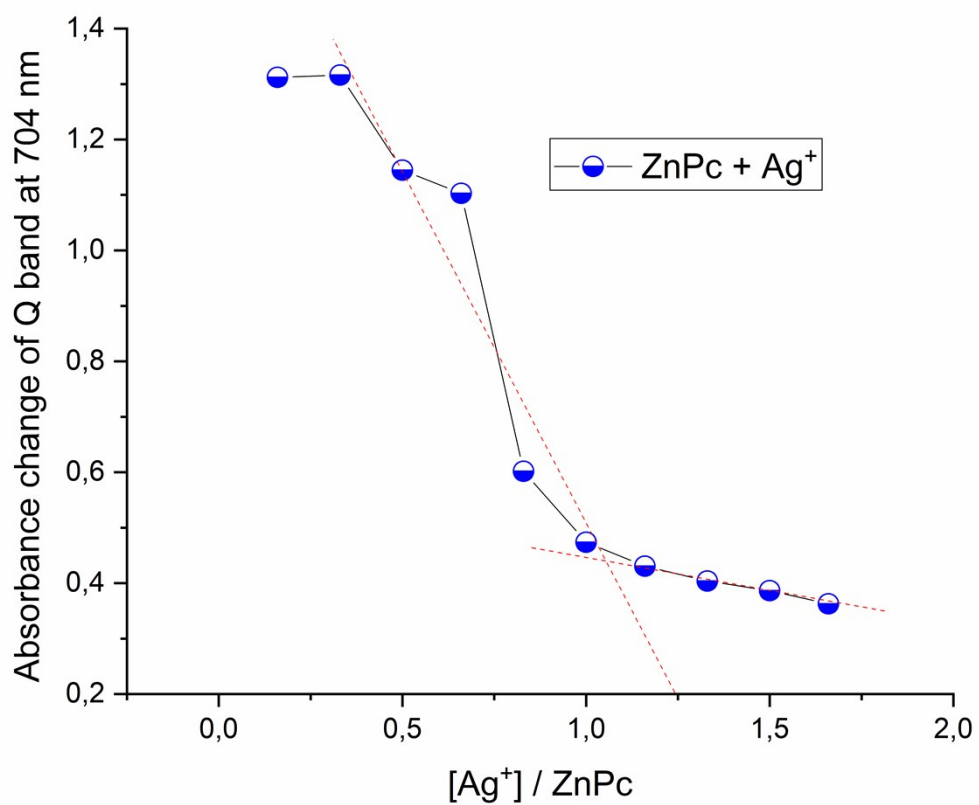


**Fig. S9** The plot of the change of Q band versus  $[\text{Ag}^+]/[\text{CuPc}]$ .

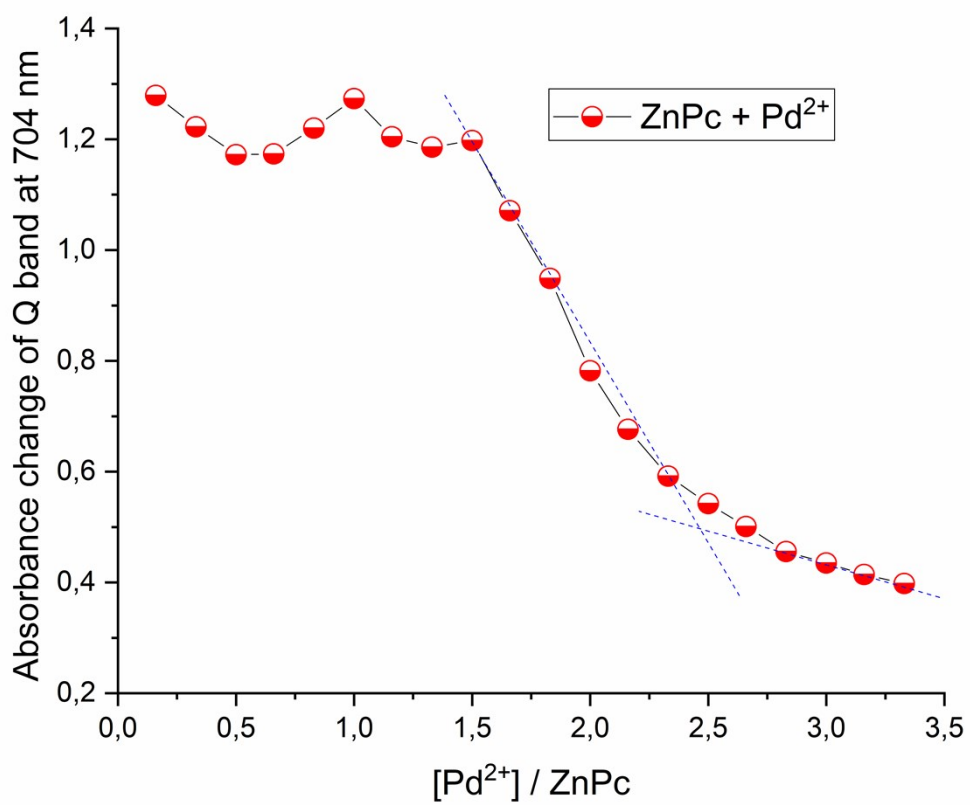


**Fig. S10** The plot of the change of Q band versus  $[Pd^{2+}]/[CuPc]$ .

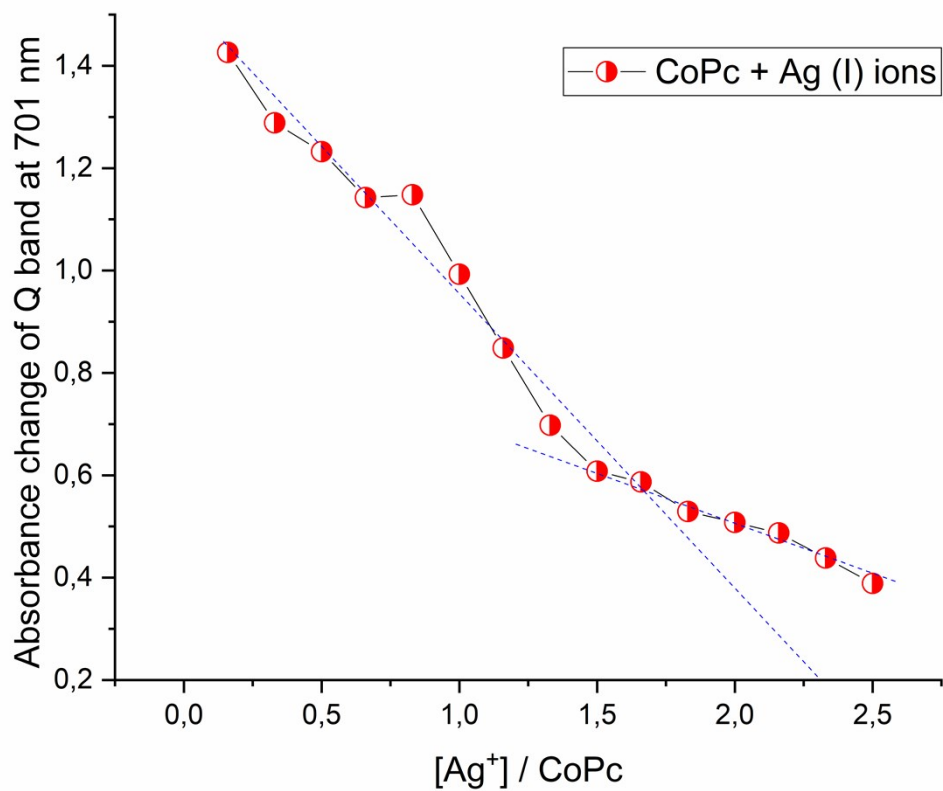




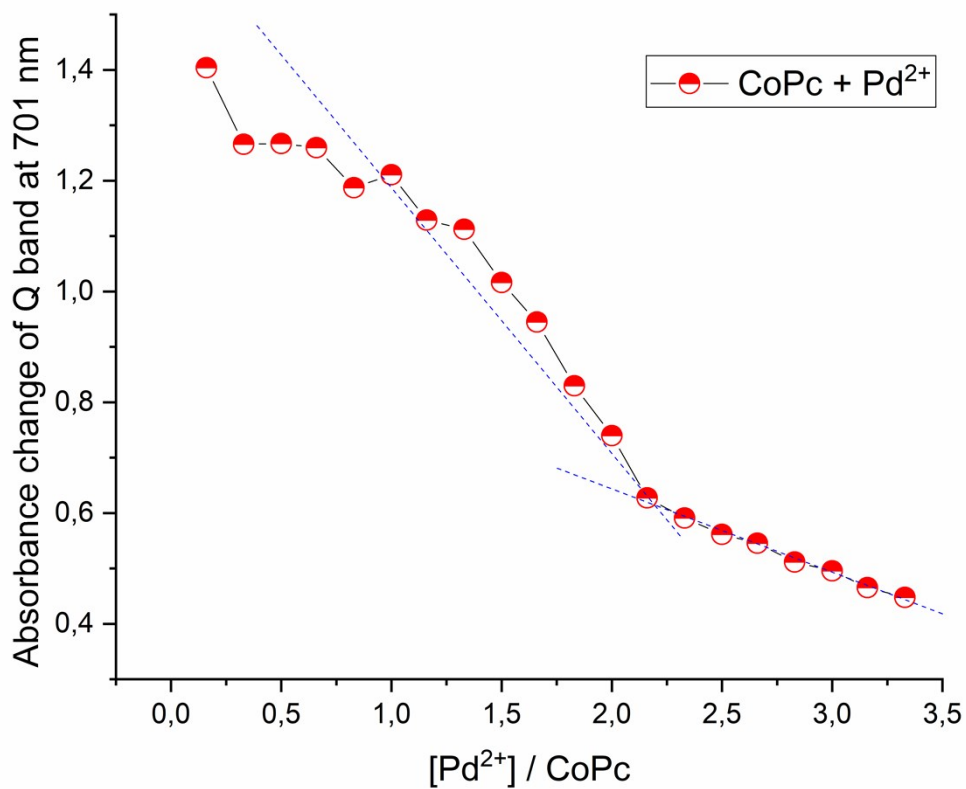
**Fig. S11** The plot of the change of Q band versus  $[Ag^+]/[ZnPc]$ .



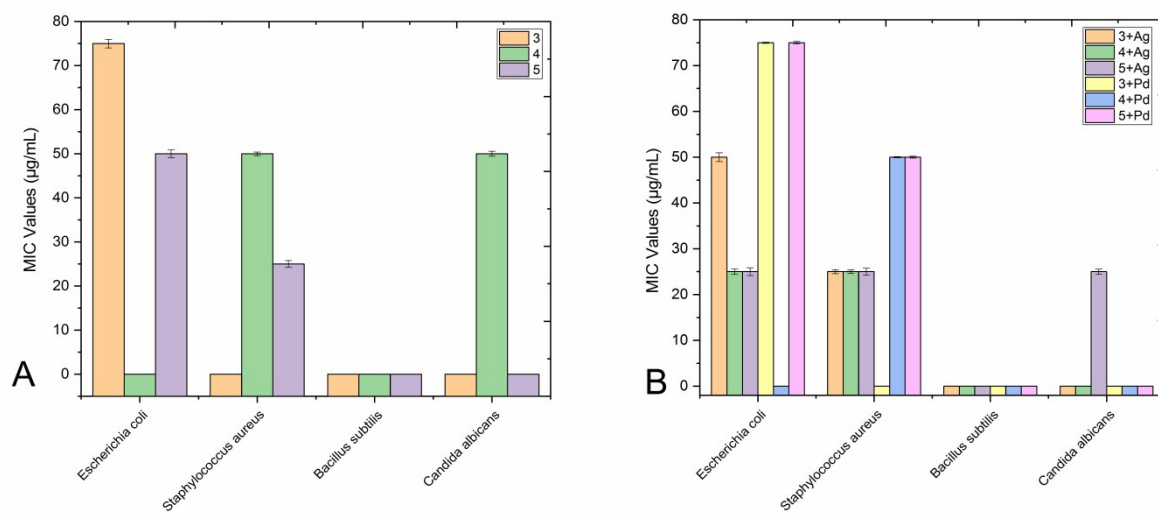
**Fig. S12** The plot of the change of Q band versus  $[\text{Pd}^{2+}]/[\text{ZnPc}]$ .



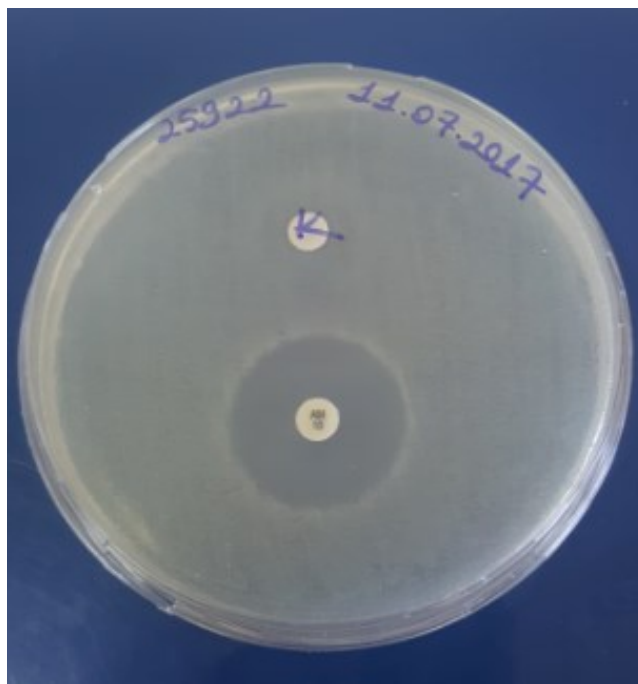
**Fig. S13** The plot of the change of Q band versus  $[\text{Ag}^+]/[\text{CoPc}]$ .



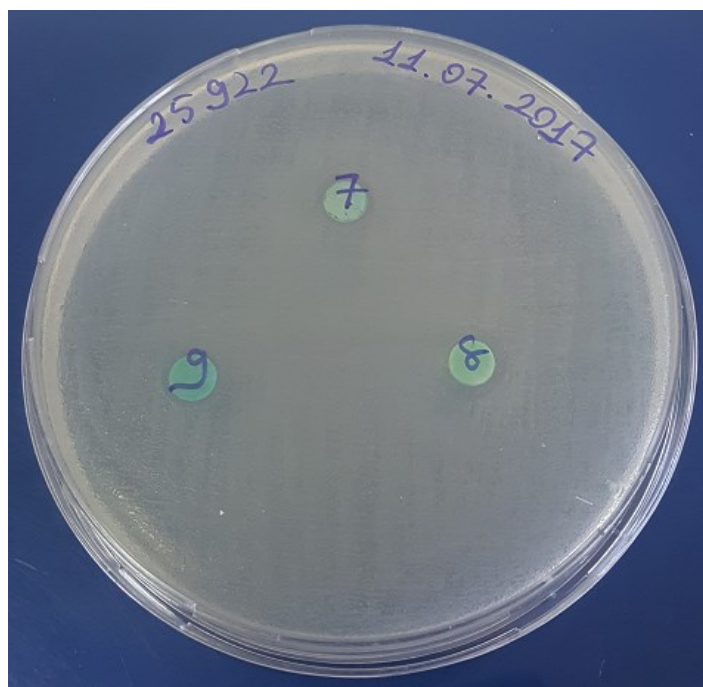
**Fig. S14** The plot of the change of Q band versus  $[Pd^{2+}]/[CoPc]$ .



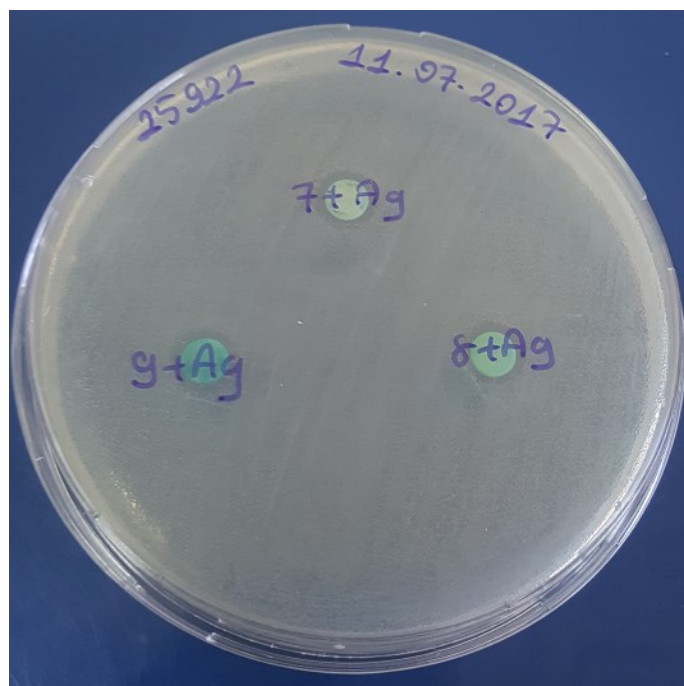
**Fig. S15** Minimum Inhibitory Concentration (MIC) results of the synthesized phthalocyanine compounds (A) and their doped Ag(I) and Pd(II) ion forms (B).



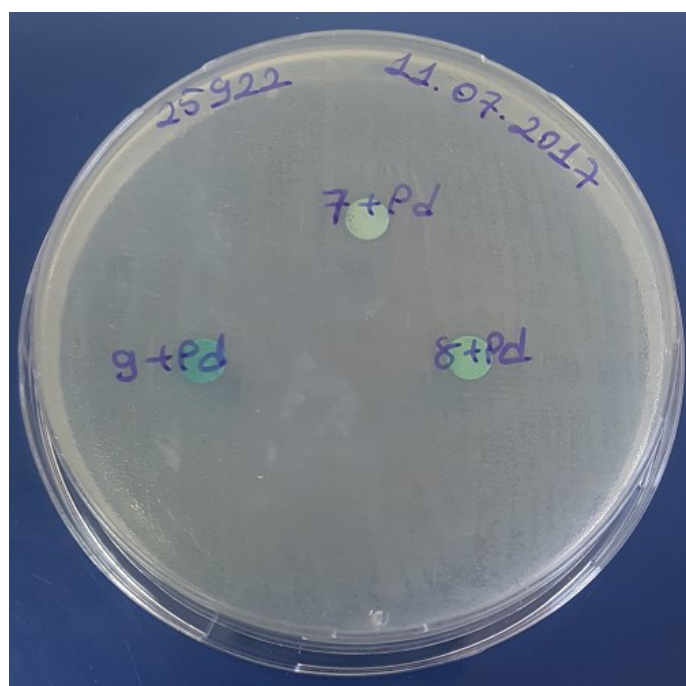
**Fig. S16.** Inhibition zones formed by DMF (control) impregnated disc and antibiotic standard disc against *E.coli*, K: control (DMF), AM10: Ampicillin 10  $\mu$ g



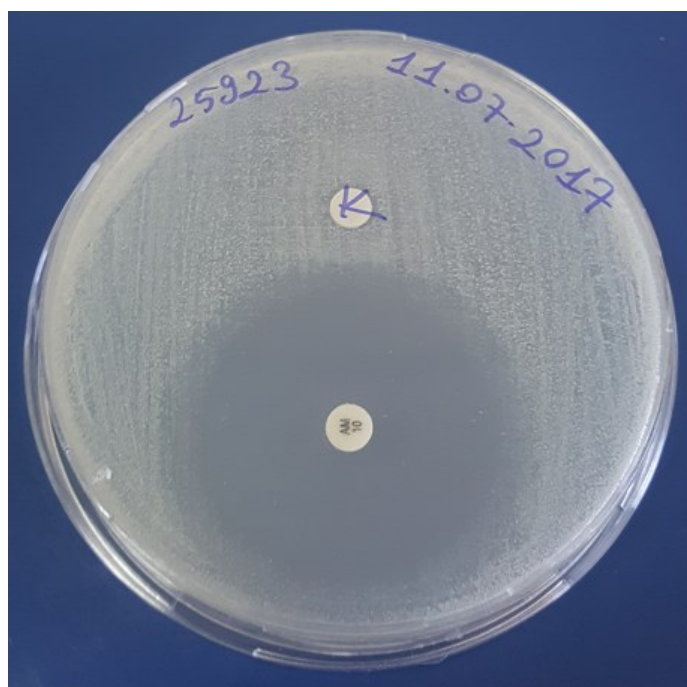
**Fig. S17.** Inhibition zones formed by discs impregnated with compound 3, 4, 5 solutions against *E. coli* (number 7, 8, 9 refer to compound 3, 4, 5, respectively)



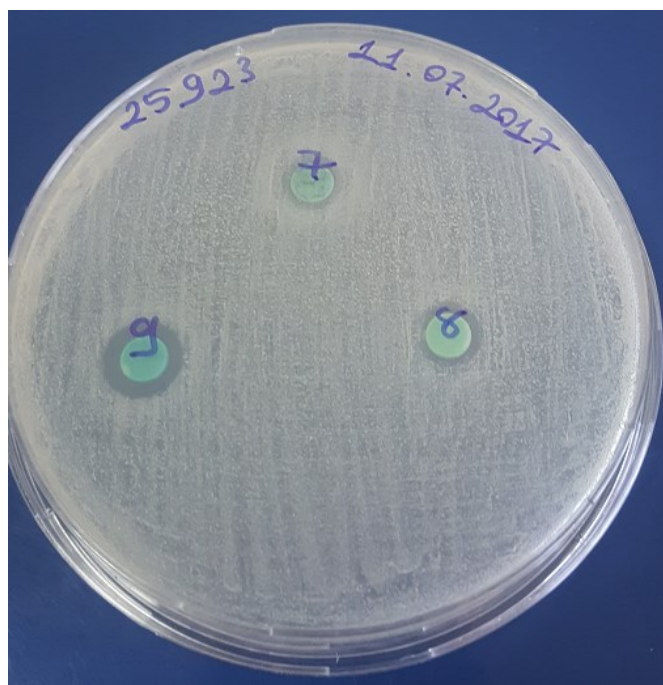
**Fig. S18.** Inhibition zones formed by discs impregnated with compound 3+Ag, 4+Ag, 5+Ag solutions against *E. coli* (number 7+Ag, 8+Ag, 9+Ag refer to compound 3+Ag, 4+Ag, 5+Ag, respectively)



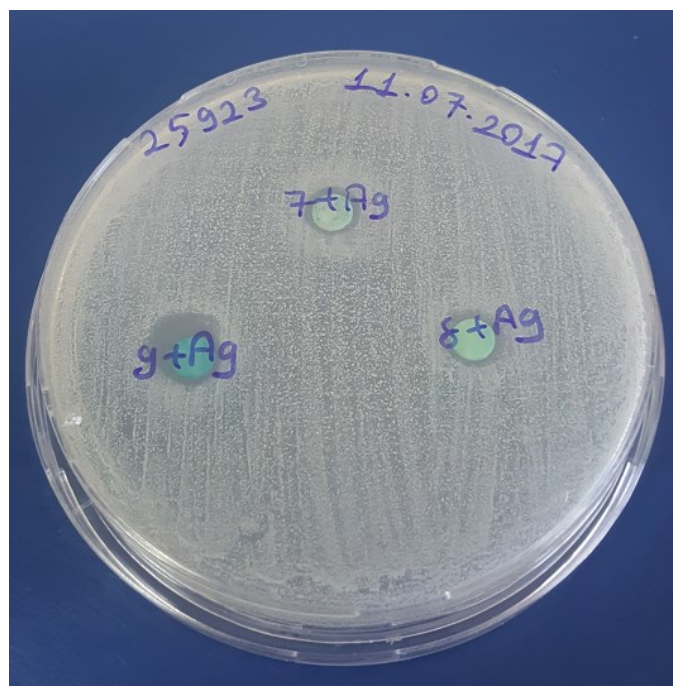
**Fig. S19.** Inhibition zones formed by discs impregnated with compound 3+Pd, 4+Pd, 5+Pd solutions against *E. coli* (number 7+Pd, 8+Pd, 9+Pd refer to compound 3+Pd, 4+Pd, 5+Pd, respectively)



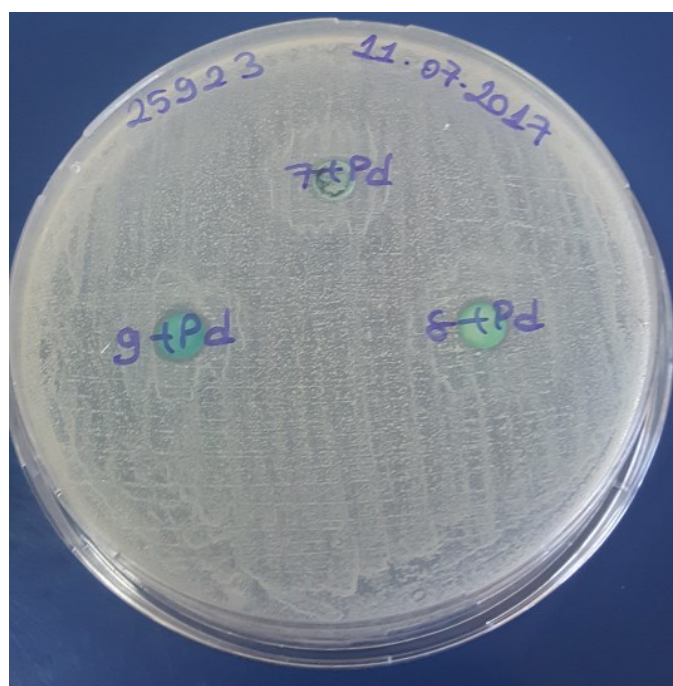
**Fig. S20.** Inhibition zones formed by DMF (control) impregnated disc and antibiotic standard disc against *S. aureus*, K: control (DMF), AM10: Ampicillin 10 µg



**Fig. S21.** Inhibition zones formed by discs impregnated with compound 3, 4, 5 solutions against *S. aureus* (number 7, 8, 9 refer to compound 3, 4, 5, respectively)

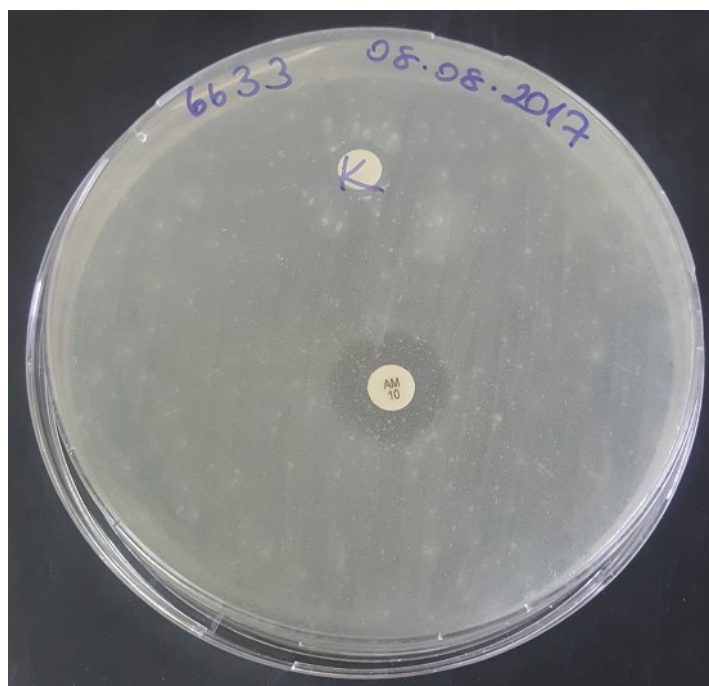


**Fig. S22.** Inhibition zones formed by discs impregnated with compound 3+Ag, 4+Ag, 5+Ag solutions against *S. aureus* (number 7+Ag, 8+Ag, 9+Ag refer to compound 3+Ag, 4+Ag, 5+Ag, respectively)

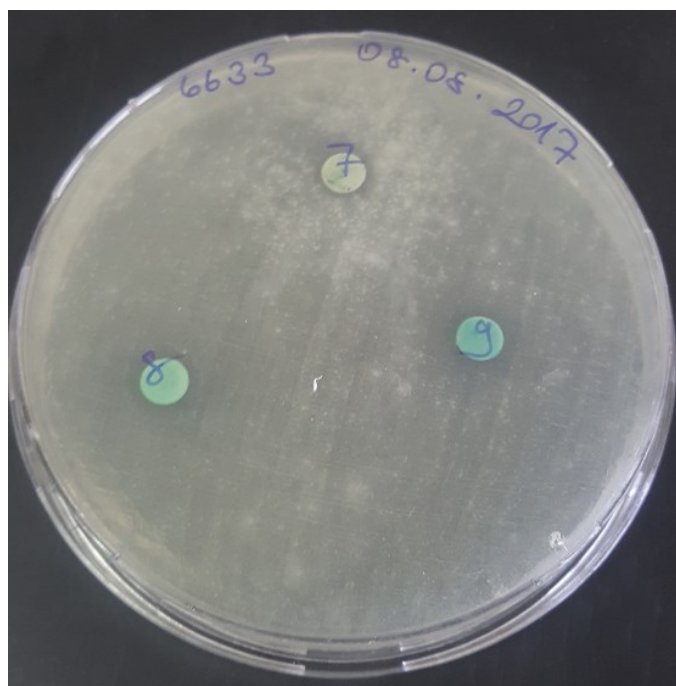


**Fig. S23.** Inhibition zones formed by discs impregnated with compound 3+Pd, 4+Pd, 5+Pd solutions against *S. aureus* (number 7+Pd, 8+Pd, 9+Pd refer to compound 3+Pd, 4+Pd, 5+Pd, respectively)

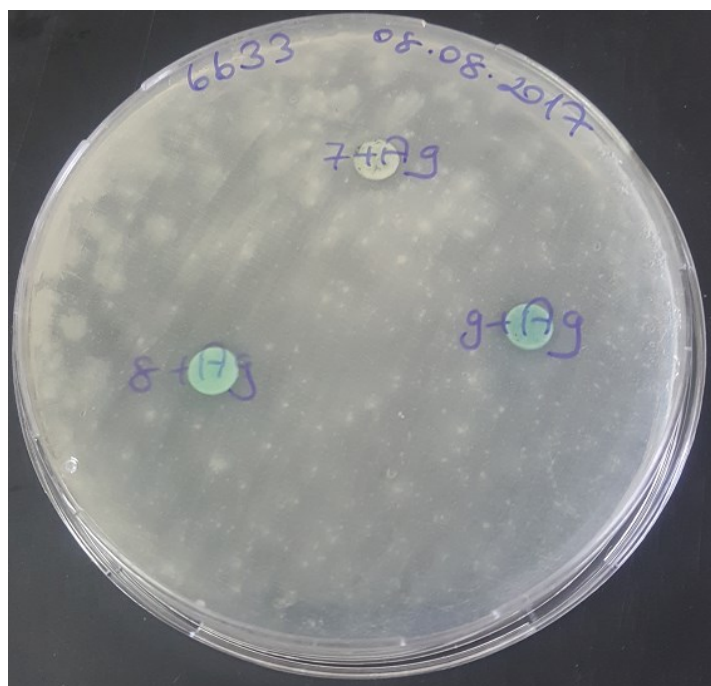




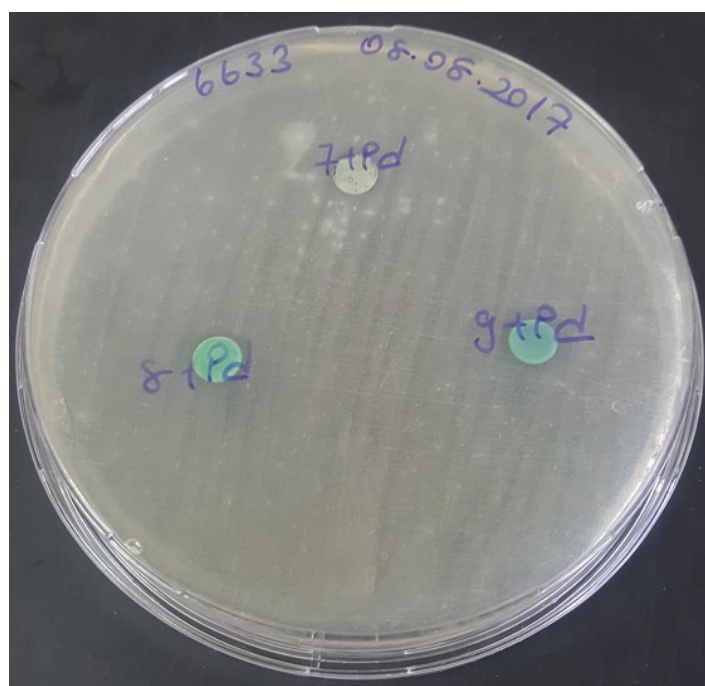
**Fig. S24.** Inhibition zones formed by DMF (control) impregnated disc and antibiotic standard disc against *B. subtilis*, K: control (DMF), AM10: Ampicillin 10  $\mu\text{g}$



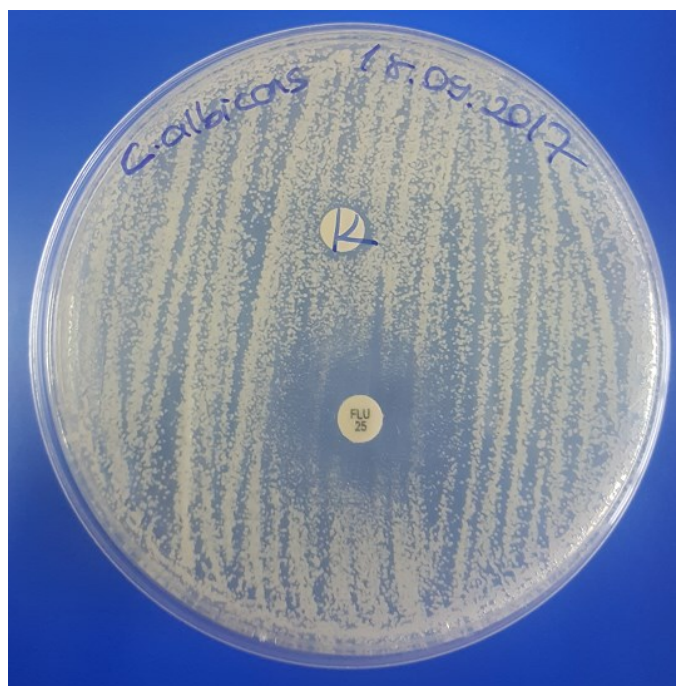
**Fig. S25.** Inhibition zones formed by discs impregnated with compound 3, 4, 5 solutions against *B. subtilis* (number 7, 8, 9 refer to compound 3, 4, 5, respectively)



**Fig. S26.** Inhibition zones formed by discs impregnated with compound 3+Ag, 4+Ag, 5+Ag solutions against *B. subtilis* (number 7+Ag, 8+Ag, 9+Ag refer to compound 3+Ag, 4+Ag, 5+Ag, respectively)



**Fig. S27.** Inhibition zones formed by discs impregnated with compound 3+Pd, 4+Pd, 5+Pd solutions against *B. subtilis* (number 7+Pd, 8+Pd, 9+Pd refer to compound 3+Pd, 4+Pd, 5+Pd, respectively)



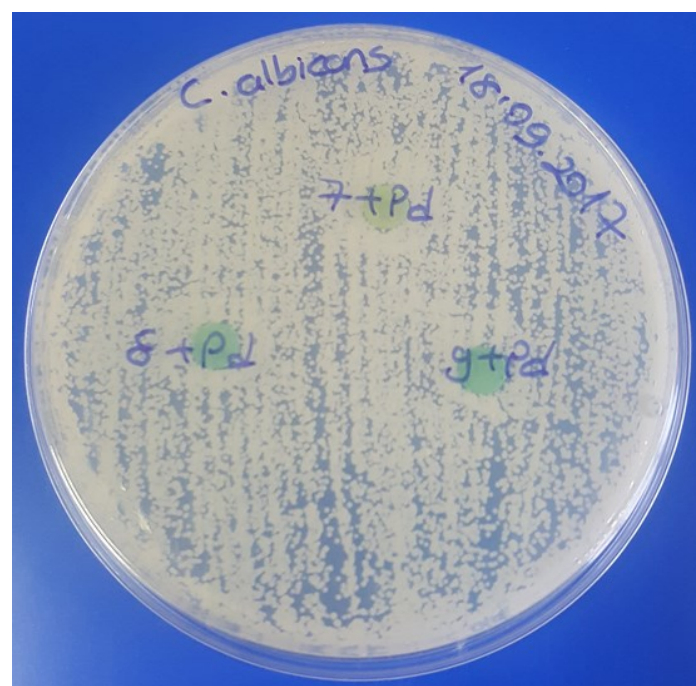
**Fig. S28.** Inhibition zones formed by DMF (control) impregnated disc and antibiotic standard disc against *C.albicans*, **K**: control (DMF), **FLU25**: Fluconazole 25 µg



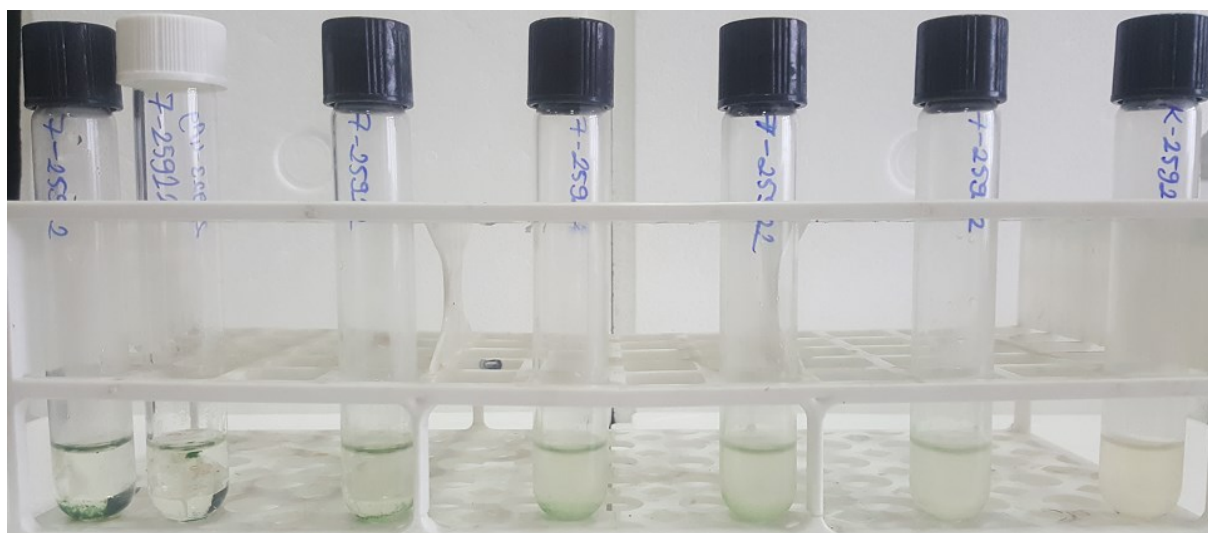
**Fig. S29.** Inhibition zones formed by discs impregnated with compound 3, 4, 5 solutions against *C.albicans* (number 7, 8, 9 refer to compound 3, 4, 5, respectively)



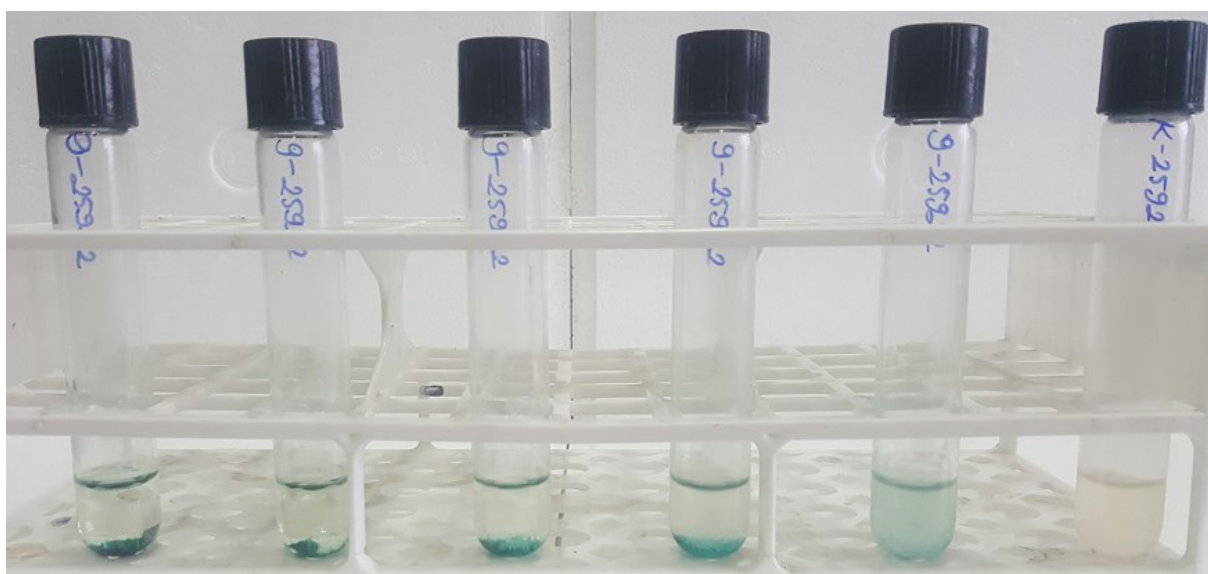
**Fig. S30.** Inhibition zones formed by discs impregnated with compound **3+Ag**, **4+Ag**, **5+Ag** solutions against *C.albicans* (number 7+Ag, 8+Ag, 9+Ag refer to compound **3+Ag**, **4+Ag**, **5+Ag**, respectively)



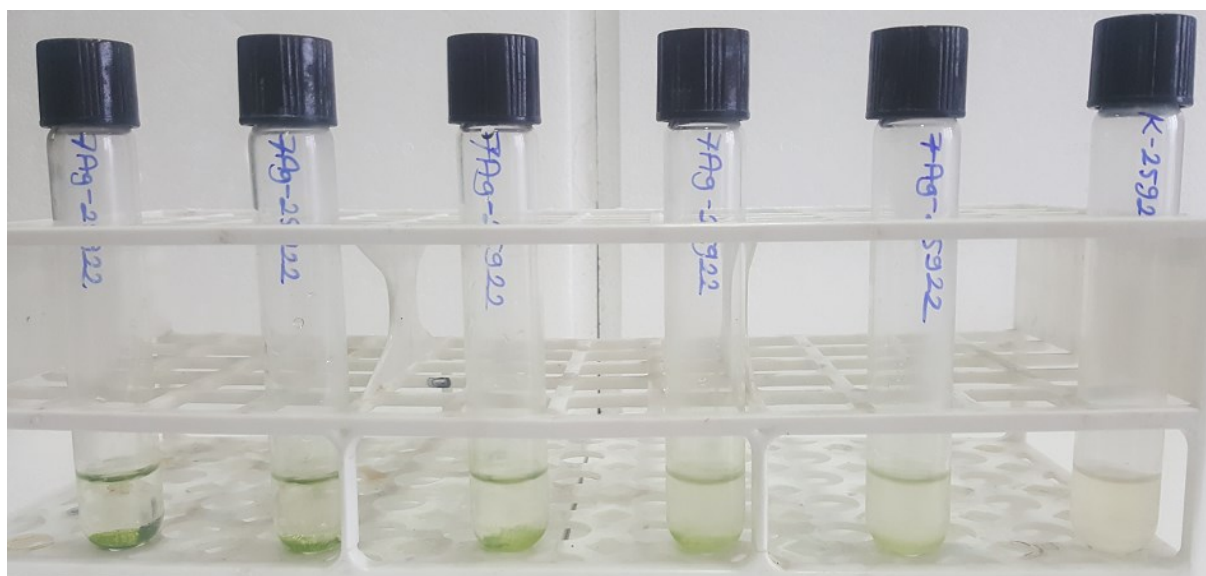
**Fig. S31.** Inhibition zones formed by discs impregnated with compound **3+Pd**, **4+Pd**, **5+Pd** solutions against *C.albicans* (number 7+Pd, 8+Pd, 9+Pd refer to compound **3+Pd**, **4+Pd**, **5+Pd**, respectively)



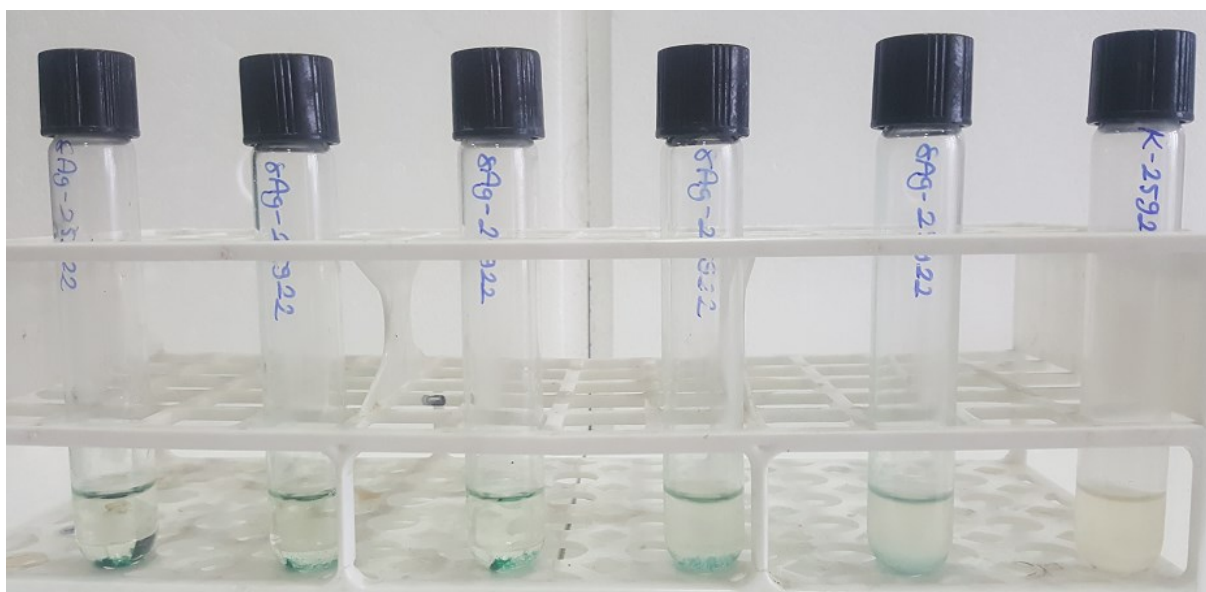
**Fig. S32.** Compound **3** - *E.coli* MIC test results (concentration of compound **3** in tubes from left to right: 100-75-50-25-12.5-6.25-0 µg/mL; K = control; number 7 refers to compound **3**)



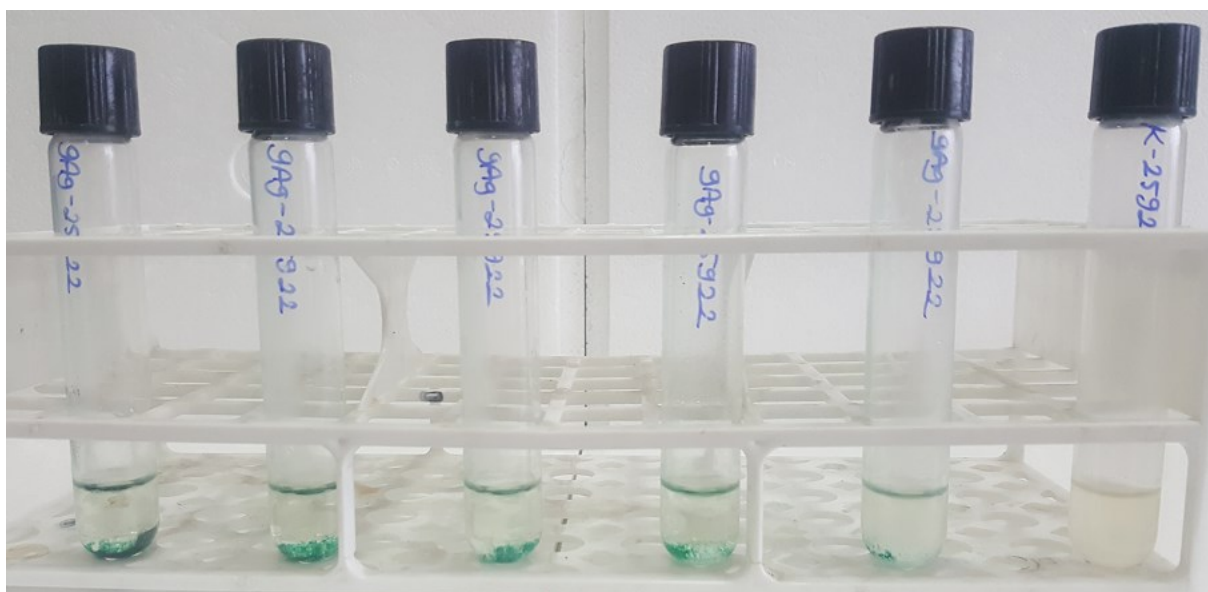
**Fig. S33.** Compound **5** - *E.coli* MIC test results (concentration of compound **5** in tubes from left to right: 100-50-25-12.5-6.25-0 µg/mL; K = control; number 9 refers to compound **5**)



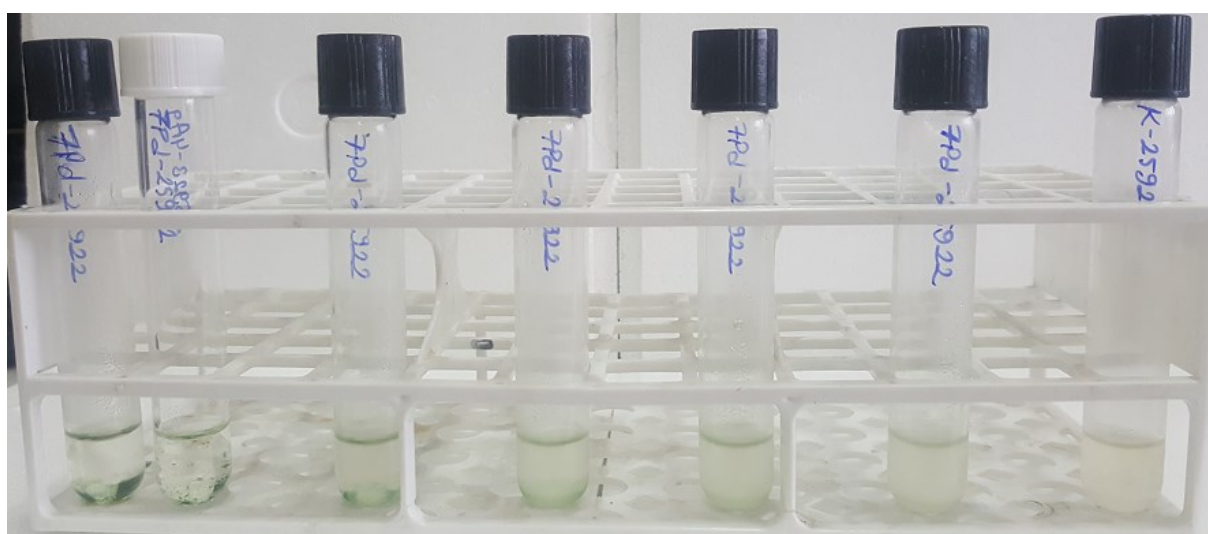
**Fig. S34.** Compound 3+Ag - *E.coli* MIC test results (concentration of compound 3+Ag in tubes from left to right: 100-50-25-12.5-6.25-0 µg/mL; K = control; number 7Ag refers to compound 3+Ag)



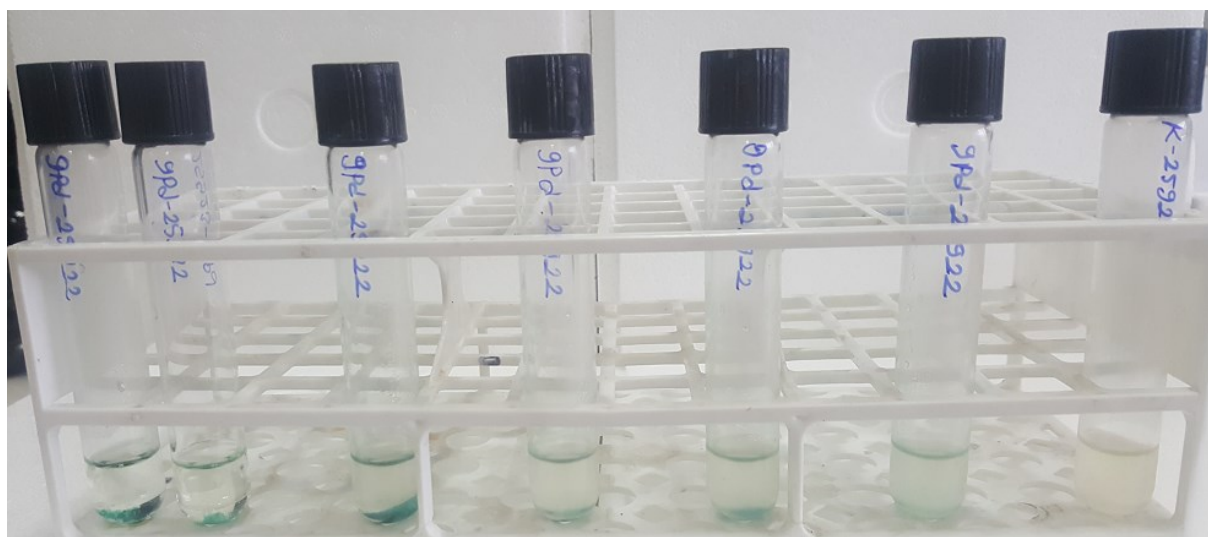
**Fig. S35.** Compound 4+Ag - *E.coli* MIC test results (concentration of compound 4+Ag in tubes from left to right: 100-50-25-12.5-6.25-0 µg/mL; K = control; number 8Ag refers to compound 4+Ag)



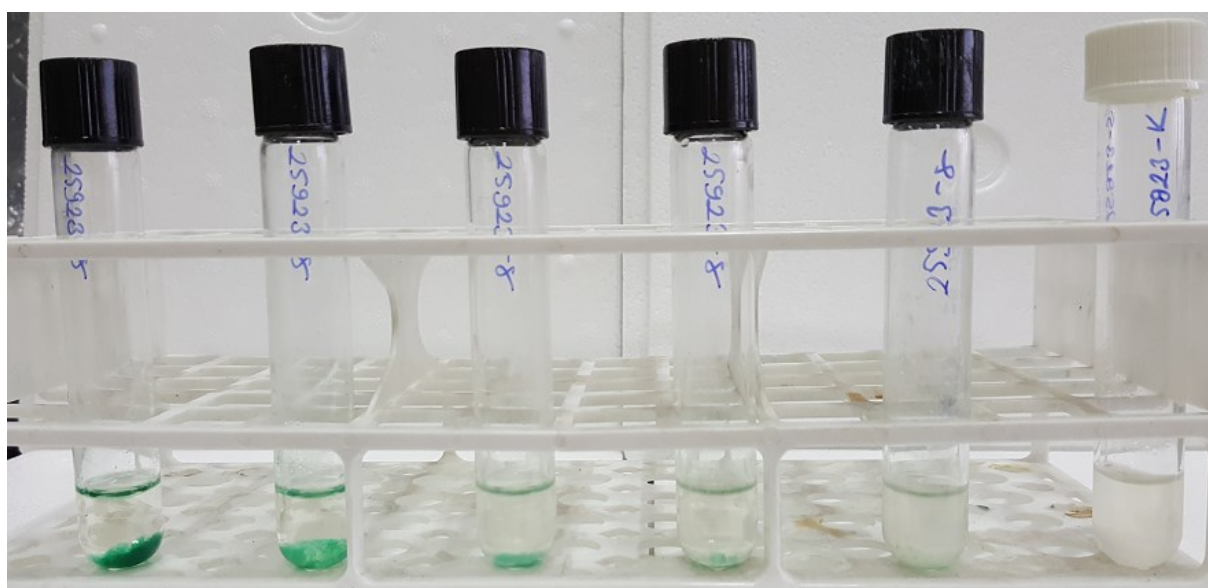
**Fig. S36.** Compound **5+Ag** - *E.coli* MIC test results (concentration of compound **5+Ag** in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 9Ag refers to compound **5+Ag**)



**Fig. S37.** Compound **3+Pd** - *E.coli* MIC test results (concentration of compound **3+Pd** in tubes from left to right: 100-75-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 7Pd refers to compound **3+Pd**)

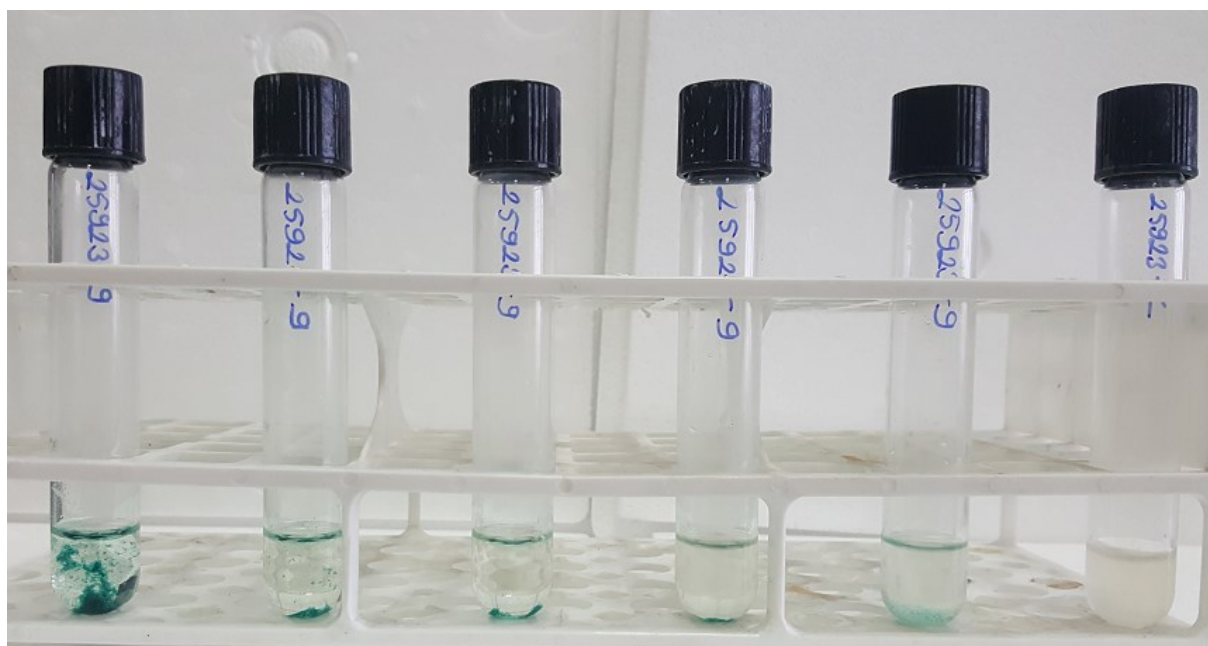


**Fig. S38.** Compound **5+Pd** - *E.coli* MIC test results (concentration of compound **5+Pd** in tubes from left to right: 100-75-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 9Pd refers to compound **5+Pd**)

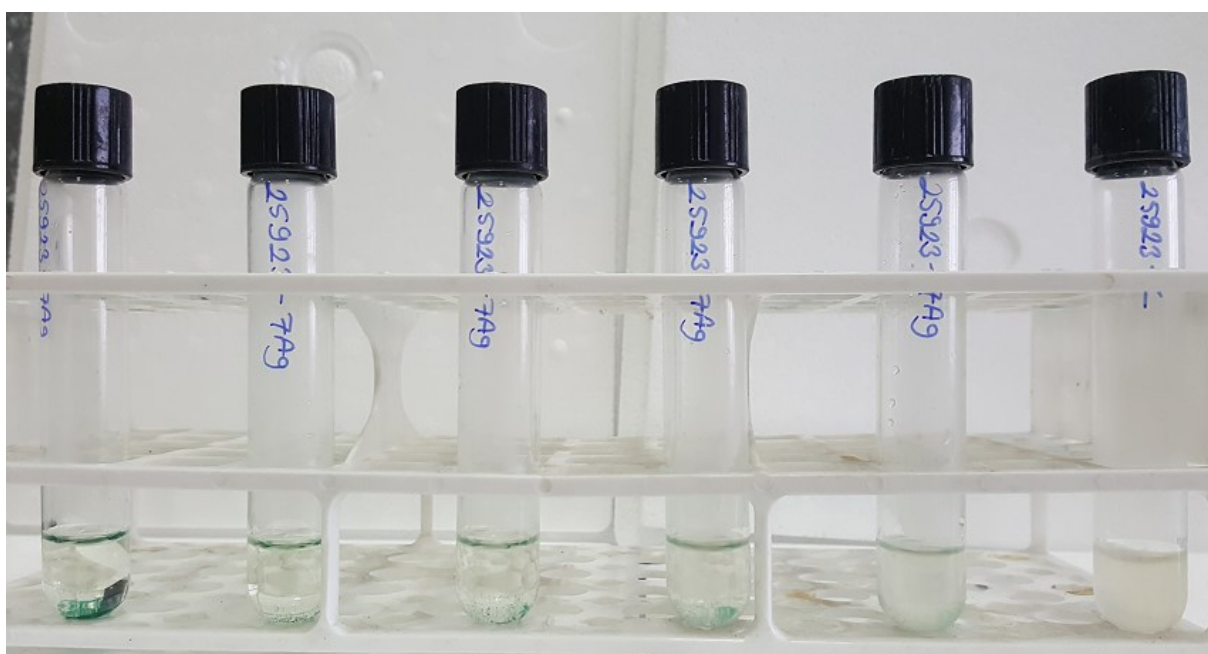


**Fig. S39.** Compound **4** - *S.aureus* MIC test results (concentration of compound **4** in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 8 refers to compound **4**)

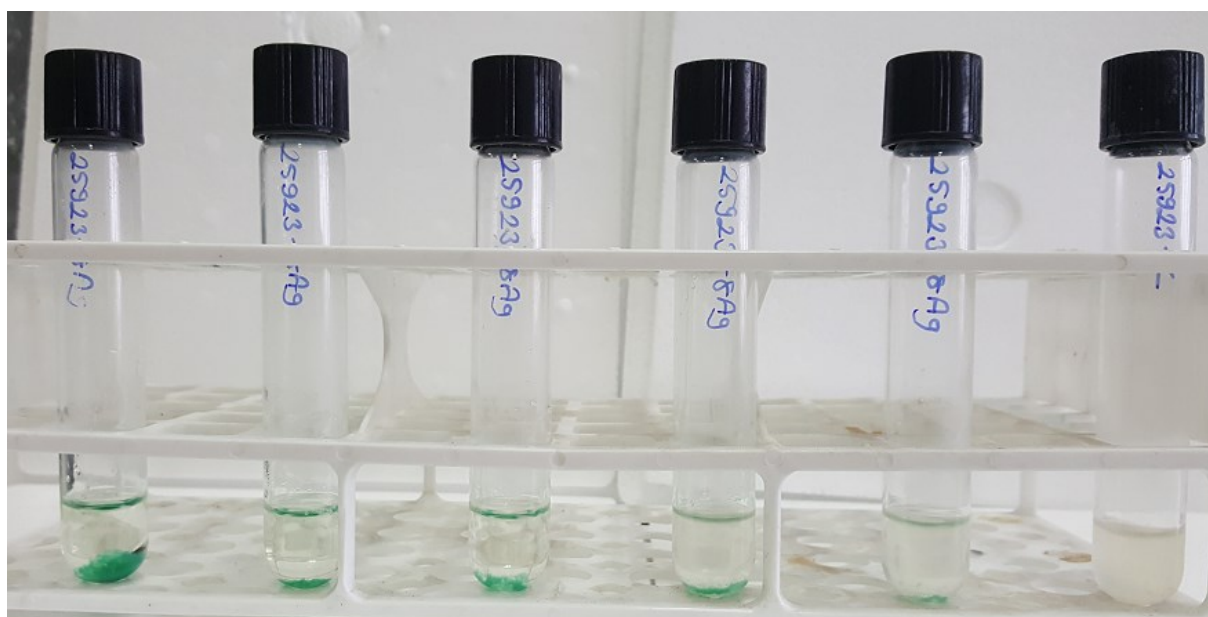




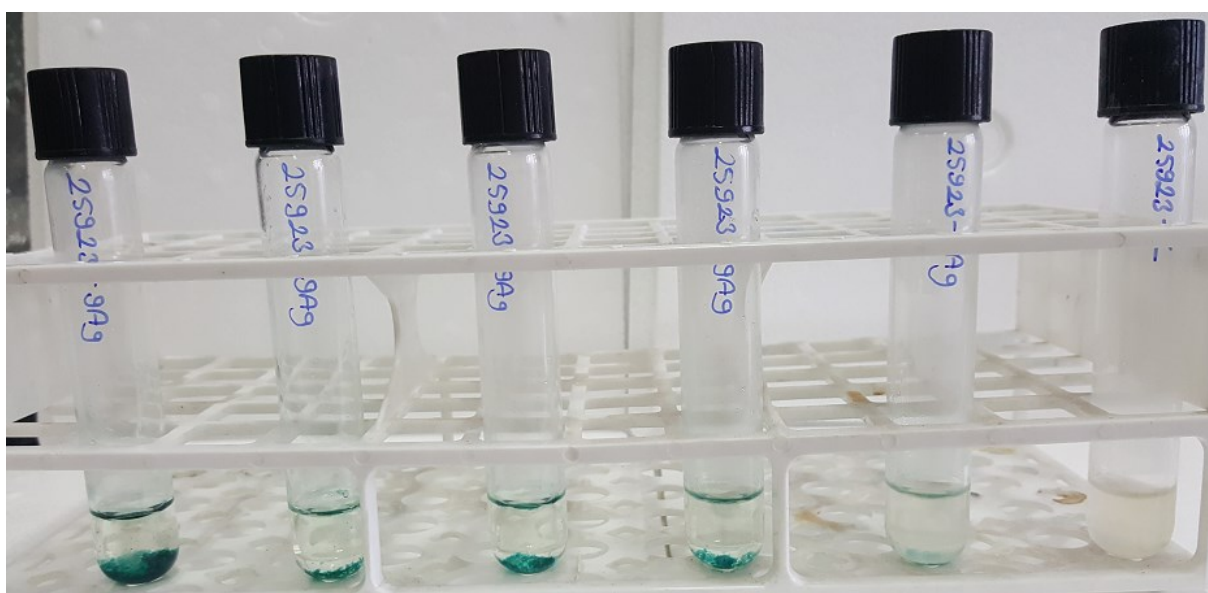
**Fig. S40.** Compound **5** - *S.aureus* MIC test results (concentration of compound **5** in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 9 refers to compound **5**)



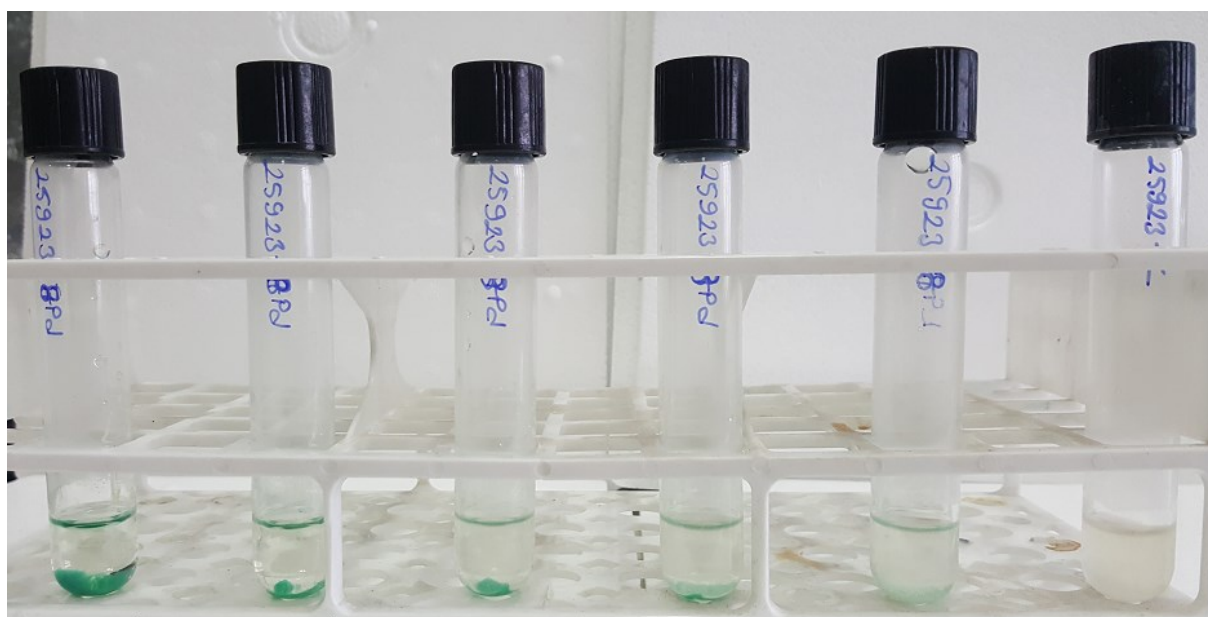
**Fig. S41.** Compound **3+Ag** - *S.aureus* MIC test results (concentration of compound **3+Ag** in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 7Ag refers to compound **3+Ag**)



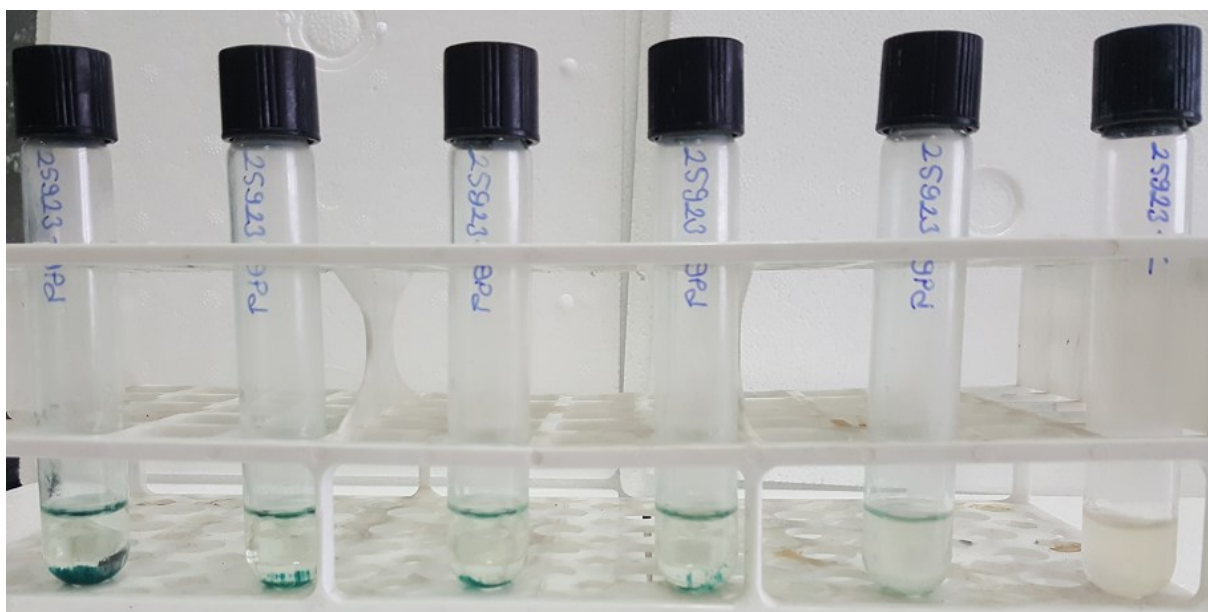
**Fig. S42.** Compound 4+Ag - *S.aureus* MIC test results (concentration of compound 4+Ag in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 8Ag refers to compound 4+Ag)



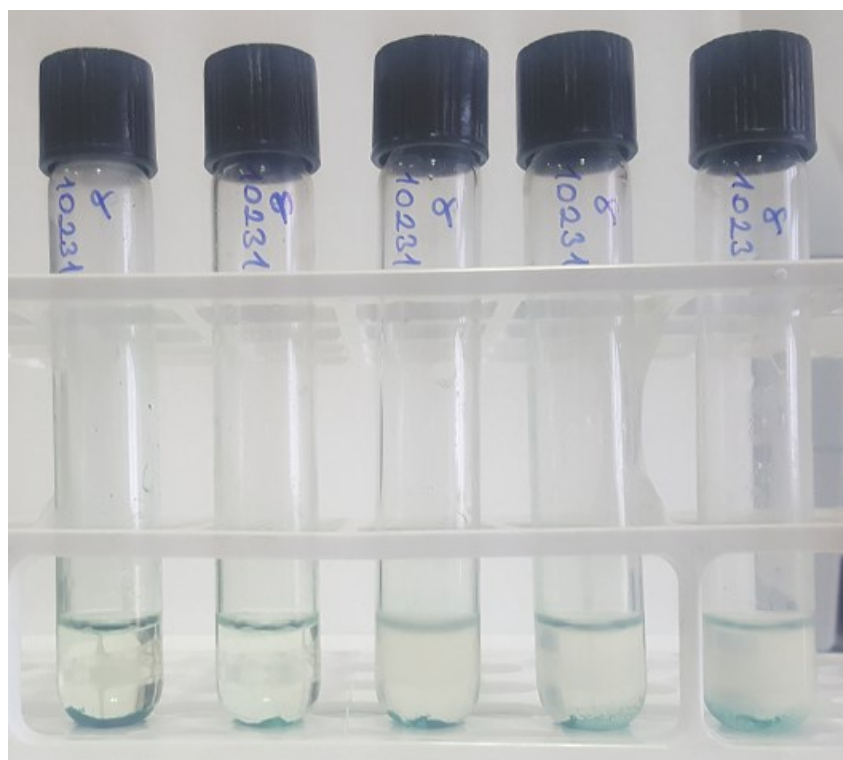
**Fig. S43.** Compound 5+Ag - *S.aureus* MIC test results (concentration of compound 5+Ag in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 9Ag refers to compound 5+Ag)



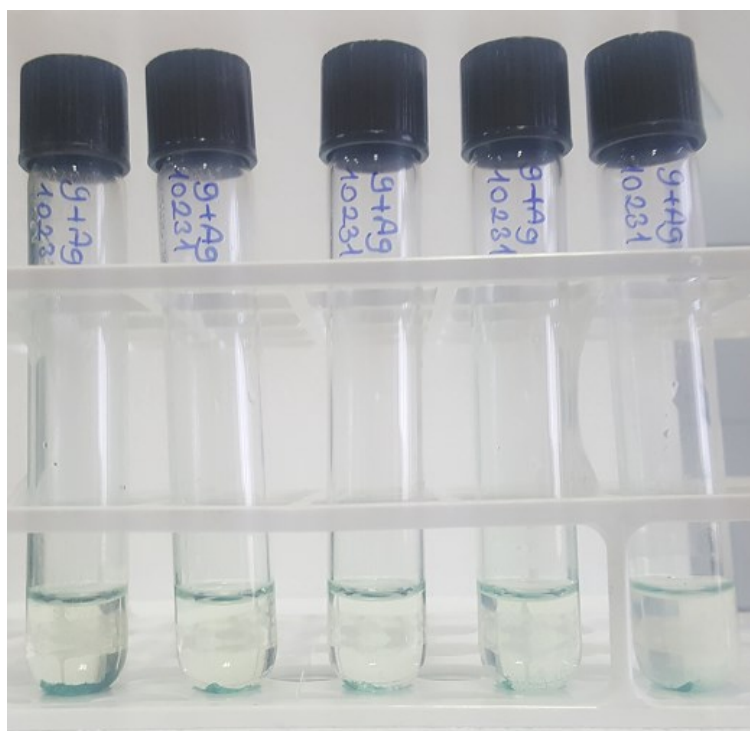
**Fig. S44.** Compound **4+Pd** - *S.aureus* MIC test results (concentration of compound **4+Pd** in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 8Pd refers to compound **4+Pd**)



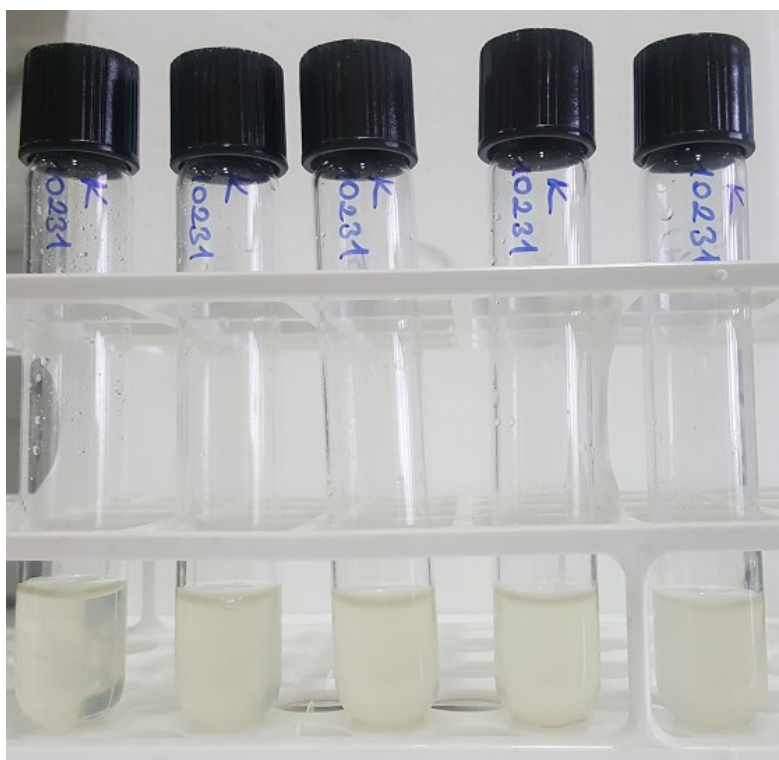
**Fig. S45.** Compound **5+Pd** - *S.aureus* MIC test results (concentration of compound **5+Pd** in tubes from left to right: 100-50-25-12.5-6.25-0  $\mu\text{g/mL}$ ; K = control; number 9Pd refers to compound **5+Pd**)



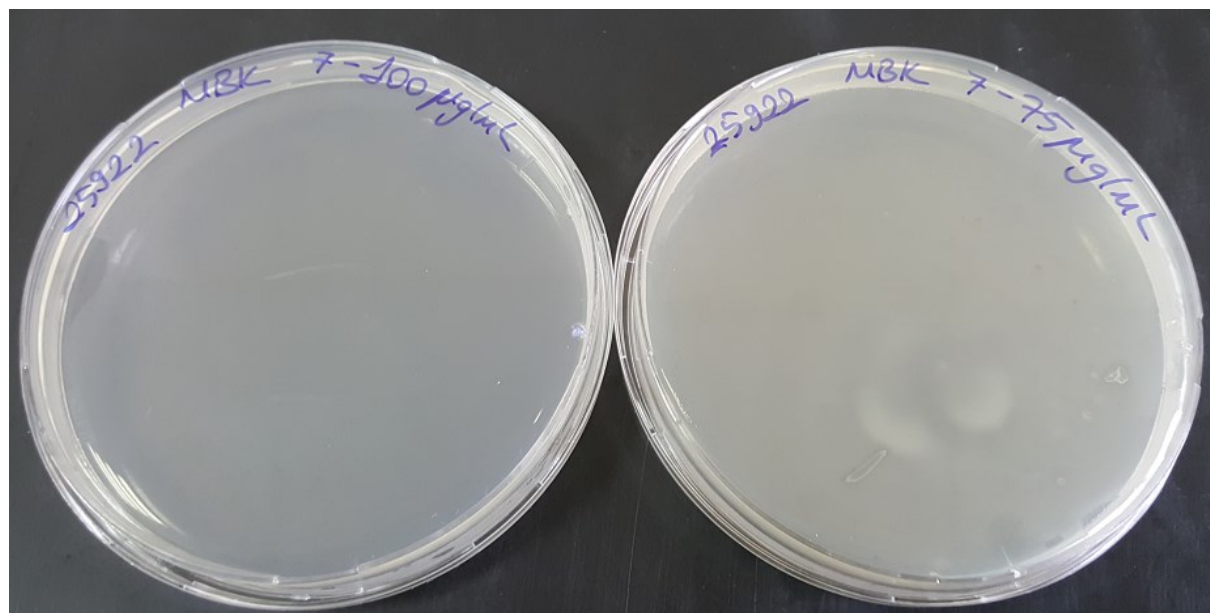
**Fig. S46.** Compound 4 - *C.albicans* MIC test results (concentration of compound 4 in tubes from left to right: 100-50-25-12.5-6.25 µg/mL; number 8 refers to compound 4)



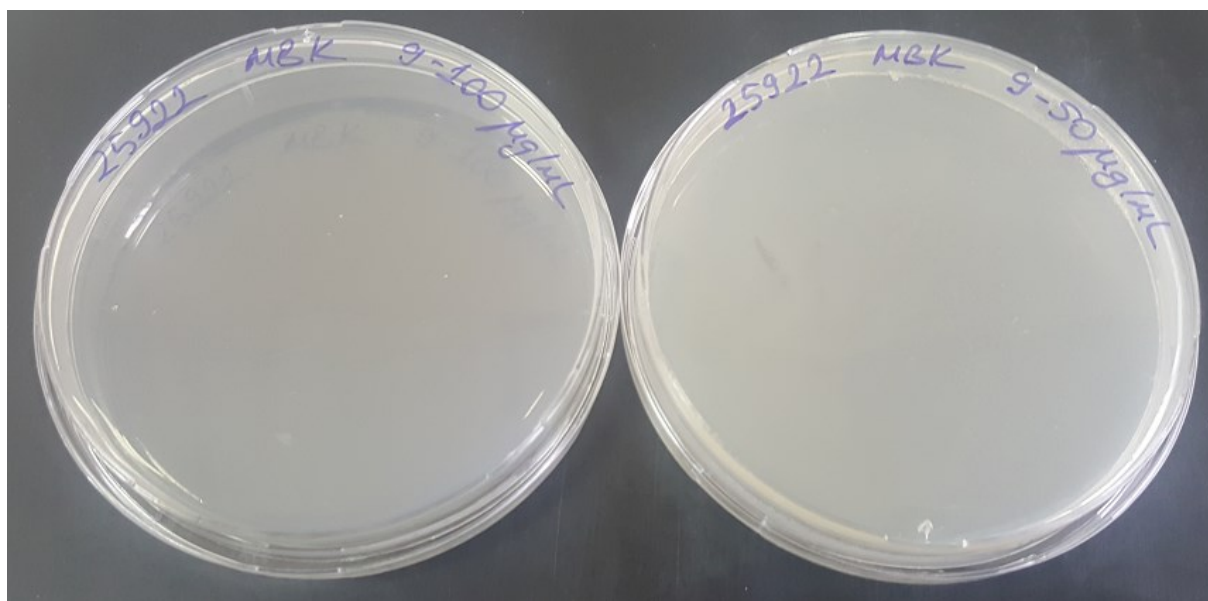
**Fig. S47.** Compound **5+Ag** - *C.albicans* MIC test results (concentration of compound **5+Ag** in tubes from left to right: 100-50-25-12.5-6.25  $\mu\text{g/mL}$ ; number 9+Ag refers to compound **5+Ag**)



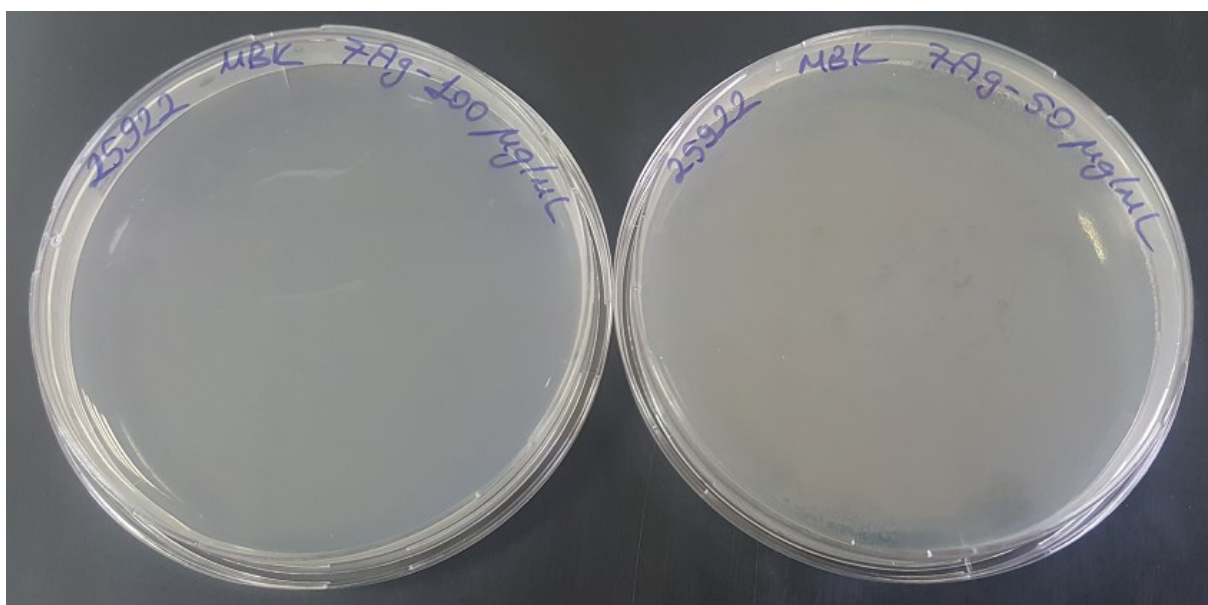
**Fig. S48.** *C.albicans* MIC test results of controls (DMF amount in tubes from left to right: adjusted to match the solvent amounts of phthalocyanine compounds at a concentration of 100-50-25-12.5-6.25  $\mu\text{g}/\text{mL}$ )



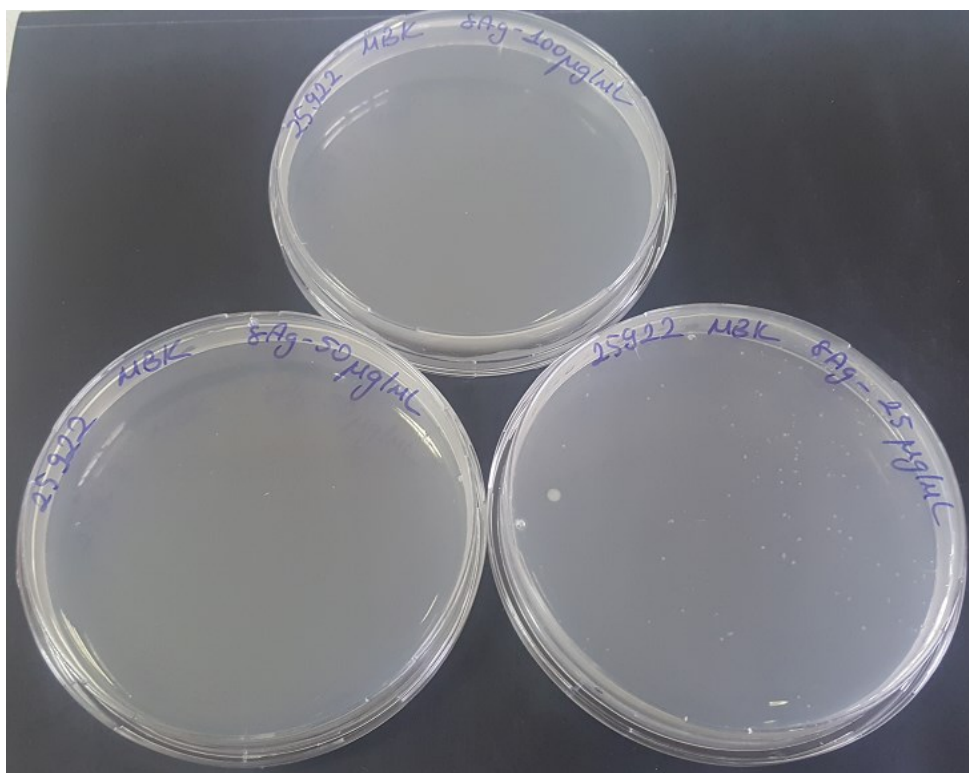
**Fig. S49.** Compound 3 - *E.coli* MBC test results (number 7 refers to compound 3)



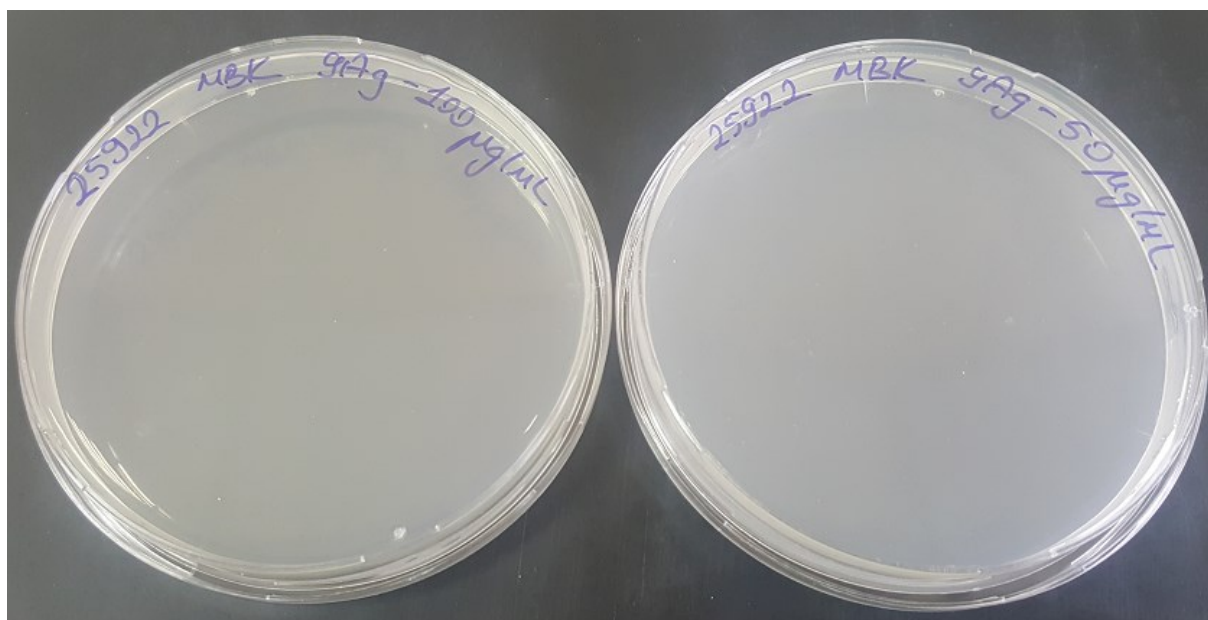
**Fig. S50.** Compound **5** - *E.coli* MBC test results (number 9 refers to compound **5**)



**Fig. S51.** Compound **3+Ag** - *E.coli* MBC test results (number 7Ag refers to compound **3+Ag**)

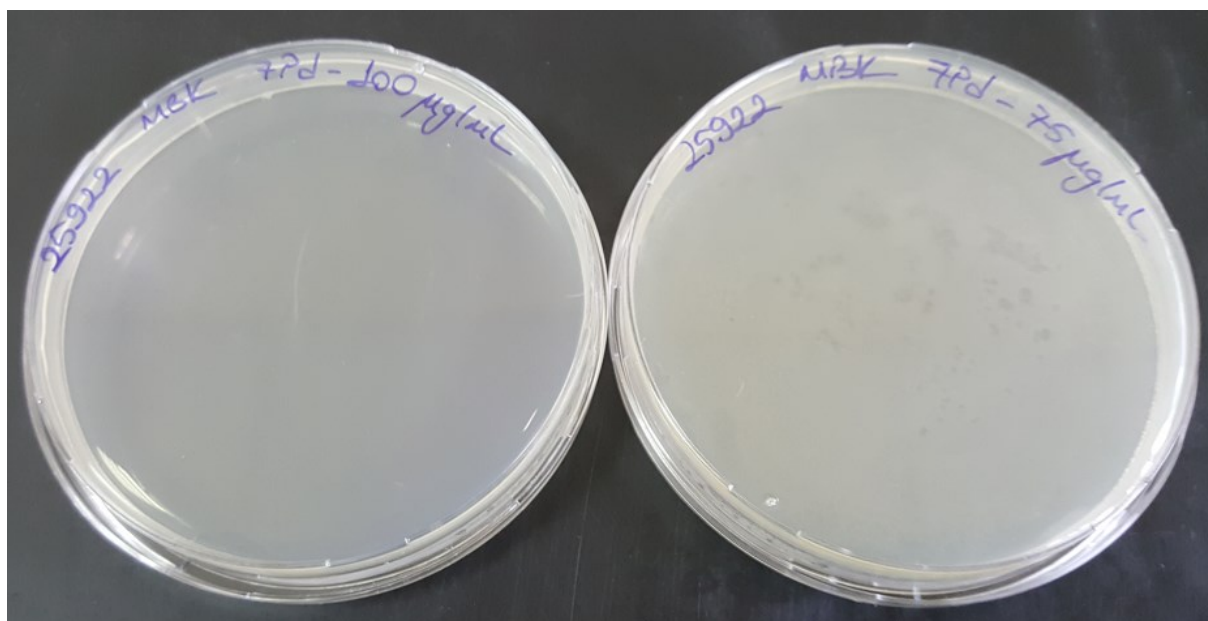


**Fig. S52.** Compound 4+Ag - *E.coli* MBC test results (number 8Ag refers to compound 4+Ag)

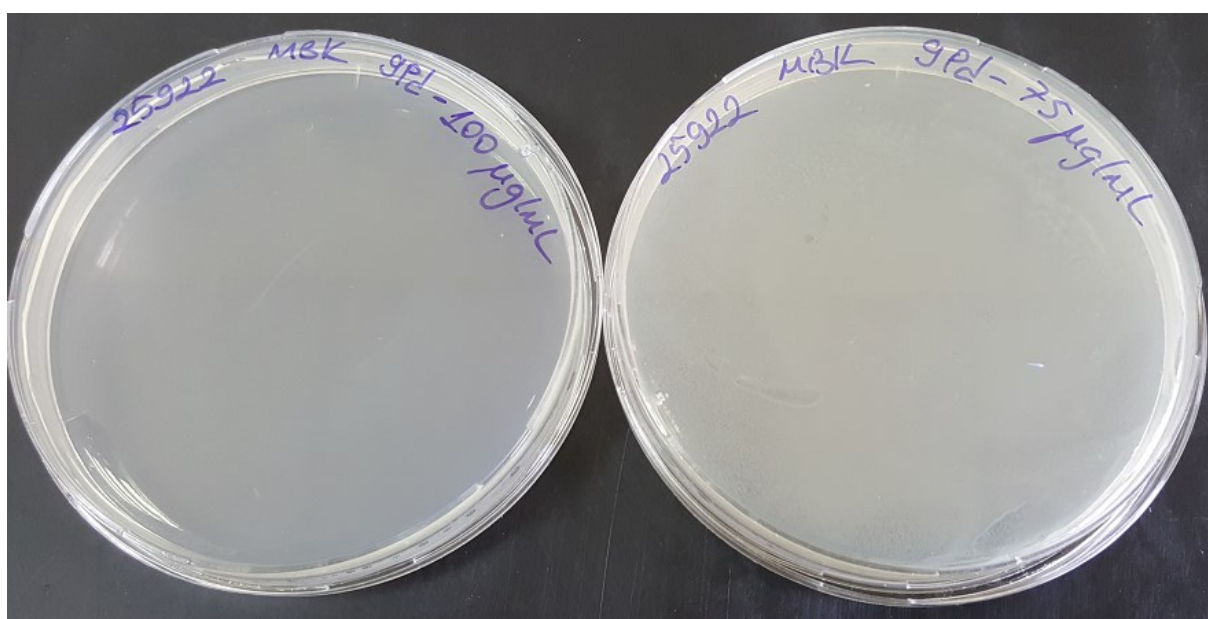


**Fig. S53.** Compound 5+Ag - *E.coli* MBC test results (number 9Ag refers to compound 5+Ag)

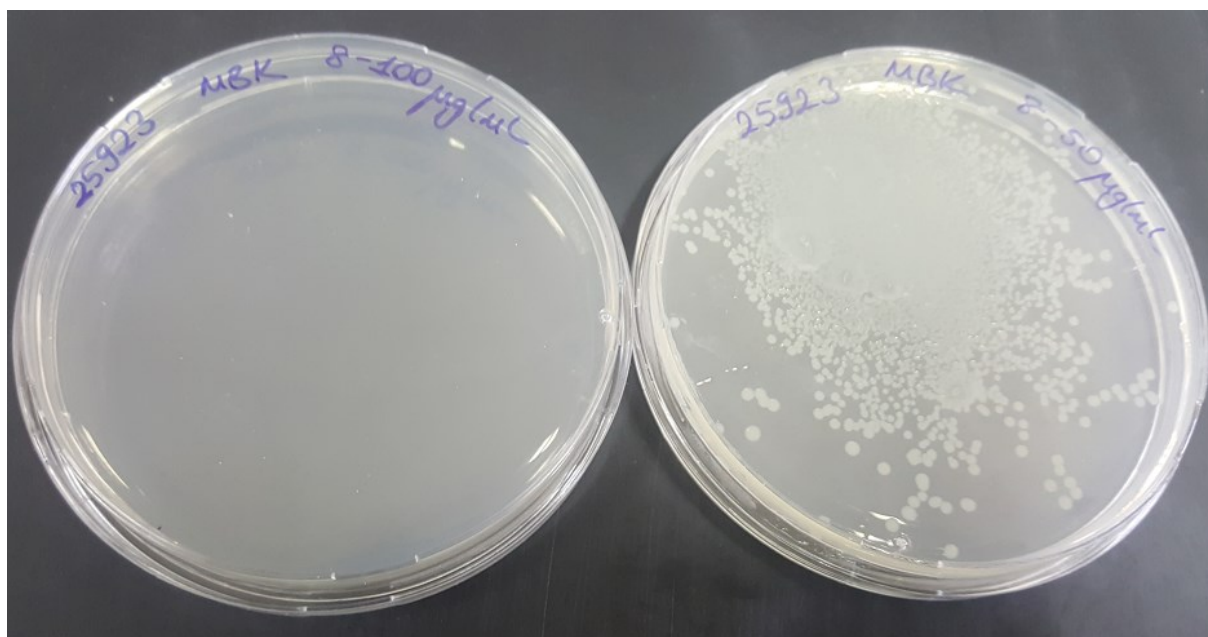




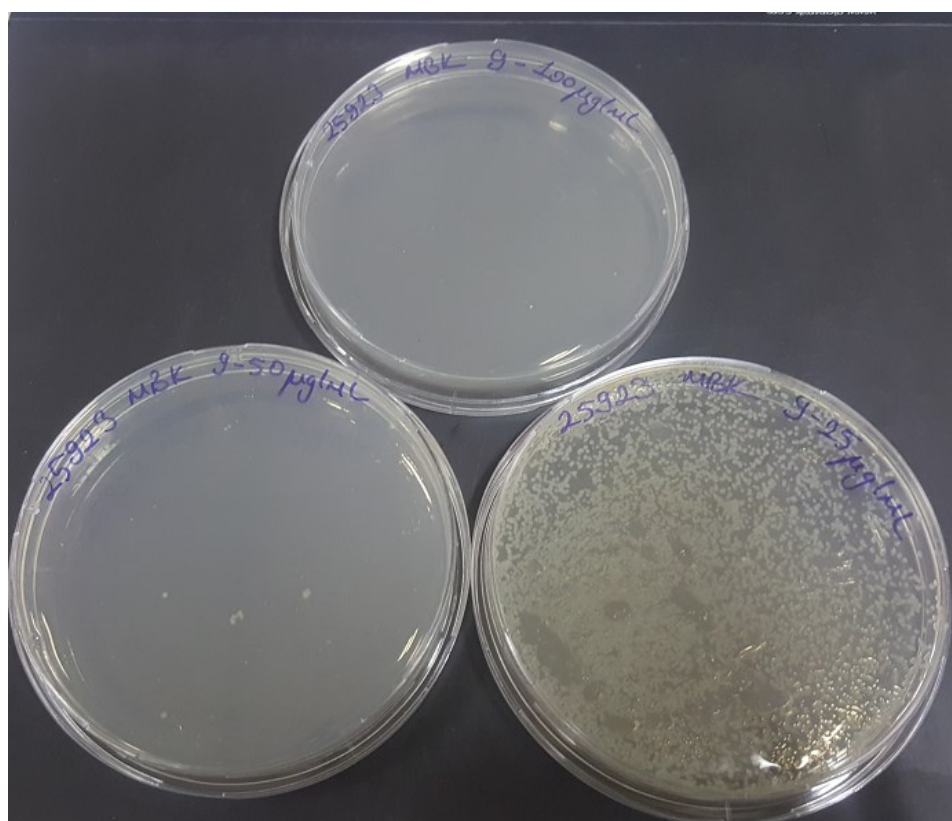
**Fig. S54.** Compound **3+Pd** - *E.coli* MBC test results (number 7Pd refers to compound **3+Pd**)



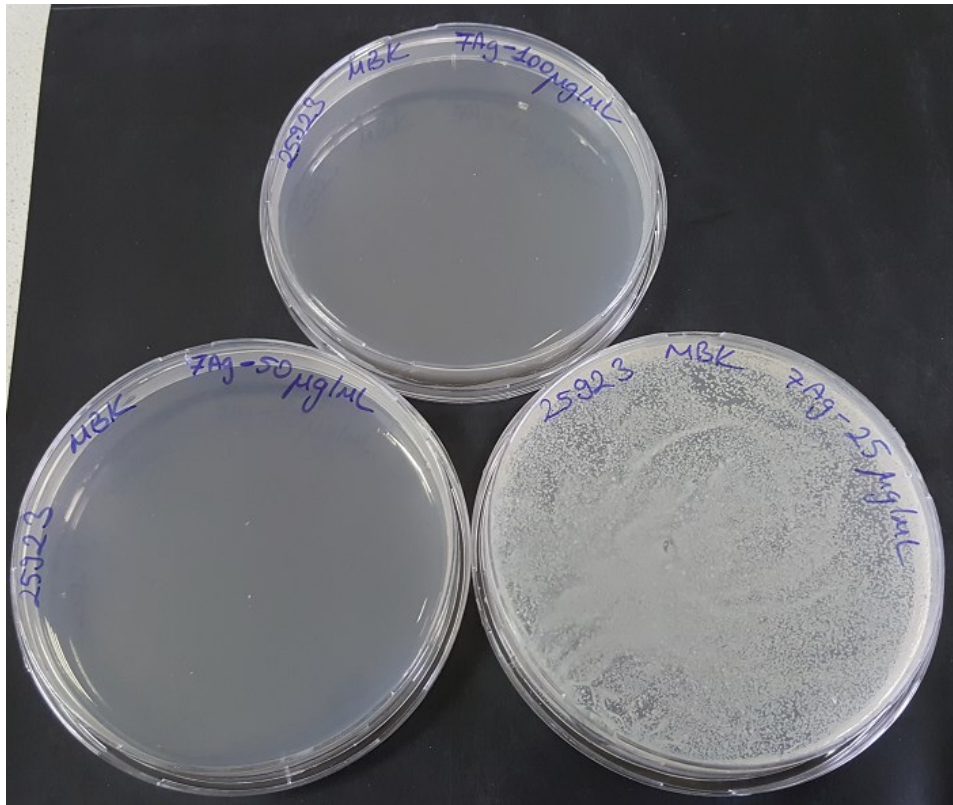
**Fig. S55.** Compound **5+Pd** - *E.coli* MBC test results (number 9Pd refers to compound **5+Pd**)



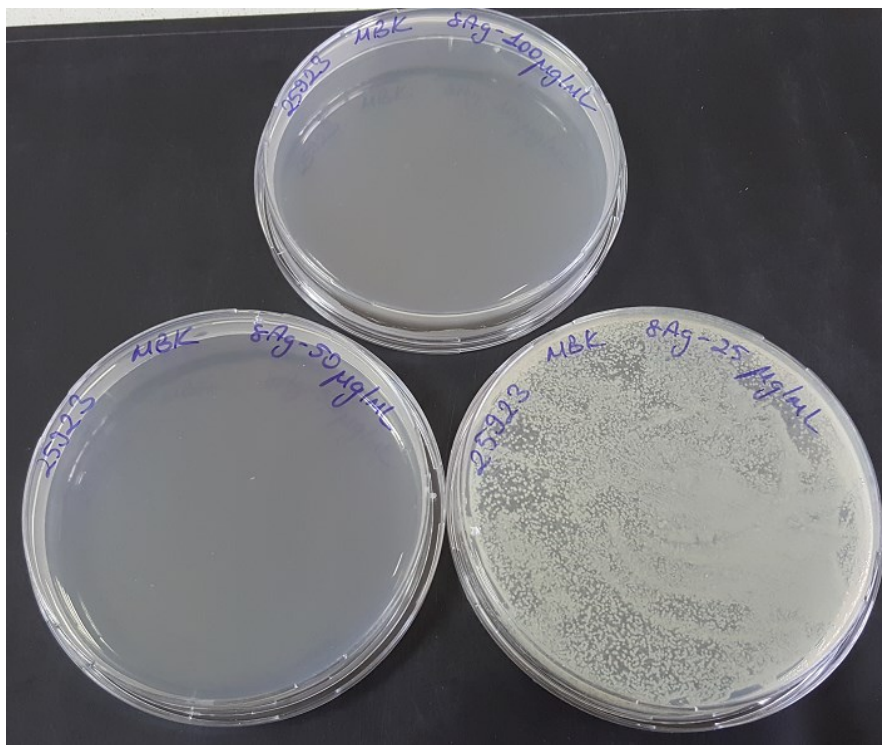
**Fig. S56.** Compound 4 *S.aureus* MBC test results (number 8 refers to compound 4)



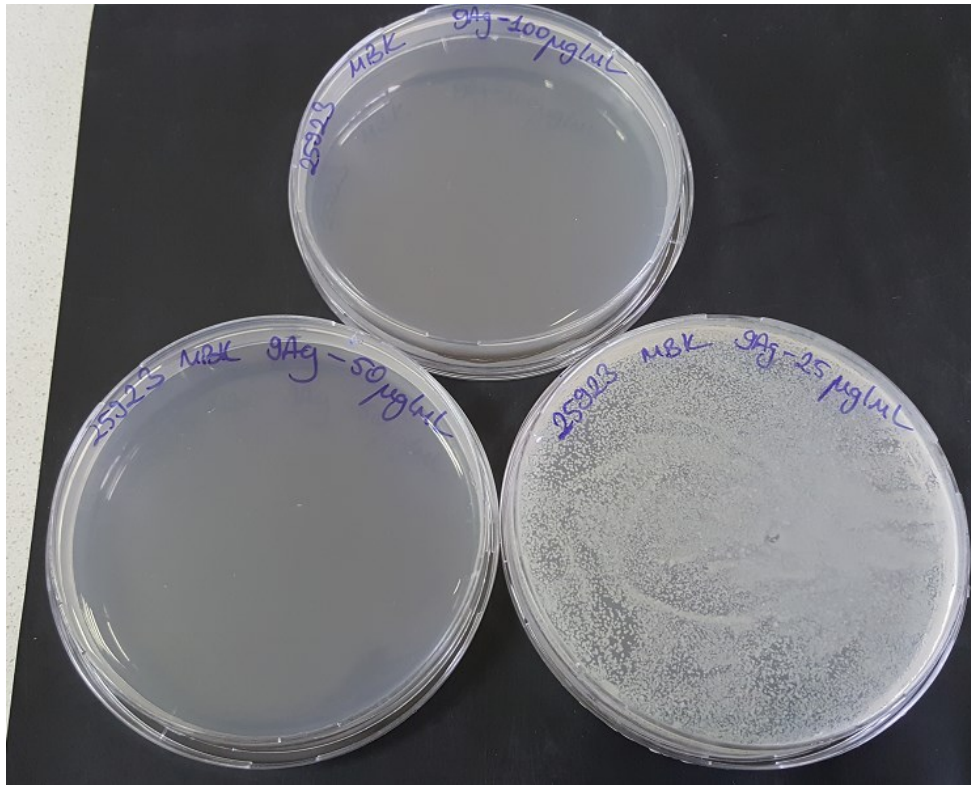
**Fig. S57.** Compound 5 *S.aureus* MBC test results (number 9 refers to compound 5)



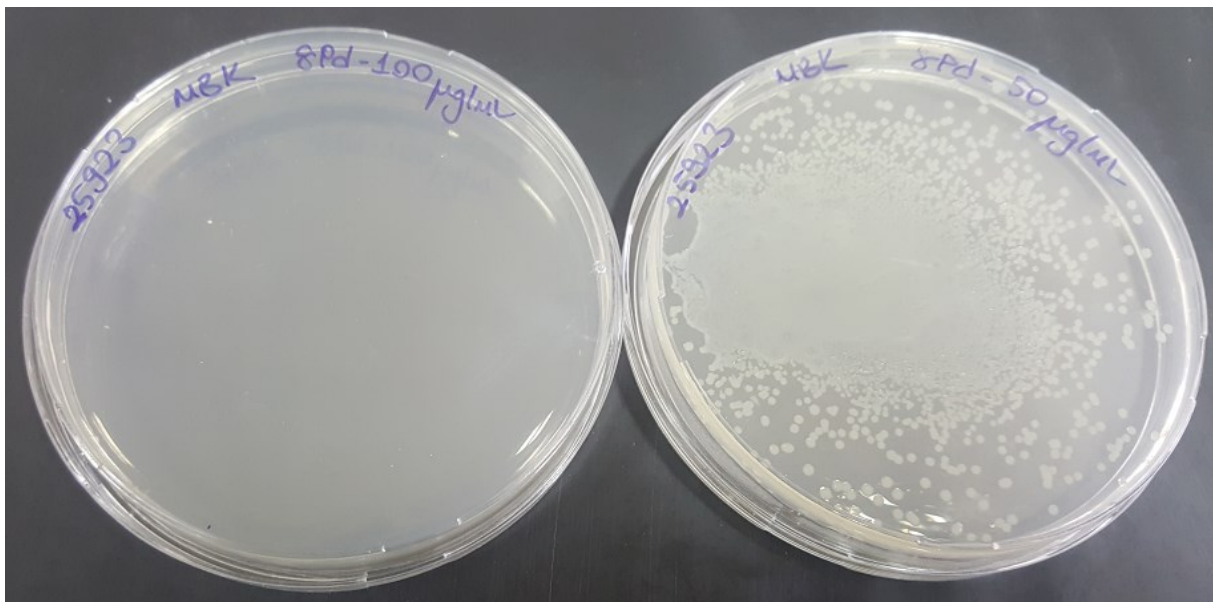
**Fig. S58.** Compound 3+Ag *S.aureus* MBC test results (number 7Ag refers to compound 3+Ag)



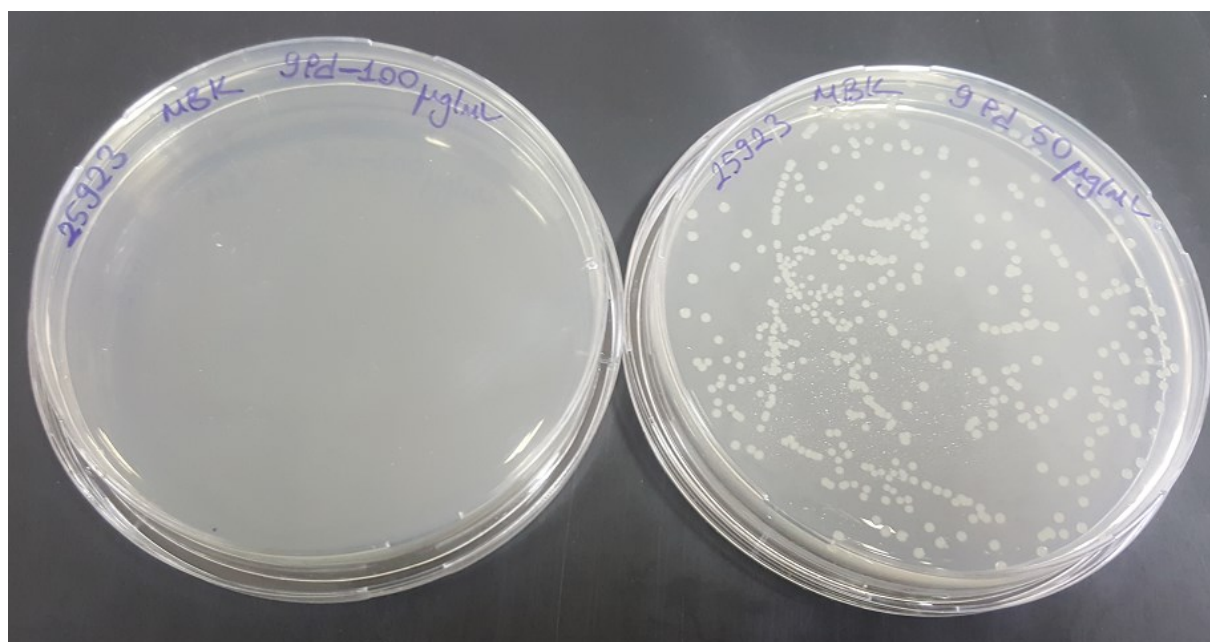
**Fig. S59.** Compound 4+Ag *S.aureus* MBC test results (number 8Ag refers to compound 4+Ag)



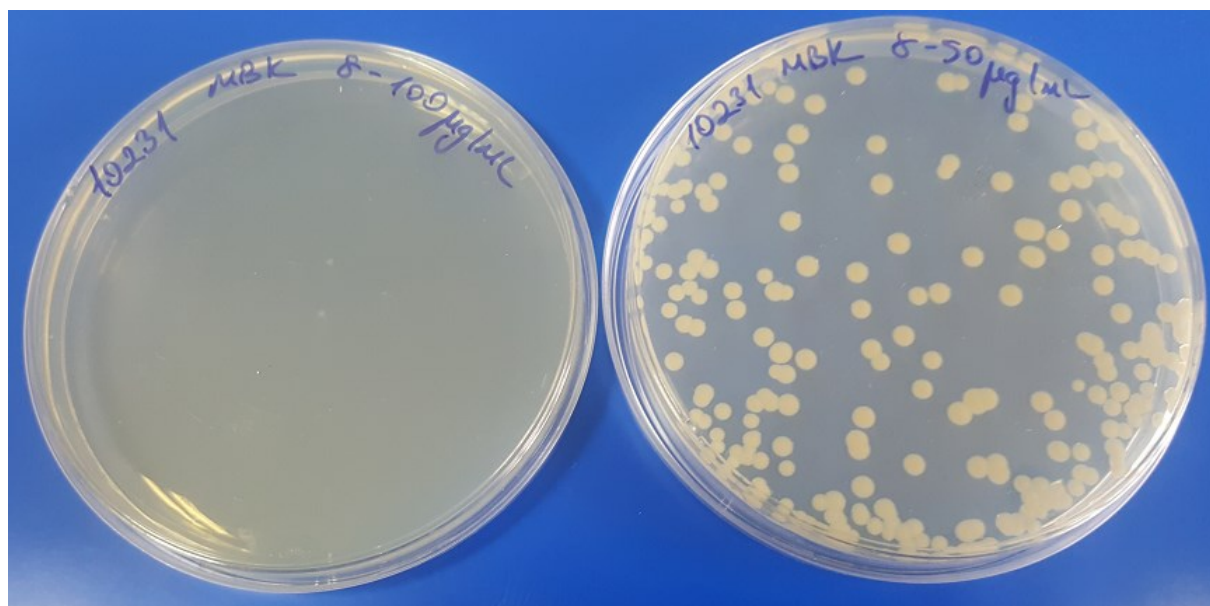
**Fig. S60.** Compound **5+Ag** *S.aureus* MBC test results (number 9Ag refers to compound **5+Ag**)



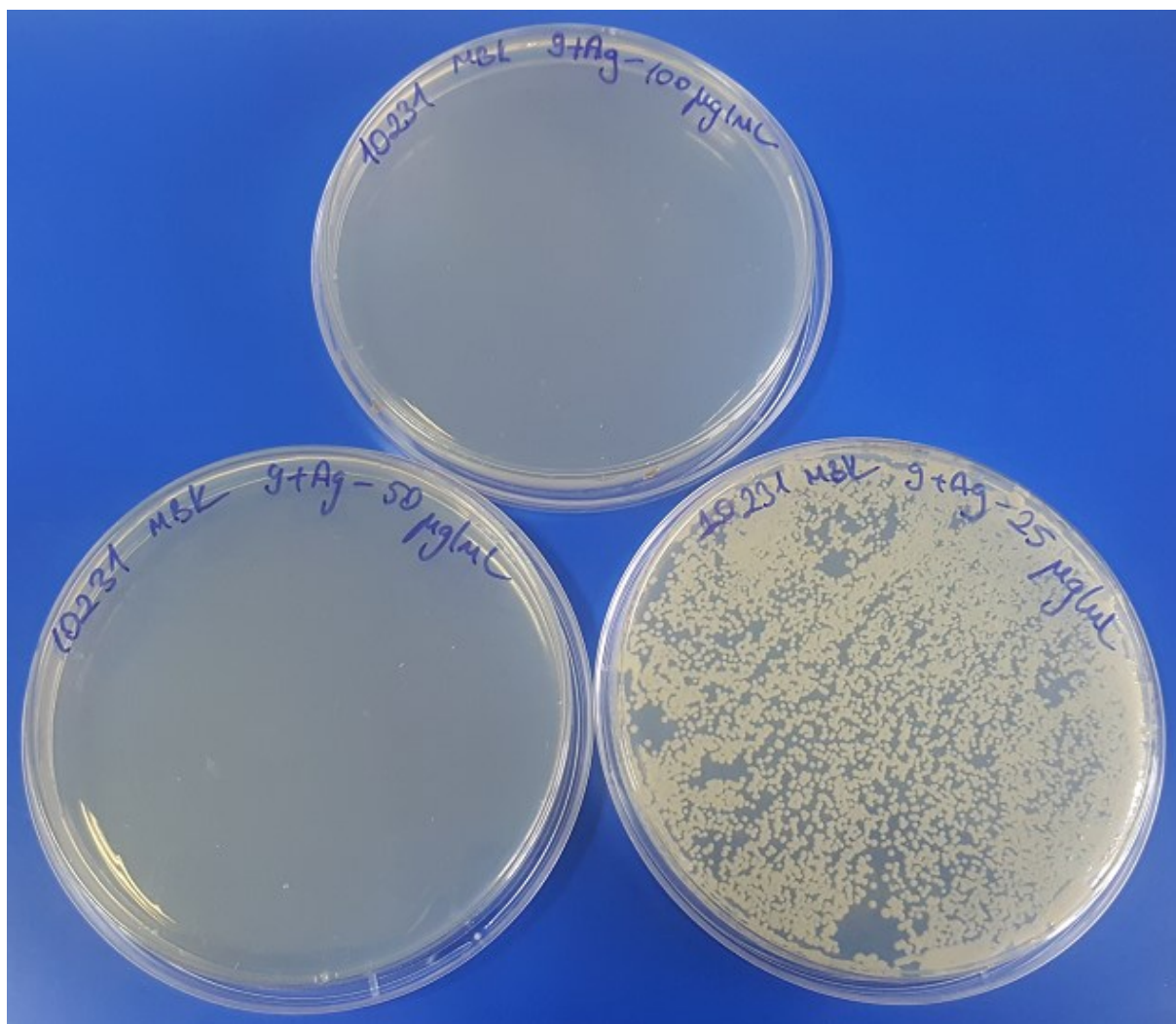
**Fig. S61.** Compound **4+Pd** *S.aureus* MBC test results (number 8Pd refers to compound **4+Pd**)



**Fig. S62.** Compound **5+Pd** *S.aureus* MBC test results (number 9Pd refers to compound **5+Pd**)



**Fig. S63.** Compound **4** *C.albicans* MBC test results (number 8 refers to compound **4**)



**Fig. S64.** Compound **5+Ag** *C.albicans* MBC test results (number 9Ag refers to compound **5+Ag**)