Electronic Supplementary Material (ESI) for CrystEngComm.

Synthesis, Structure diversity, and Antimicrobial Studies of Ag(I) Complexes with Quinoline-type Ligands

Amal Yousry[1], Matti Haukka[2], Morsy A. M. Abu-Youssef[1*], Mohammed Salah Ayoup[1*], Magda M. F. Ismail [3], Nagwan G. El Menofy[4], Saied M. Soliman[1], Assem Barakat[5], Francoise M. Amombo Noa[6], Lars Öhrström[6*]

[1] Department of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Ibrahimia, Alexandria 21321, Egypt. Emails: saied1soliman@yahoo.com (SMS) and morsy5@alexu.edu.eg (MAMA).

[2] Department of Chemistry, University of Jyväskylä, P.O. Box 35, FI-40014 Jyväskylä, Finland; matti.o.haukka@jyu.fi

[3]Department of pharmaceutical Medicinal Chemistry, Faculty of Pharmacy (Girls), Al-Azhar University, Cairo, Egypt. m.elalfy101@gmail.com

[4]Department of Microbiology and Immunology, Faculty of Pharmacy (Girls), Al-Azhar University, Cairo, Egypt.

[5] Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia; ambarakat@ksu.edu.sa

[6]Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-41296 Gothenburg, Sweden

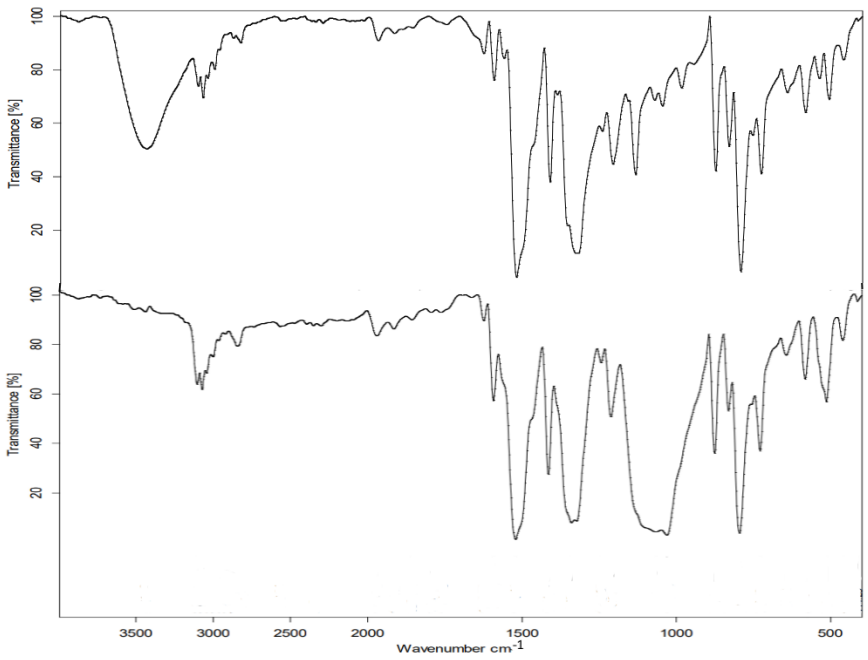
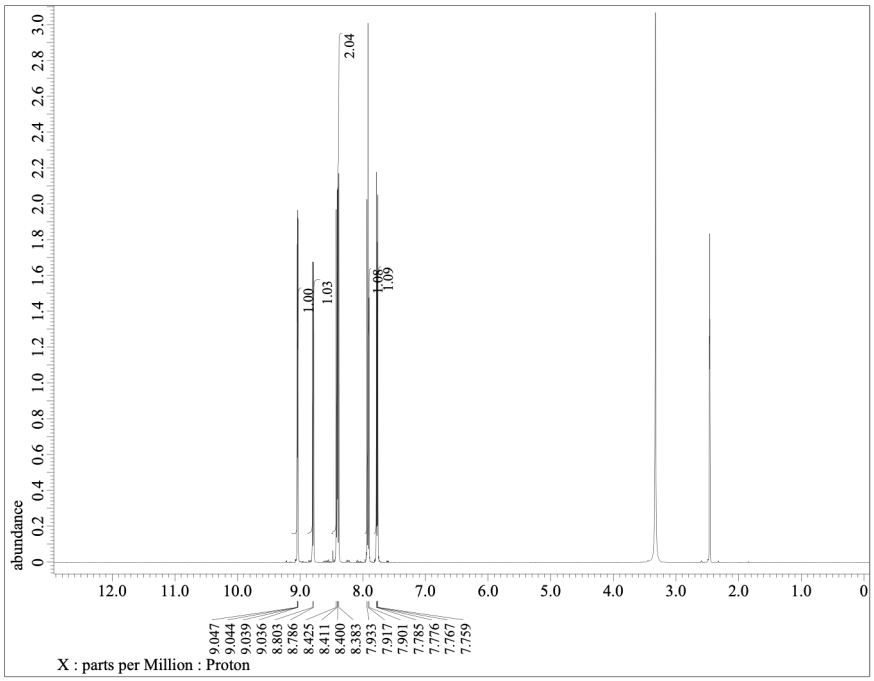


Figure S1. FTIR spectra of the free ligand (**5NO$_2$Qu**); (upper) and; the [Ag(5NO$_2$Qu)$_2$]BF$_4$ (**1**) complex (lower).



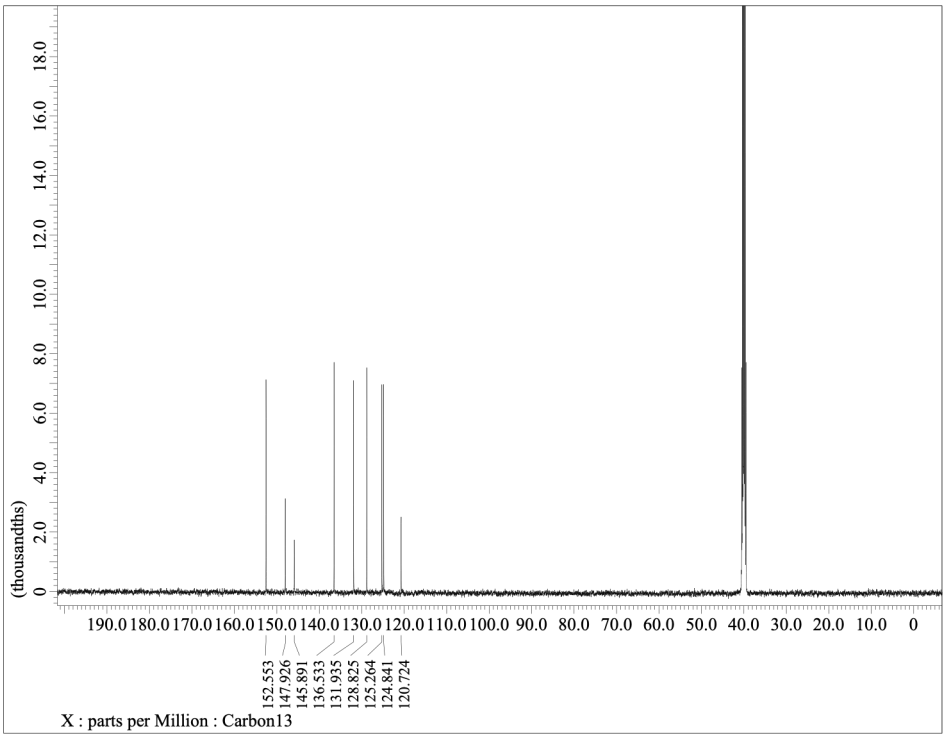
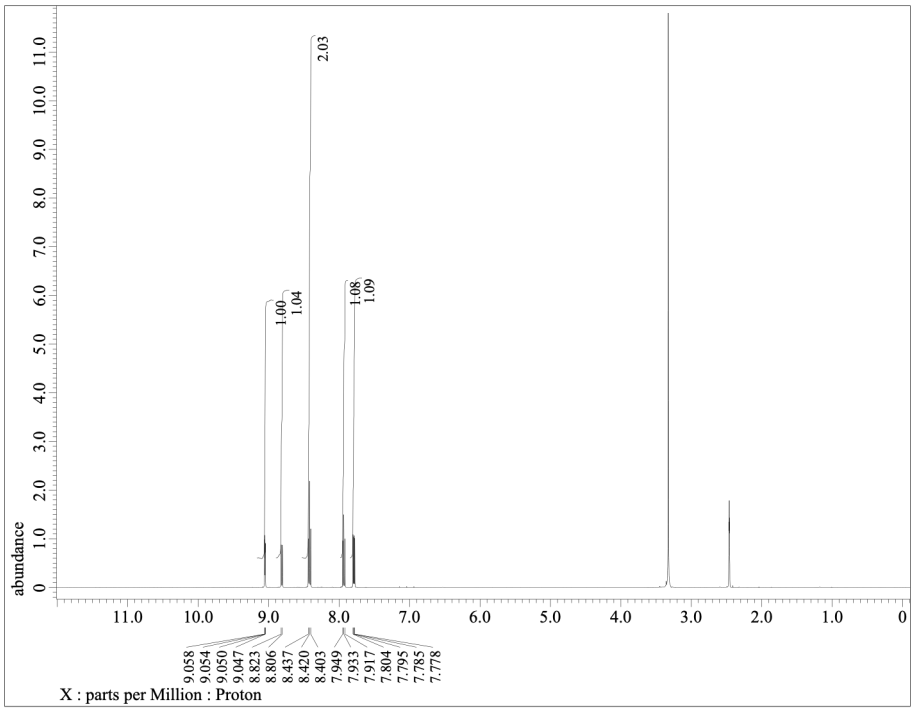


Figure S2 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of the free ligand **$5NO_2Qu$**.



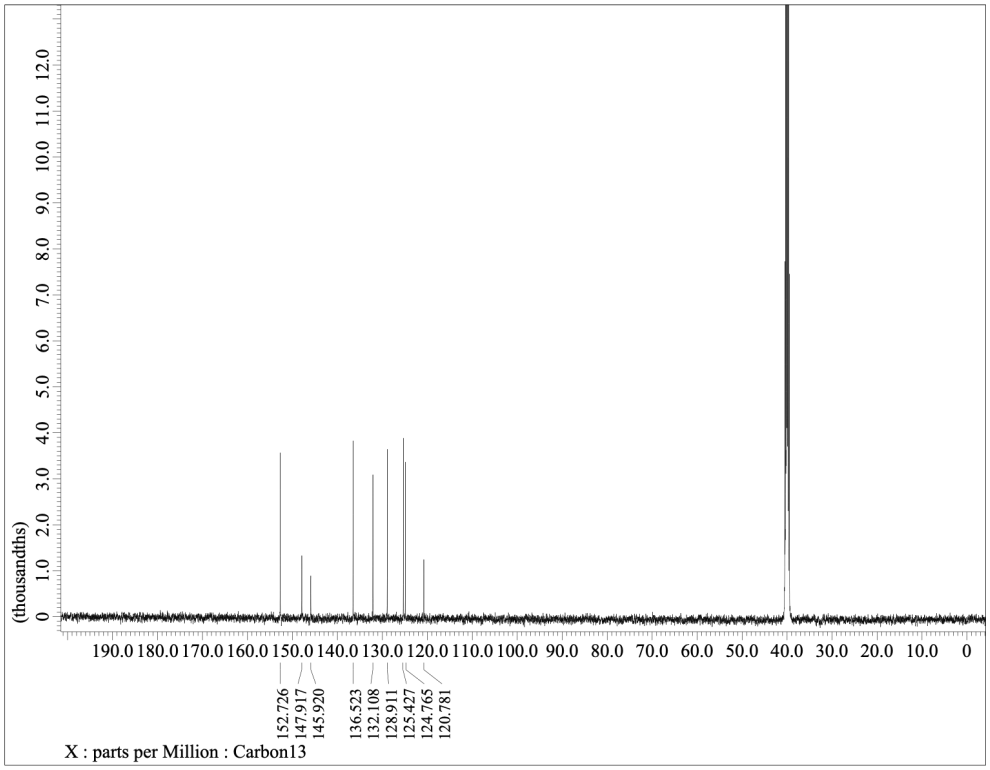
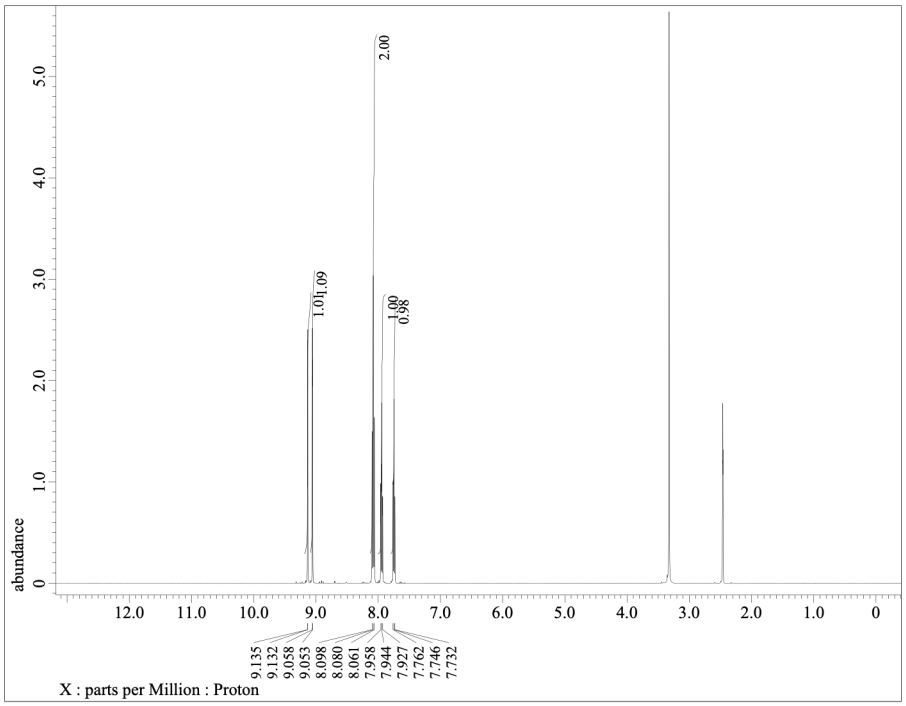


Figure S3 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of the $[Ag(5NO_2Qu)_2]BF_4$ (**1**) complex.


abundance
0
1.0
2.0
3.0
4.0
5.0
2.00
1.01
1.09
1.00
0.98
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.135
9.132
9.058
9.053
8.098
8.080
8.061
7.958
7.944
7.927
7.762
7.746
7.732
X : parts per Million : Proton

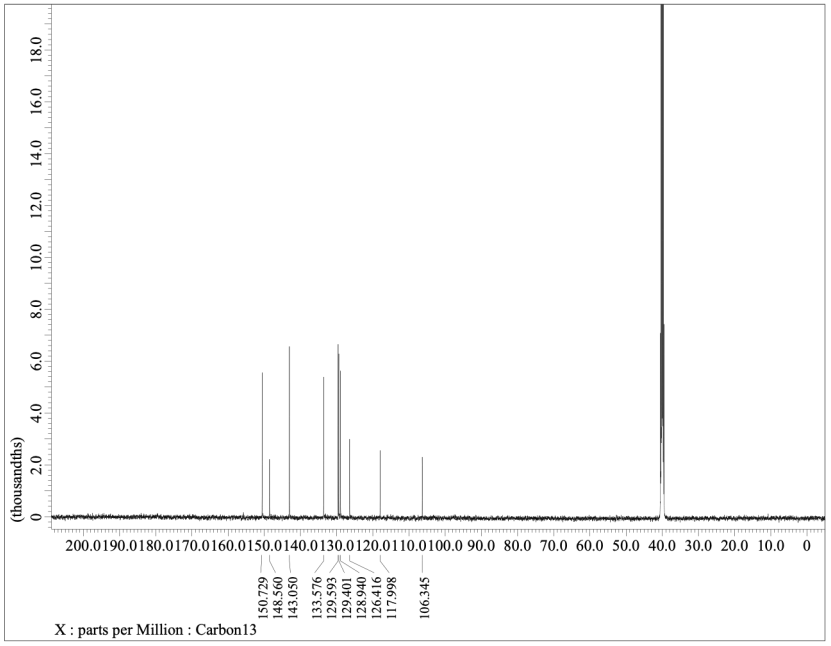

(thousandths)
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
150.729
148.560
143.050
133.576
129.593
129.401
128.940
126.416
117.998
106.345
X : parts per Million : Carbon13

Figure S4 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of the free ligand (**Qu3CN**).

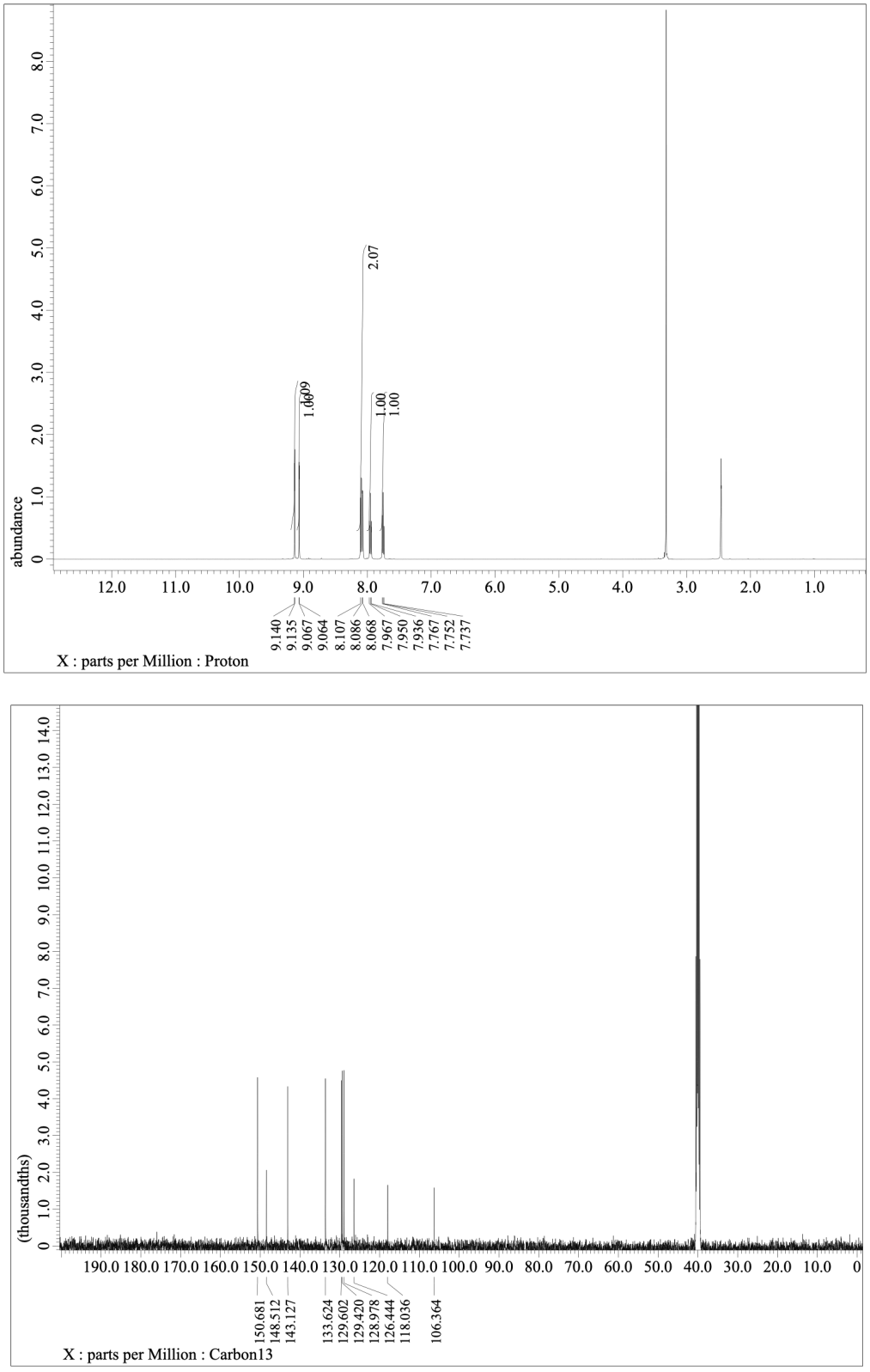


Figure S5 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of the $[Ag(Qu3CN)(H_2O)]_n(BF_4)_n$ (**2**) complex.

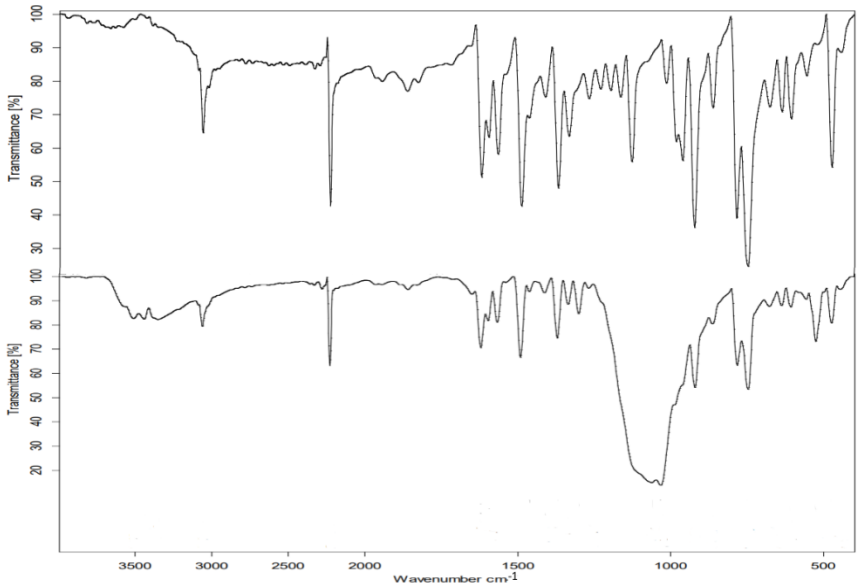


Figure S6 FTIR spectra of the free ligand (**Qu3CN**); (upper) and; the $[Ag(Qu3CN)(H_2O)]_n(BF_4)_n$ (**2**) polymer (lower).

CSD analysis of C-NO2 … Ag interactions

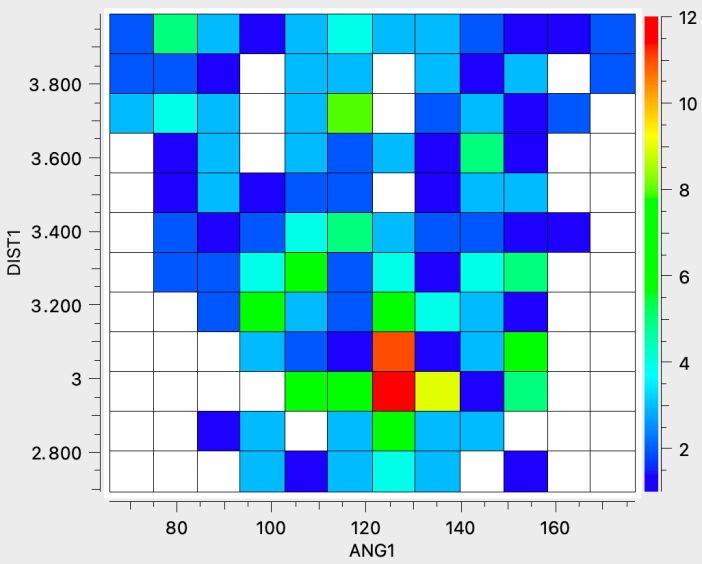


Figure S7 FTIR Heat plot of Ag…O distances and N-O…Ag angles, a clear peak 120°-130° at distances 2.9 Å – 3.1 Å

Method S1

Antimicrobial activity of the two Ag(I) complexes and the free ligand was screened against Gram-positive bacteria ; *Staphylococcus aureus* (ATCC 25923), Methicillin-resistant *Staphylococcus aureus* (MRSA ATCC 43300), MRSA *(1)* clinical isolates and multidrug resistant (MDR) *Enterococcus fecium* (31) clinical isolates and against Gram-negative bacteria including; *Klebsiella pneumonia* (ATCC 700603), *Pseudomonas aeruginosa* (ATCC 29853), *Escherichia coli* (ATCC 25922), *Acinetobacter baumannii* (ATCC 19606), MDR clinical isolates including two *Klebsiella pneumonia* isolates (50 & R124), one *Pseudomonas aeruginosa* (5) isolate, *Proteus mirabilis* and one *Acinetobacter baumannii (8)* in addition to one fungal isolate; *Candida albicans* for determination of their minimum inhibitory concentration according to the CLSI reference standards. The most active compounds were further tested for determination of their minimum bactericidal concentration.

Determination of minimum inhibitory concentration (MIC)

Investigation of antimicrobial activity of the studied compounds was performed by microbroth dilution assay for determination of minimum inhibitory concentration (MIC). In summary, 100 µL of Muller-Hinton broth (MHB) (Oxoid® Limited, Basingstoke, UK) were disseminated in 96 multi-well microtiter plates, followed by the addition of 100 µL of the tested compound into the first row of the microtiter plate. Then, from the first to the twelfth well, serial dilutions was performed. Each well received 7 µL of freshly prepared bacterial or fungi suspension (1.5×10^8 cfu/mL). For each bacterial or fungi strain, positive and negative controls were carried out. Plates were incubated for 18-24 hours at 37 ˚C, with Amoxicillin 1000 µg/mL serving as reference standard antibiotic. The MIC was estimated as the minimum concentration that demonstrated no detectable bacterial growth.

Determination of minimum bactericidal concentrations (MBC)

The minimum bactericidal concentrations (MBC), was determined by inoculating 10 µL from each corresponding wells that showed no apparent growth in multi-well microtiter plates onto Muller-Hinton agar (MHA) and incubating the agar plates at 37°C for 24 hours. MBC was determined as the lowest concentration that demonstrated no bacterial growth on the agar surfaces.