Electronic Supplementary Information (ESI)

for

Water-soluble silver(I) complexes with N-donor benzimidazole ligands containing imidazolium core: Stability and preliminary biological studies

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Table S1. Selected geometric parameters for **4**.

Bond lengths (Å)			
Ag1─N1	2.135(4)	N4─C12	1.241(9)
Ag1─N5	2.144(4)	N5─C14	1.311(6)
N1─C1	1.316(6)	N6─C14	1.347(6)
N2─C1	1.339(7)	N7─C25	1.319(6)
N3─C12	1.264(9)	N8─C25	1.322(7)
Bond angles (°)			
N1─Ag1─N5	164.33(15)	C11─N4─C10	121.3(7)
N1─C1─N2	111.5(5)	C14─N5─C15	106.4(4)
C1─N1─C2	106.1(4)	C14─N6─C20	107.8(4)
C1─N2─C7	108.5(4)	C25─N7─C22	109.3(5)
C12─N3─C8	135.2(7)	C25─N7─C21	126.1(5)
C12─N3─C9	104.9(7)	C22─N7─C21	124.5(5)
C8─N3─C9	119.7(6)	C25─N8─C23	108.8(5)
C12─N4─C11	134.6(8)	C25─N8─C24	126.1(6)
C12─N4─C10	103.8(7)	C23─N8─C24	125.0(6)

Table S2. Crystal data and structure refinement parameters for **4**.

CCDC depository	2062835
Colour/shape	Colorless/prism
Chemical formula	$C_{26}H_{30}AgN_{11}O_9$
Formula weight	748.48
Temperature (K)	296(2)
Wavelength (Å)	0.71073 Mo Kα
Crystal system	Monoclinic
Space group	$P2_1/c$ (No. 14)
Unit cell parameters	
a, b, c (Å)	14.8453(6), 15.1725(7), 14.2740(6)
α, β, γ (°)	90, 105.931(3), 90
Volume (Å^3)	3091.6(2)
Z	4
$D_{calc.}$ (g/cm^3)	1.608
μ (mm^{-1})	0.723
Absorption correction	Integration
$T_{min.}$, $T_{max.}$	0.8166, 0.9663
F_{000}	1528
Crystal size (mm^3)	0.70 × 0.49 × 0.10
Diffractometer	STOE IPDS II
Measurement method	ω scan
Index ranges	$-19 \le h \le 19$, $-19 \le k \le 19$, $-18 \le l \le 17$
θ range for data collection (°)	$1.959 \le \theta \le 27.677$
Reflections collected	25008
Independent/observed reflections	7191/3818
$R_{int.}$	0.0904
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7191/0/428
Goodness-of-fit on F^2	0.994
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0683$, $wR_2 = 0.1196$
R indices (all data)	$R_1 = 0.1406$, $wR_2 = 0.1411$
$\Delta\rho_{max.}$, $\Delta\rho_{min.}$ (e/Å^3)	0.87, −0.27

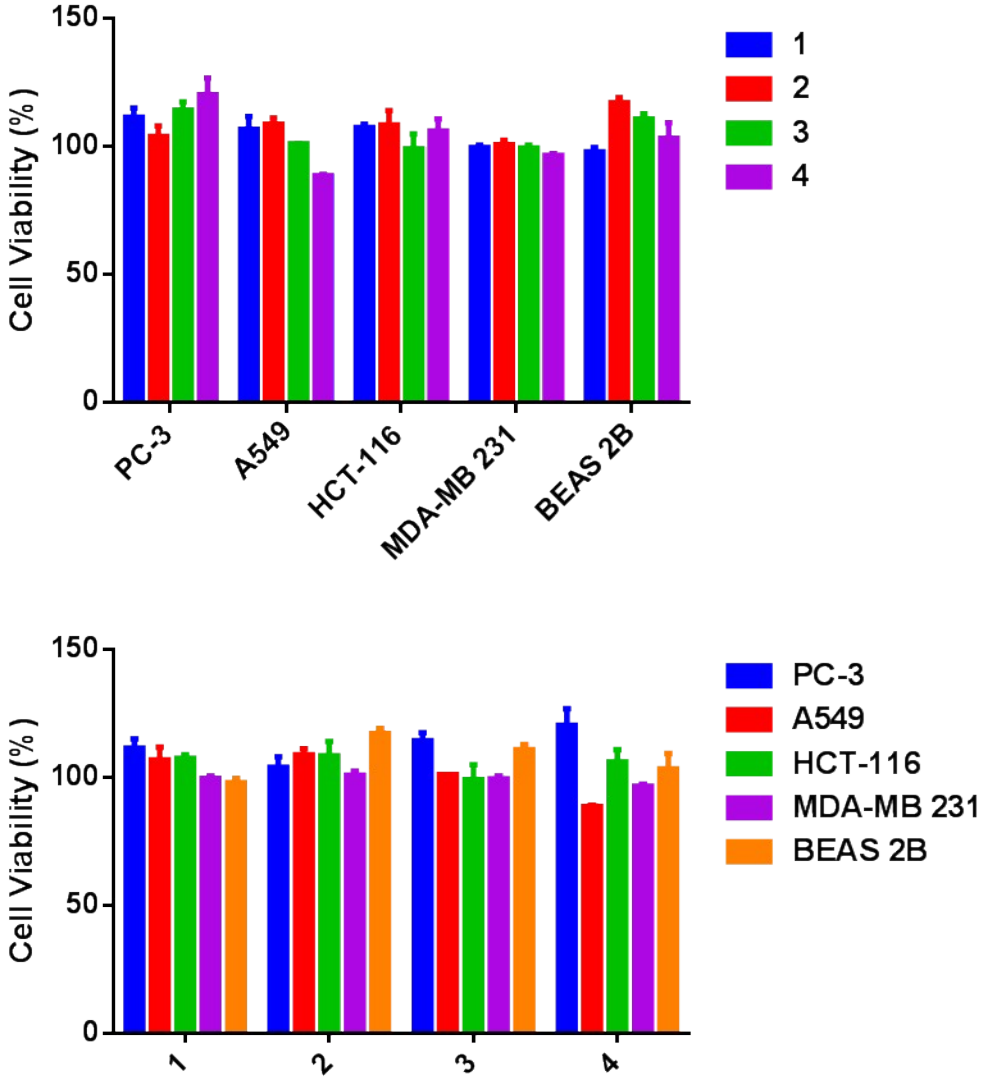

Figure S1. The cell viability detected by SRB assay after treatment with 10 μM of compounds for 48 hours.

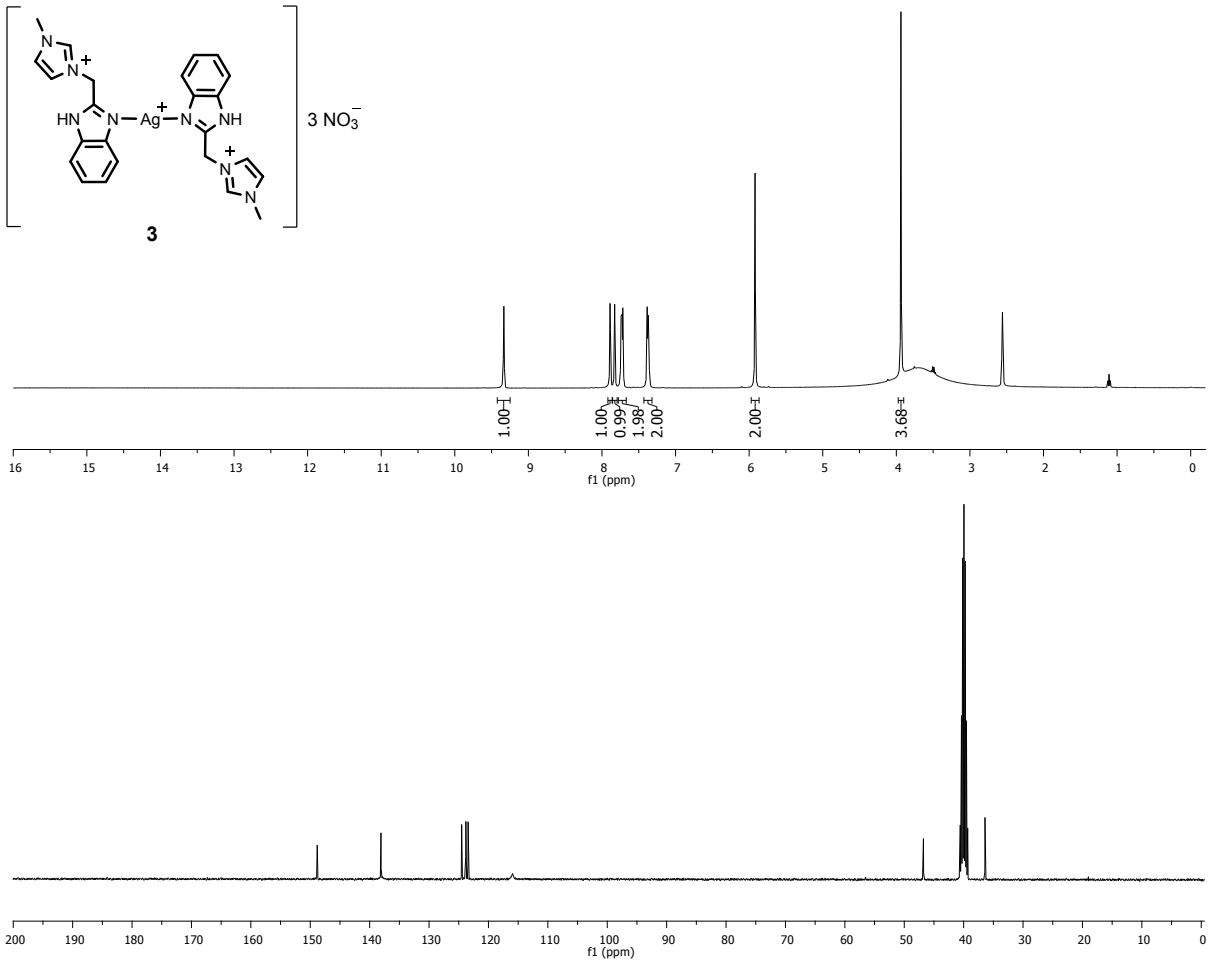

Figure S2. ^{1}H and ^{13}C NMR spectra of **3**.

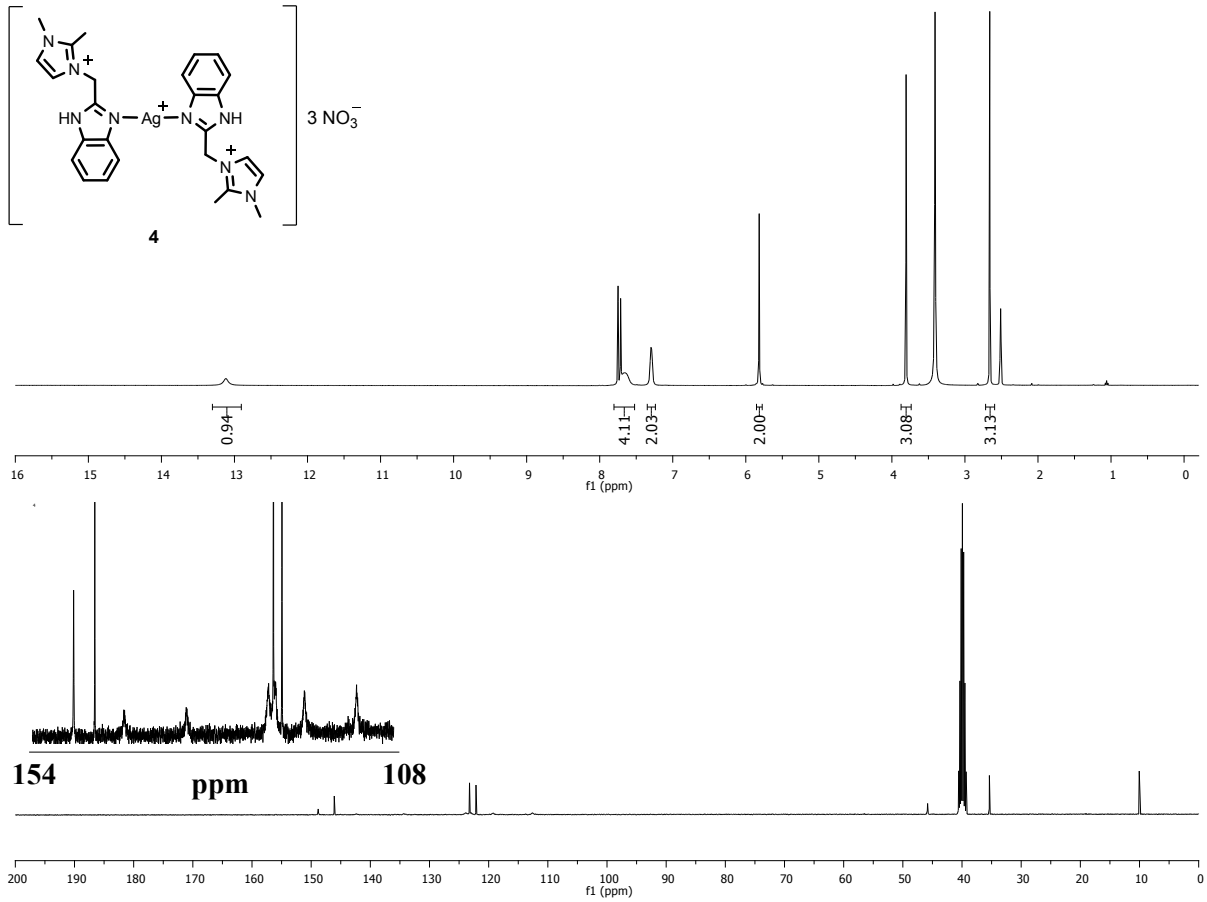

Figure S3. ^{1}H and ^{13}C NMR spectra of **4**.

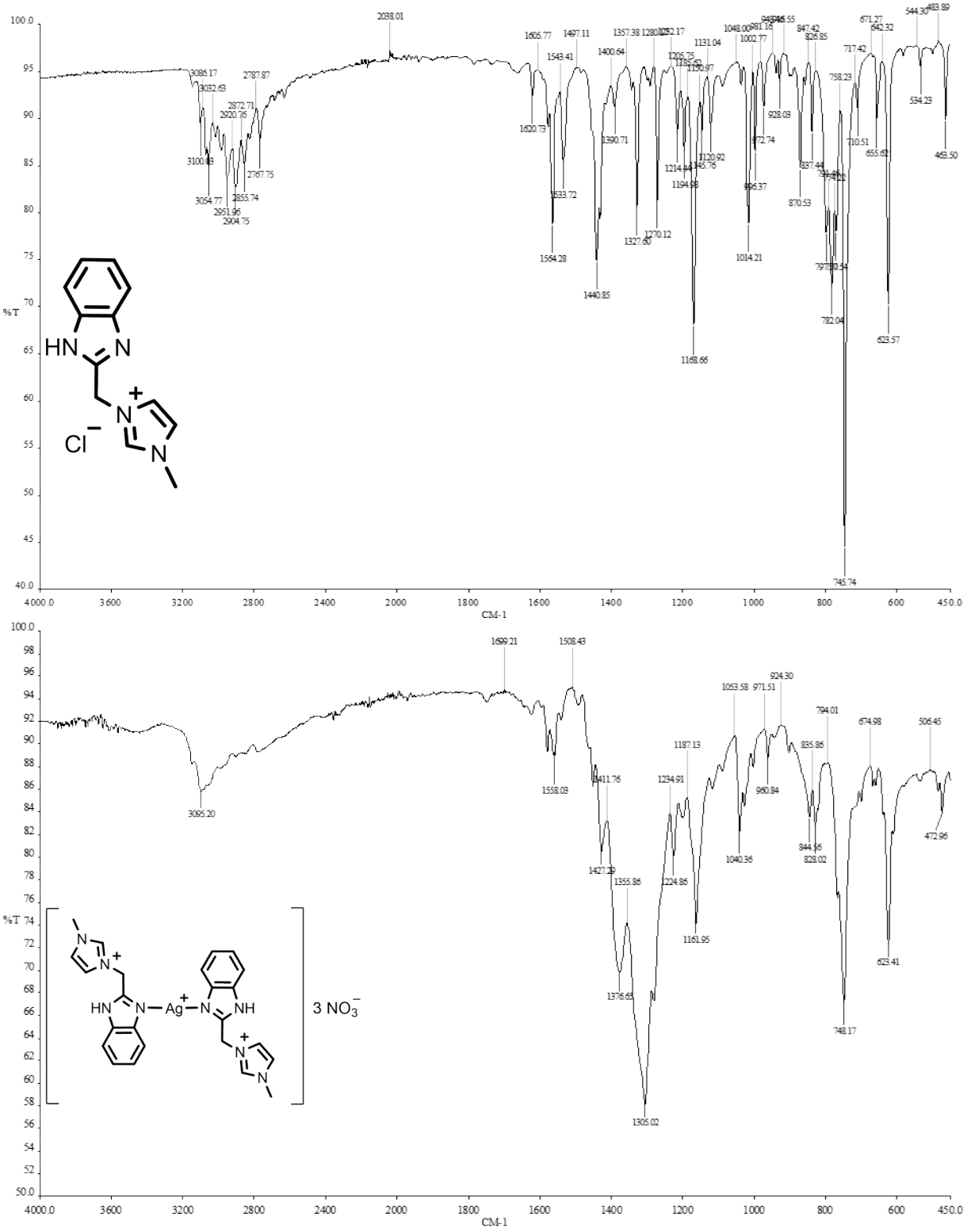

Figure S4. IR spectra of **3** (bottom) and corresponding ligand **1** (top).

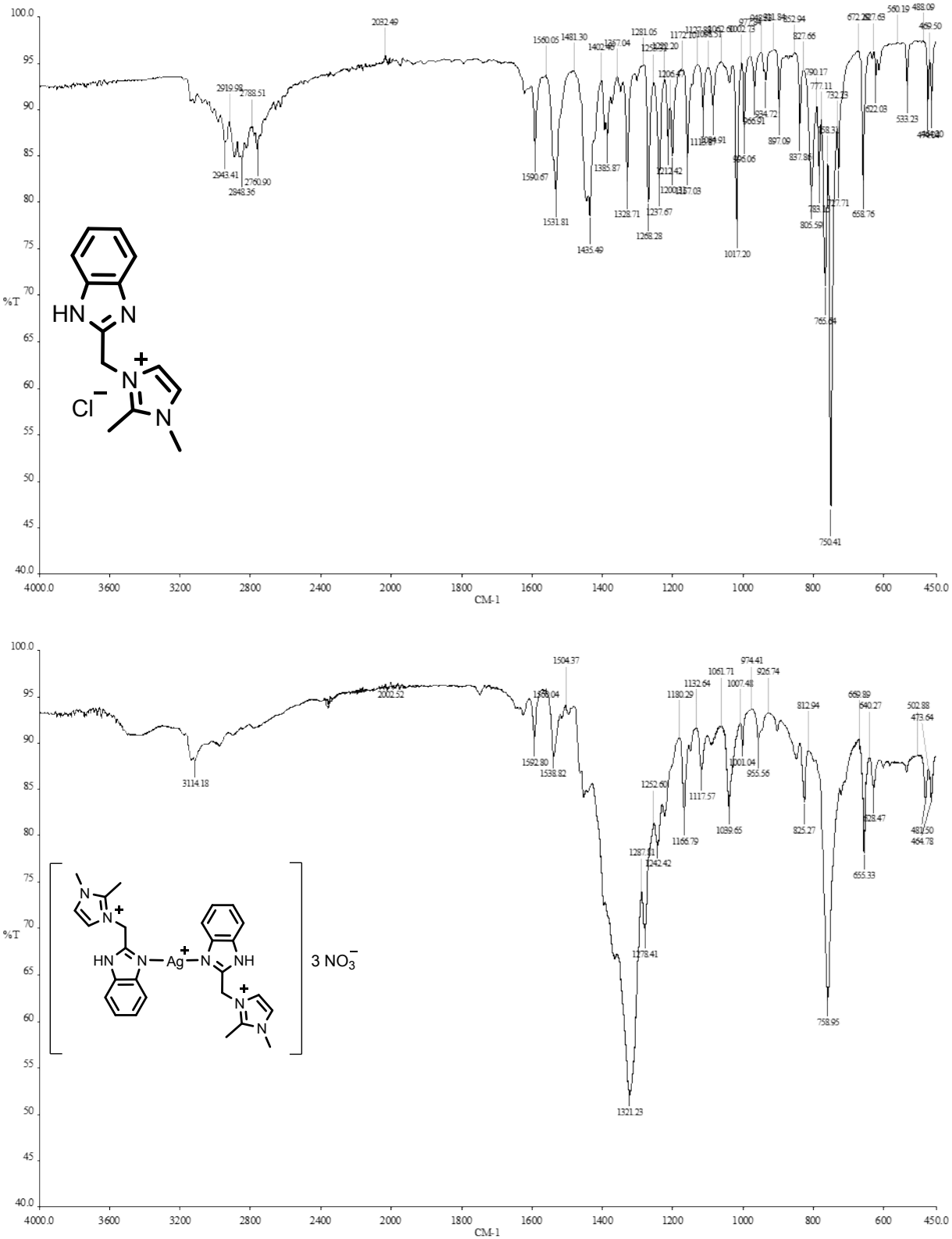

Figure S5. IR spectra of **4** (bottom) and corresponding ligand **2** (top).

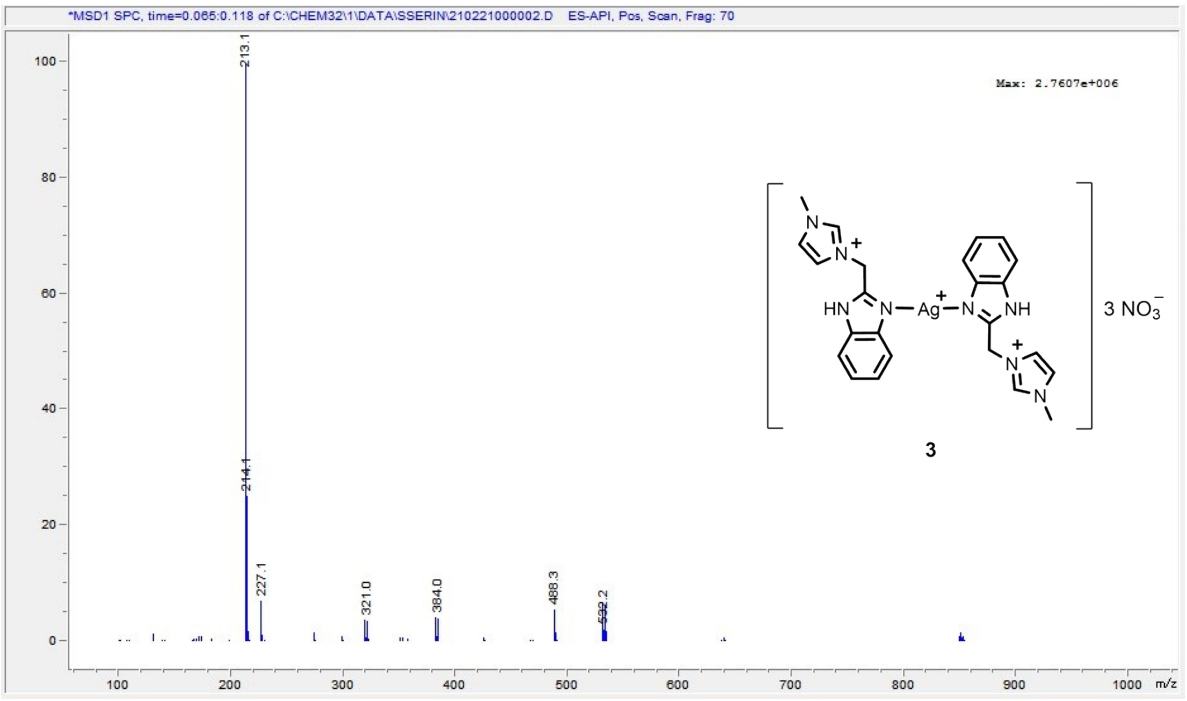

Figure S6. LC-MS spectrum of **3**.

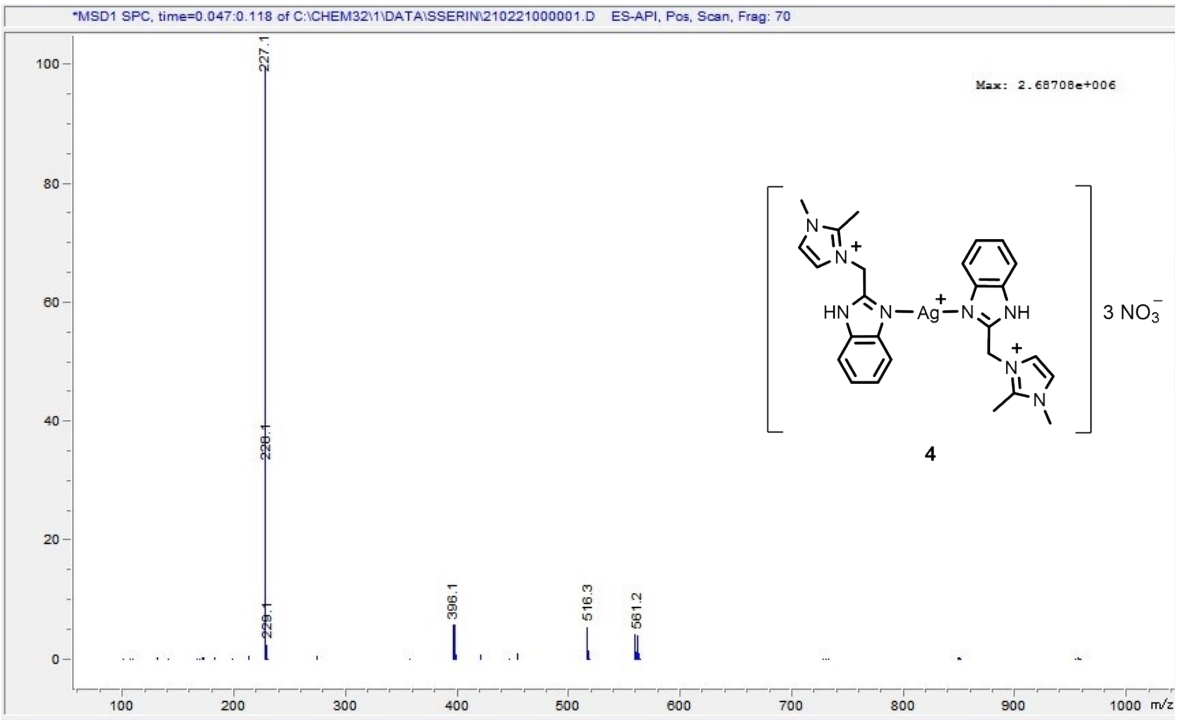

Figure S7. LC-MS spectrum of **4**.

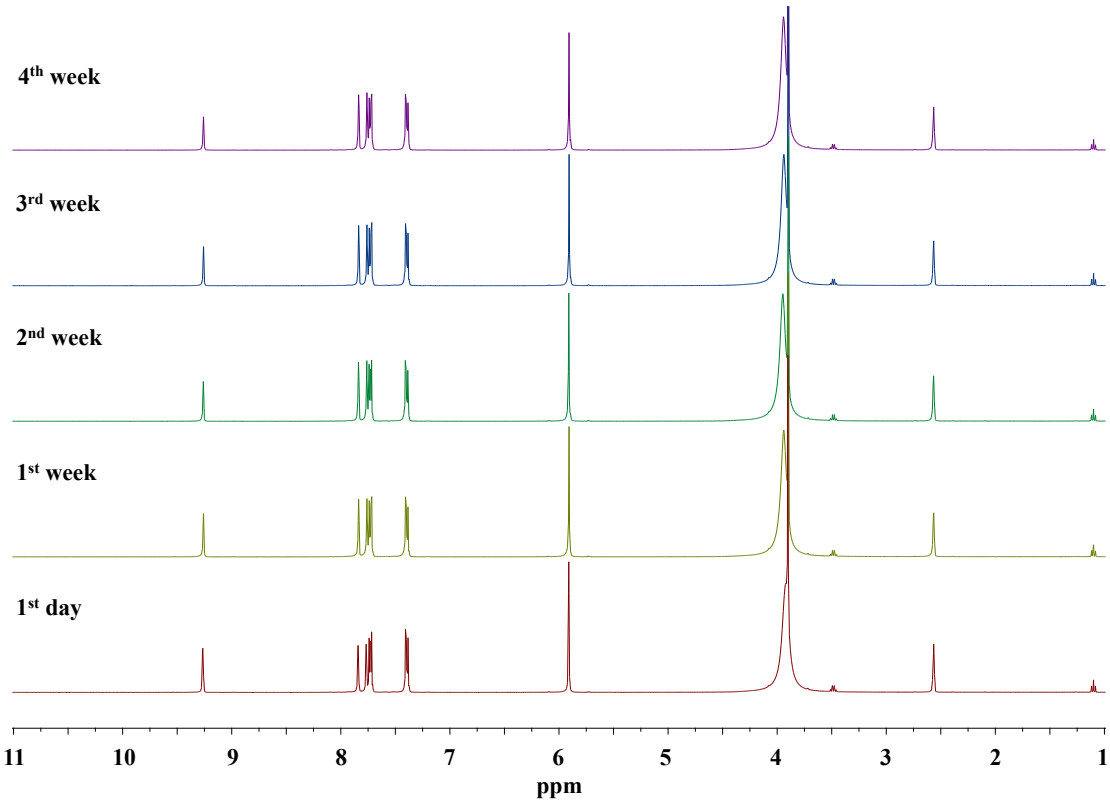

Figure S8. ^{1}H NMR spectra of **3** in DMSO-d_6/D_2O (4:1) at different time intervals.

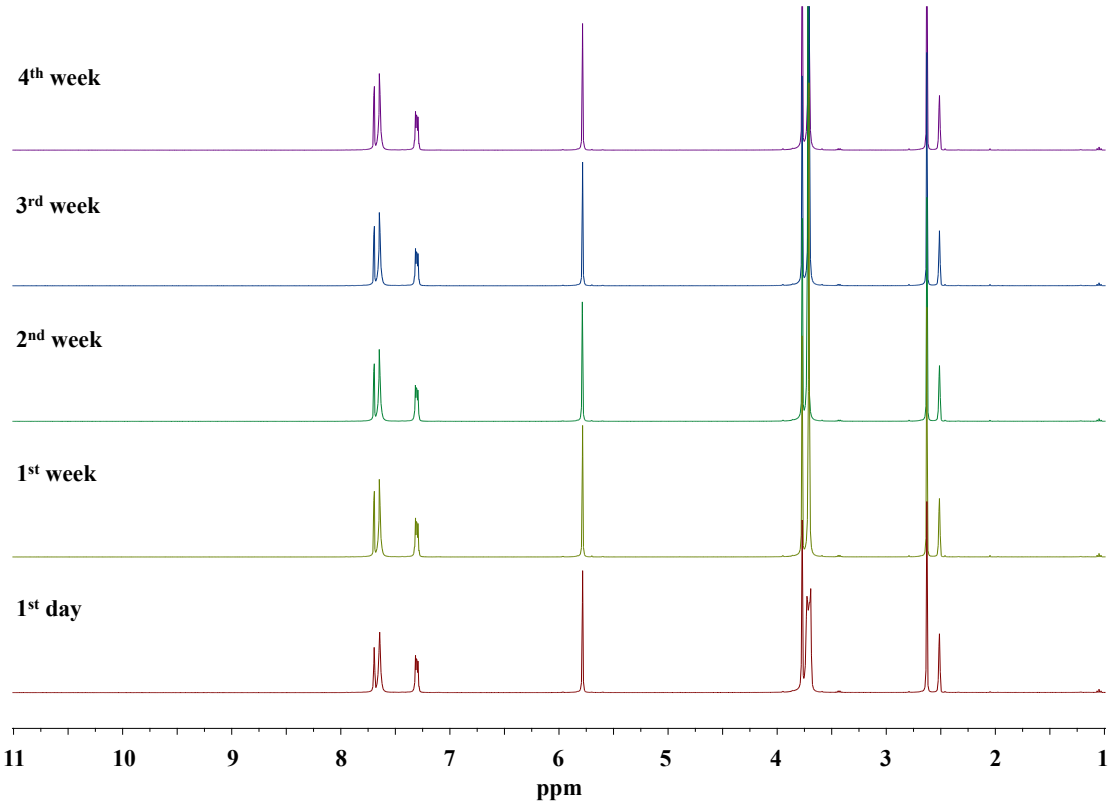

Figure S9. ^{1}H NMR spectra of **4** in DMSO-d_6/D_2O (4:1) at different time intervals.

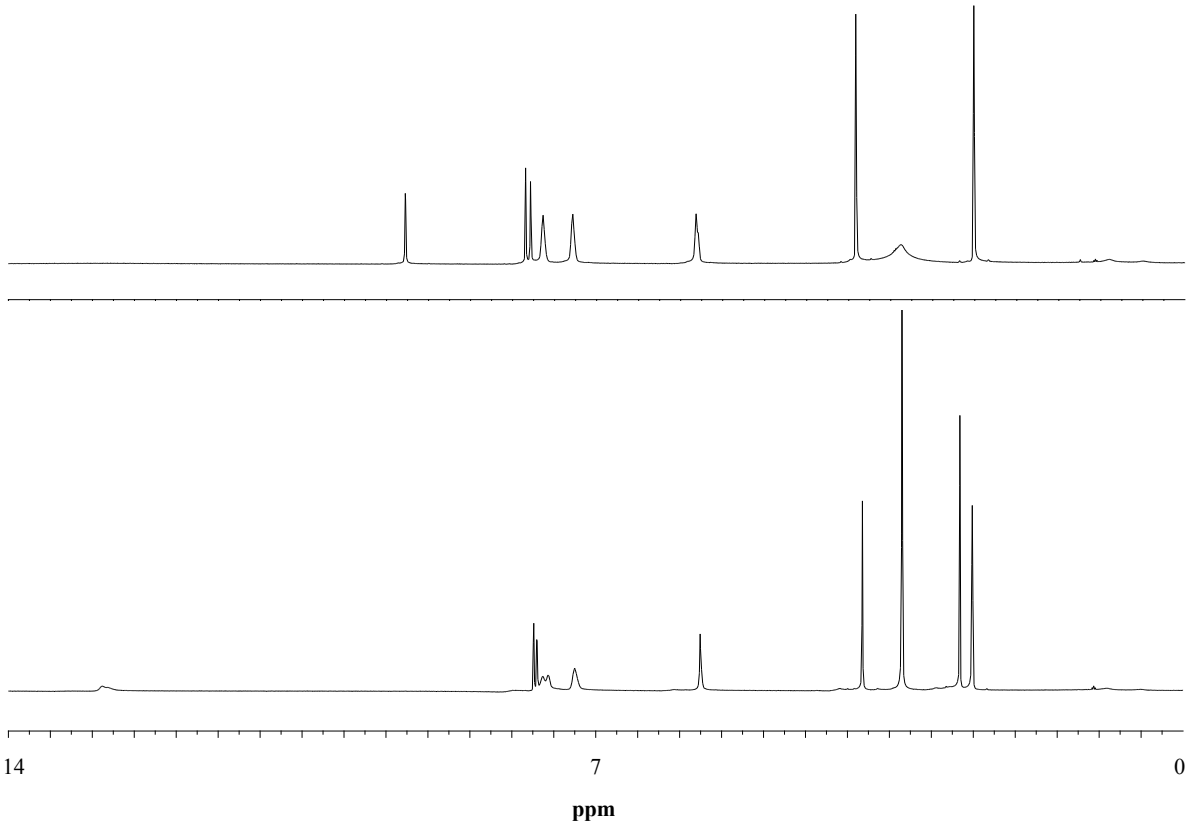

Figure S10. ^{1}H NMR spectra of **3** (top) and **4** (bottom) in DMSO-d_6 after 48 hours of exposing with white LED light.

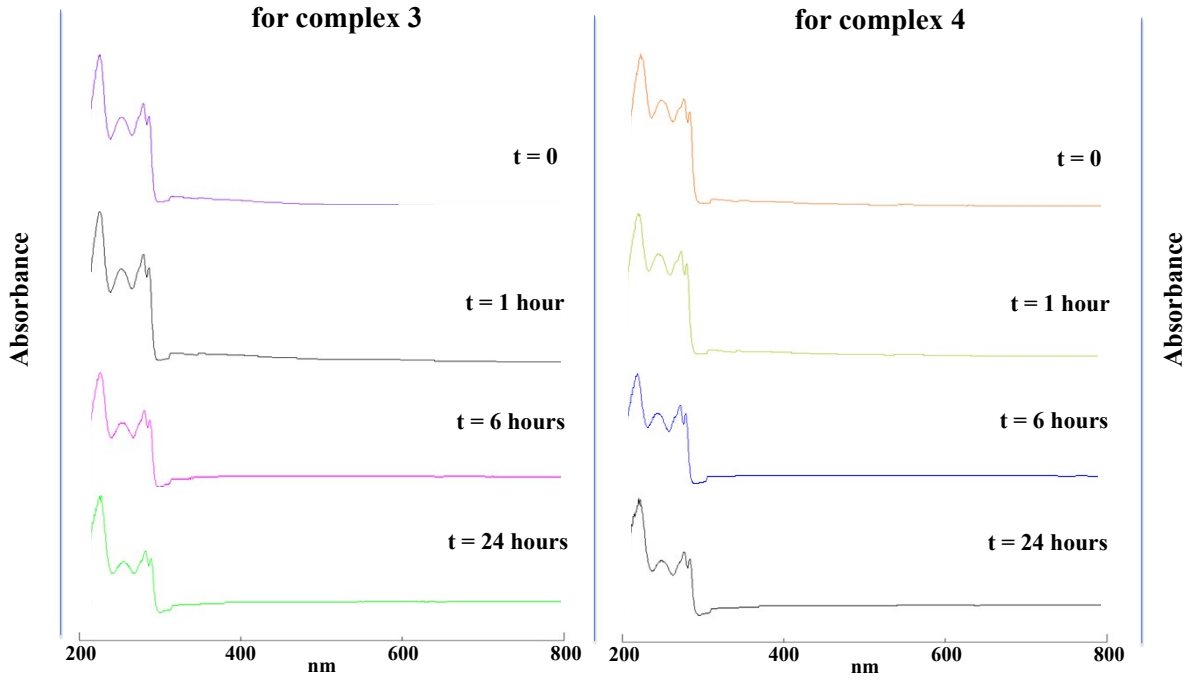

Figure S11. Time dependant UV-Visible absorption spectra of **3** and **4** in the presence of 0.05 mL of 0.15 M NaCl. Total volume is 1 mL.

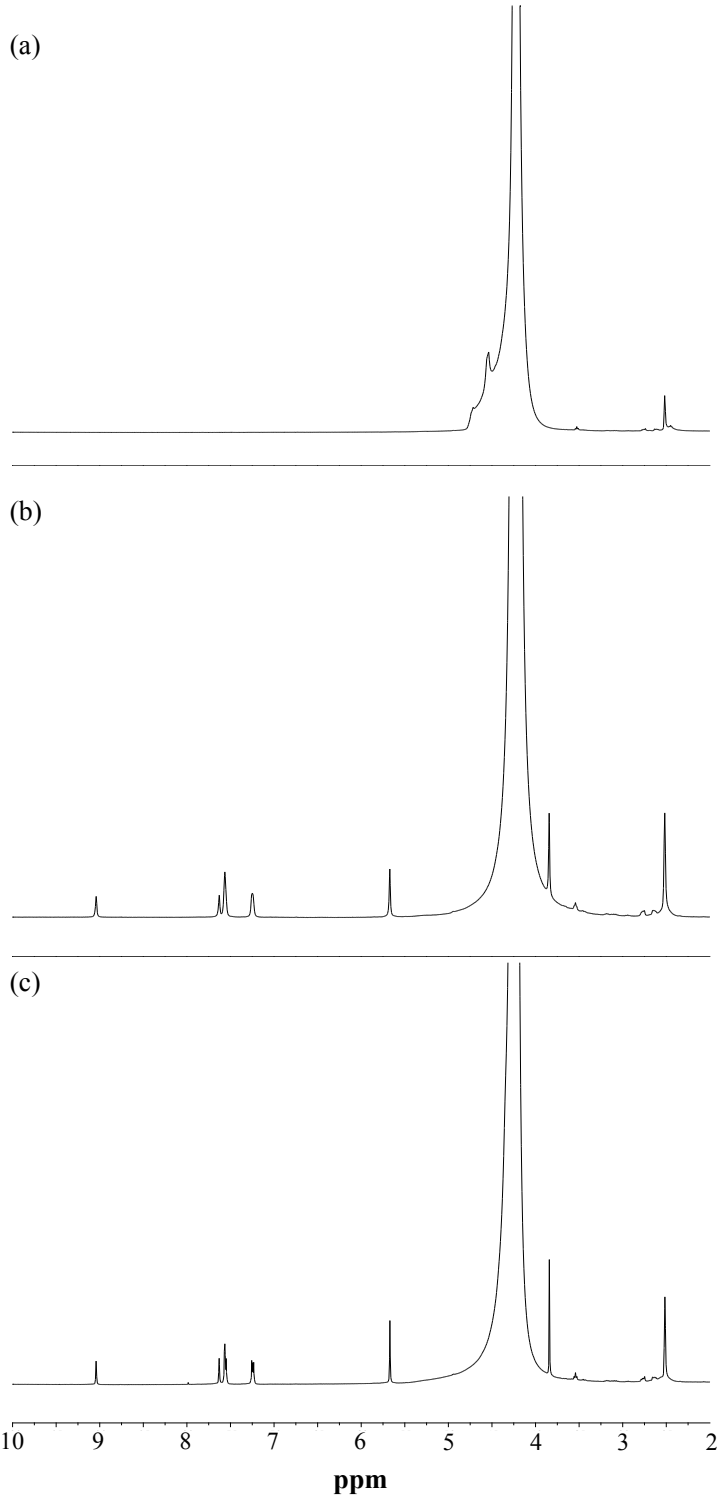

Figure S12. (a) ^{1}H NMR spectrum of 200 µL of culture medium in 400 µL of DMSO-d_6, (b) ^{1}H NMR spectrum of **3** in 400 µL of DMSO-d_6 in the presence of 200 µL of culture medium (t = 0), (c) ^{1}H NMR spectrum of **3** in 400 µL of DMSO-d_6 in the presence of 200 µL of culture medium (t = 48 h). (Culture medium is RPMI-1640 with L-glutamine containing 1% streptomycin and 10% fetal bovine serum)

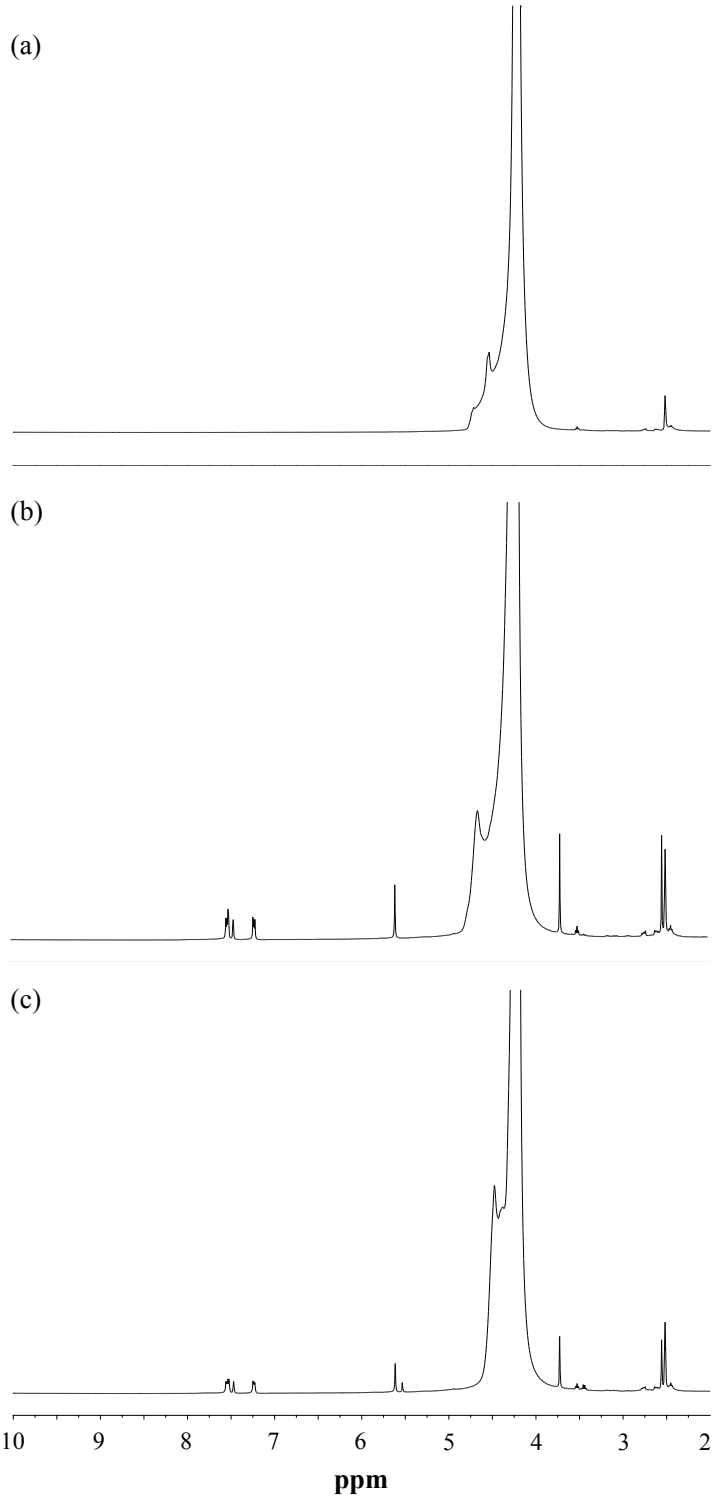

Figure S13. (a) ^{1}H NMR spectrum of 200 µL of culture medium in 400 µL of DMSO-d_6, (b) ^{1}H NMR spectrum of **4** in 400 µL of DMSO-d_6 in the presence of 200 µL of culture medium (t = 0), (c) ^{1}H NMR spectrum of **4** in 400 µL of DMSO-d_6 in the presence of 200 µL of culture medium (t = 48 h). (Culture medium is RPMI-1640 with L-glutamine containing 1% streptomycin and 10% fetal bovine serum)