Supporting information for:

Harvesting greenish blue luminescence in Gold(I) complexes and their application as promising bioactive molecules and cellular bioimaging agents.

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Table S1. Crystal data and structure refinement for complexes **1**, **2** and **3**

Compound	**1**	**2**	**3**
Empirical formula	$C_{36}H_{36}AuF_6N_3OP_2S$	$C_{35}H_{34}AuF_6N_3OP_2S$	$C_{36}H_{36}AuO_2N_3SP_2F_6$
Formula weight	931.64	917.62	947.70
Temperature (K)	296(2)	296(2)	296(2)
Radiation, λ (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic ($P2_1/n$)	Monoclinic ($P2_1/n$)	Monoclinic ($P2_1/n$)
Unit cell dimensions			
a (Å)	15.6260(6)	15.5446(3)	15.730(4)
b (Å)	15.1781(6)	14.8994(3)	14.896(5)
c (Å)	16.3393(6)	16.1594(4)	16.543(5)
α (º)	90.000(0)	90.000(0)	90.000(0)
β (º)	104.658(2)	105.9130(10)	105.515(10)
γ (º)	90.000(0)	90.000(0)	90.000(0)
Volume (Å^3)	3749.1(2)	3599.18(13)	3734.8(19)
Z / density calculated (g cm^{-3})	4/1.651	4/1.693	4/1.402
Absorption coefficient (mm^{-1})	4.128	4.298	4.087
F(000)	1840	1808	1528
Crystal size (mm)	0.41 × 0.18 × 0.18	0.82 × 0.56 × 0.28	0.22 × 0.22 × 0.14
Range for data collection, θ (º)	1.86 to 26.42	1.61 to 26.41	2.495 to 30.176
Index ranges	–19 ≤ h ≤ 19 –18 ≤ k ≤ 18 –20 ≤ l ≤ 20	–16 ≤ h ≤ 19 –15 ≤ k ≤ 18 –16 ≤ l ≤ 20	–22 ≤ h ≤ 22 –20 ≤ k ≤ 20 –22 ≤ l ≤ 23
Reflections collected	28644	27388	53312
Independent reflections	7690[R(int) = 0.0244]	7382[R(int) = 0.0364]	10998[R(int) = 0.0408]
Completeness to θ_{max}	99.7%	99.9 %	99.7%
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Data/restraints/parameters	7690 / 0 / 518	7382 / 36 / 444	10998 / 0 / 460
Goodness-of-fit, F^2	1.019	1.027	1.032
Final *R* indices ($I>2\sigma(I)$)	R_1 = 0.0254 wR_2 = 0.0670	R_1 = 0.0302 wR_2 = 0.0720	R_1 = 0.0405 wR_2 = 0.0980
R indices (all data)	R_1 = 0.0333 wR_2 = 0.0718	R_1 = 0.0391 wR_2 = 0.0756	R_1 = 0.0732 wR_2 = 0.1122
Largest peak-and-hole difference (*e* Å^{-3})	1.192 and –0.694	0.921 and –0.875	1.021 and –0.644

*$R_1 = |F_0 - F_c|/|F_0|$; $wR_2 = [w(F_0^2 - F_c^2)^2/(wF_0^2)]^{-1/2}$

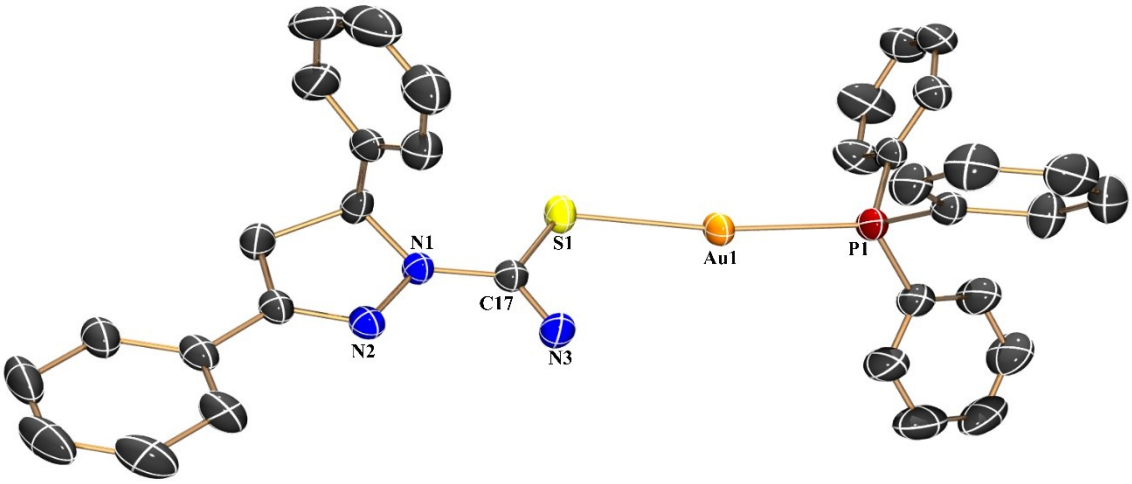


Figure S1. Crystalline structure of **2**. Hydrogen atoms, PF_6 anion, and methanol solvate omitted for clarity. Thermal ellipsoids drawn at a 50% probability level.

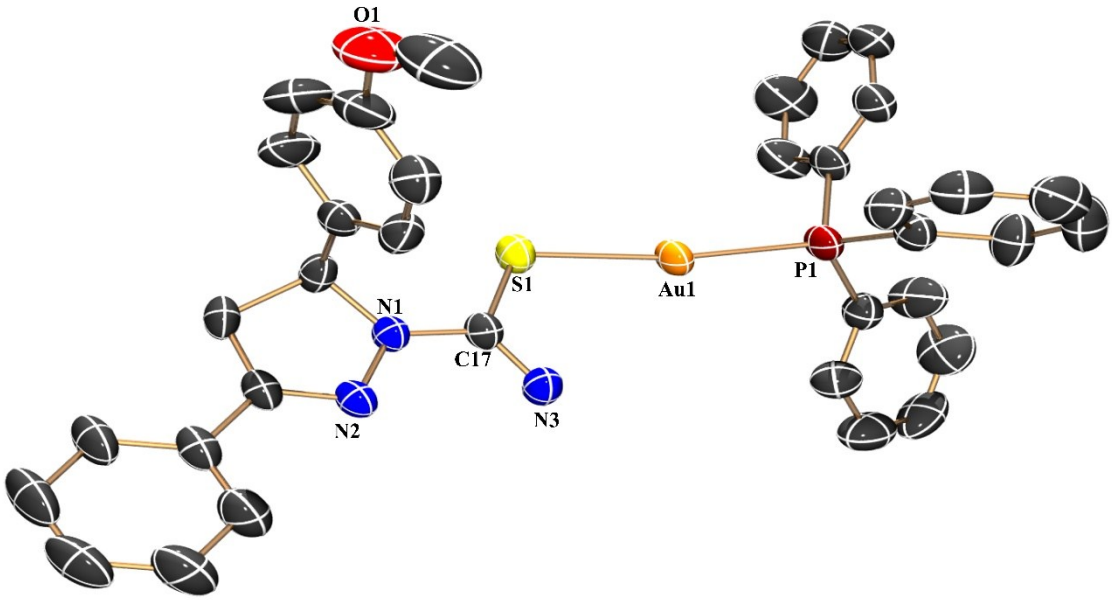


Figure S2. Crystalline structure of **3**. Hydrogen atoms, PF_6 anion, and methanol solvate omitted for clarity. Thermal ellipsoids drawn at a 50% probability level.

Table S2. Selected bond distances (Å) and bond angles (°) for complexes **1**, **2** and **3**.

	Complex 1	**Complex 2**	**Complex 3**
Distances (Å)			
P(1)-Au(1)	2.2729(8)	2.2680(9)	2.2600(12)
S(1)-Au(1)	2.3053(8)	2.3018(9)	2.2950(12)
C(17)-S(1)	1.724(3)	1.719(4)	1.721(4)
C(17)-(N1)	1.331(4)	1.329(4)	1.326(5)
C(17)-N(3)	1.309(4)	1.314(5)	1.303(5)
N(1)-N(2)	1.410(3)	1.409(4)	1.406(4)
Angles (°)			
P(1)-Au(1)-S(1)	169.83(3)	169.63(4)	170.64(4)

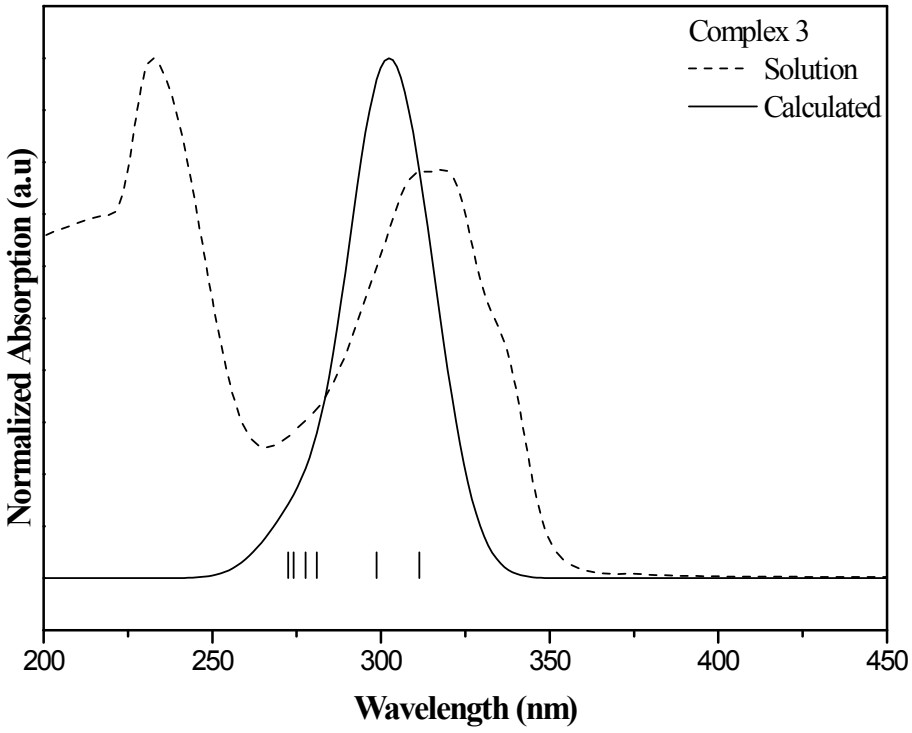


Figure S3. Experimental (solid line) and calculated (dashed line) absorption spectra of complex **3**.

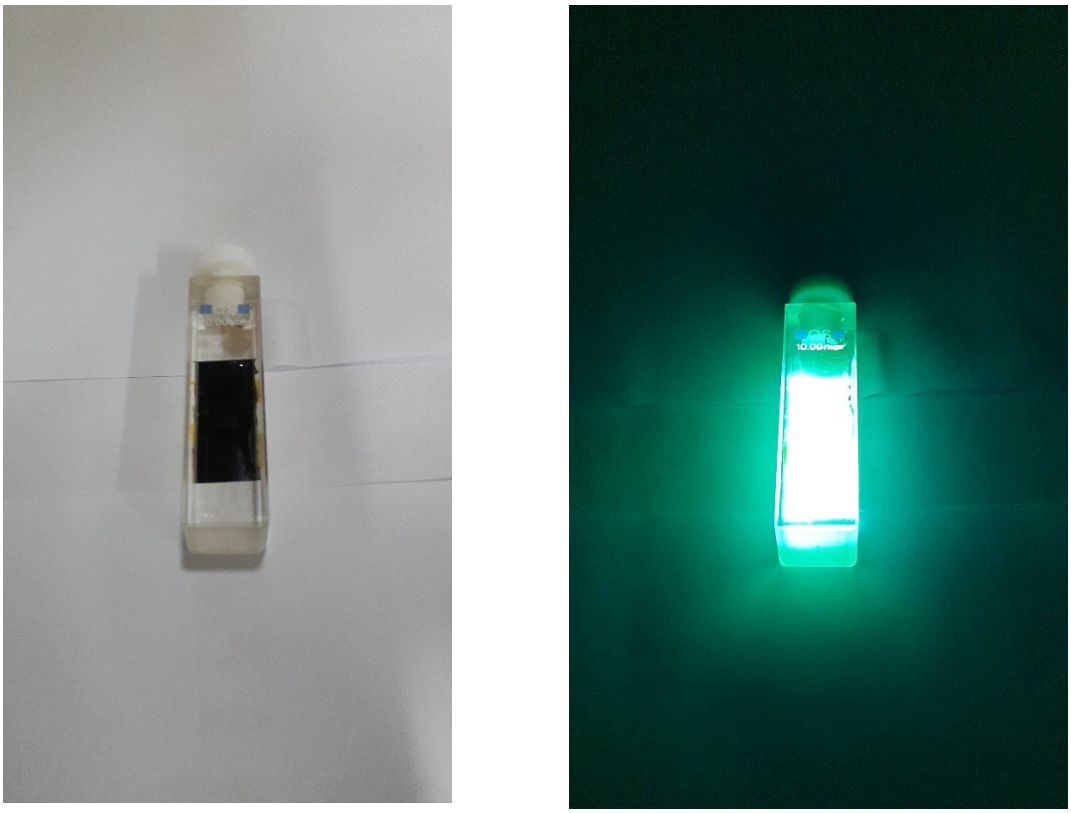


Figure S4. Dichloromethane solution (1.0×10^{-5} M) of complex **3**. Left: under natural light; right: with 306 nm (UV) passing through solution. Complexes **1** and **2** exhibited similar behavior.

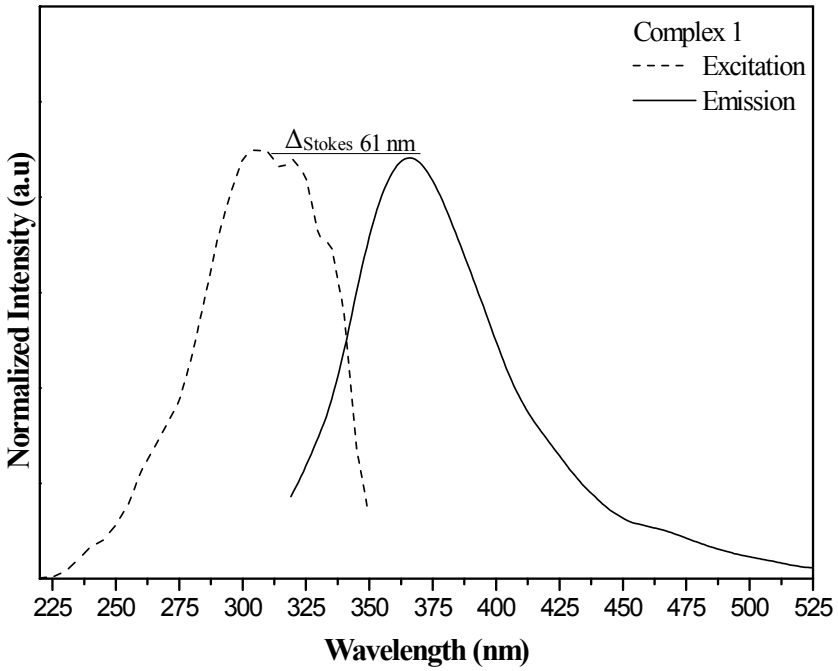


Figure S5. Excitation and emission spectra of complex **1** measured in CH_2Cl_2 solution (≈1.0×10^{-5} M) at 298 K (λ_{ex} = 305 nm).

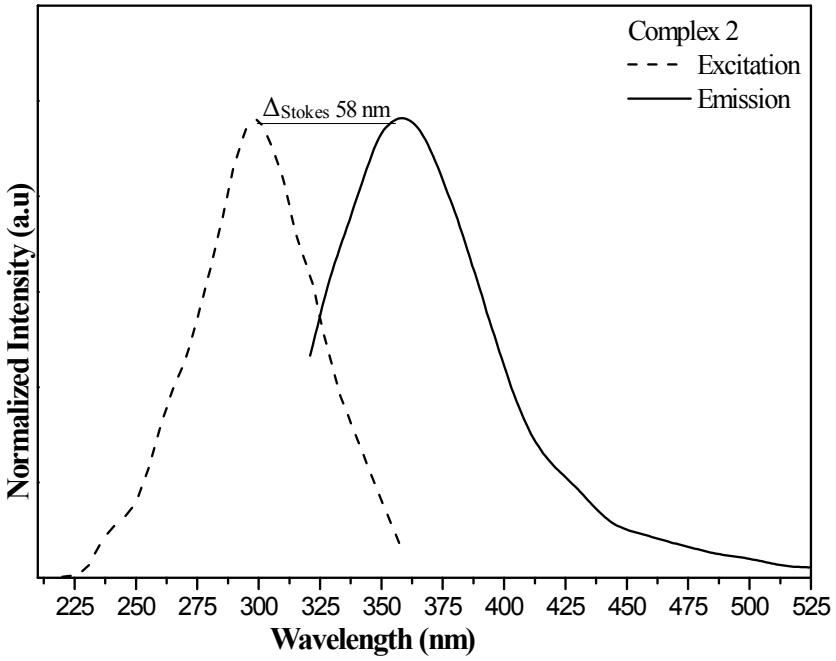


Figure S6. Excitation and emission spectra of complex **2** measured in CH_2Cl_2 solution (≈1.0×10^{-5} M) at 298 K (λ_{ex} = 300 nm).

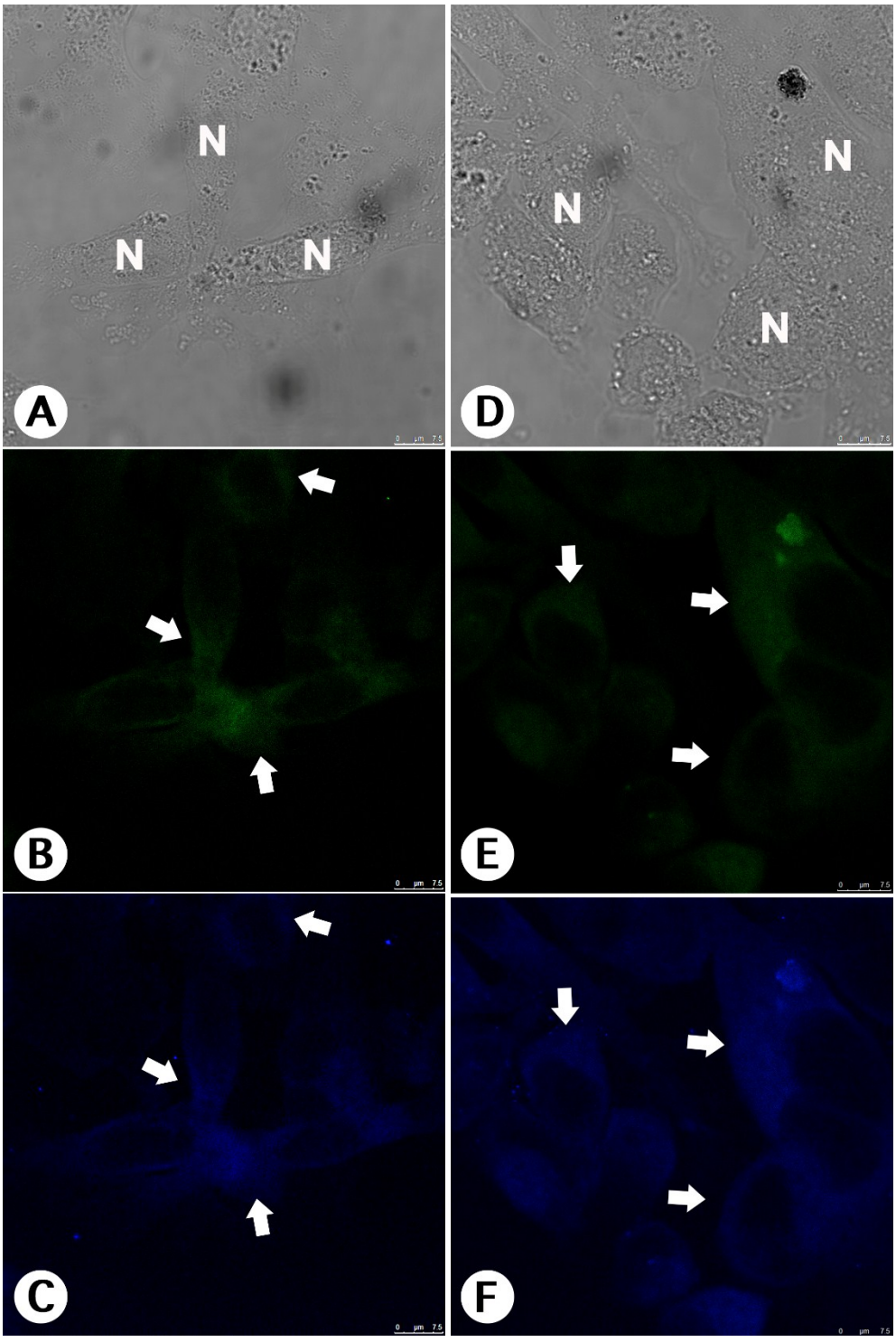


Figure S7. Confocal fluorescence microscopy images of MCF-7 cells stained with **1**. Images A, B and C live cells, imagens D, E and F fixed cells. The complex **1** have dual fluorescence emission, green (λ_{exc} = 405 nm) showed in images B and E and blue (λ_{exc} = 305 nm) showed in imagens C and F. The fluorescence was distributed into the cells cytoplasm (white arrow). The cells nuclei were not stained by this compound, which are showed as black voids in the cells. Images A and D show the normal cells morphology by phase contrast microscopy. Reference scale bar = 75 µm.

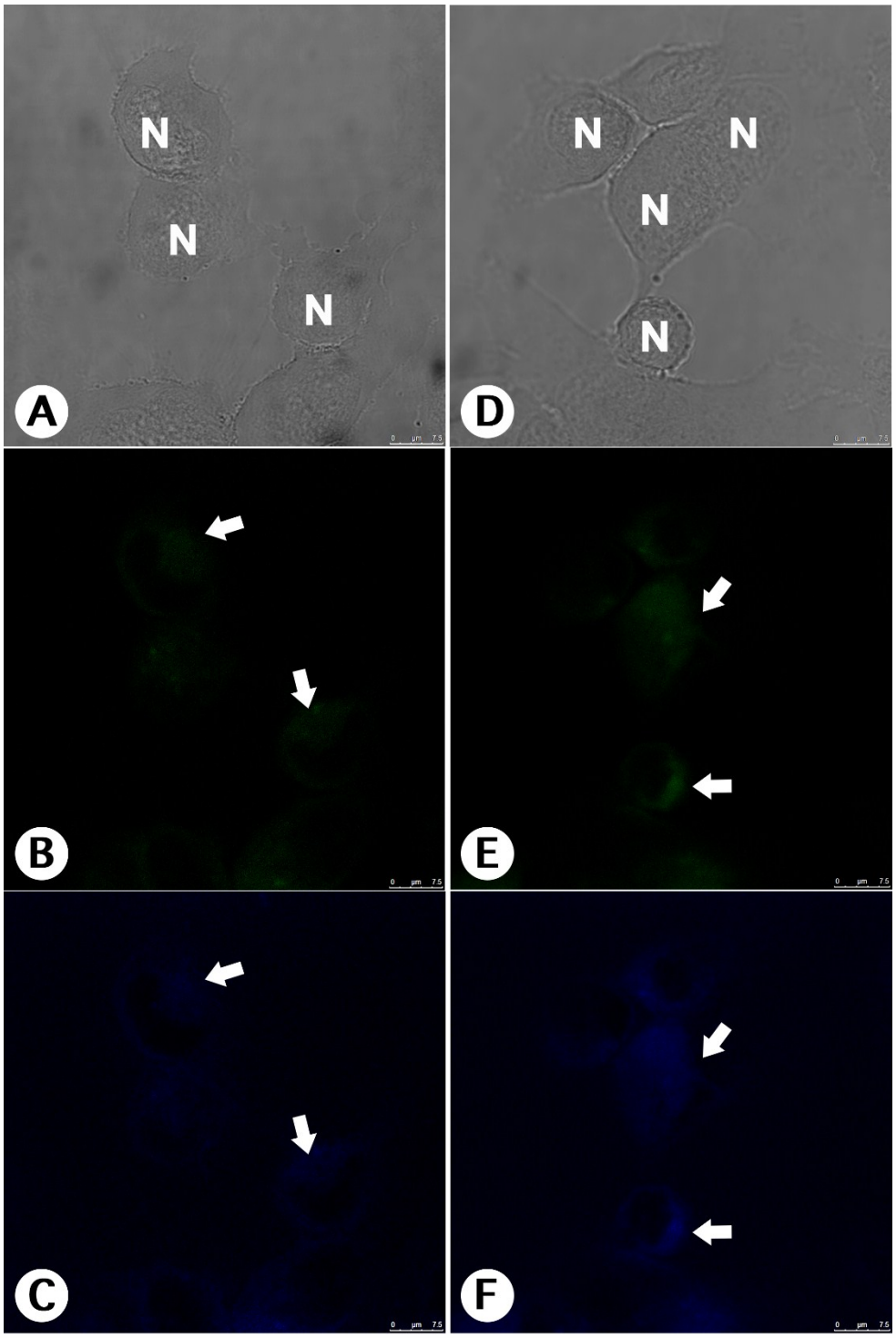


Figure S8. Confocal fluorescence microscopy images of MCF-7 cells stained with **2**. Images A, B and C live cells, imagens D, E and F fixed cells. The complex **2** presented dual fluorescence emission, green (λ_{exc} = 405 nm) showed in images B and E and blue (λ_{exc} = 305 nm) showed in imagens C and F. The fluorescence was distributed into the cells cytoplasm (white arrow). The fluorescent signal was less intense to those observed in cell stained with **2**. The cells nuclei were not stained by this compound, which are showed as black voids in the cells. Images A and D show the normal cells morphology by phase contrast microscopy. Reference scale bar = 75 µm.

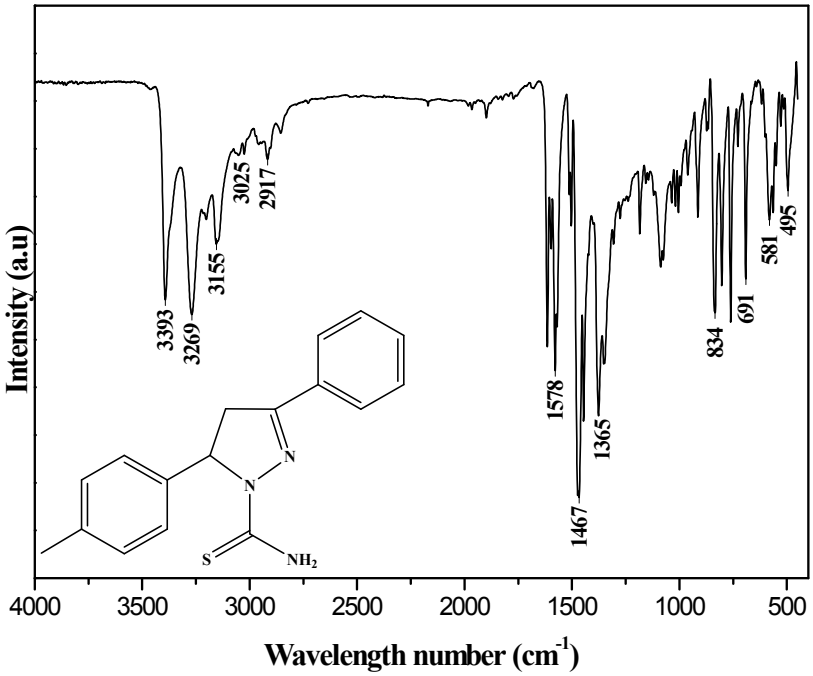


Figure S9. Infrared spectrum of ligand **1**.

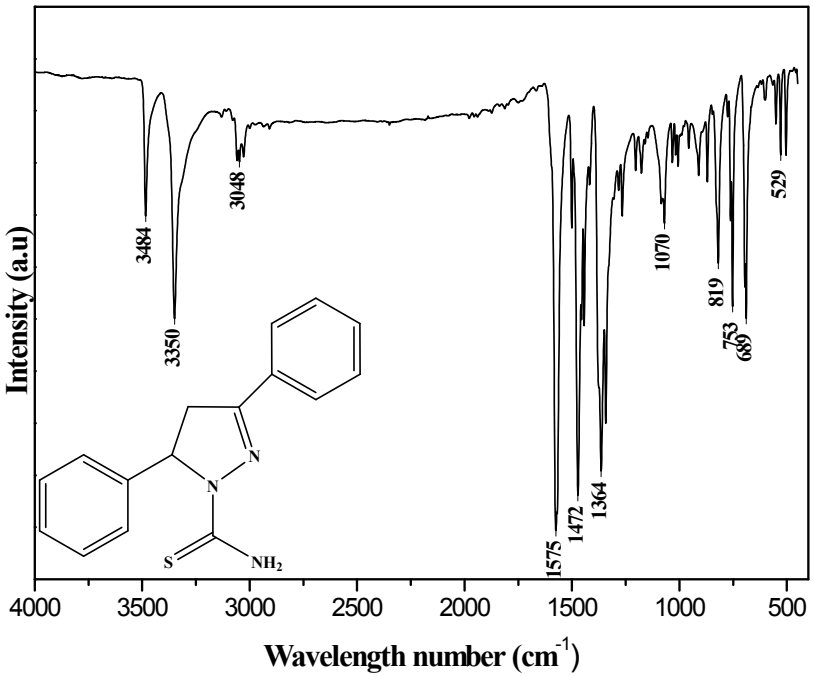


Figure S10. Infrared spectrum of ligand **2**.

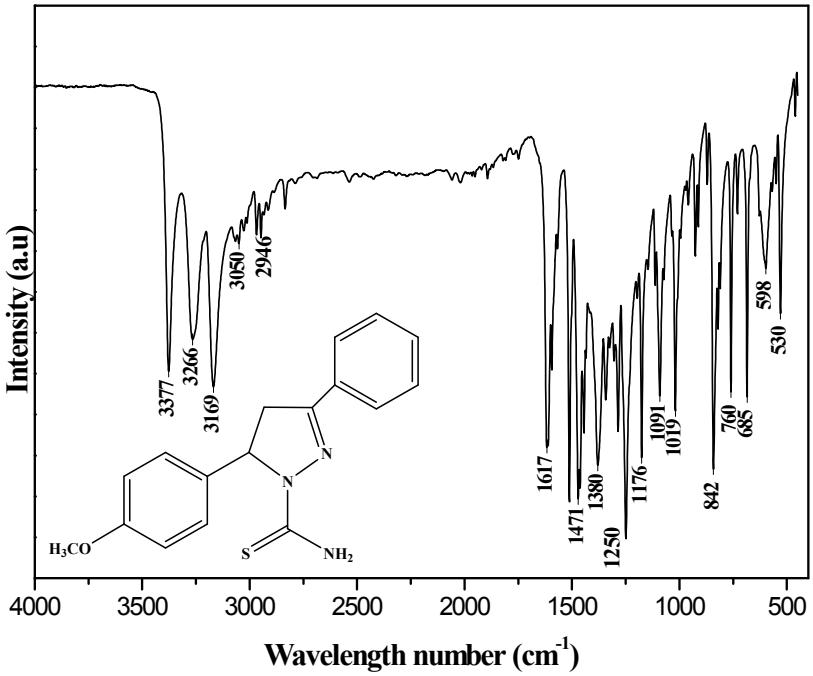


Figure S11. Infrared spectrum of ligand **3**.

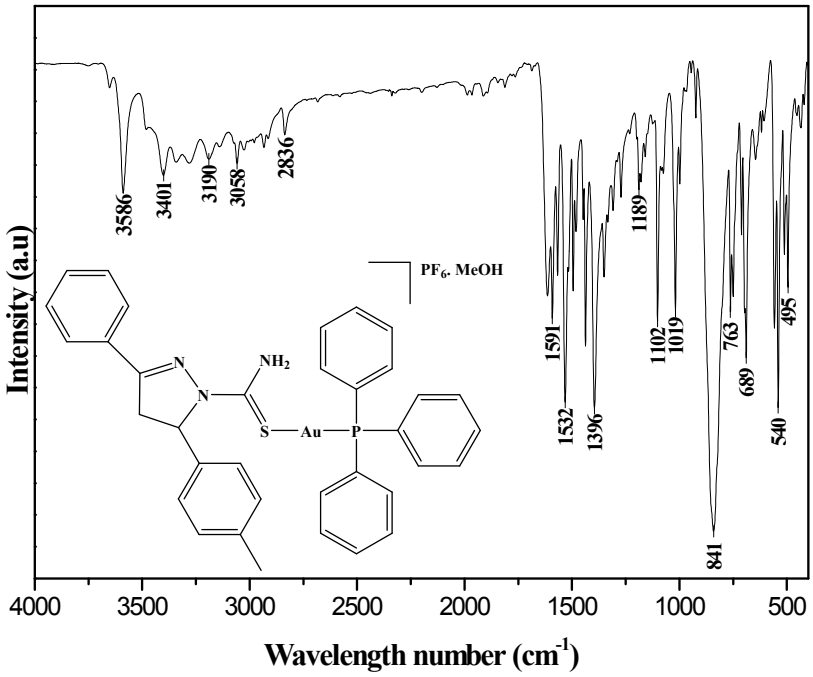


Figure S12. Infrared spectrum of complex **1**.

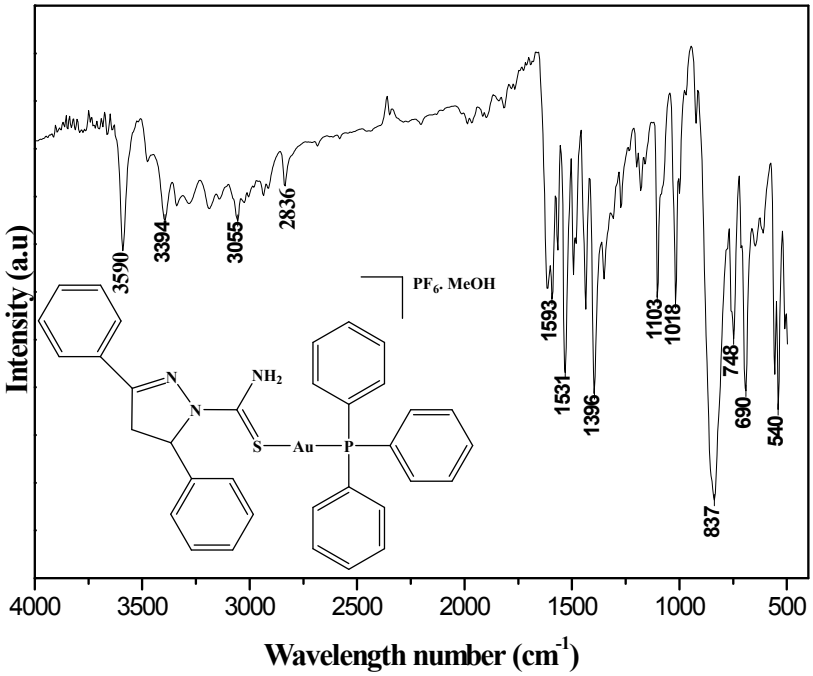


Figure S13. Infrared spectrum of complex **2**.

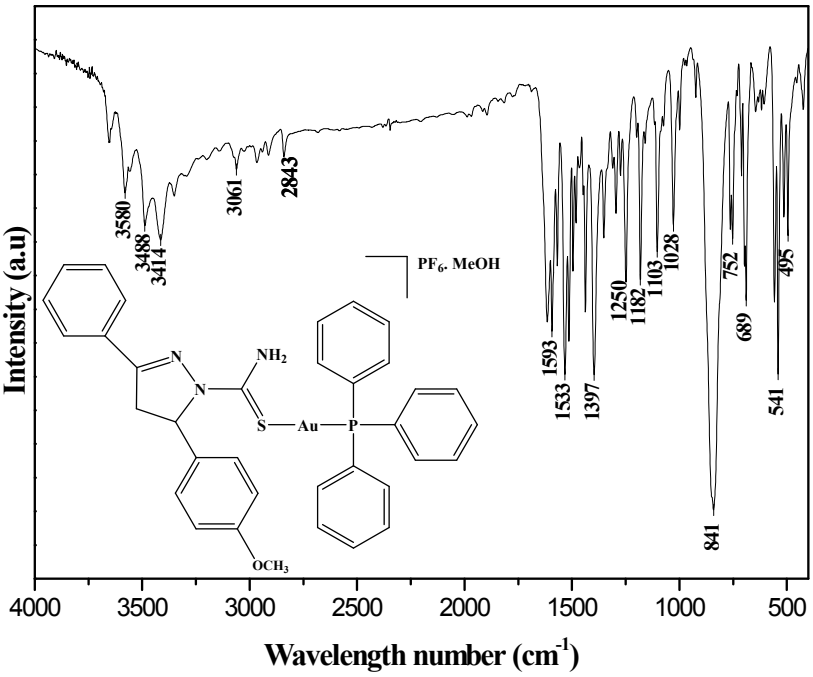
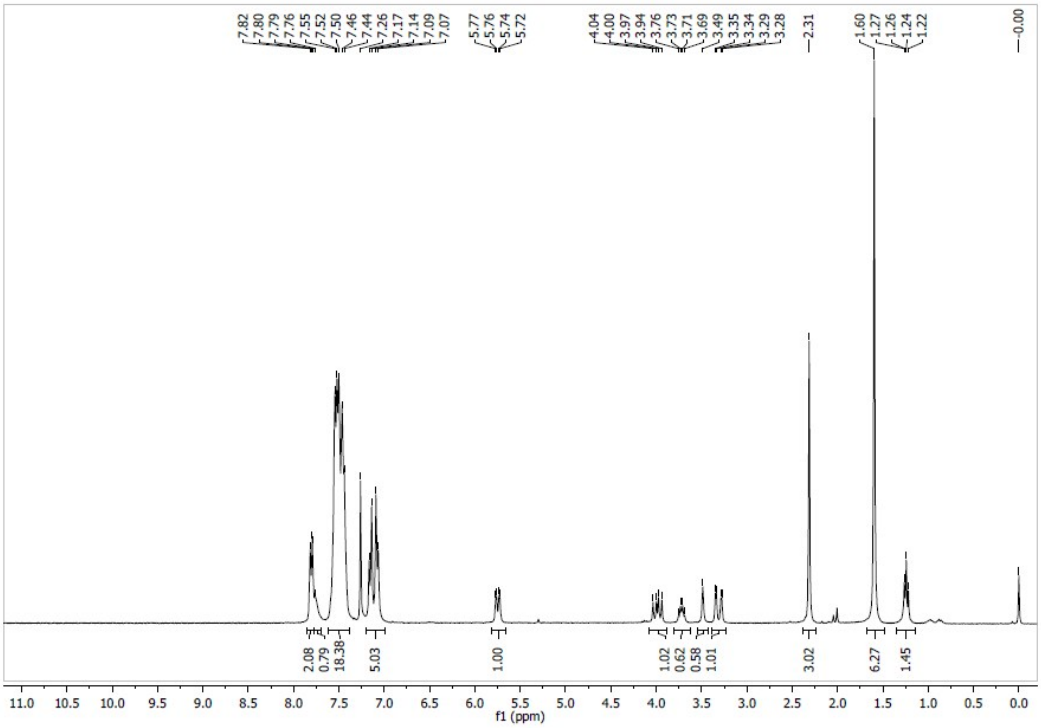


Figure S14. Infrared spectrum of complex **3**.

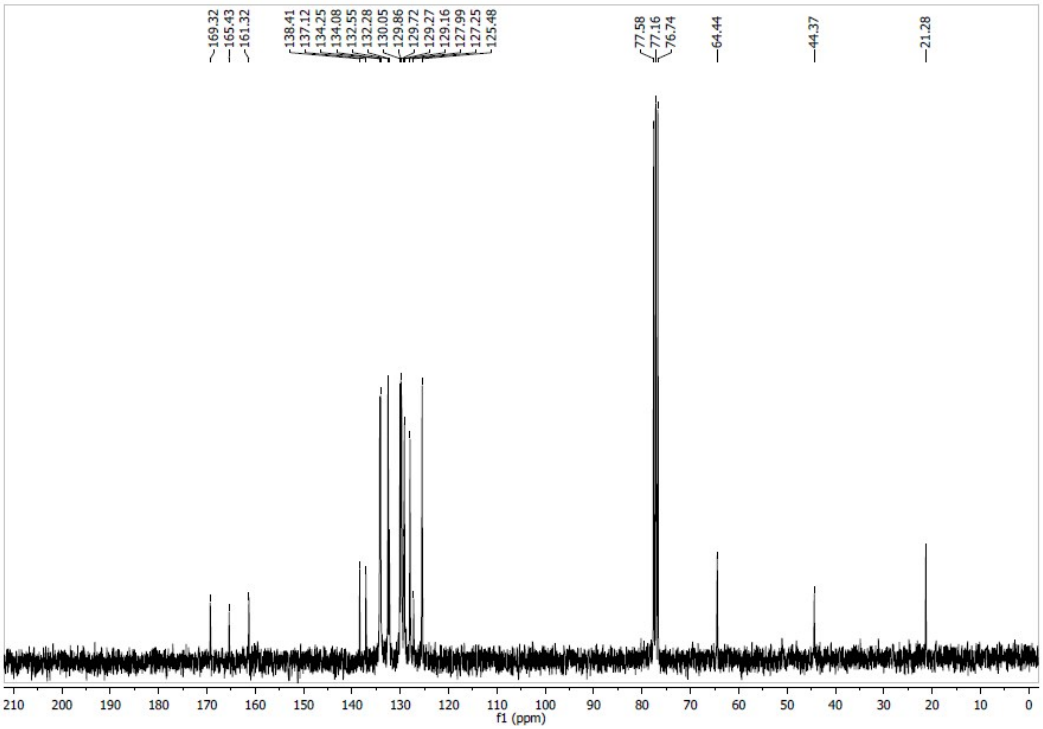
Table S3. Modes and vibrational frequencies of the precursor, ligands and complexes.

	Vibrational frequency (cm^{-1})						
	[Ph_3PAuCl]	Ligand **1**	Ligand **2**	Ligand **3**	Complex **1**	Complex **2**	Complex **3**
ν (N-H)	–	3393-3155	3484-3350	3337-3169	3586-3190	3580-3414	3580-3414
$\nu(C\text{-}H)_{Ar}$	3062	3025	3048	3050	3058	3055	3061
ν(C-H)	–	2917	NO	2956	2836	2836	2843
$\nu(C{=}C)_{Ar}$	1480-1384	1467	1472	1471	1532	1531	1533
ν(C=N)	–	1578	1575	1617	1591	1593	1593
ν(C=S)	–	1365	1364	1380	1396	1396	1397
δ(C-H)	990-750	990-750	990-750	990-750	990-760	990-760	990-760
ν(P-F)	–	–	–	–	841	837	841
ν(C-P)	1098	–	–	–	1102	1103	1103
$\delta(C\text{-}H)_{Ar}$	748	691	689	685	689	690	689
$\nu(C\text{-}O\text{-}CH_3)$	–	–	–	1250	–	–	1250
ν(O-H)	–	–	–	–	3586	3590	3580

NO: not observed.

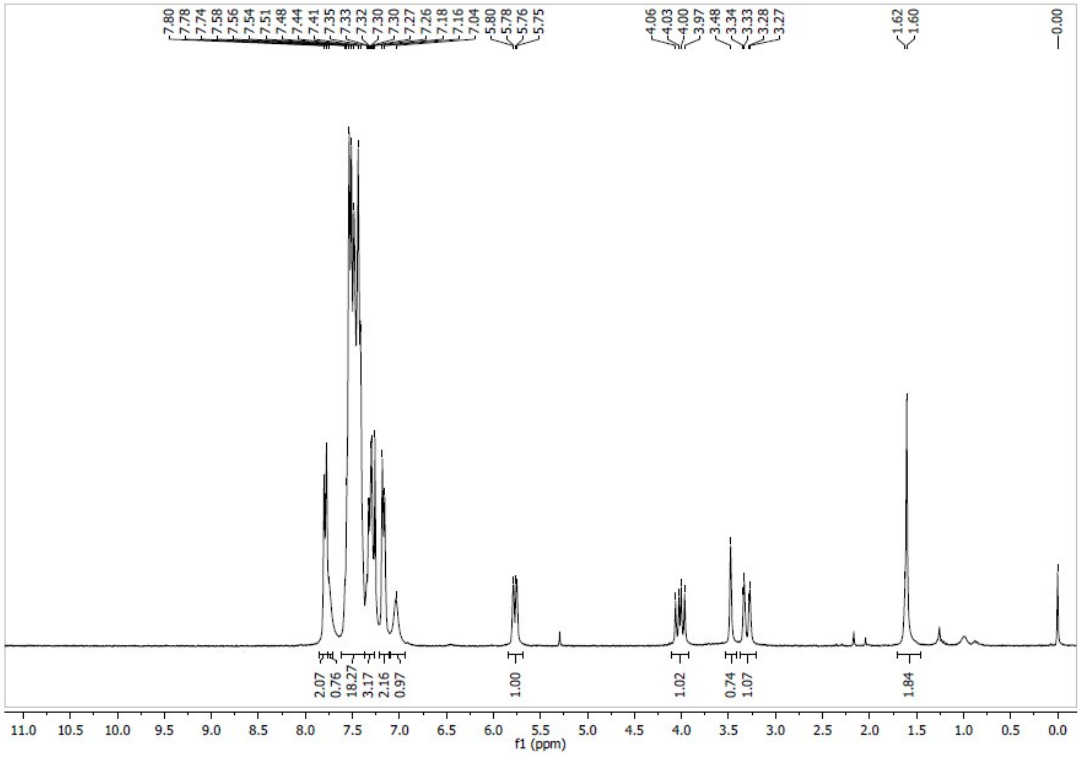


Complex **1**. 1H NMR (300 MHz, CDCl3) δ 7.82-7.79 (m, 2H, Ar), 7.76 (bs, 1H, NH), 7.55-7.44 (m, 18H, Ar), 7.26-7.07 (m, 5H, Ar + NH), 5.75 (dd, J = 11.0, 3.5 Hz, 1H), 3.99 (dd, J = 18.0, 11.0 Hz, 1H), 3.31 (dd, J = 18.0, 3.6 Hz, 1H). 2.31 (s, 3H, CH3).

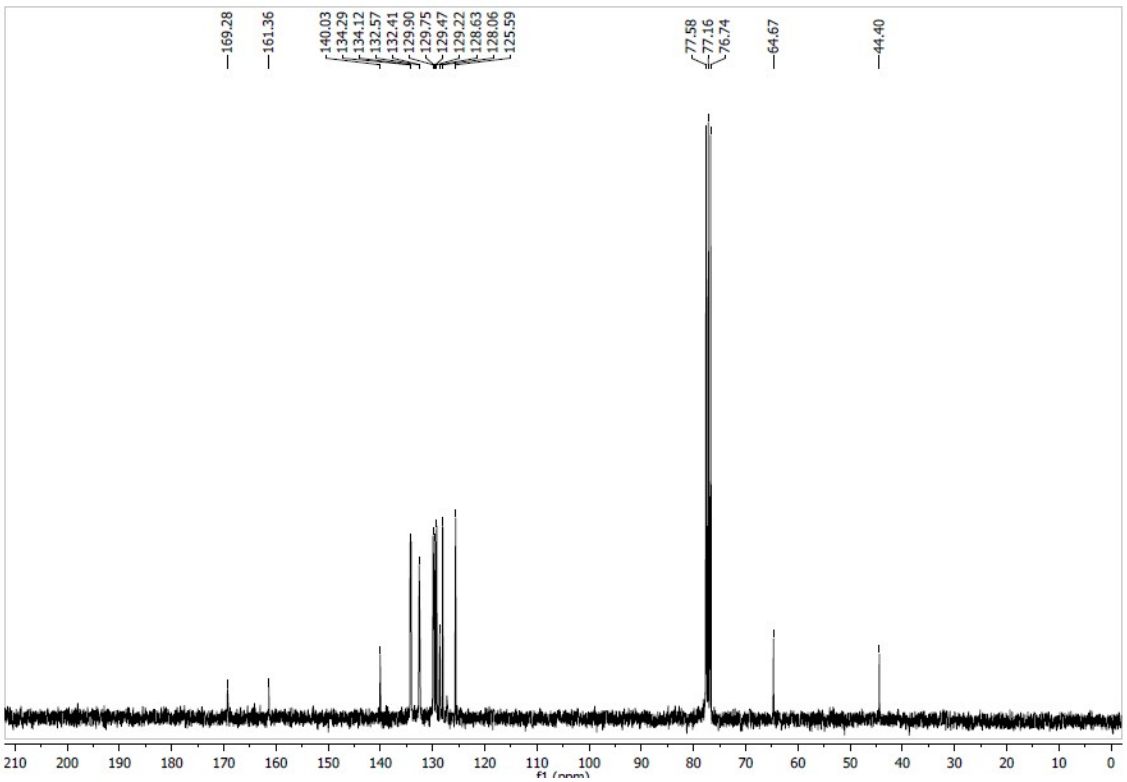


Complex **1**. 13C NMR (75 MHz, CDCl3) δ 169.3, 165.4, 161.3, 137.7 (d, JC-P = 96.8 Hz), 134.2 (d, JC-P = 12.9 Hz), 132.6, 132.3, 130.0, 130.0 (d, JC-P = 13.9 Hz), 129.3, 129.2, 128.0, 127.2, 125.5,

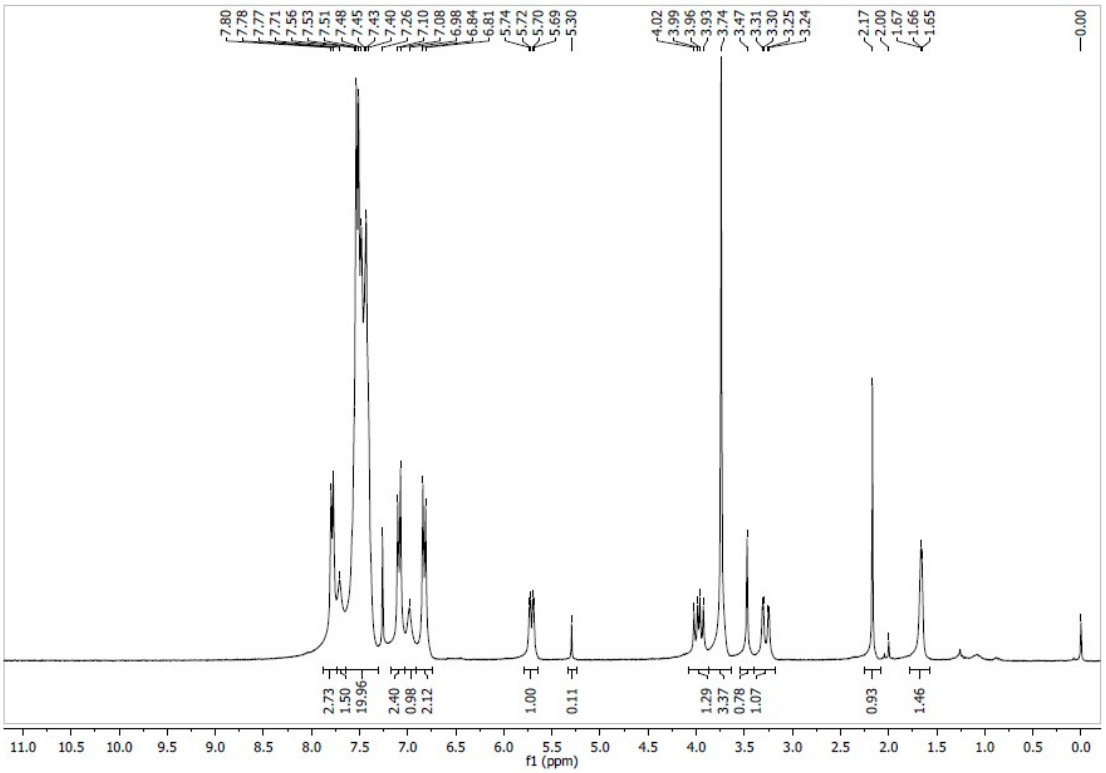
64.4, 44.4, 21.3.



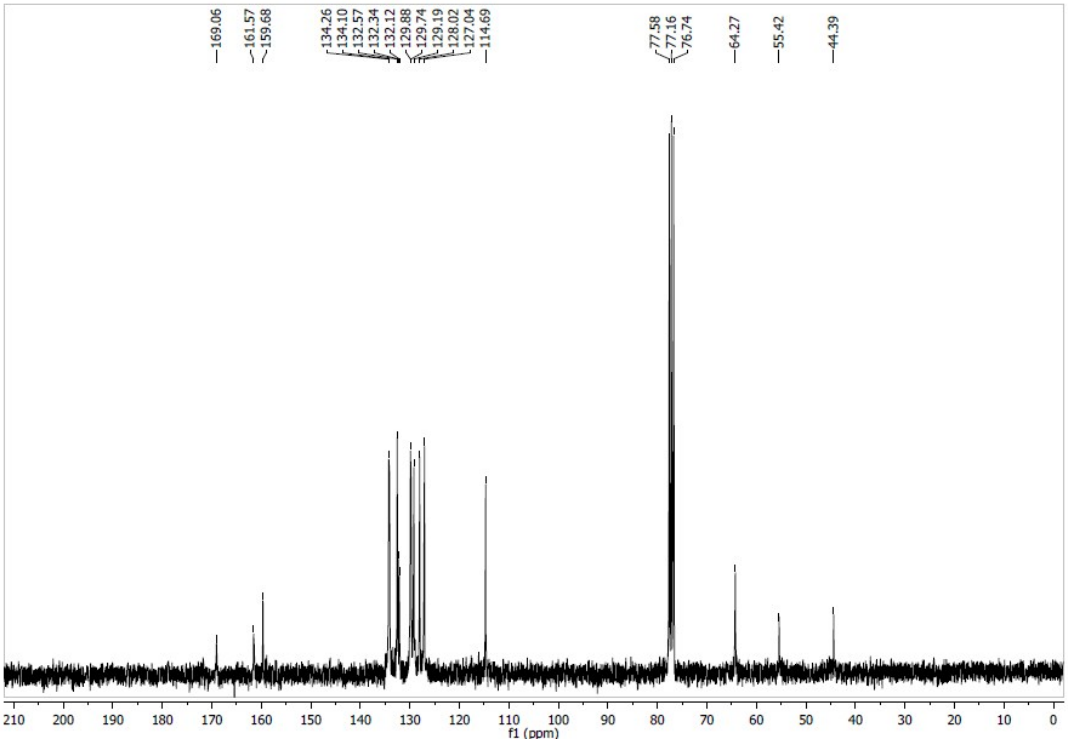
Complex **2**. 1H NMR (300 MHz, CDCl3) δ 7.80-7.78 (m, 2H, Ar), 7.74 (bs, 1H, NH), 7.58-7.41 (m, 18H, Ar), 7.35-7.26 (m, 3H, Ar), 7.18-7.16 (m, 2H, Ar), 7.04 (bs, 1H, NH), 5.77 (dd, J = 11.0, 3.6 Hz), 4.02 (dd, J = 18.2, 11.0 Hz), 3.31 (dd, J = 18.1, 3.4 Hz).



Complex **2**. 13C NMR (75 MHz, CDCl3) δ 169.3, 161.4, 140.0, 134.3, 134.1, 132.6, 132.4, 129.9, 129.8, 129.5, 129.2, 128.6, 128.1, 125.6, 64.7, 44.4.



Complex **3**. 1H NMR (300 MHz, CDCl3) δ 7.80-7.77 (m, 2H, Ar), 7.71 (bs, 1H, NH), 7.56-7.40 (m, 18H, Ar), 7.10-7.08 (m, 2H, Ar), 6.98 (bs, 1H, NH), 6.84-6.81 (m, 2H, Ar), 5.71 (dd, J = 11.0, 3.6 Hz, 1H), 3.97 (dd, J = 18.2, 11.0 Hz, 1H), 3.74 (s, 3H, OCH3), 3.28 (dd, J = 18.2, 3.6 Hz, 1H).



Complex **3**. 13C NMR (75 MHz, CDCl3) δ 169.1, 161.6, 159.7, 134.3, 134.1, 132.6, 132.3, 132.1, 129.9, 129.7, 129.2, 128.0, 127.0, 114.7, 64.3, 55.4, 44.4.