

SUPPORTING INFORMATION

for

New selective thiolate gold(I) complexes inhibit proliferation of different human cancer cells and induce apoptosis in primary cultures of mouse colon tumors.

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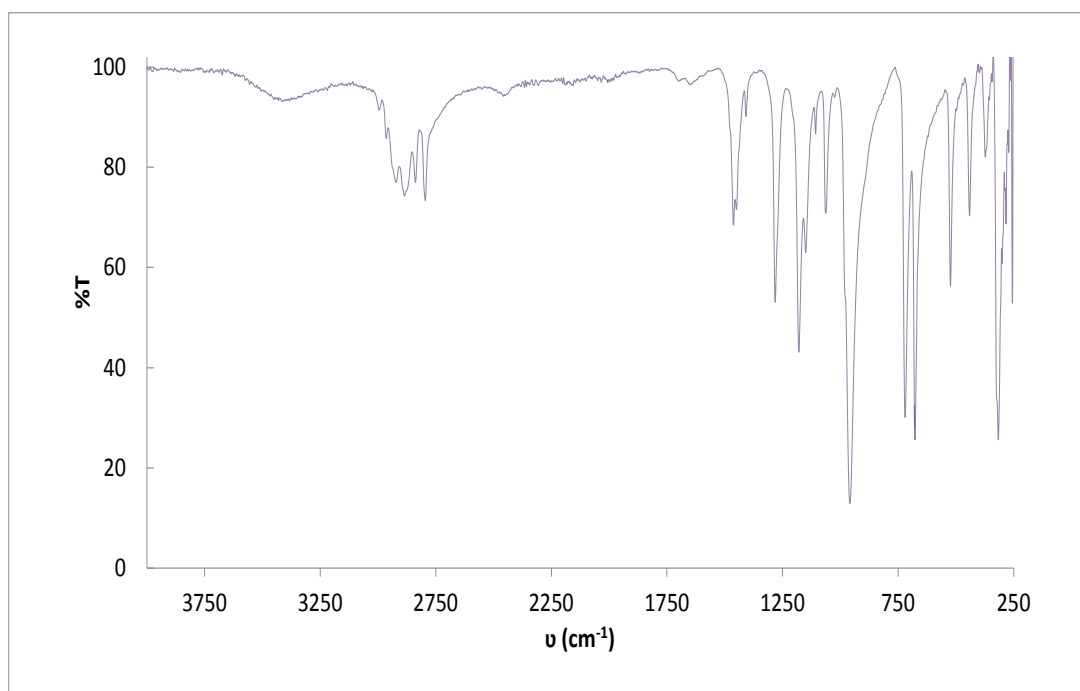


Figure S1. Infrared spectrum of complex 1.

Table S1. Details of data collection and structure refinement for complexes **4**, **5** and **8**.

	Complex 4	Complex 5	Complex 8
<i>Chemical Formula</i>	C ₁₂ H ₂₅ AuN ₃ PS	C ₅₂ H ₈₈ Au ₄ N ₁₆ P ₄ S ₈	C ₁₀ H ₂₁ AuN ₅ OPS
<i>CCDC number</i>	1938214	1938215	<i>Supp. Information</i>
<i>Molecular Weight</i>	499.36	2105.60	487.31
<i>Temperature (K)</i>	293(2)	293(2)	293(2)
<i>Crystal system, Cspace group</i>	Triclinic, P -1	Monoclinic, P 21/c	Monoclinic, P 21/c
Cell unit dimensions			
<i>a(Å)</i>	7.9330(4)	7.7454(2)	16.0623(9)
<i>b(Å)</i>	9.2516(4)	13.1136(3)	21.3110(10)
<i>c(Å)</i>	13.6133(8)	18.2077(5)	19.9610(13)
<i>α (°)</i>	72.501(5)	90	90
<i>β (°)</i>	80.034(4)	107.215(2)	103.728(6)
<i>γ (°)</i>	68.630(4)	90	90
<i>Volumen</i>	885.10(9)	1766.51(8)	6637.5(7)
<i>Z</i>	2	1	16
<i>Calculated density (g/cm³)</i>	1.874	1.979	1.951
<i>F(000)</i>	484	1016	3744
<i>Collected/unique reflexions</i>	13818	13769	51002
<i>Data/retrains/parametres</i>	3792/0/182	3703/0/196	14143/102/685
<i>F²</i>	1.040	1.094	0.999
<i>Final R values</i>	R ₁ 0.0336 wR ₂ 0.0653	R ₁ 0.0268 wR ₂ 0.0569	R ₁ 0.0912 wR ₂ 0.1221
<i>R all data</i>	R ₁ 0.0428 wR ₂ 0.0697	R ₁ 0.0308 wR ₂ 0.0588	R ₁ 0.2587 wR ₂ 0.1795

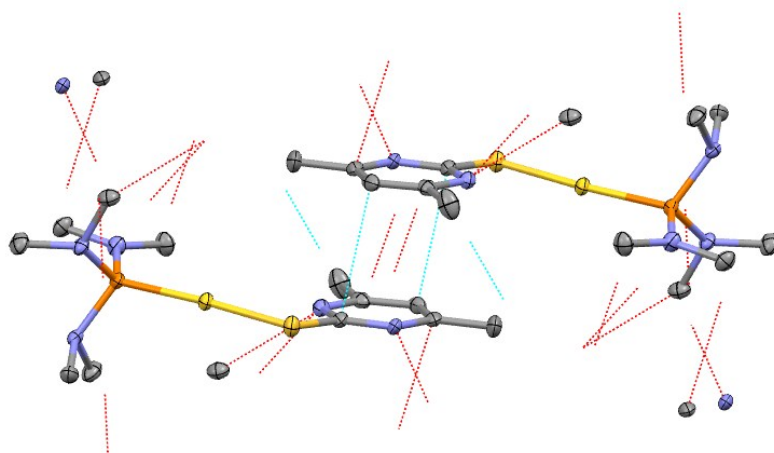


Figure S2. Stacking interactions between aromatic rings of complex **4**.

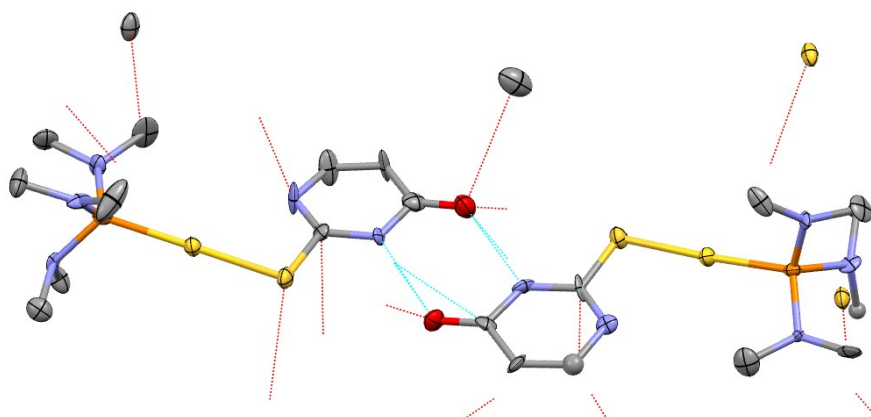


Figure S3. Hydrogen bond interactions between N6-O3 y N11-O2 atoms, presents in complex **8**.

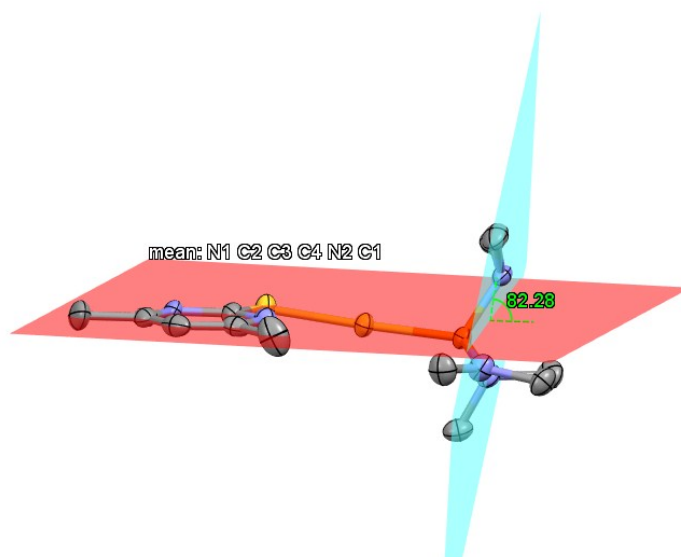


Figure S4. Angle of 82.28° between the plane containing the benzene ring and the defined plane for nitrogen atoms pertaining to the HMPT ligand.

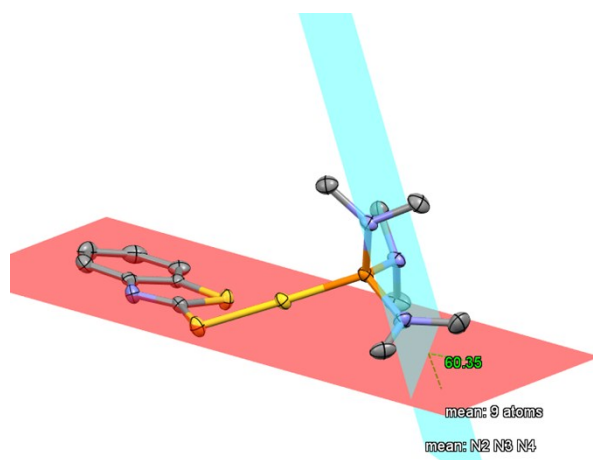
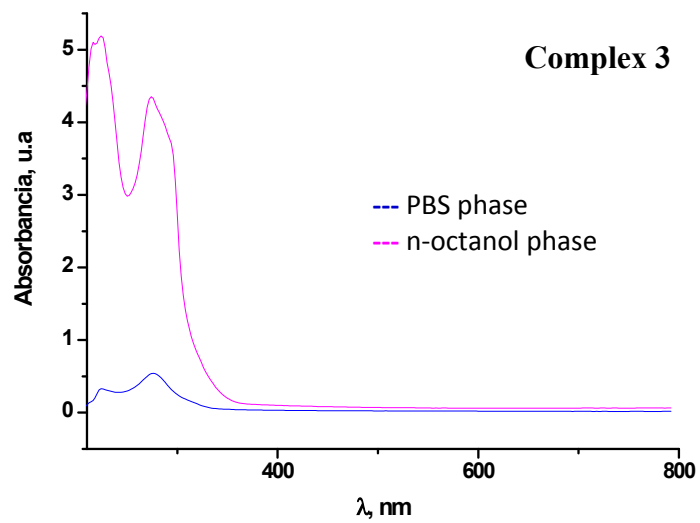
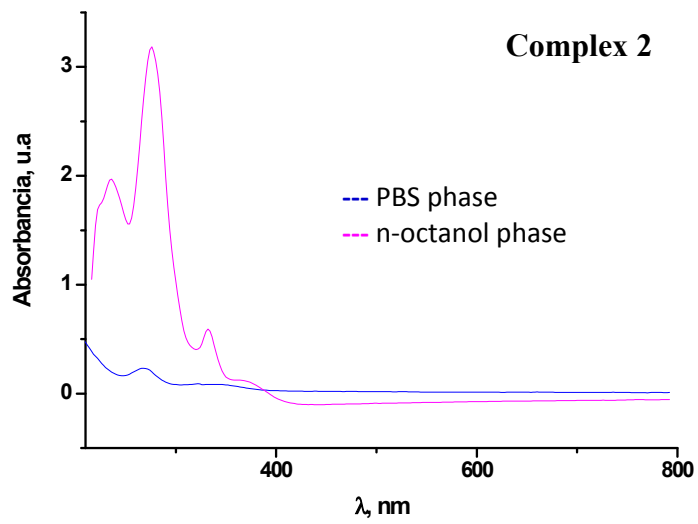
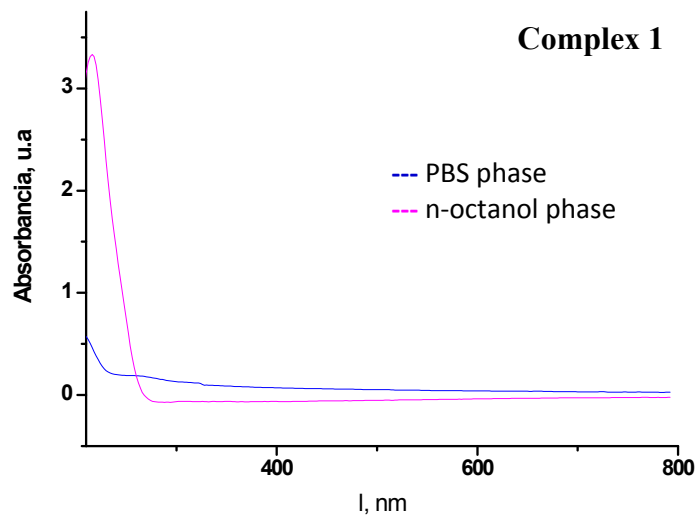
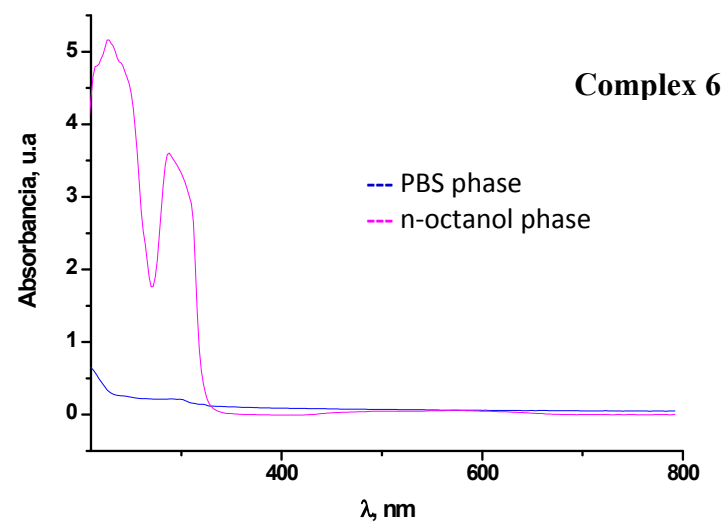
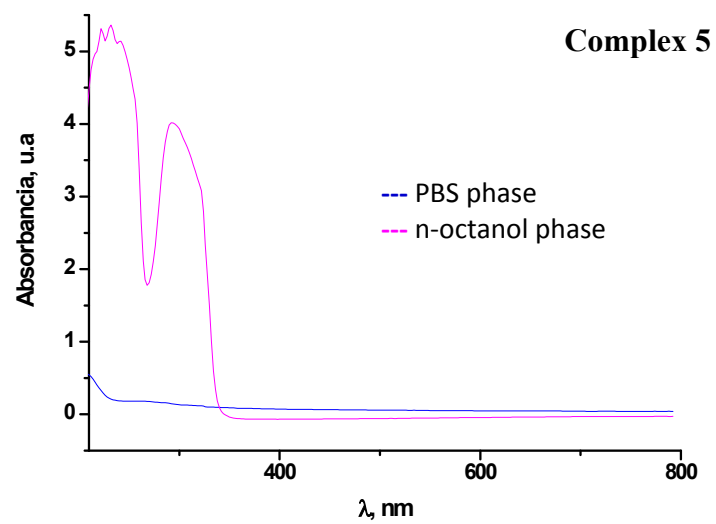
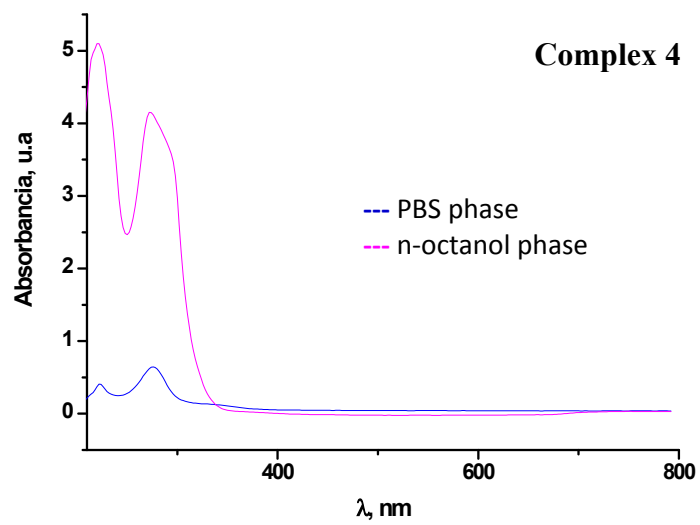


Figure S5. Angle of 60.35° between the plane containing the benzene ring and the defined plane for nitrogen atoms pertaining to the HMPT ligand.





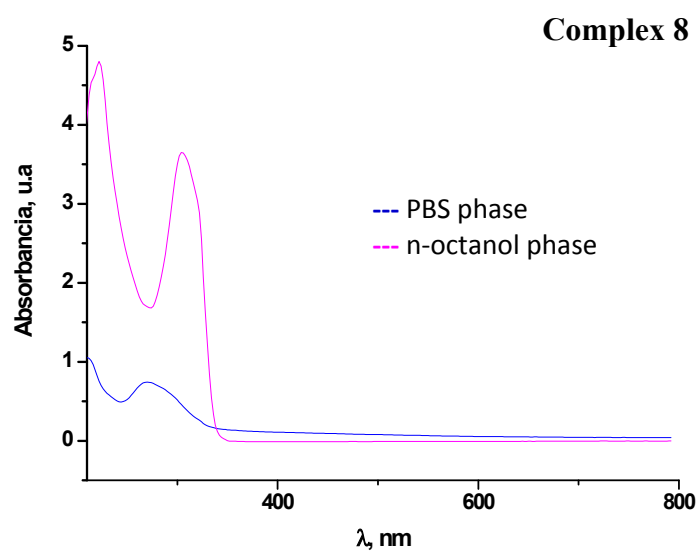
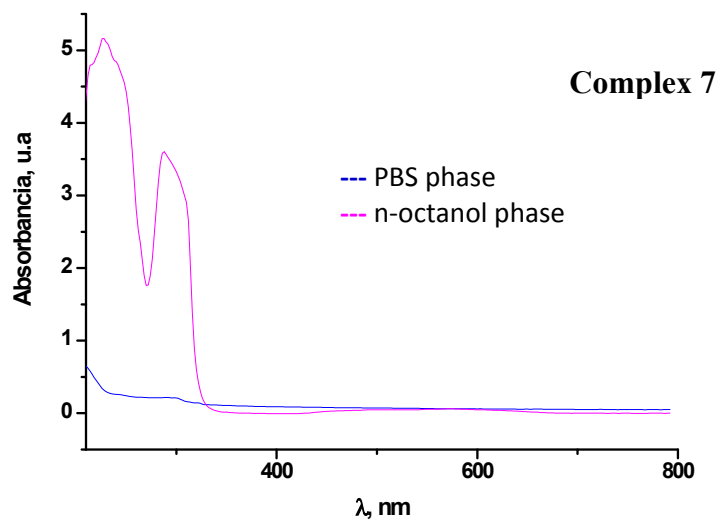
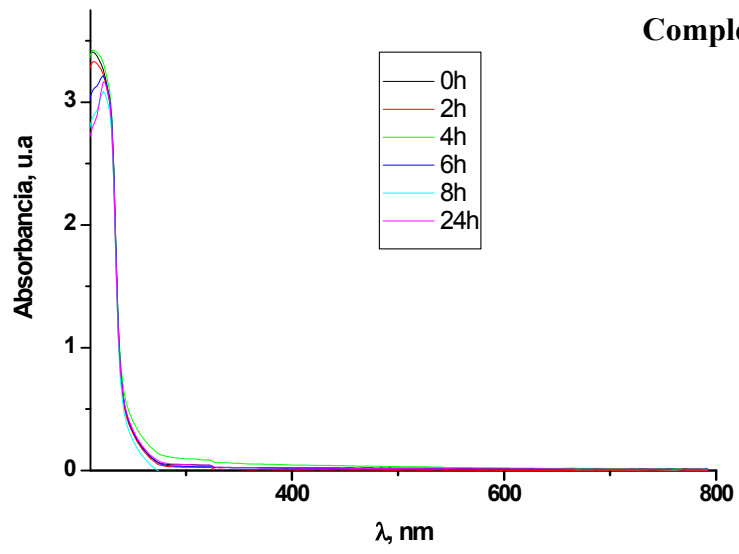
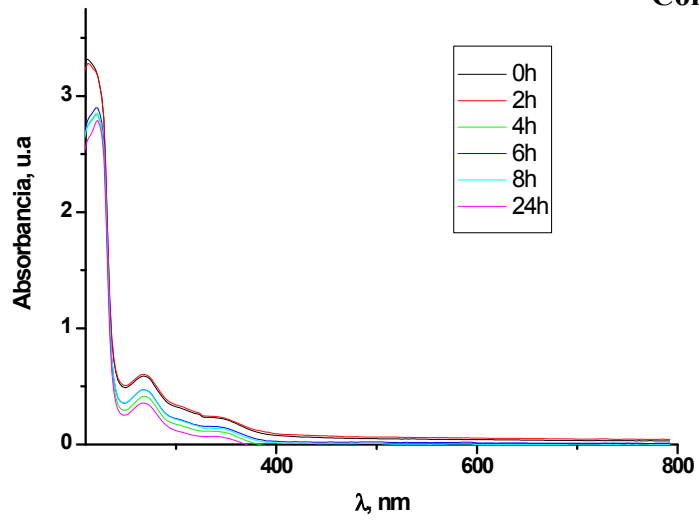


Figure S6. UV-Vis spectra of **1-8** complexes recorded in PBS and n-octanol at 37°C.

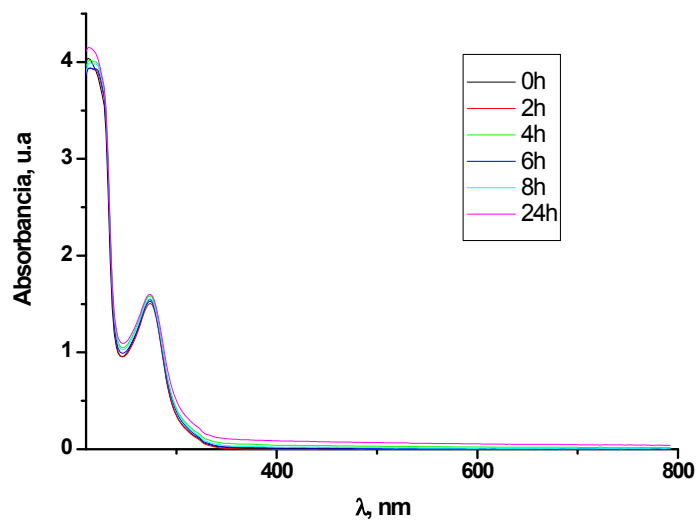
Complex 1

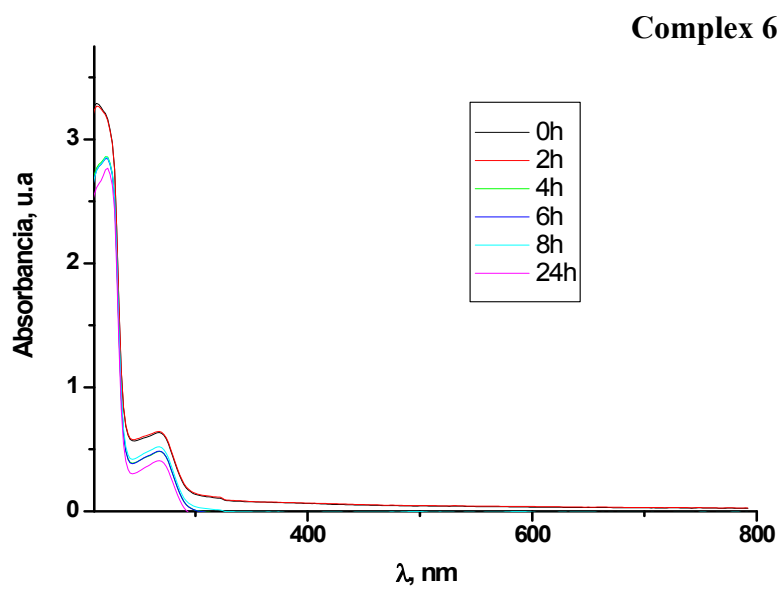
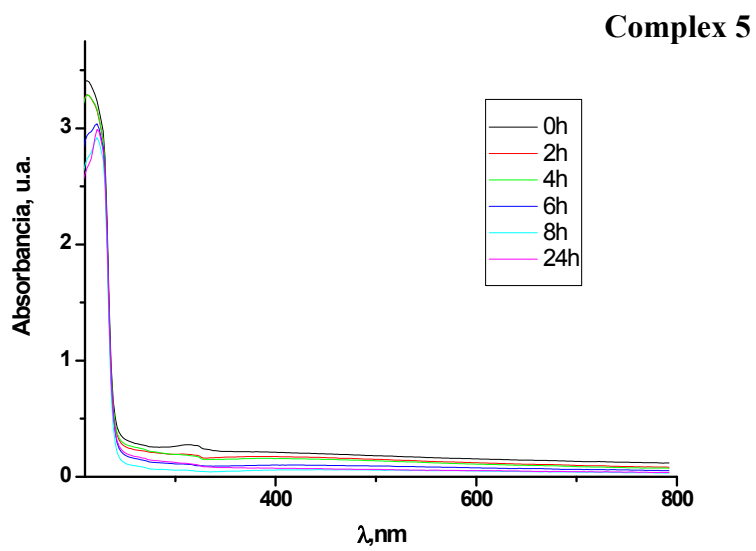
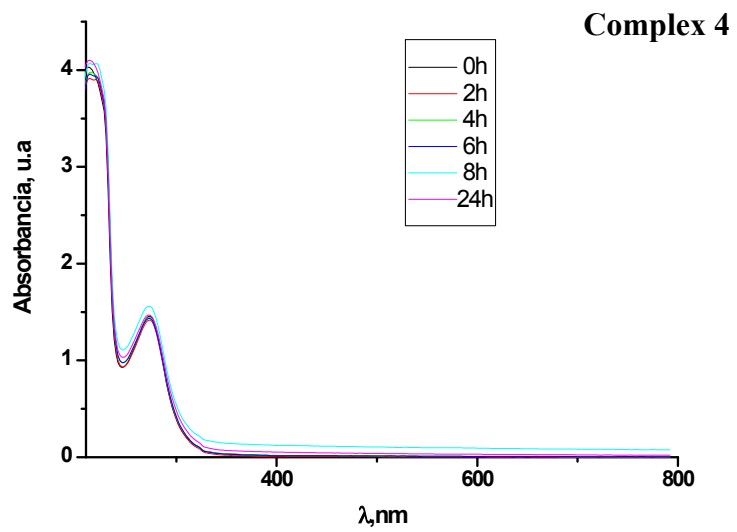


Complex 2

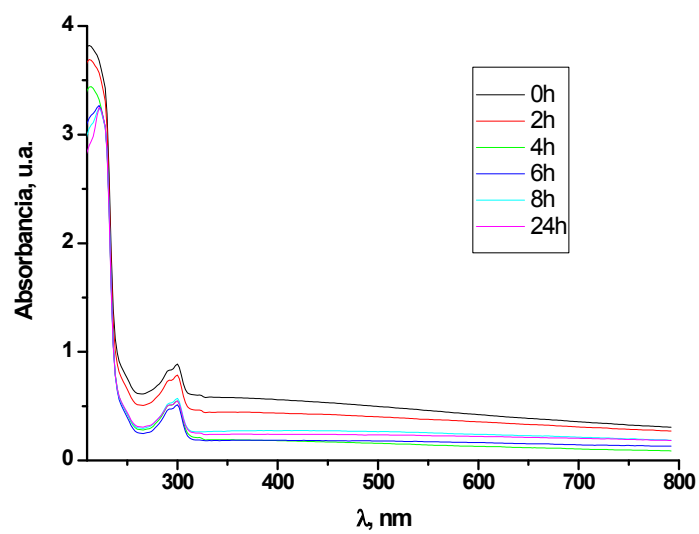


Complex 3





Complex 7



Complex 8

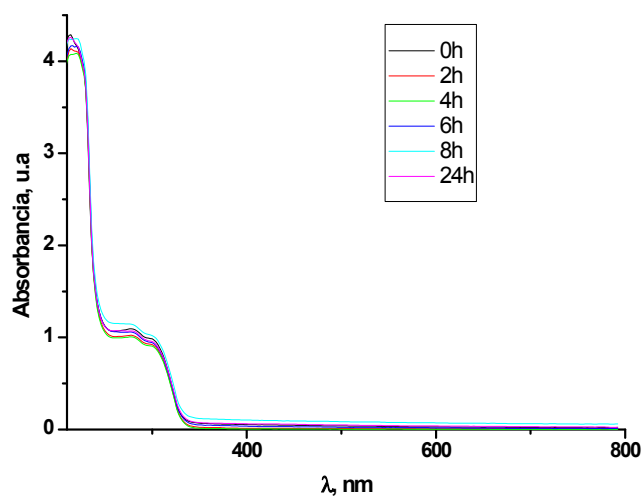
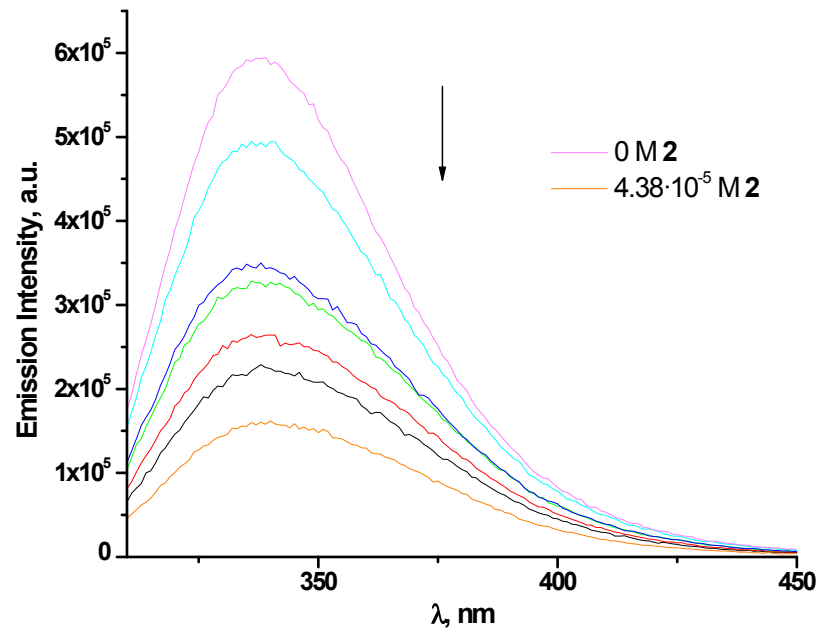
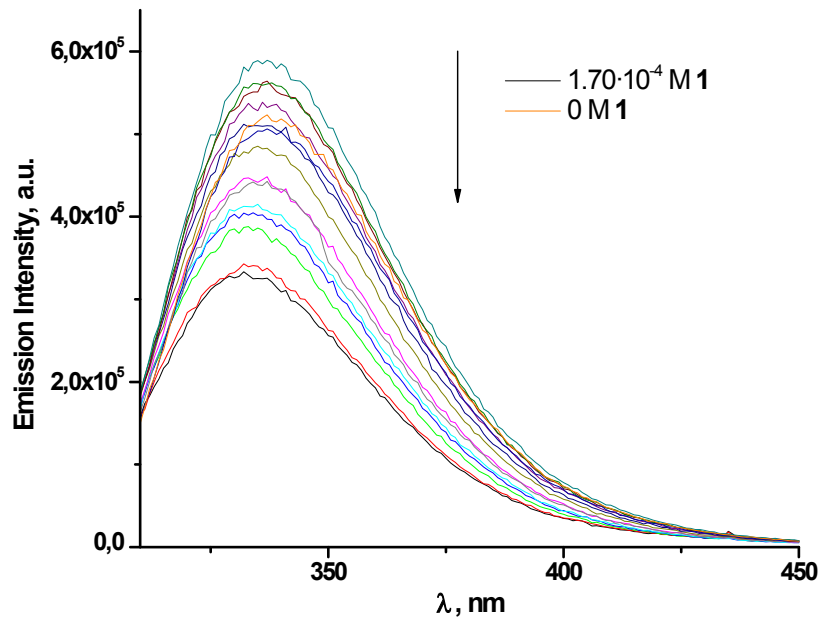
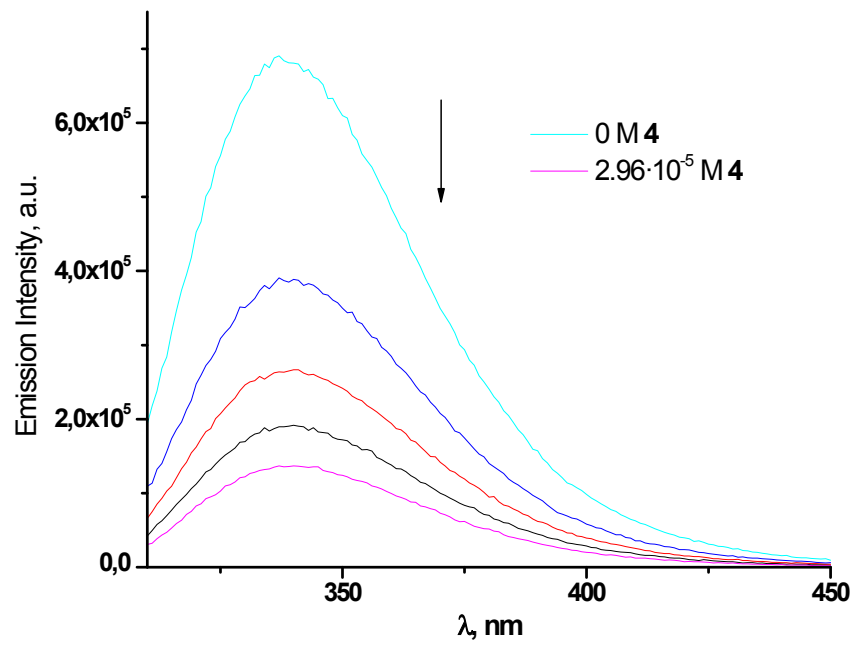
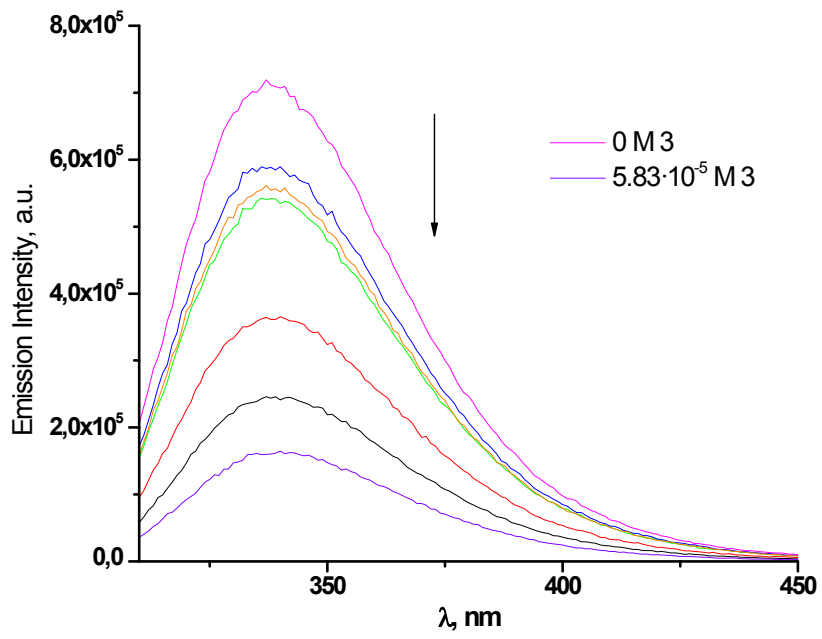
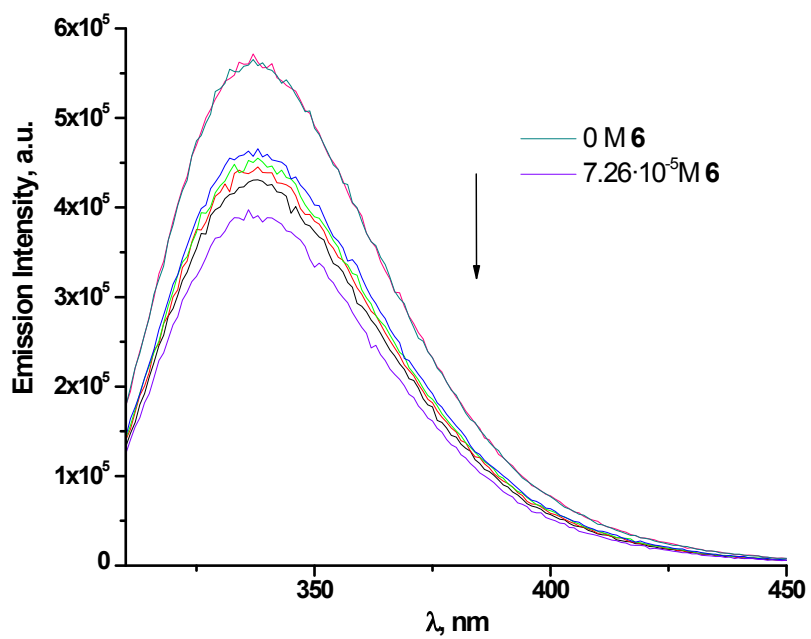
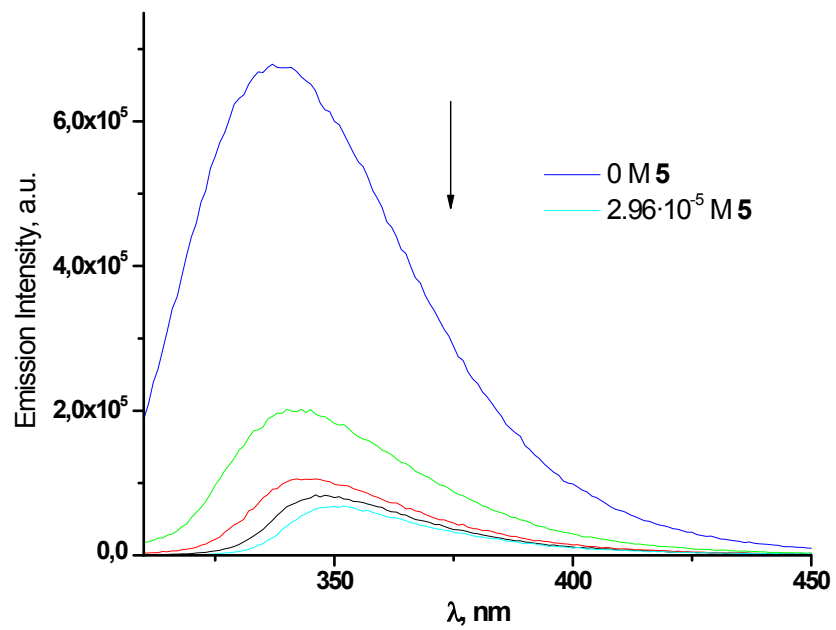


Figure S7. UV-Vis spectra of **1-8** complexes recorded at different times for 24 h in PBS at 37°C.







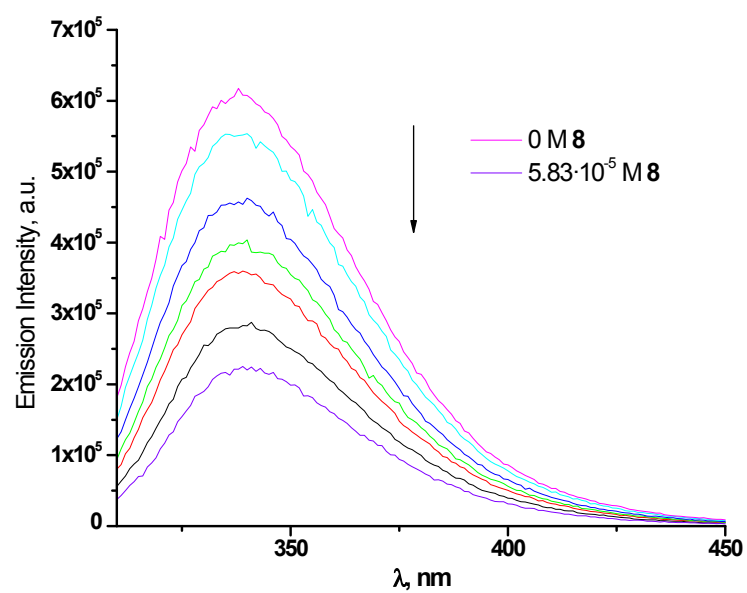
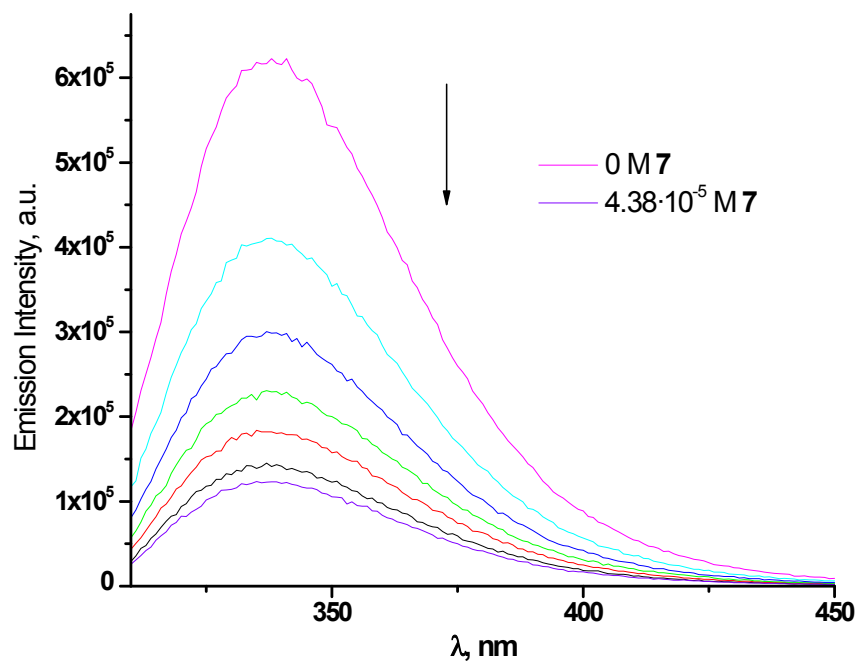


Figure S8. Fluorescence emission spectra of BSA at 298 K in the presence of increasing amounts of the gold(I) complexes.

