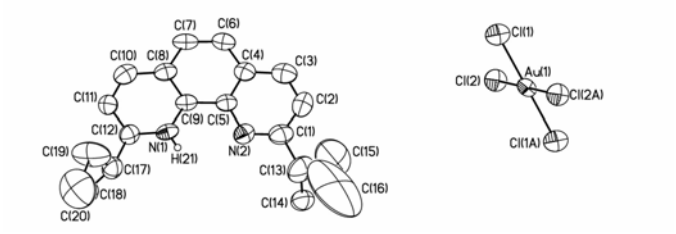
Synthesis and characterization of gold(III) complexes possessing 2,9-dialkylphenanthroline ligands: to bind or not to bind?

A



B

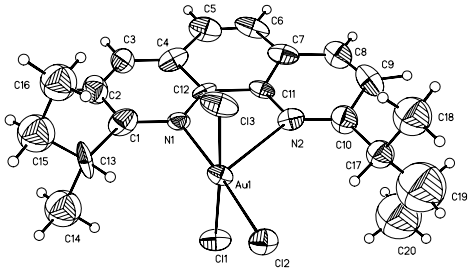
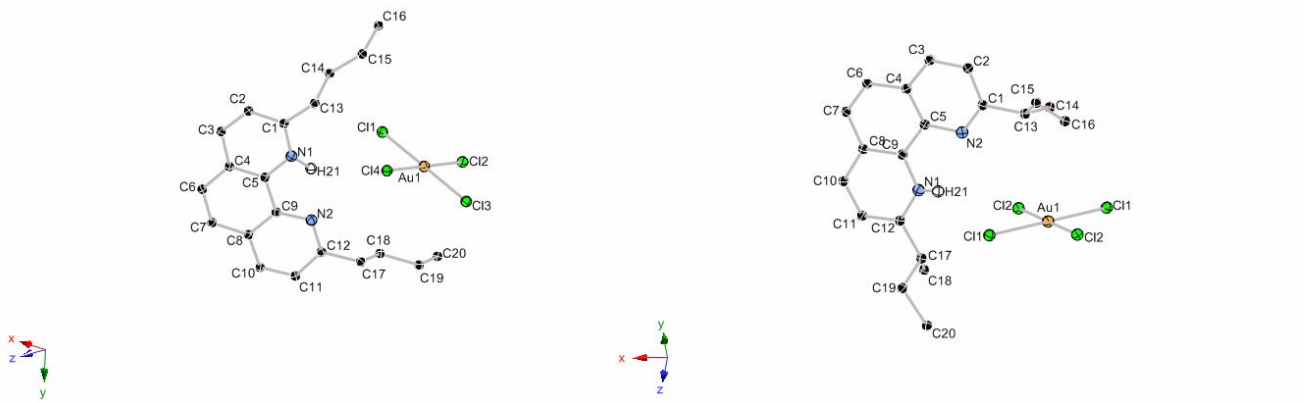


Figure S1. Molecular structures and numbering schemes for **A**) $[^{sec\text{-}Bu}phenH]^{+}[AuCl_4]^{-}$ (**2**) and **B**) $[Au(^{sec\text{-}Bu}phen)Cl_3]$ (**4**). Thermal ellipsoids drawn at 35% probability for **B**; thermal ellipsoids drawn at 50% probability for **A**. Hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (°) for **2**: Au-Cl···H–N 3.000, Au(1)–Cl(1) 2.278(2), Au(1) –Cl(2) 2.2807(18), Au(2)–Cl(3) 2.273(2), Au(2)–Cl(4) 2.277(2), Cl(1) –Au(1) –Cl(2) 90.34(7) and **4:** Au(1)–N(1) 2.063(15), Au(1)–N(2) 2.598(18), Au(1)–Cl(1) 2.285(5), Au(1)–Cl(2) 2.265(5), Au(1)–Cl(3) 2.275(6), N(1)–Au(1)–Cl(1) 90.7(5), N(1)–Au(1)–Cl(2) 175.6(6), Cl(1)–Au(1)–Cl(2)89.9(2), N(1)–Au(1)–Cl(3)88.9(5), Cl(1)–Au(1)–Cl(3)176.3(3).

Table S1. Crystal and refinement data for complex **4.**

Empirical formula	C20 H24 Au Cl3 N2	
Formula weight	595.73	
Temperature	172(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.5833(9) Å	α= 92.228(9)°.
	b = 16.761(2) Å	β= 98.611(9)°.
	c = 17.214(2) Å	γ = 98.813(8)°.
Volume	2133.5(5) $Å^3$	
Z	4	
Density (calculated)	1.855 Mg/m^3	
Absorption coefficient	7.278 mm^{-1}	
F(000)	1152	
Crystal size	0.45 x 0.03 x 0.02 mm^3	
Theta range for data collection	1.66 to 26.62°.	
Index ranges	-9<=h<=9, -20<=k<=20, 0<=l<=21	
Reflections collected	8771	
Independent reflections	8771 [R(int) = 0.1103]	
Completeness to theta = 26.62°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8681 and 0.1382	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8771 / 1 / 394	
Goodness-of-fit on F^2	1.103	
Final R indices [I>2sigma(I)]	R1 = 0.1077, wR2 = 0.2403	
R indices (all data)	R1 = 0.2039, wR2 = 0.2751	
Largest diff. peak and hole	5.588 and -2.108 e.$Å^{-3}$	



A **B**

Figure S2: Ellipsoid plot of **A**) $[^{n\text{-Bu}}\text{phenH}]^+$ $[AuCl_4]^-$ (**1**) crystal structure and **B**) $[^{sec\text{-Bu}}\text{phenH}]^+$ $[AuCl_4]^-$ (**2**) crystal structure; these better depict the Au-Cl···H-N interactions. The interatomic distance between H21 and Cl4 in **1** is 2.096 Å and H21 and Cl2 in **2** is 3.000 Å.

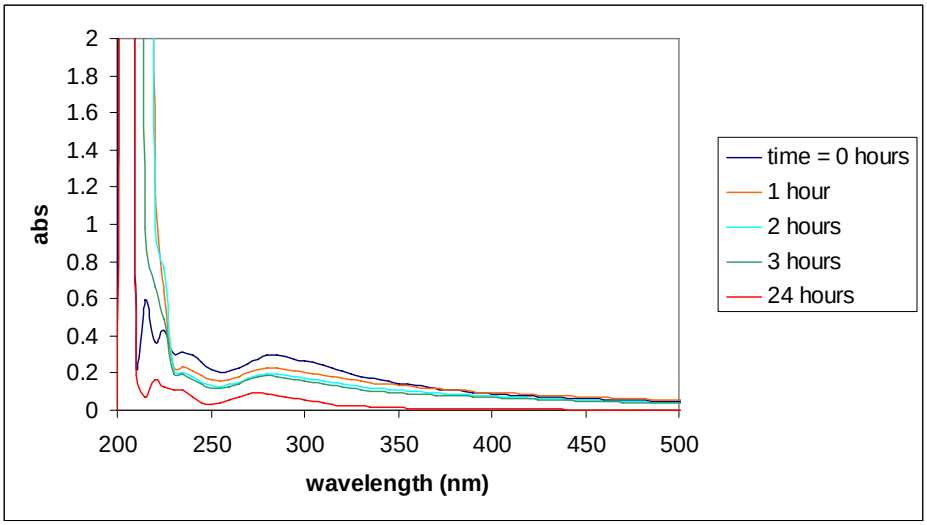


Figure S3: UV/vis spectra of compound **2** in phosphate buffer pH 7.2 over a 24 hour period (0.010 g of the solid gold complex was dissolved in 4.00 mL of a 3:1 2-propanal/acetonitrile solvent mixture temperature; an 8.0 uL aliquot of this solution was diluted in phosphate buffer to a final volume of 3.50 mL, which yielded a gold concentration of 1.0×10^{-5} M; spectra were collected at 20ºC).