

Supplementary Information

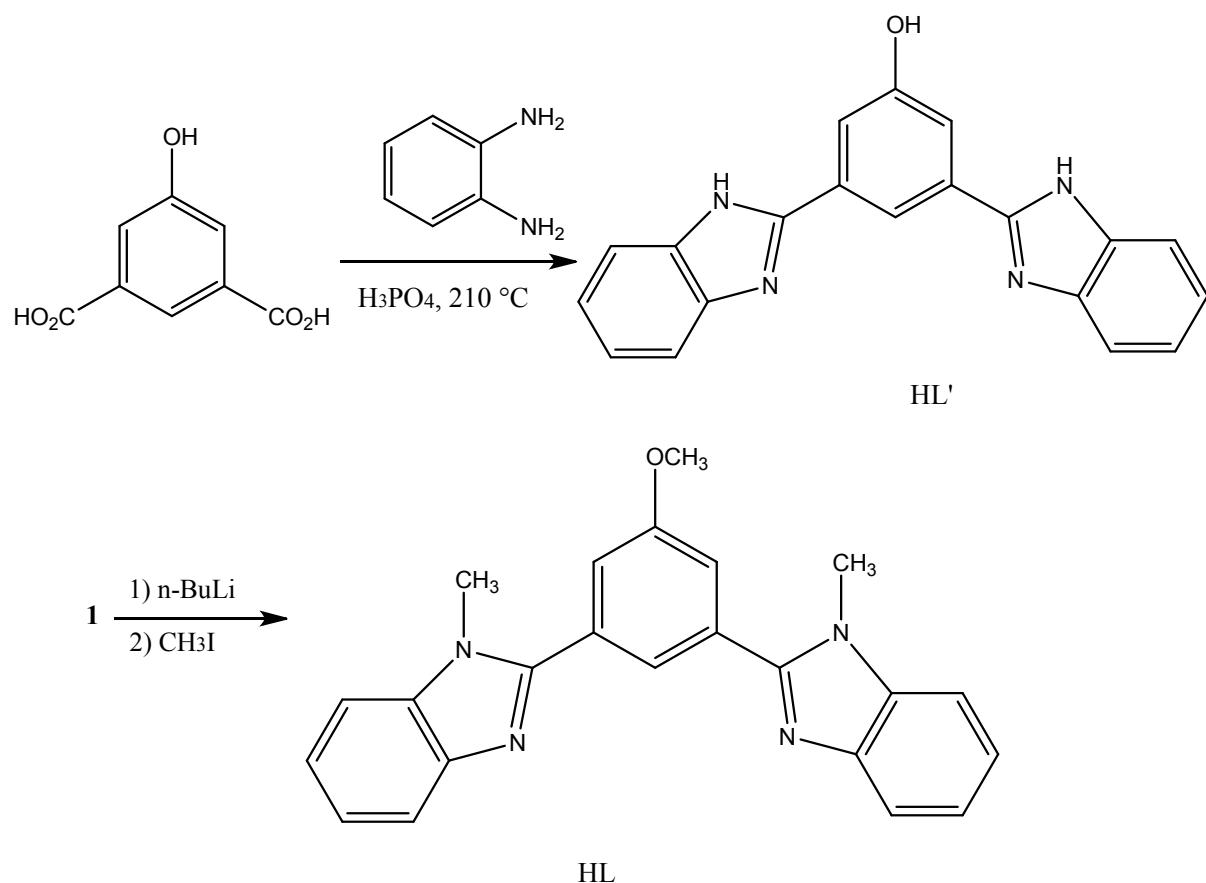
A New Water-Soluble Heteronuclear Pd^{II}-Au^I Pincer Complex as Two-Photon Luminescent Probe for Biological Co²⁺ Detection

Leila Tabrizi *, Hossein Chiniforoshan*

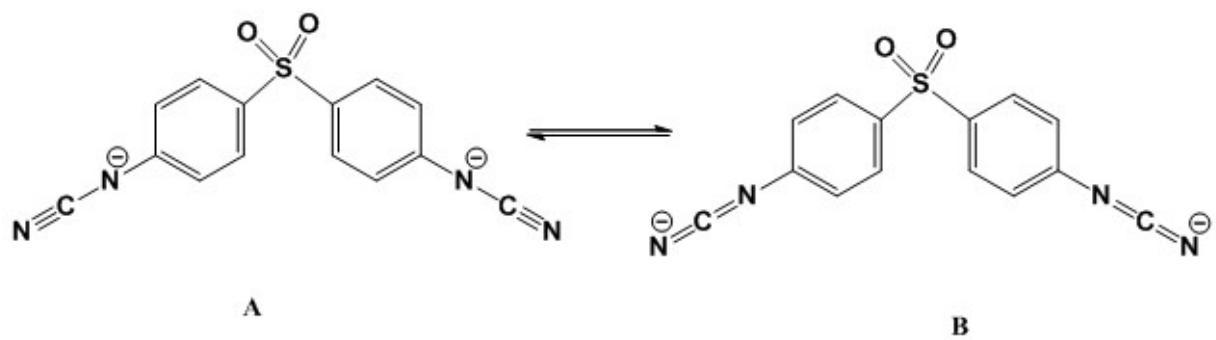
Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran

* Corresponding author: Leila Tabrizi; Email: l.tabrizi@ch.iut.ac.ir

*Corresponding author: H. Chiniforoshan; Email: Chinif@cc.iut.ac.ir



Scheme S1. Synthesis of ligand **HL**.



Scheme S2. Resonance structures of DPS²⁻ anionic ligand.

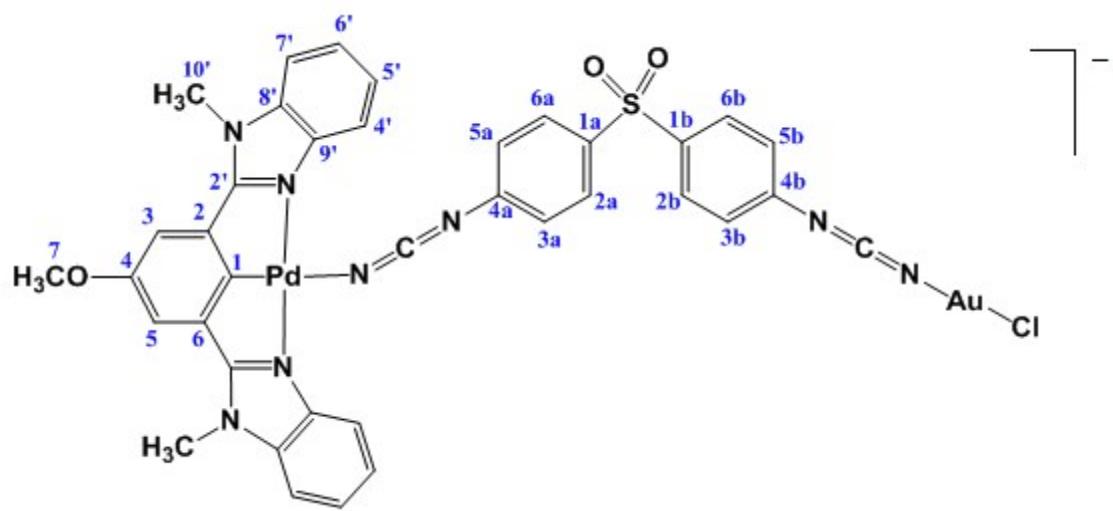


Fig.S1. The structure of complex 1.

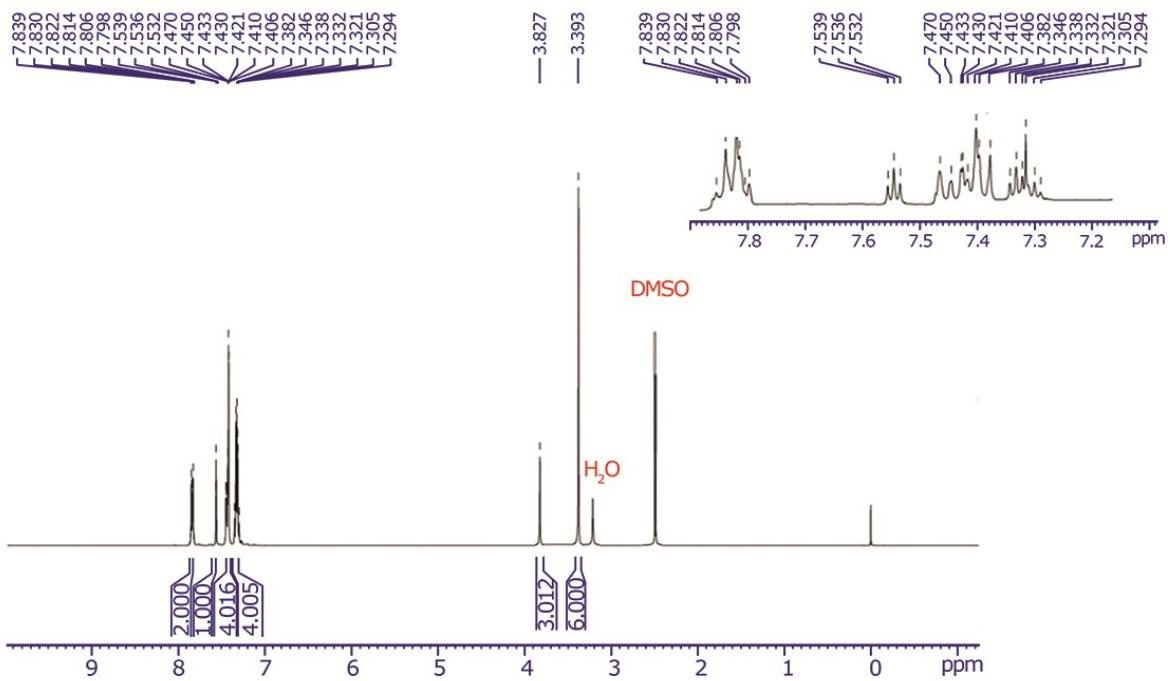


Fig. S2. ^1H NMR spectrum of ligand HL.

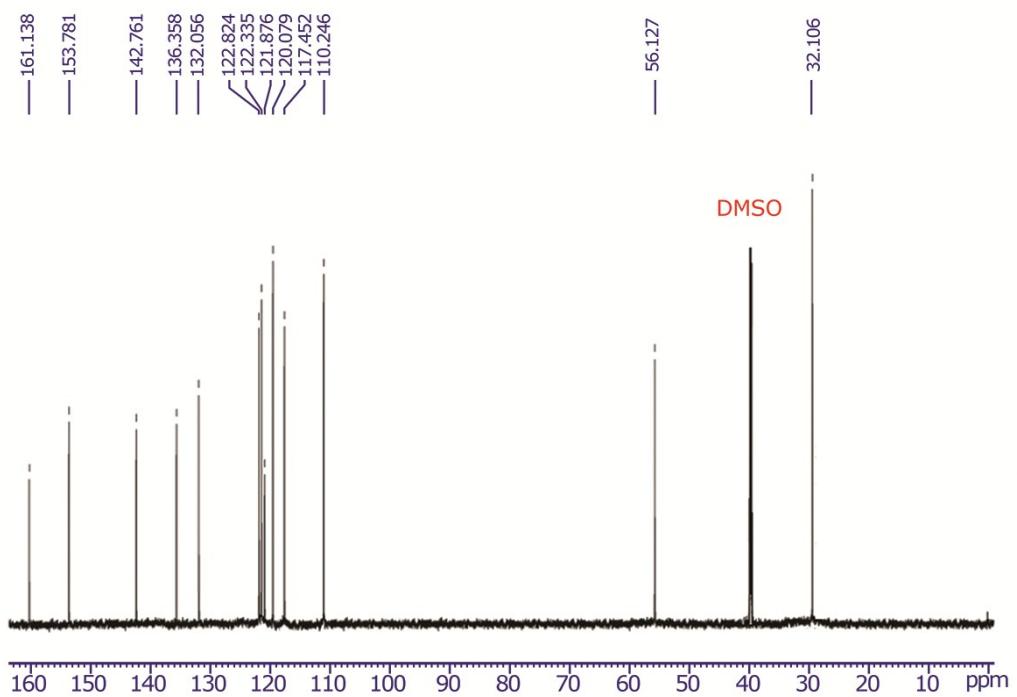


Fig. S3. ¹³C NMR spectrum of ligand HL.

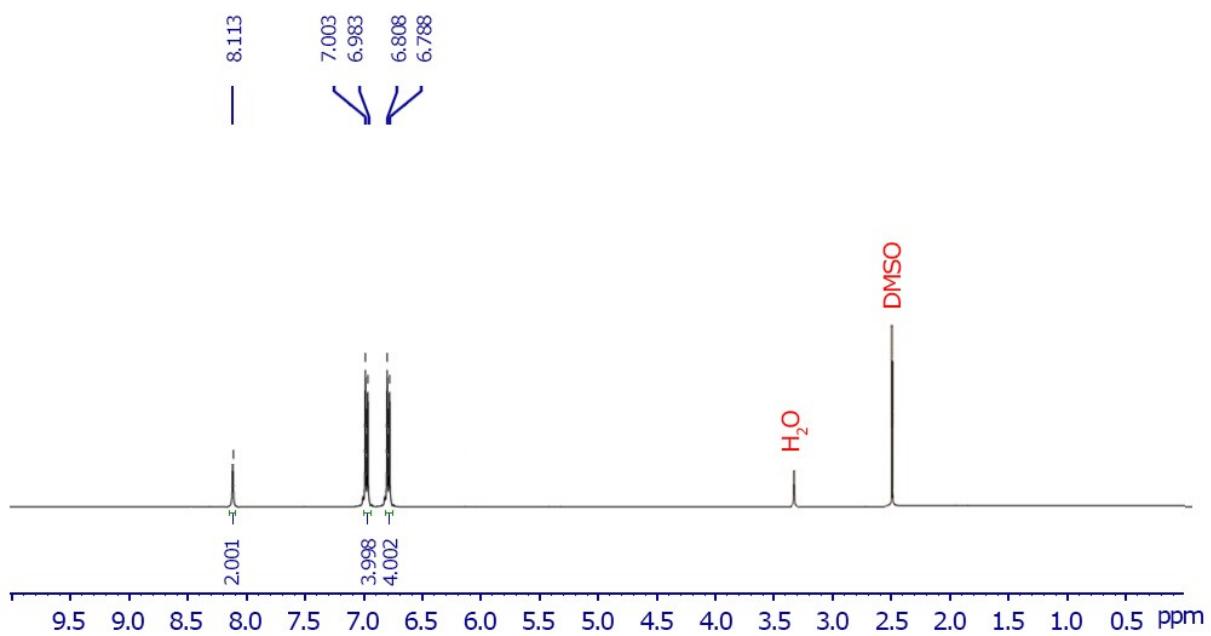


Fig. S4. ^1H NMR spectrum of ligand DPSH₂.

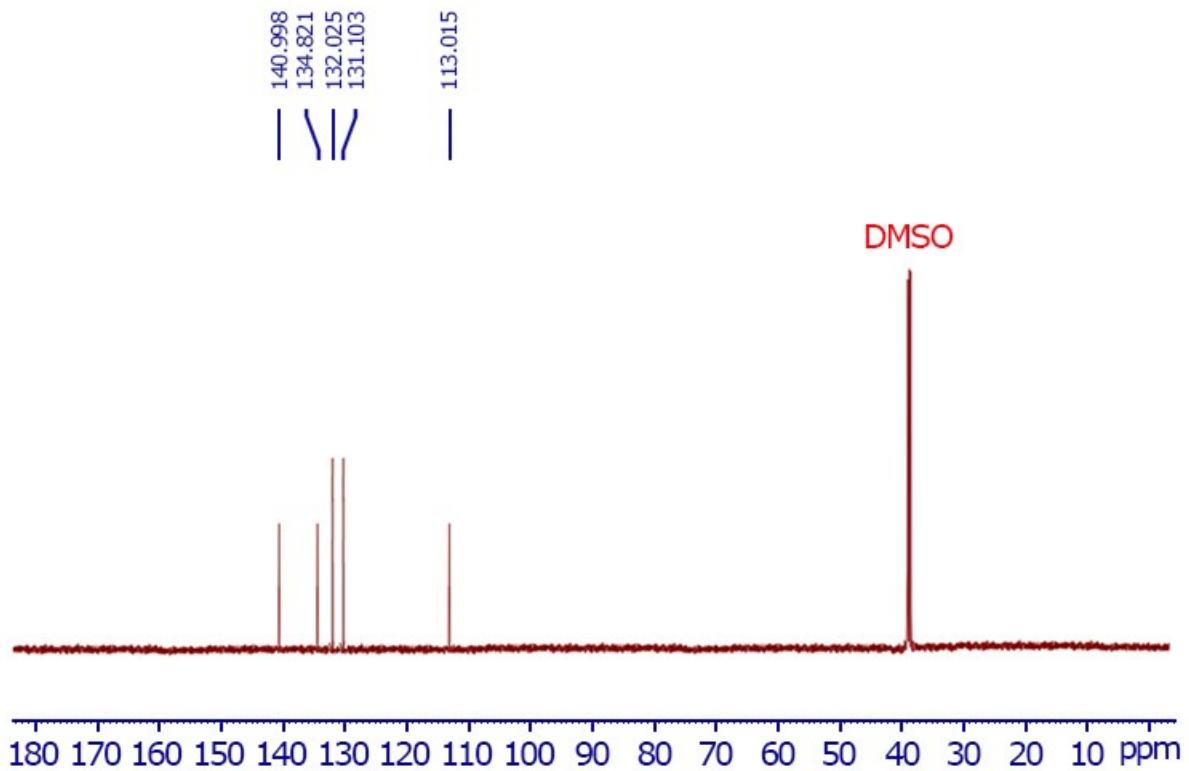


Fig. S5. ^{13}C NMR spectrum of ligand DPSH₂.

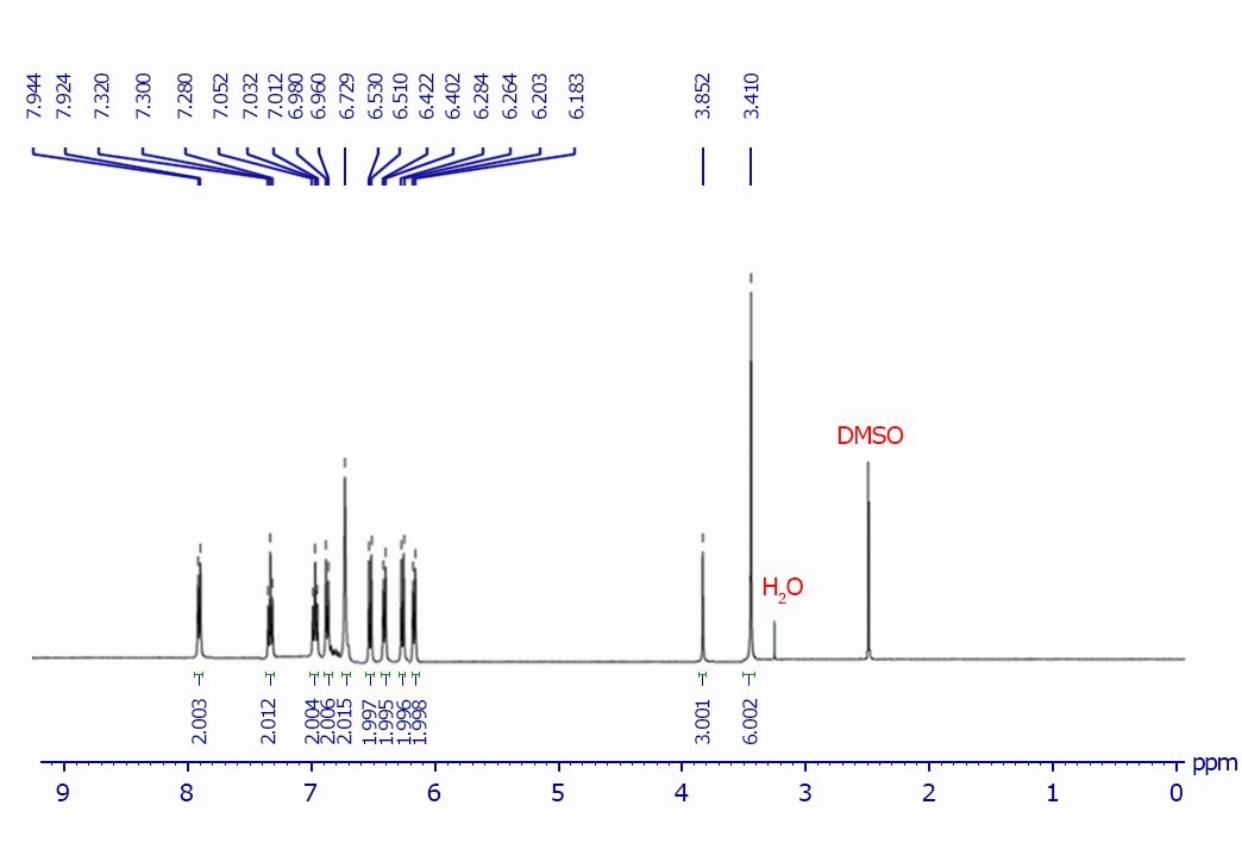


Fig. S6. ¹H NMR spectrum of complex 1.

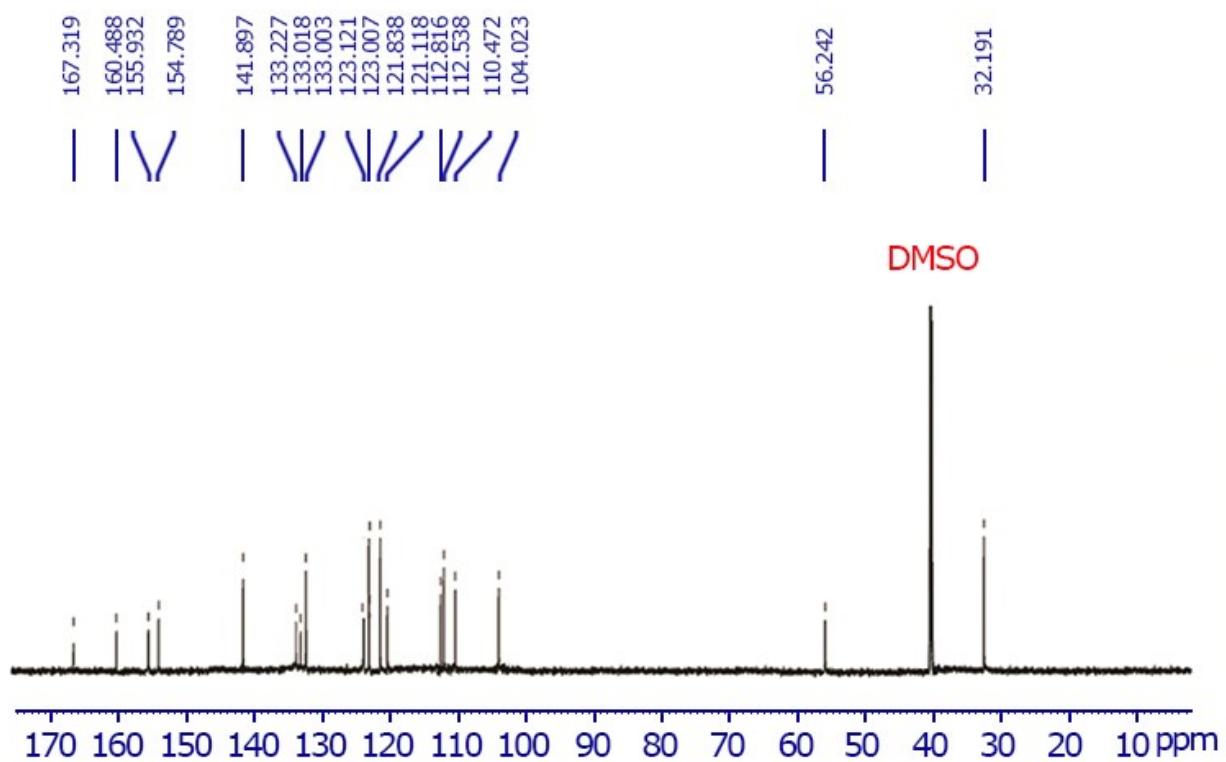


Fig. S7. ^{13}C NMR spectrum of complex **1**.

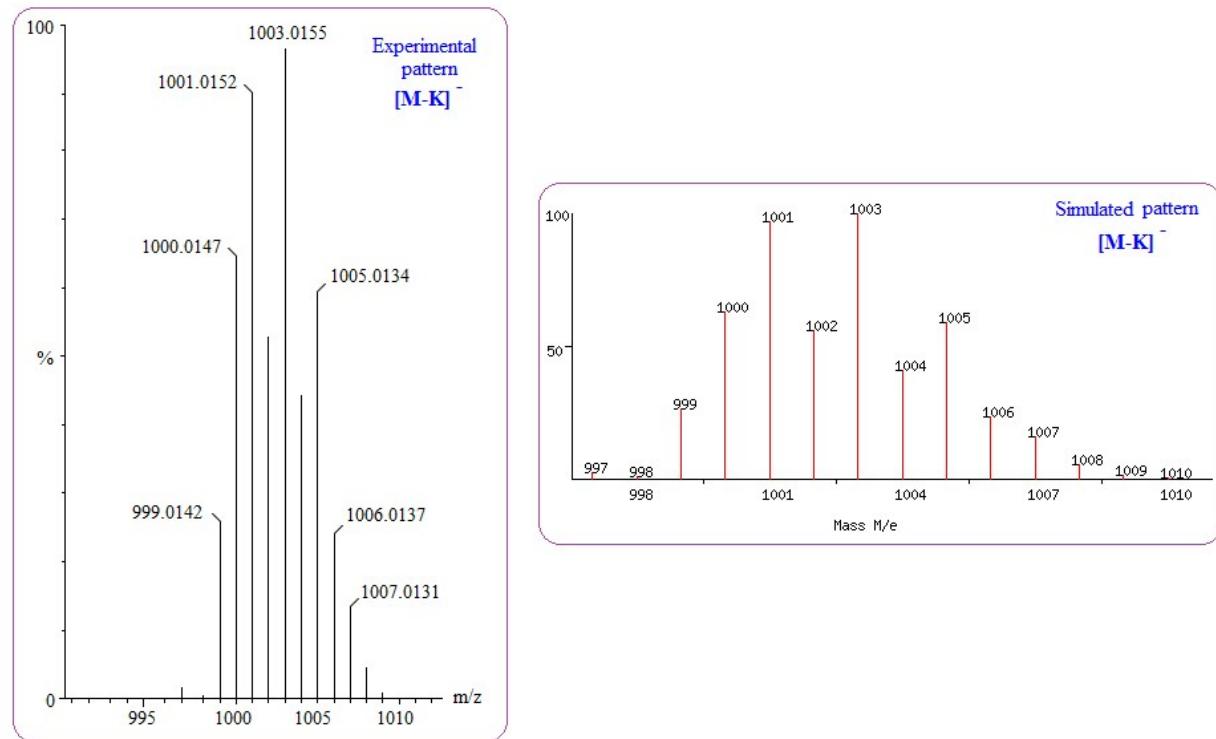


Fig. S8. TOF MS spectrum of complex 1

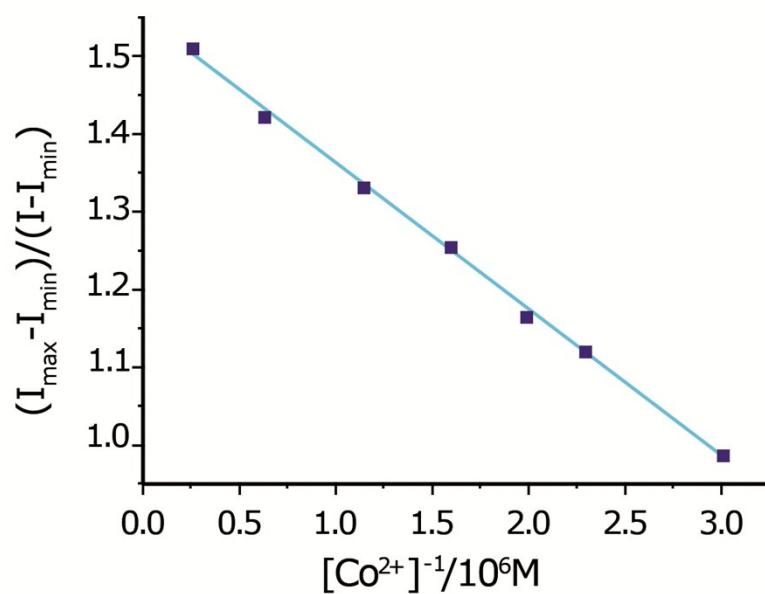


Fig. S9. The binding constant value of Co^{2+} with **1** has been determined from the luminescence titration data following the modified Benesi-Hildebrand equation.

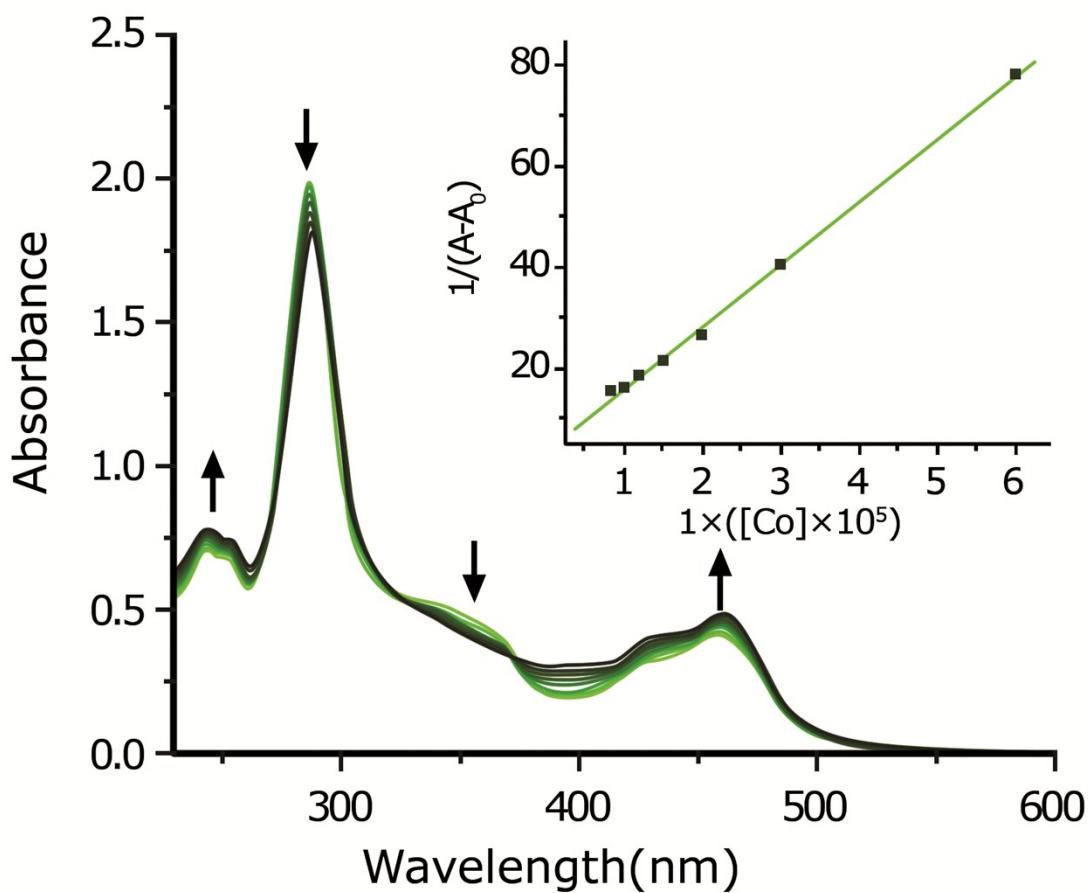


Fig.S10. UV-Vis spectral changes of **1** (10 μM) upon the addition of Co^{2+} (0-50 μM) in aqueous solution (HEPES buffer solution, 10 mM, pH = 7.4).

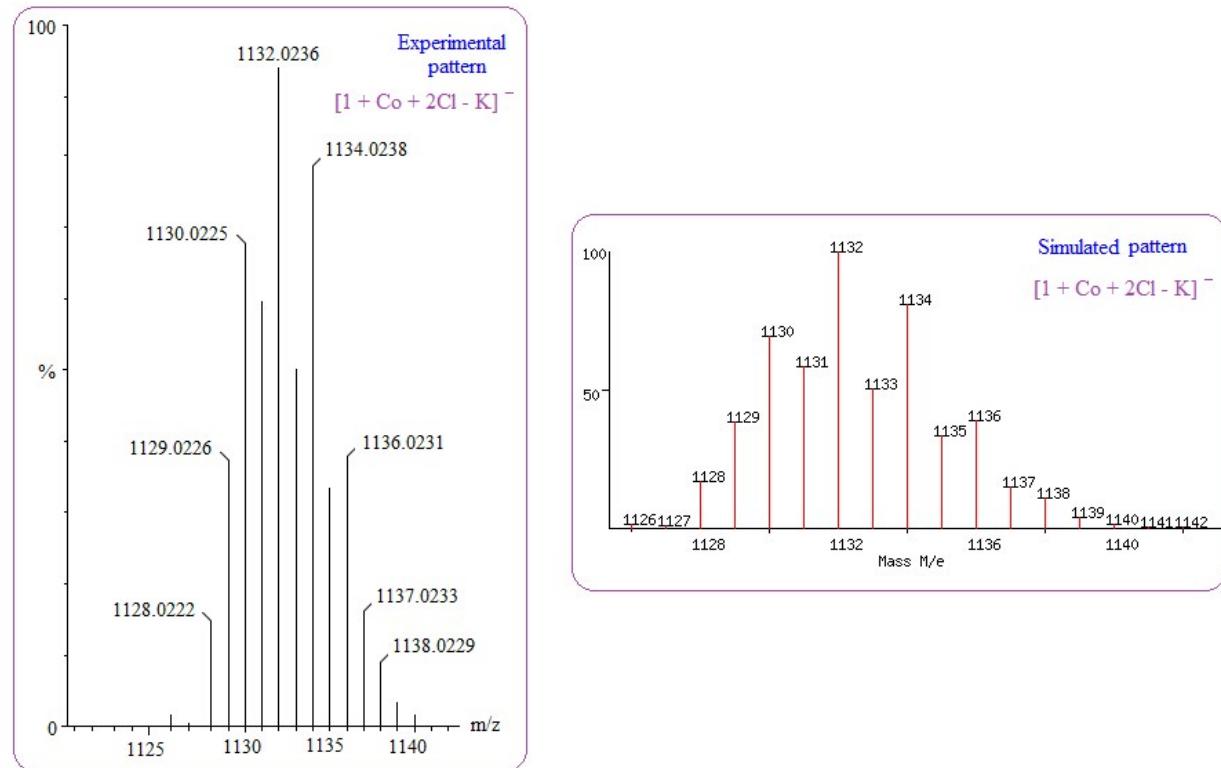


Fig. S11. TOF MS spectrum of complex $\text{K}[1+\text{CoCl}_2]$

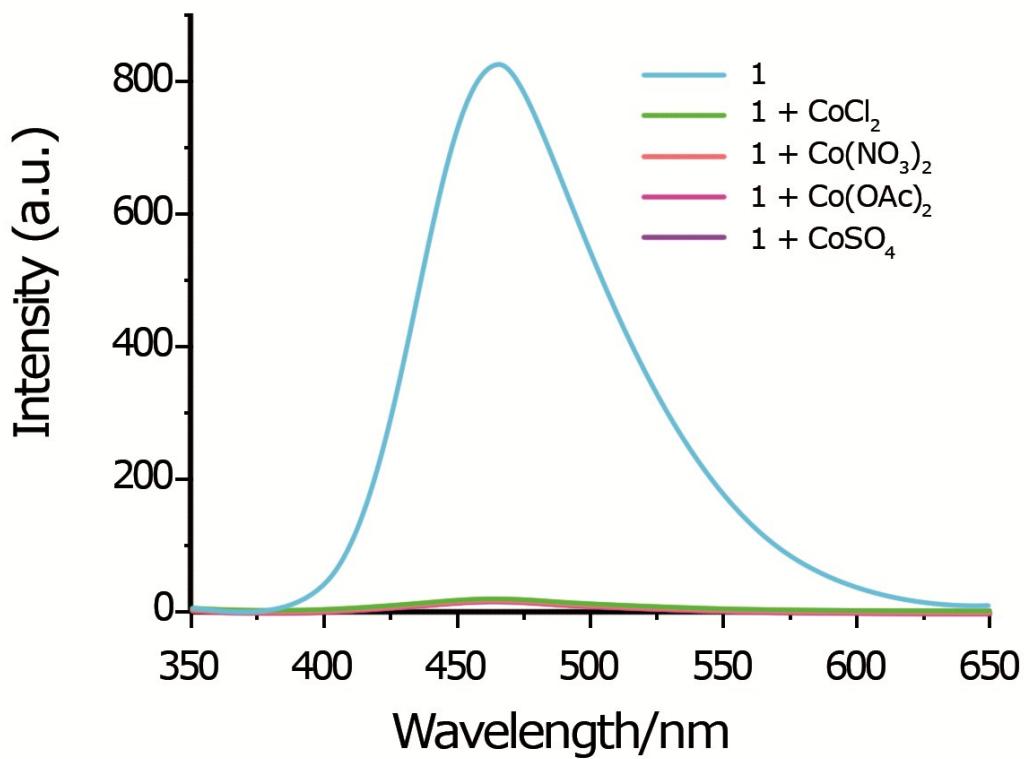


Fig. S12. The emission spectral changes of 10 μM complex **1** upon the addition of 50 μM of different types of cobalt salts in HEPES buffer solution (CoCl_2 , $\text{Co}(\text{NO}_3)_2$, $\text{Co}(\text{OAc})_2$, CoSO_4) in aqueous solution.

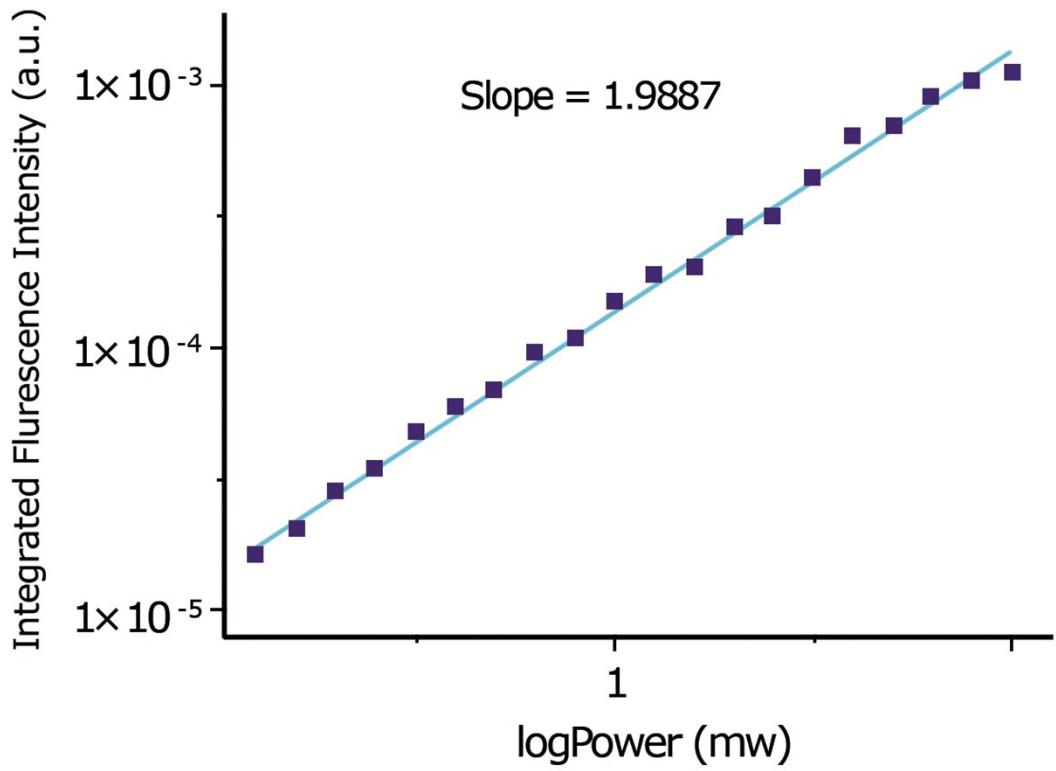


Fig. S13. The logarithmic plots of the power dependence of relative two-photon induced luminescence intensity of **1** as a function of pump power at an excitation wavelength of 850 nm. The solid lines are the best-fit straight lines with gradient $n = 1.9887$, indicating that **1** is two-photon excitation active.

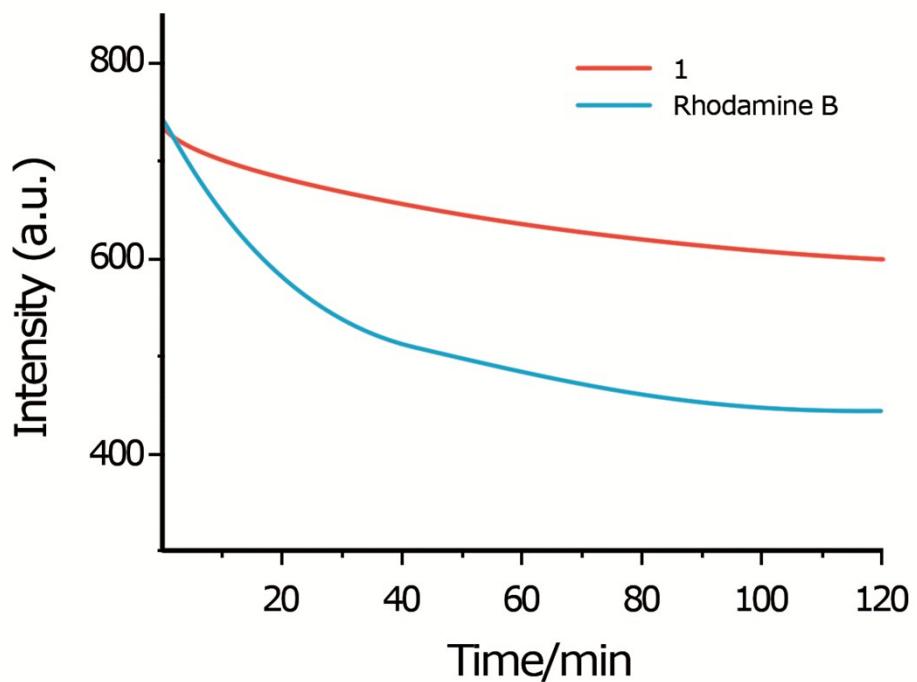


Fig. S14. Time courses of **1** and Rhodamine B by fluorescence spectrophotometer ($\lambda_{\text{ex}} = 365$ nm, $\lambda_{\text{em}} = 450$ nm for **1** and 582 nm for Rhodamine B).

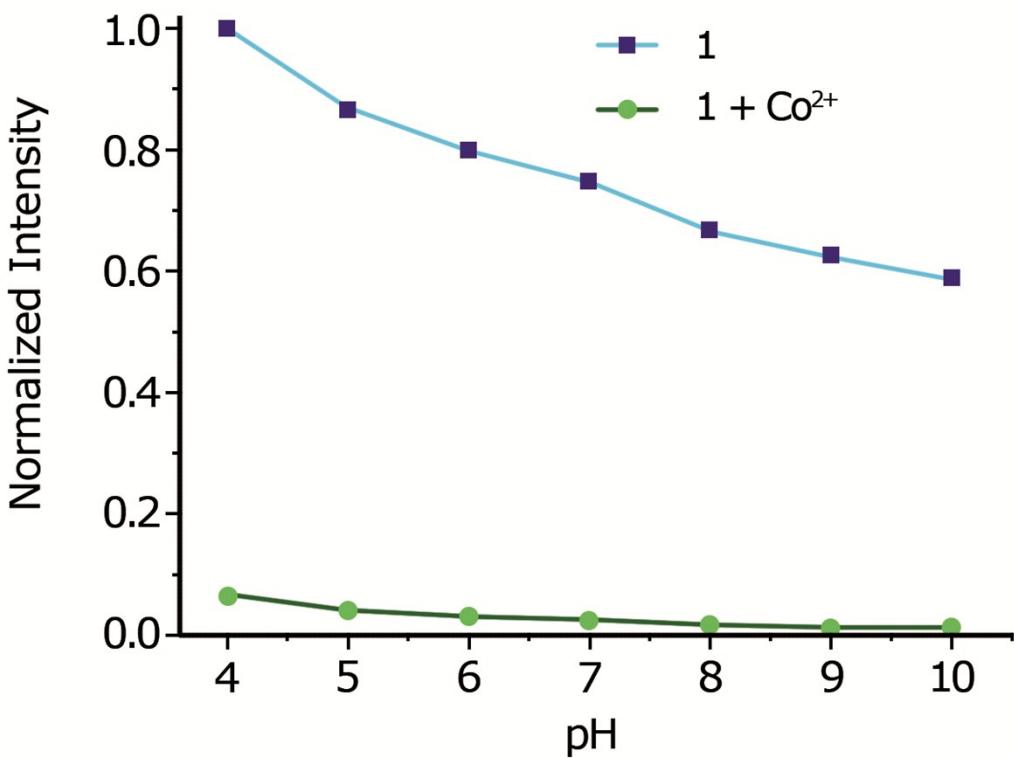


Fig. S15. The luminescence intensity of **1** (10 μM) with and without Co^{2+} (50 μM) as a function of pH in aqueous solution.

Table S1. Selected ^1H NMR data of HL, **1** and **2** (in $\text{DMSO}-d_6$, δ : ppm)

Protons	HL	DPSH ₂	1
H-4'	7.84-7.79 (m, 2H)	-	7.93 (d, 2H, 3J 8.0)
H-1	7.54 (t, 1H, 4J 1.4)	-	-
H-5'	7.47-7.38 (m, 4H)	-	7.03 (t, 2H, 3J 8.0)
H-6'			7.30 (t, 2H, 3J 8.0)
H-3,5	7.35-7.29 (m, 2H)	-	6.72 (s, 2H)
H-7'			6.97 (d, 2H, 3J 8.0)
H-7	3.83 (s, 3H)	-	3.85 (s, 3H)
H-10'	3.39 (s, 6H)	-	3.41 (s, 6H)
H-Ar (DPSH ₂)	-	6.79 (d, 4H, 3J 8.0)	6.19 (d, 2H, 3J 8.0)
H-Ar (DPSH ₂)	-	6.99 (d, 4H, 3J 8.0)	6.27 (d, 2H, 3J 8.0)
H-Ar (DPSH ₂)	-	-	6.41 (d, 2H, 3J 8.0)
H-Ar (DPSH ₂)	-	-	6.52 (d, 2H, 3J 8.0)
H-NH (DPSH ₂)	-	8.11 (s, 1H)	-