

Synthesis, Characterization, and Anticancer Activity of Phosphanegold(i) Complexes of 3-Thiosemicarbano-butan-2-one Oxime

Sani A. Zarewa ^{1,†}, Lama Binobaid ^{2,†}, Adam A. A. Sulaiman ^{1,3,*}, Homood M. As Sobeai ², Moureq Alotaibi ², Ali Alhoshani ² and Anvarhusein A. Isab ^{1,4,*}

¹ Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia; g202101570@kfupm.edu.sa

² Department of Pharmacology and Toxicology, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia; 442202864@student.ksu.edu.sa (L.B.); hassobeai@ksu.edu.sa (H.M.A.S.); mralotaibi@ksu.edu.sa (M.A.); ahoshani@ksu.edu.sa (A.A.)

³ Core Research Facilities (CRF), King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

⁴ Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

* Correspondence: adamahmed@kfupm.edu.sa (A.A.A.S.); aisab@kfupm.edu.sa (A.A.I.)

† These authors contributed equally to this work.

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Table S1: CHNS analysis of ligand and gold(I) complexes **1-4**

Complex	Found (Calculated) %			
	%C	% H	%N	%S
C ₅ H ₁₀ N ₄ SO (Ligand) (TBO)	34.75(34.47)	5.39(5.79)	31.50(32.16)	18.22(18.40)
[(CH ₃) ₃ PAu(I)(C ₅ H ₁₀ N ₄ SO)].PF ₆ (1)	15.79(16.22)	2.97(3.23)	9.02(9.46)	5.14(5.41)
[(CH ₃ CH ₂) ₃ PAu(I)(C ₅ H ₁₀ N ₄ SO)].PF ₆ (2)	20.77(20.83)	3.85(3.97)	9.06(8.83)	5.13(5.06)
[[C(CH ₃) ₃] ₃ PAu(I)(C ₅ H ₁₀ N ₄ SO)].PF ₆ (3)	28.81(28.42)	4.91(5.19)	7.96(7.80)	4.85(4.46)
[(Ph) ₃ PAu(I)(C ₅ H ₁₀ N ₄ SO)].PF ₆ (4)	35.37(35.49)	3.02(3.24)	7.16(7.20)	3.96(4.12)

Table S2. Mid FT-IR wavenumbers (cm⁻¹) of ligand and gold(I) complexes (**1-4**)

Compound	$\nu(\text{OH})$	$\nu(\text{NH}_2)$	$\nu(\text{NH})$	$\nu(\text{C=N-OH})$	$\nu(\text{C=N})$	$\nu(-\text{N-C=S})$
Ligand(TBO)	3415	3264,3238	3156	1598	1494	1374, 1286, 845
1	3427	3248, 3222	3165	1605	1507	1365, 1294, 845
2	3429	3247, 3220	3165	1607	1508	1367, 1297, 842
3	3429	3248, 3220	3165	1607	1508	1370, 1297, 838
4	3428	3246, 3221	3158	1605	1507	1367, 1295, 841

Table S3: ^{31}P NMR chemical shifts of phosphanegold(I) precursors and their complexes with TBO ligand in DMSO.

Compound	^{31}P	δ_{shift}	PF_6^-
$(\text{CH}_3)_3\text{PAuCl}$	-9.662		
$[(\text{CH}_3)_3\text{PAu(I)}(\text{C}_5\text{H}_{10}\text{N}_4\text{SO})]\text{PF}_6$ (1)	0.089	9.751	-143.591
$[(\text{CH}_3\text{CH}_2)_3\text{PAuCl}$	32.077		
$[(\text{CH}_3\text{CH}_2)_3\text{PAu(I)}(\text{C}_5\text{H}_{10}\text{N}_4\text{SO})]\text{PF}_6$ (2)	36.899	4.822	-143.591
$[\text{C}(\text{CH}_3)_3]\text{PAuCl}$	91.155		
$[\{\text{C}(\text{CH}_3)_3\}_3\text{PAu(I)}(\text{C}_5\text{H}_{10}\text{N}_4\text{SO})].\text{PF}_6$ (3)	97.021	5.866	
$\text{Ph}_3\text{PAu(I)Cl}$	33.818		
$[\text{Ph}_3\text{PAu(I)}(\text{C}_5\text{H}_{10}\text{N}_4\text{SO})].\text{PF}_6$ (4)	36.792	2.974	-143.591

FT-IR spectra data

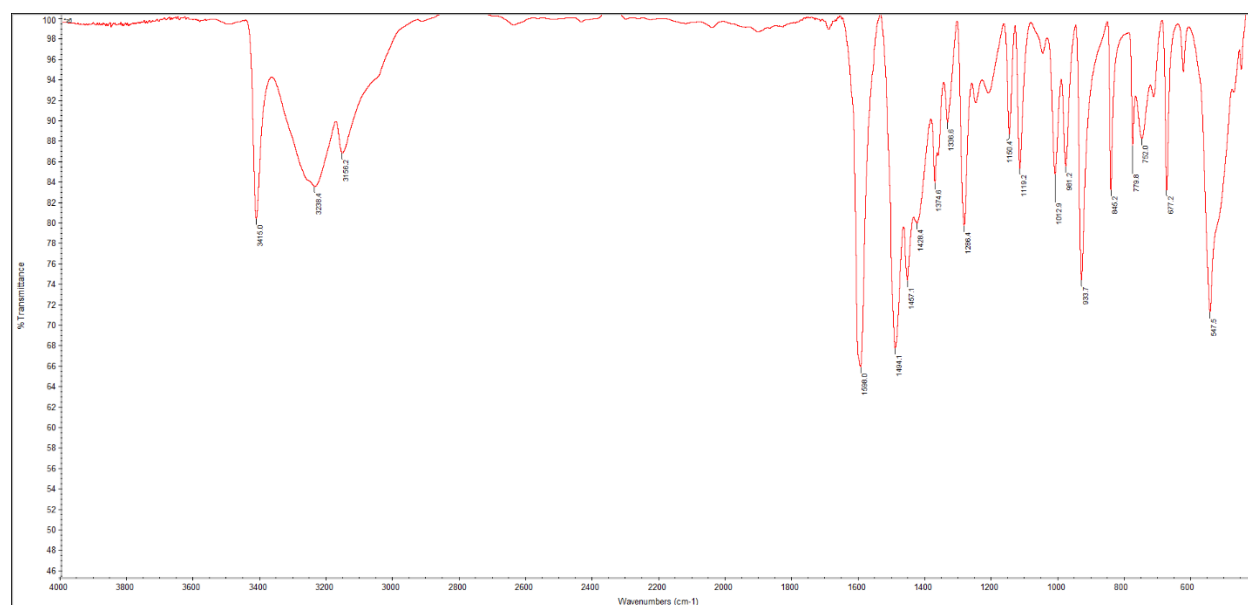
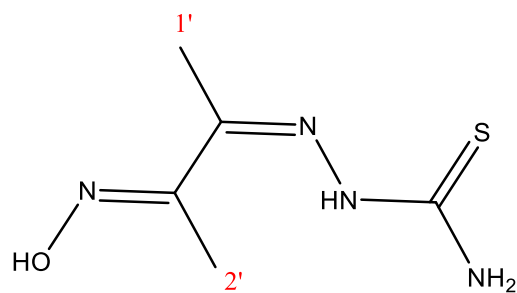


Figure S1: IR spectra of Ligand (TBO)

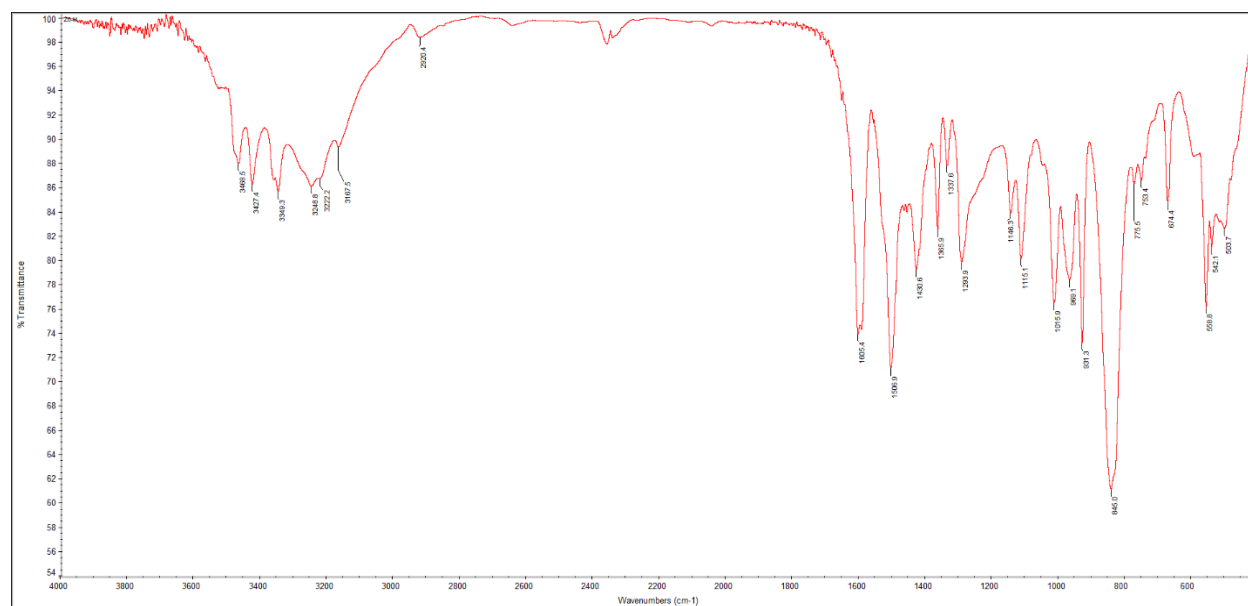
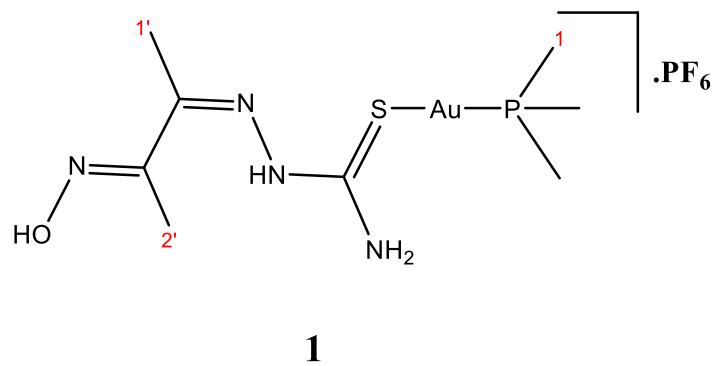


Figure S2: IR spectra of complex **1**

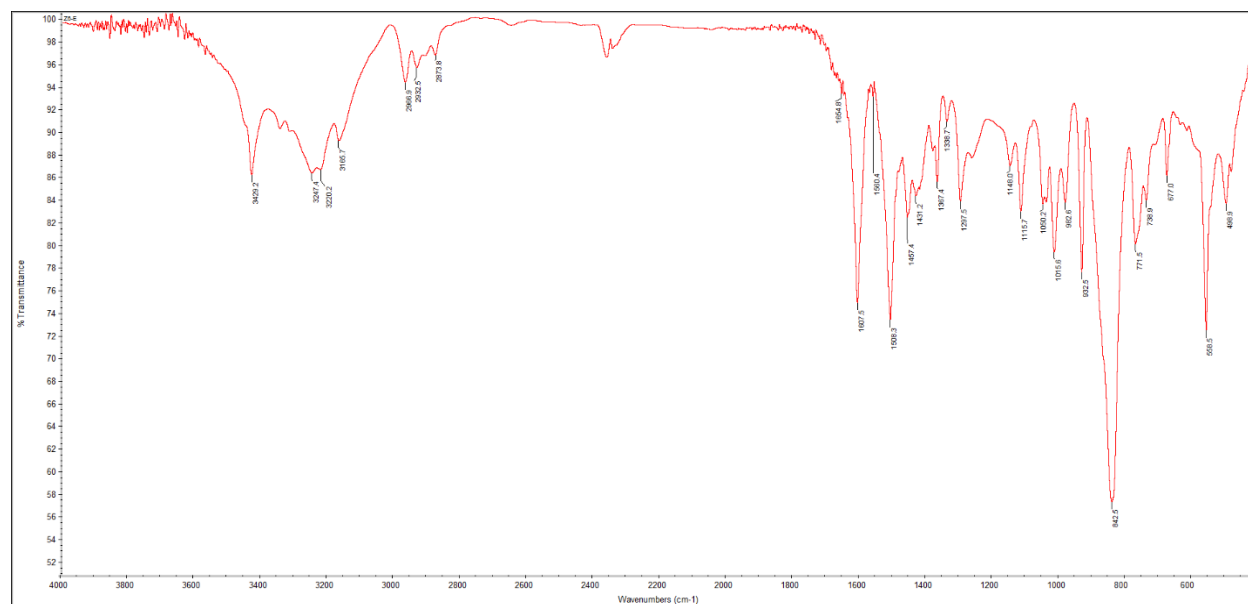
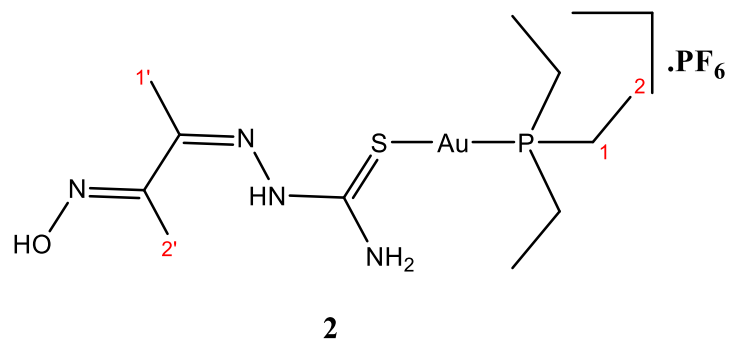
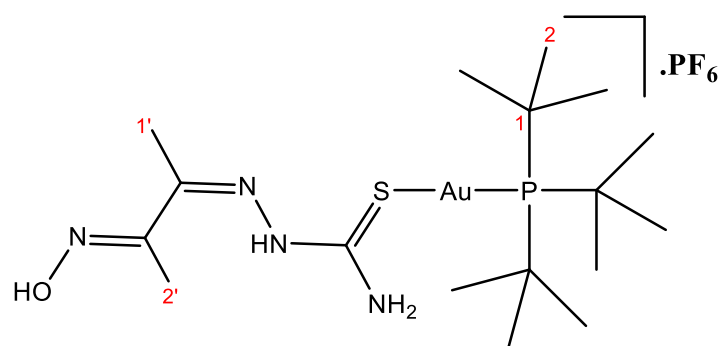


Figure S3: IR spectra of complex **2**



3

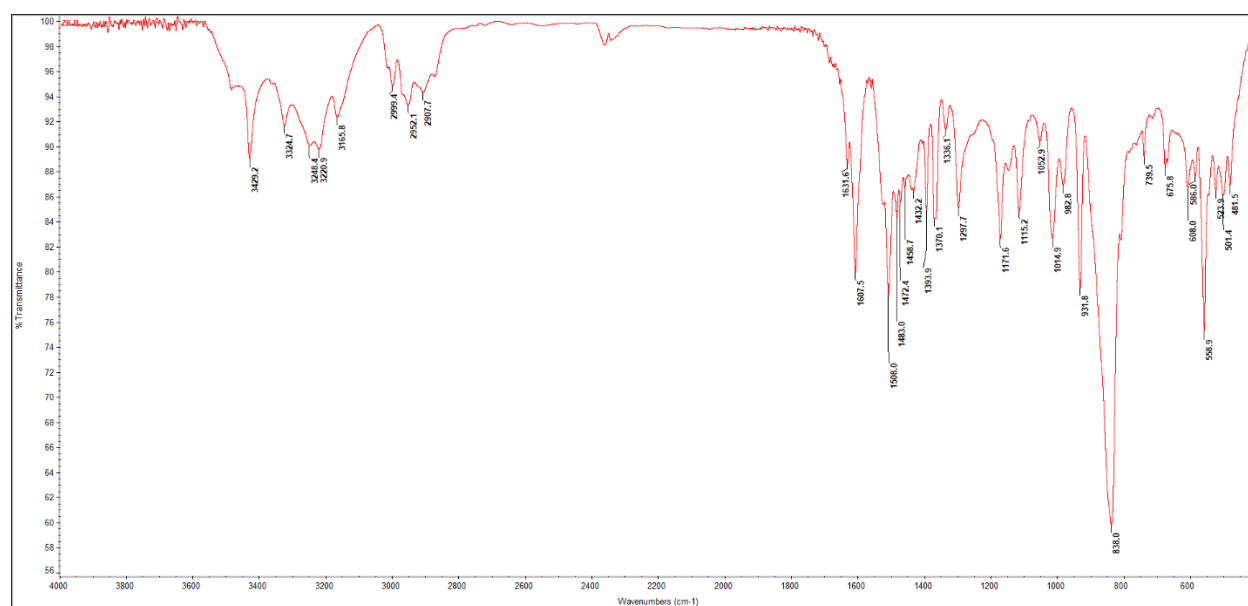


Figure S4: IR spectra of complex 3

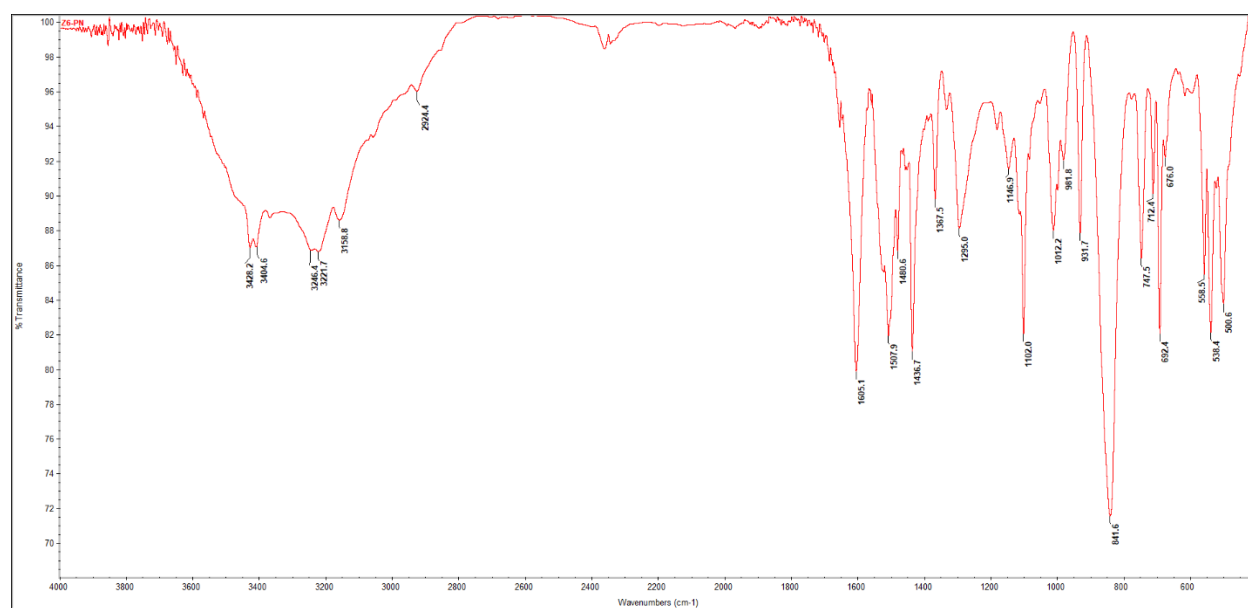
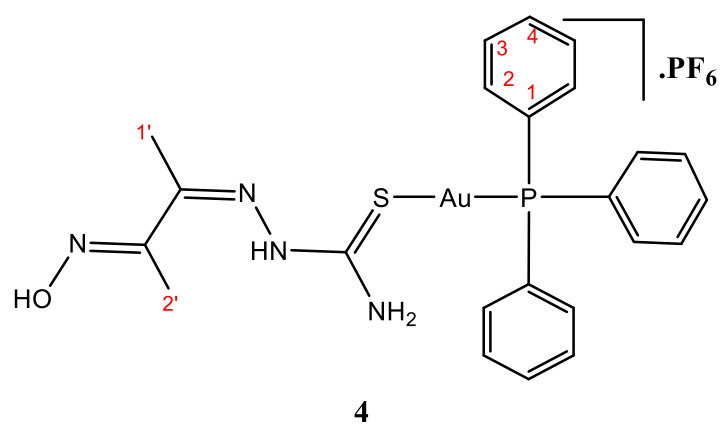


Figure S5: IR spectra of complex **4**

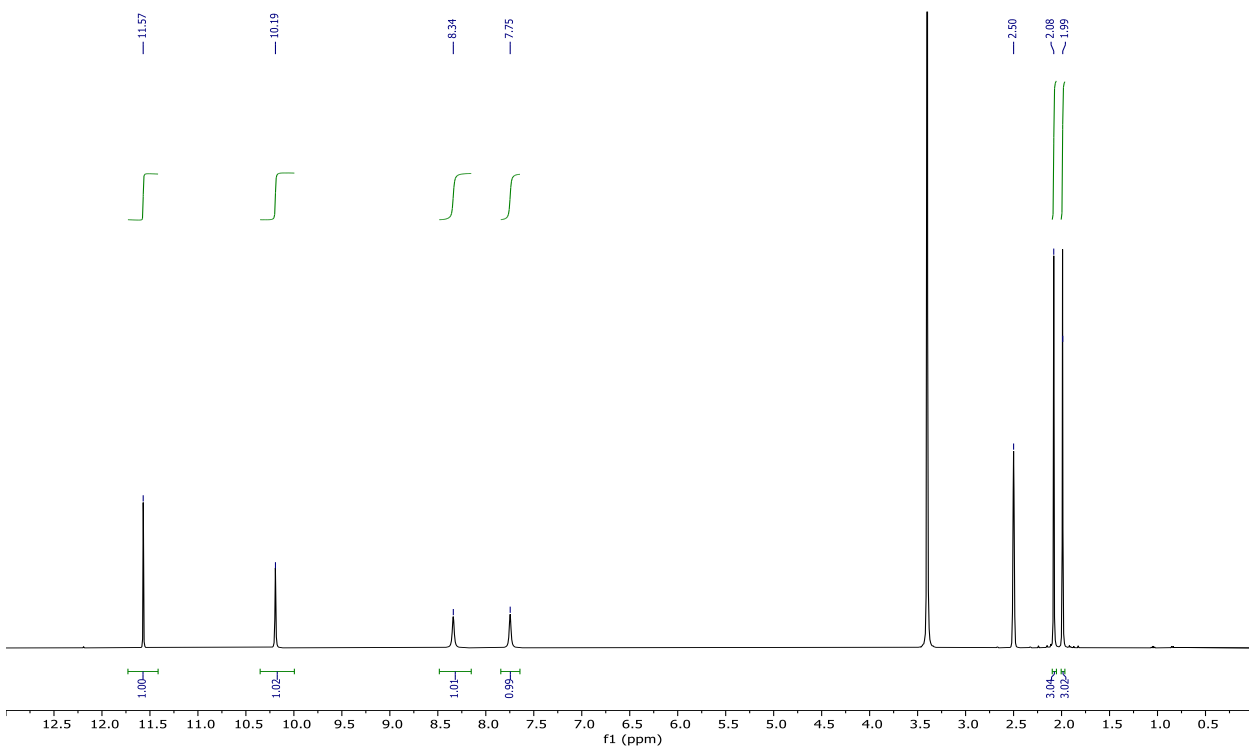


Figure S6: ^1H NMR spectrum of Ligand (TBO) in DMSO- d_6

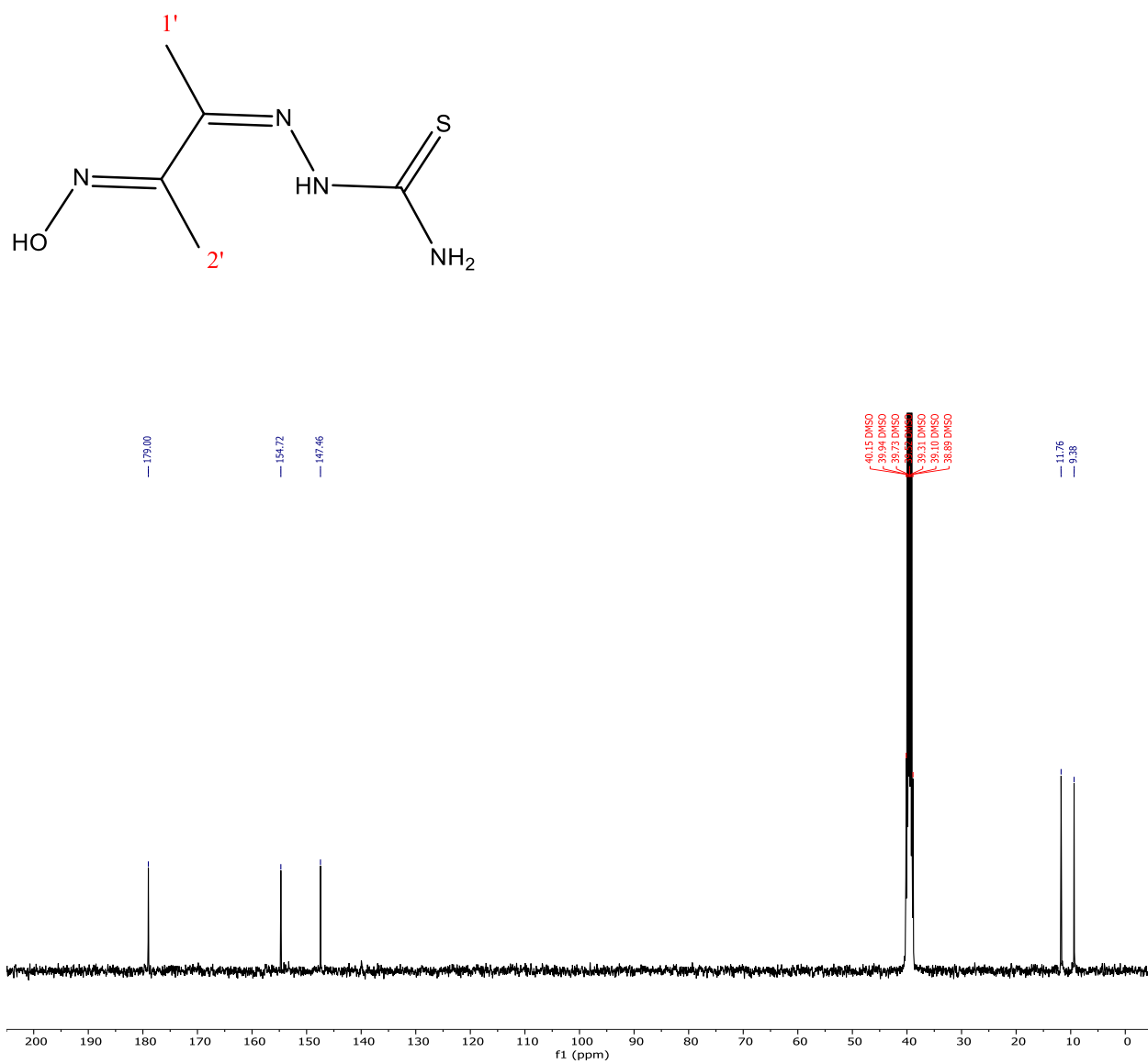


Figure S7: ^{13}C NMR spectrum of Ligand (TBO) in DMSO-d₆.



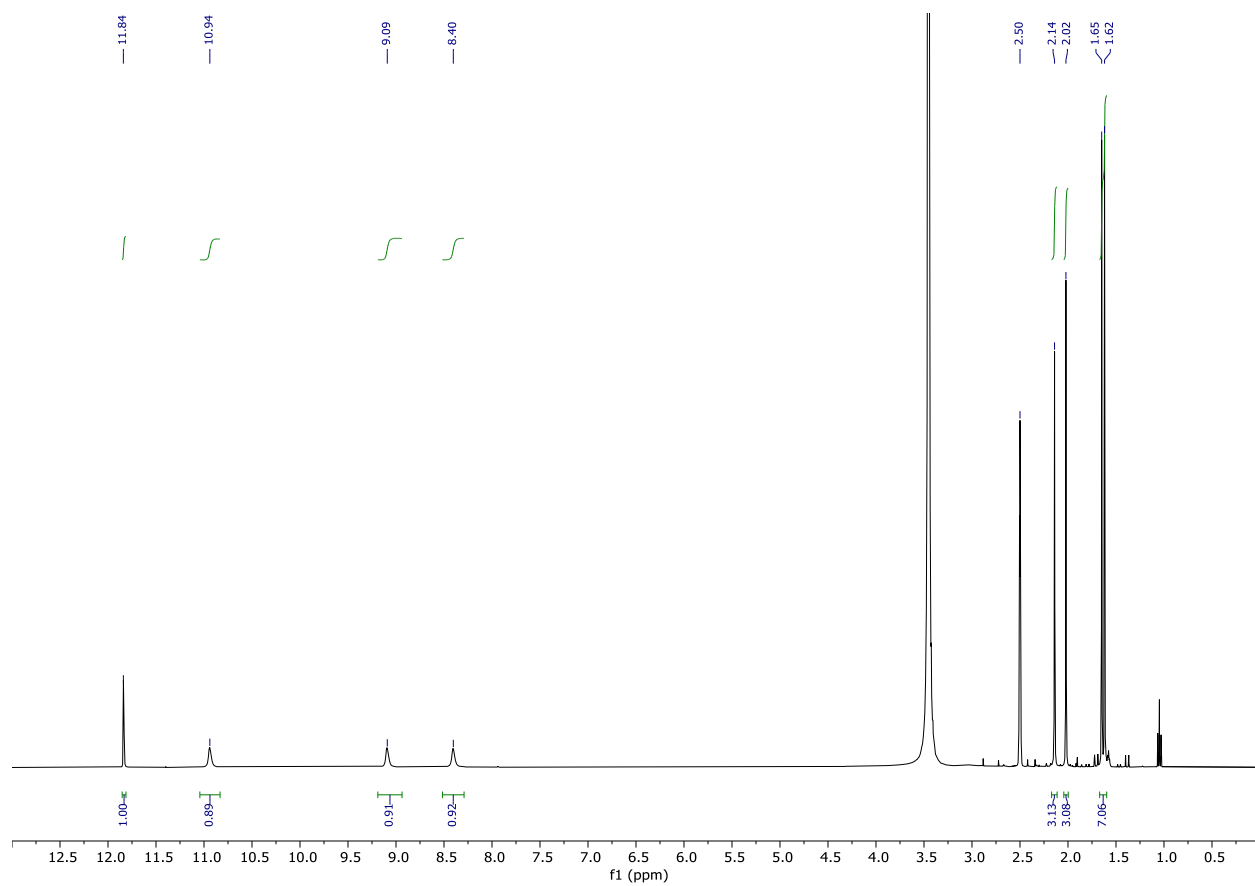
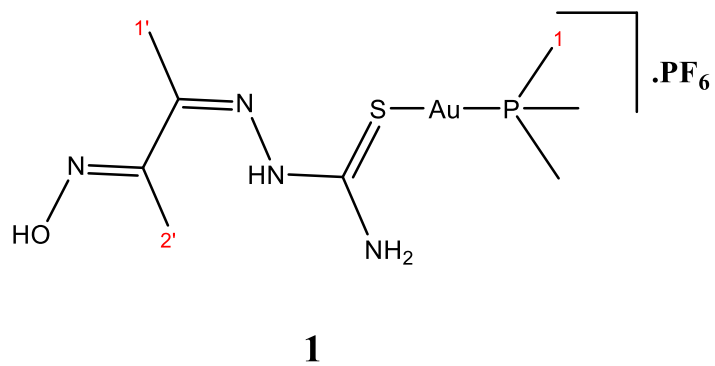


Figure S8: ¹H NMR spectrum of Complex **1** in DMSO-d₆.



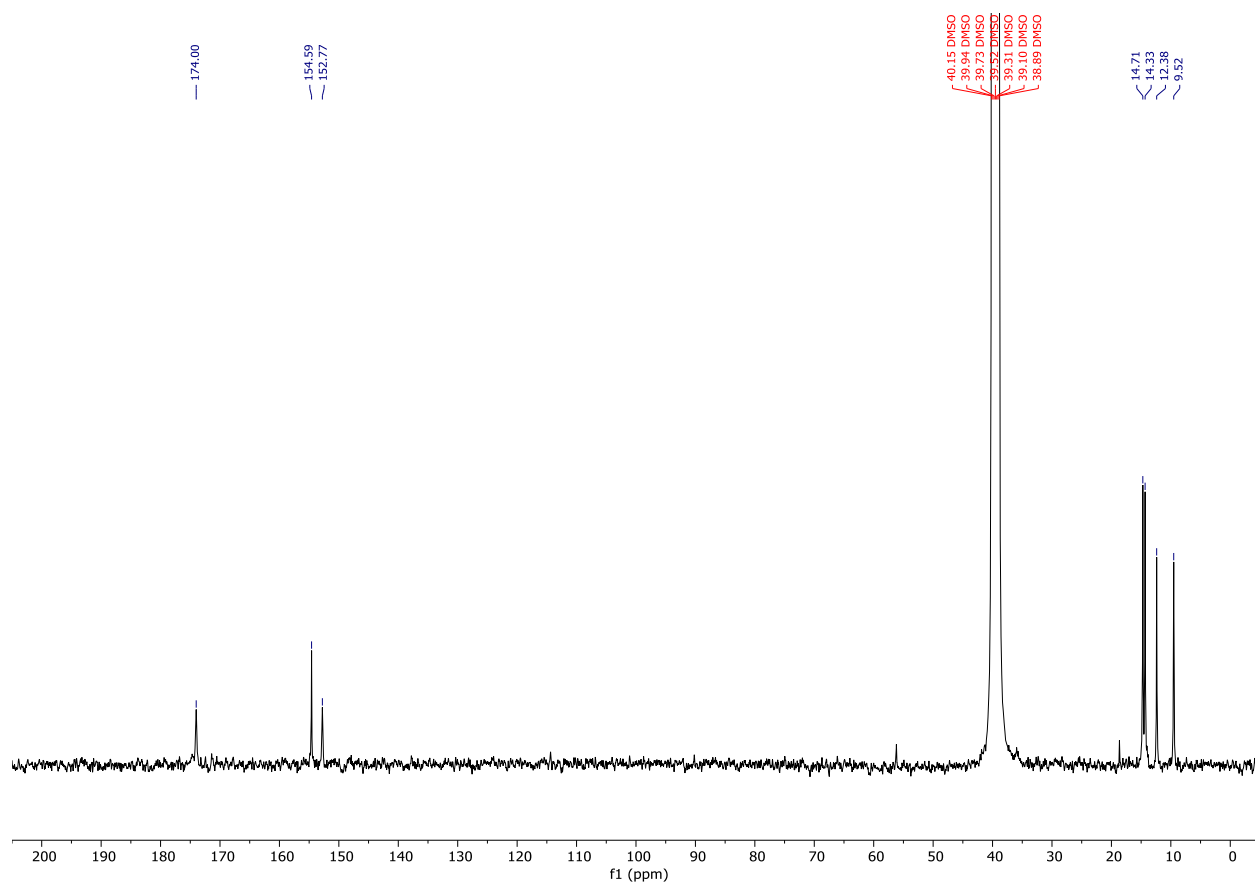
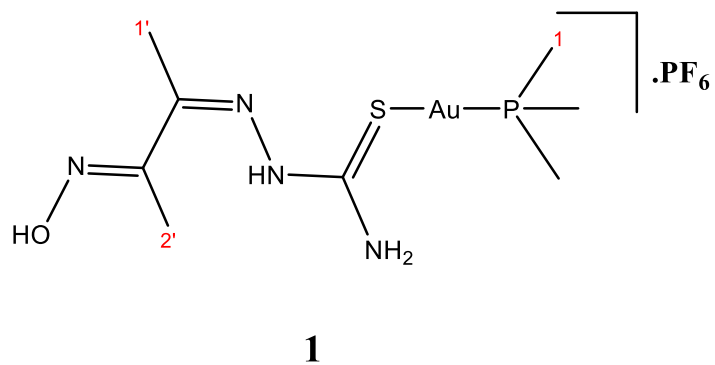


Figure S9: ^{13}C NMR spectrum of Complex **1** in DMSO- d_6 .



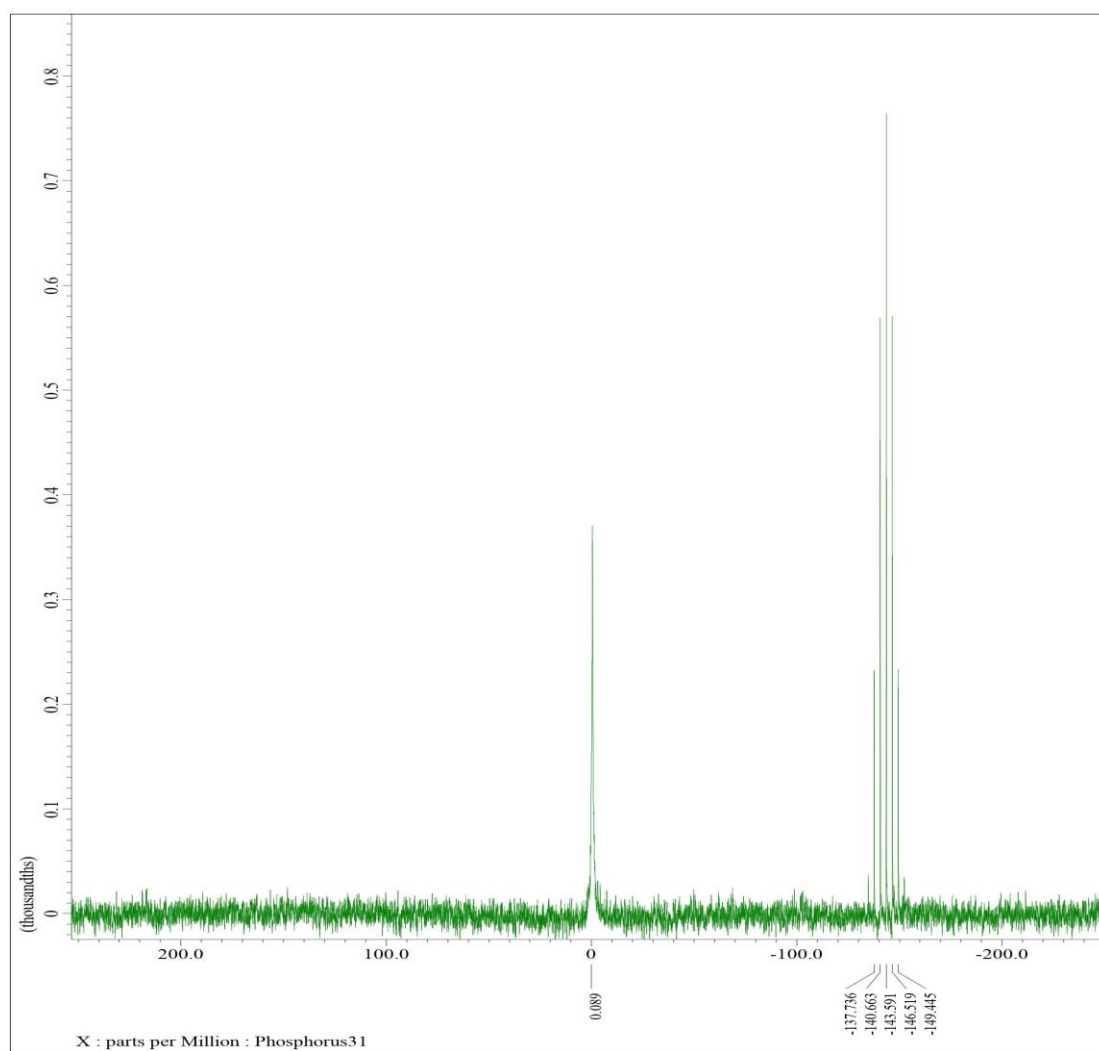


Figure S10: ^{31}P NMR spectrum of complex **1** in DMSO- d_6 .

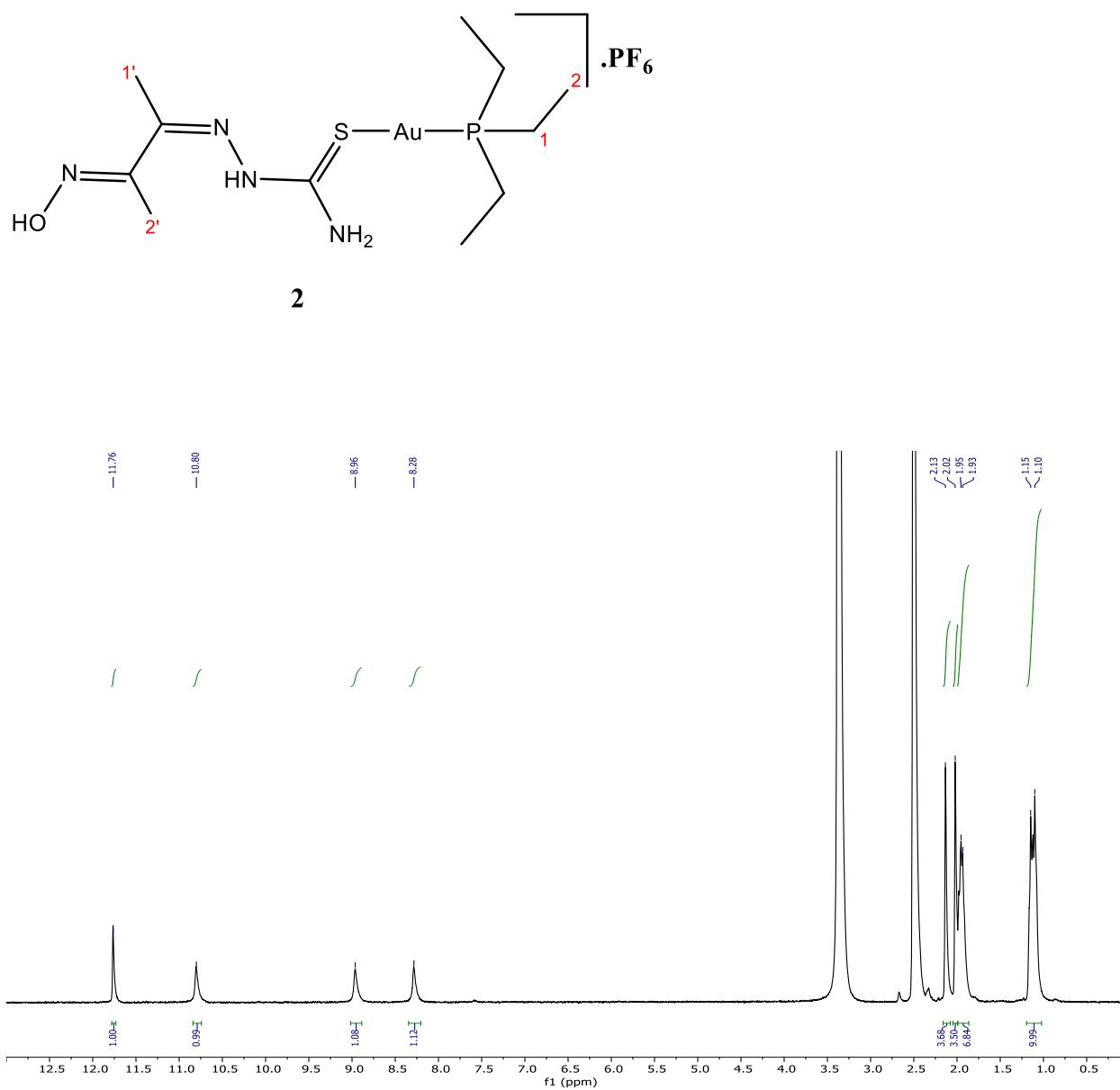


Figure S11: ^1H NMR spectrum of Complex 2 in DMSO- d_6 .

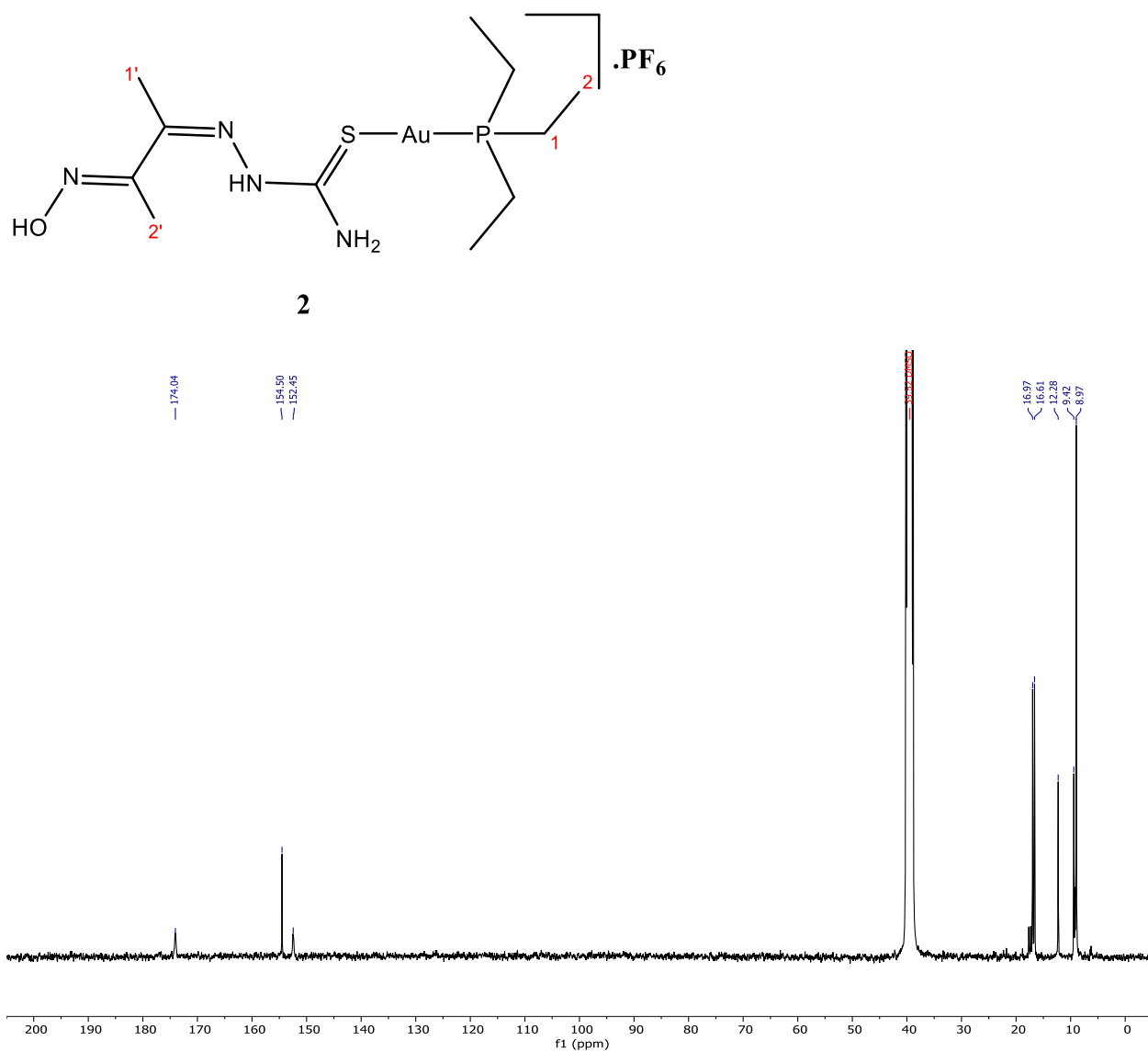


Figure S12: ^{13}C NMR spectrum of Complex 2 in DMSO-d_6 .

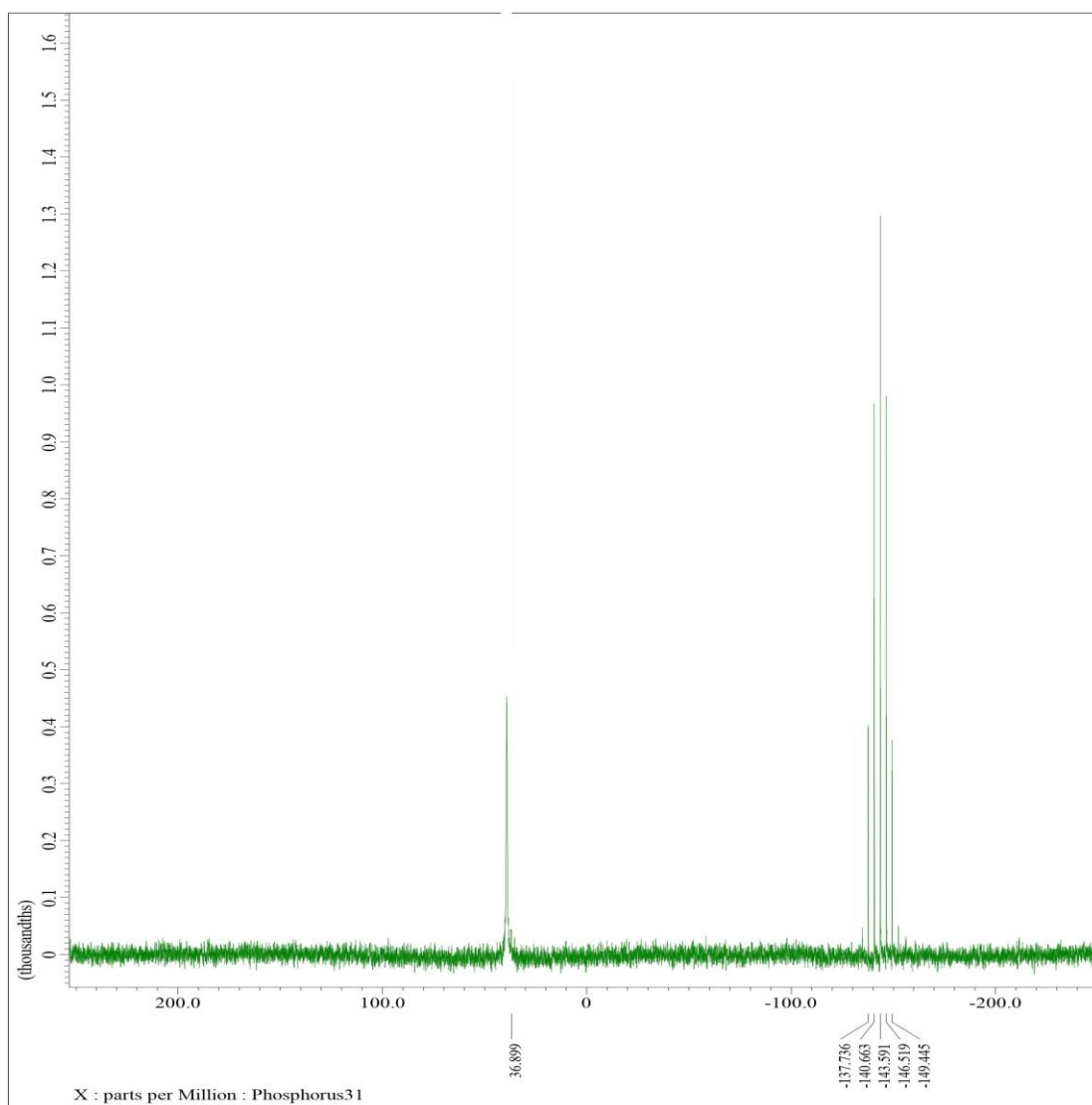
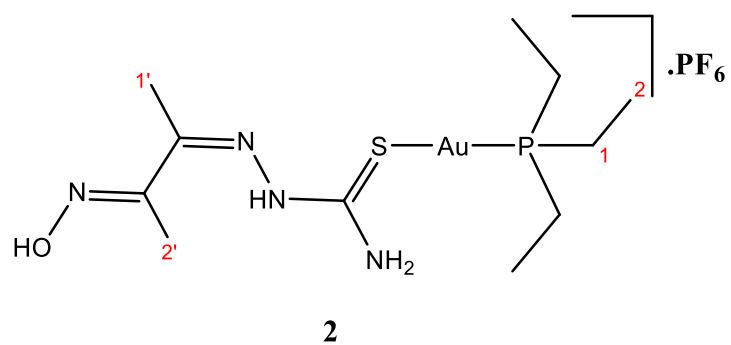


Figure S13: ³¹P NMR spectrum of complex **2** in DMSO-d₆.

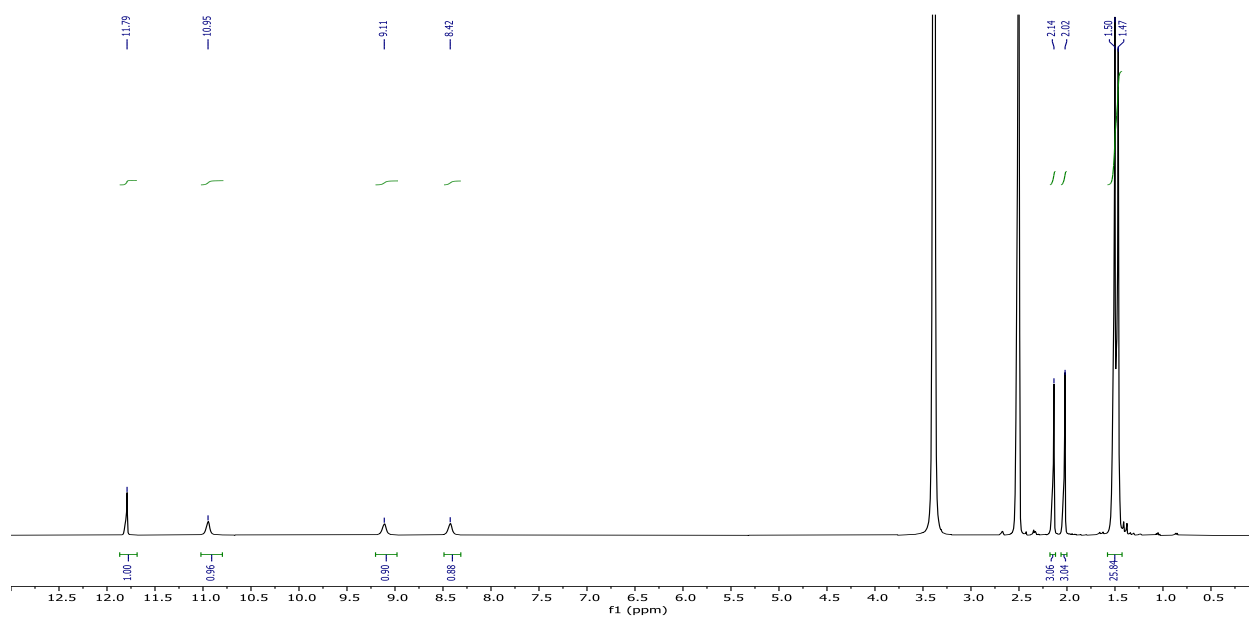
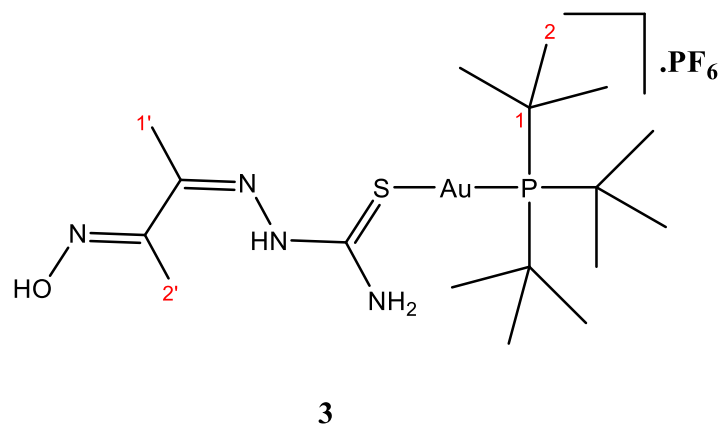
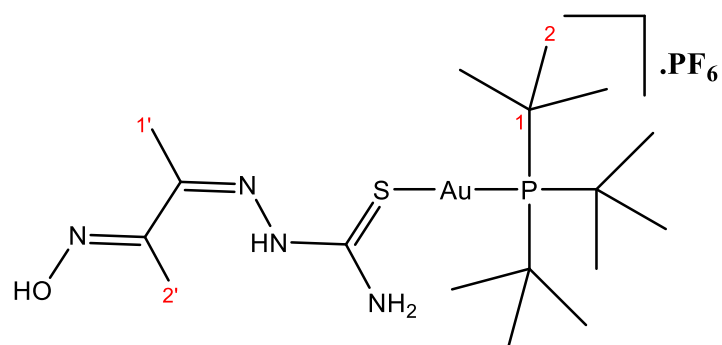


Figure S14: ^1H NMR spectrum of Complex 3 in DMSO-d_6 .



3

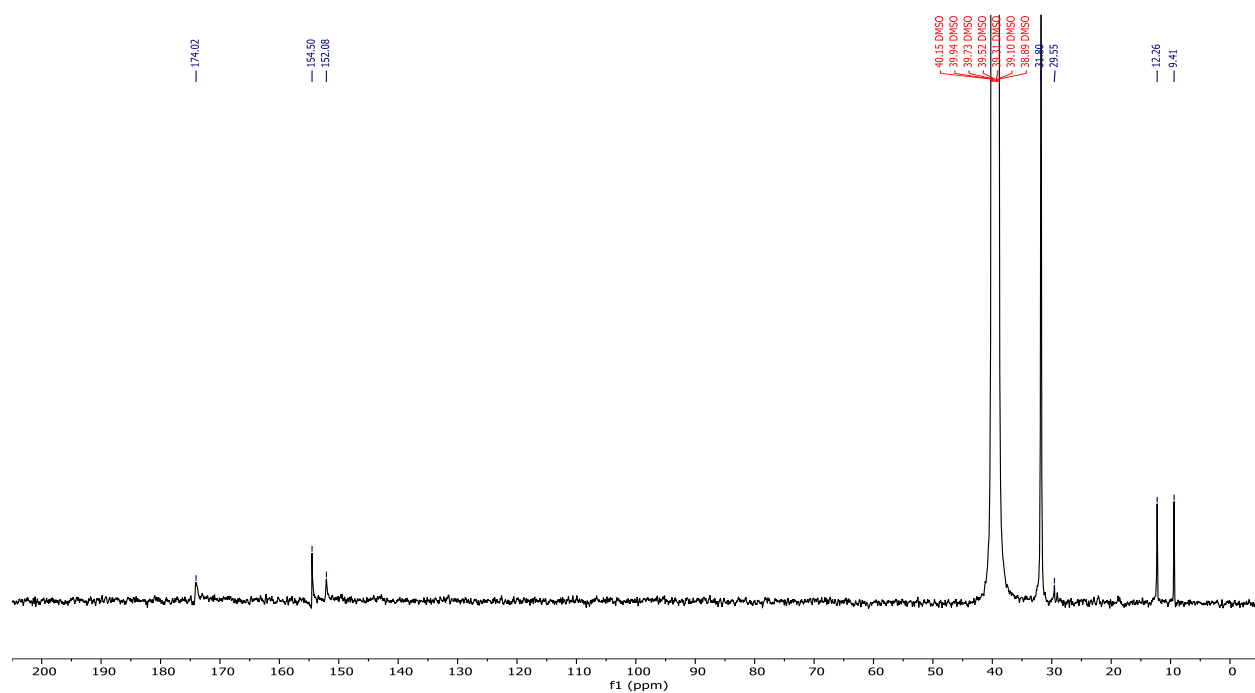
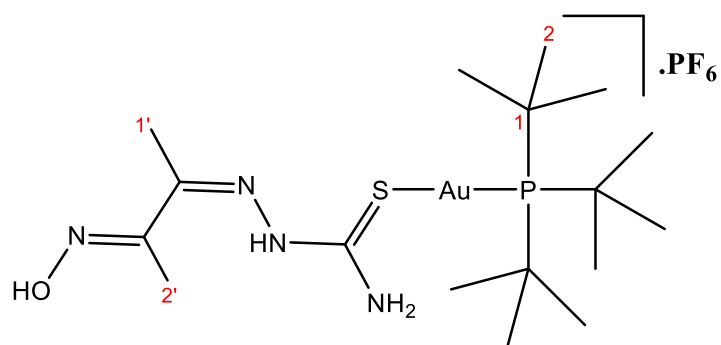


Figure S15: ¹³C NMR spectrum of Complex **3** in DMSO-d₆.



3

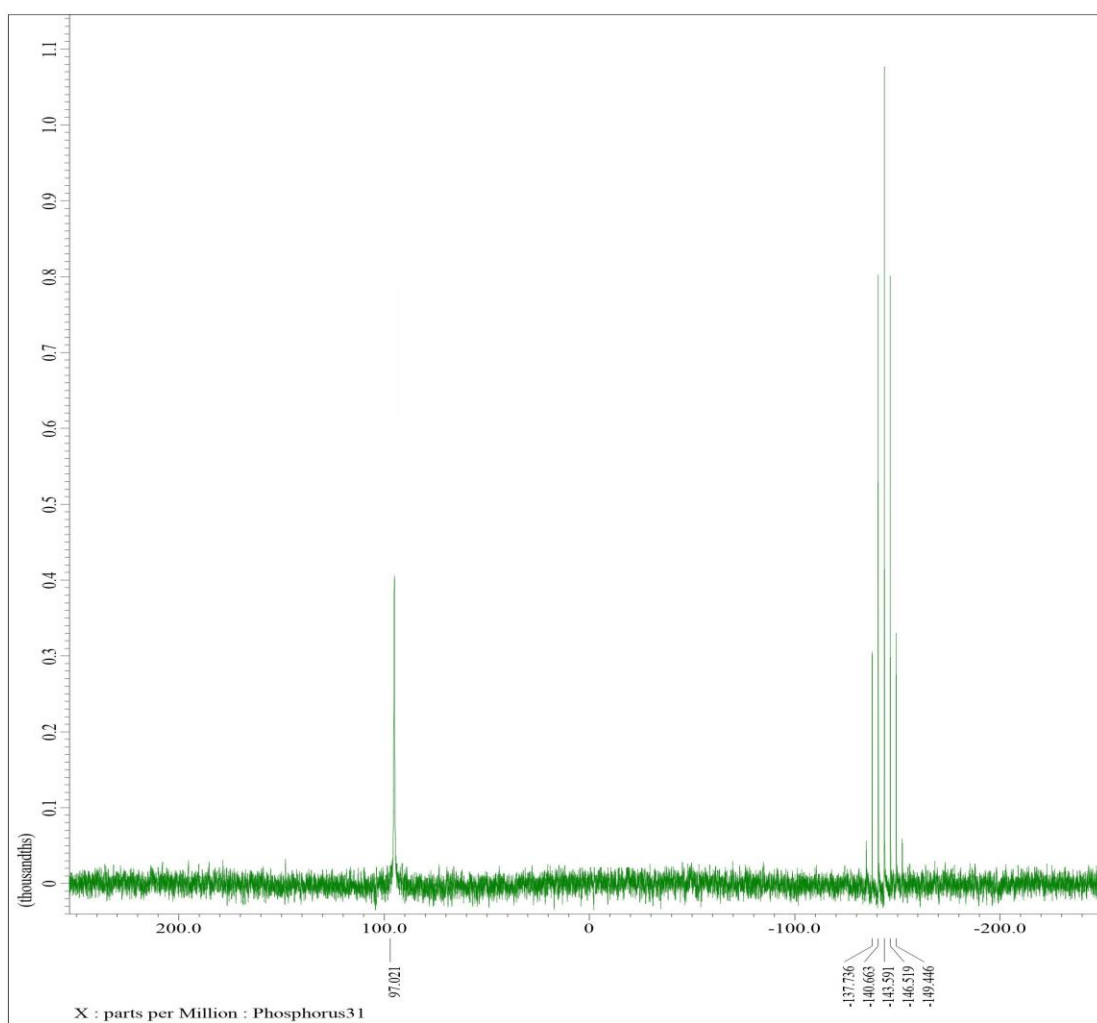


Figure S16: ³¹P NMR spectrum of complex **3** in DMSO-d₆

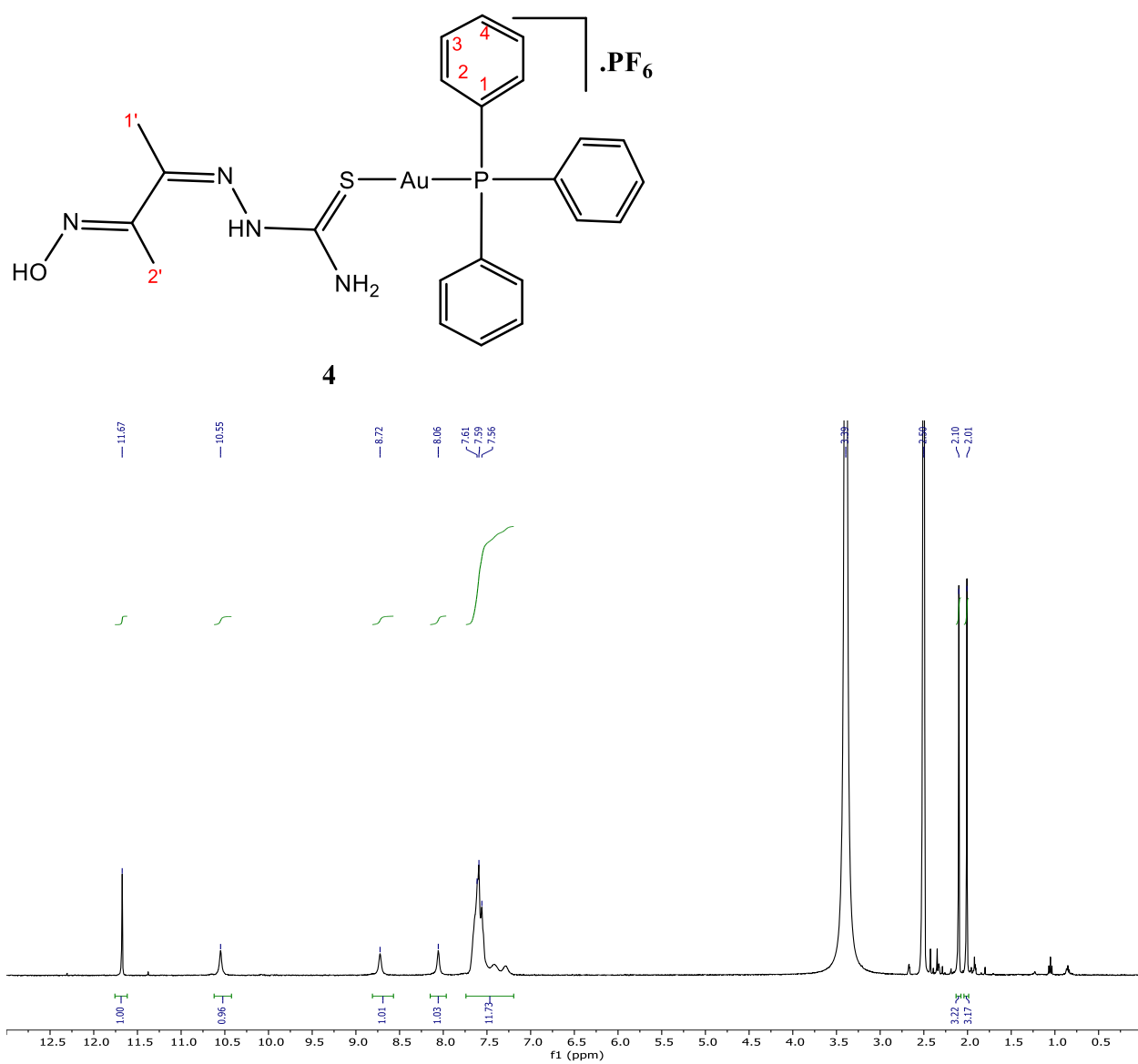


Figure S17: ¹H NMR spectrum of Complex 4 in DMSO-d₆.

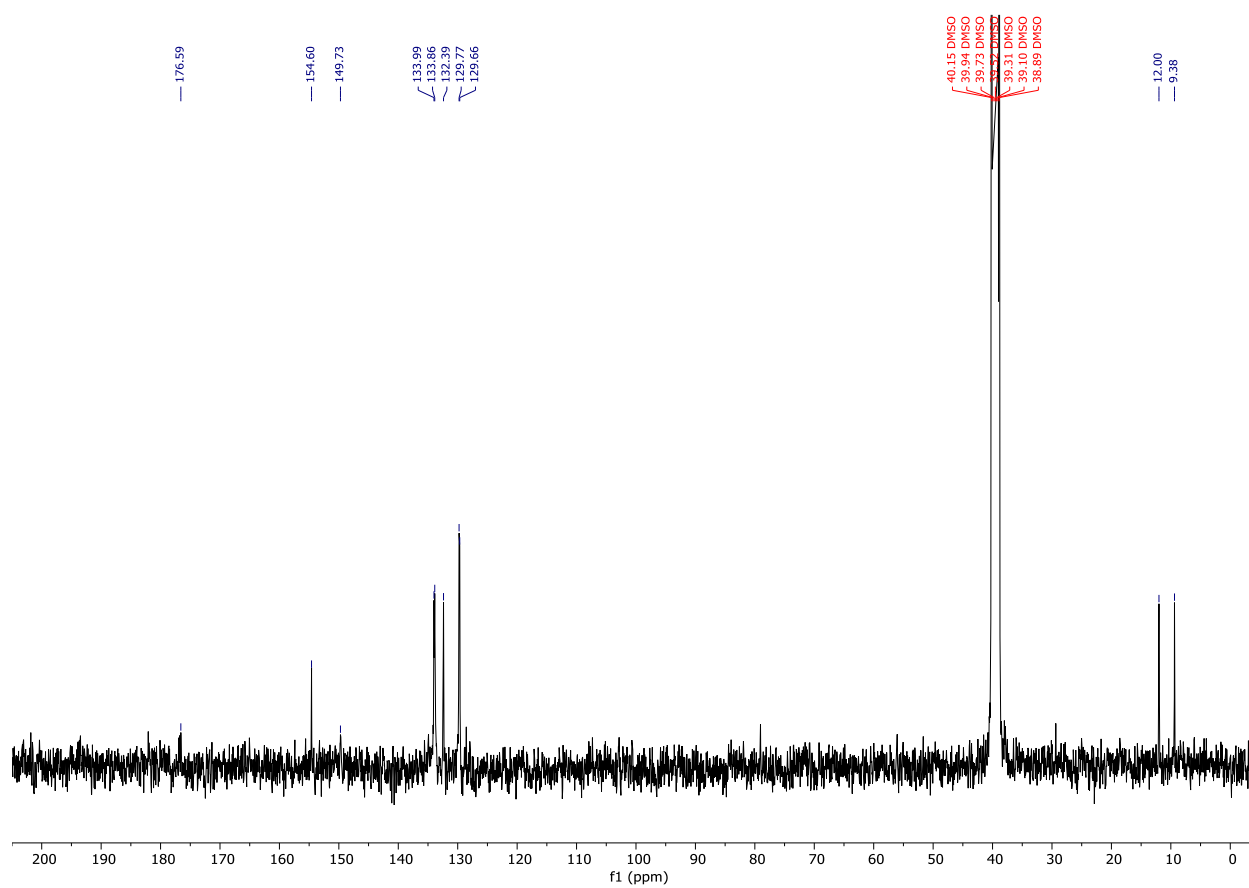
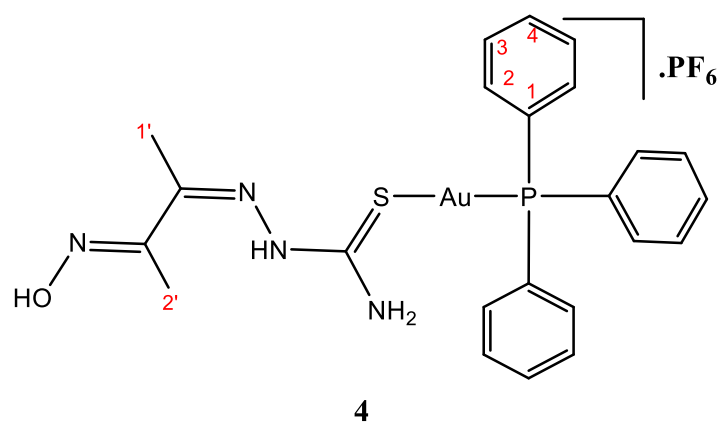


Figure S18: ^{13}C NMR spectrum of Complex 4 in DMSO- d_6 .

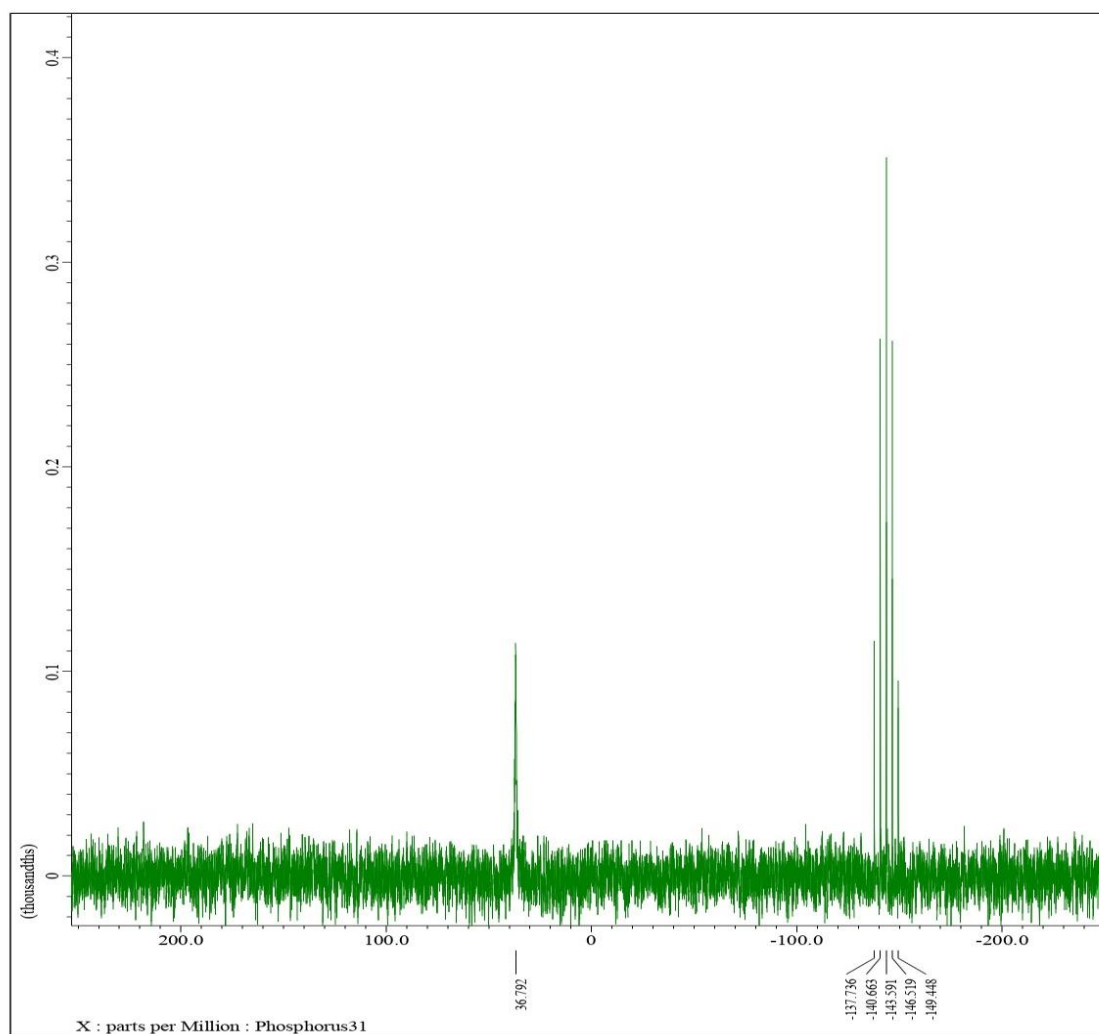
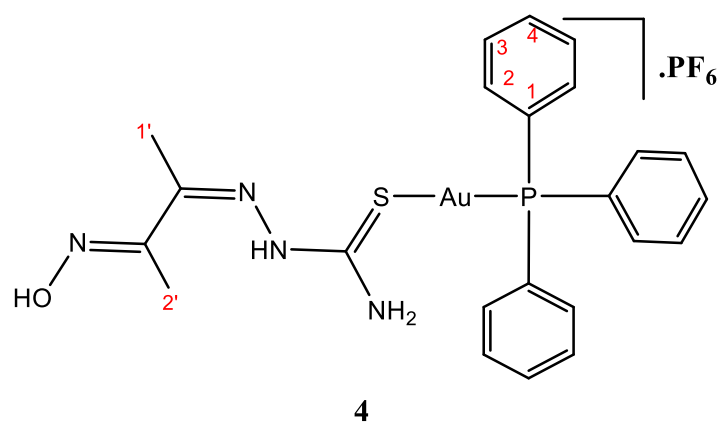
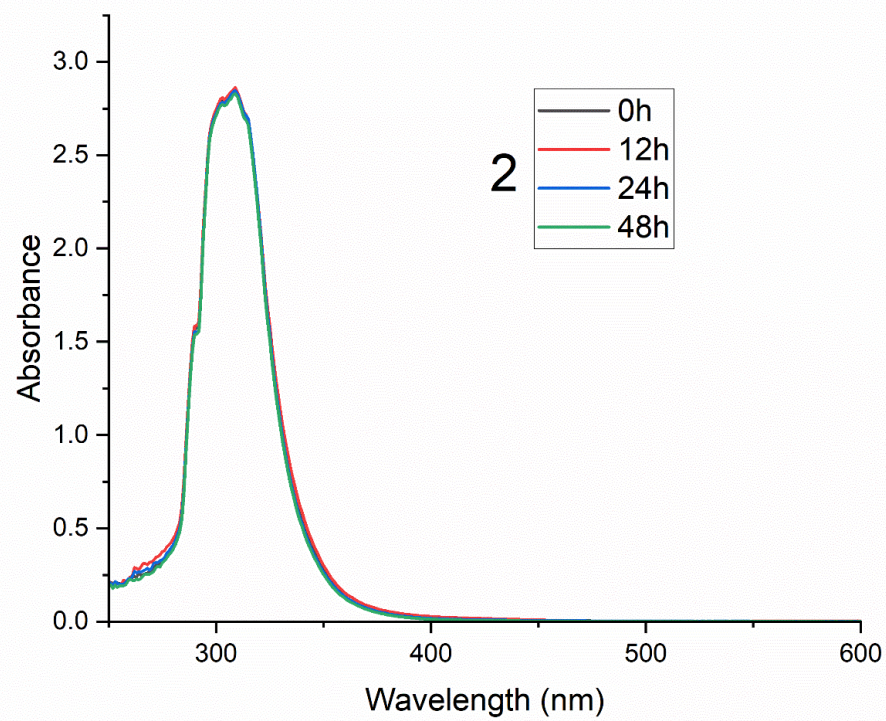
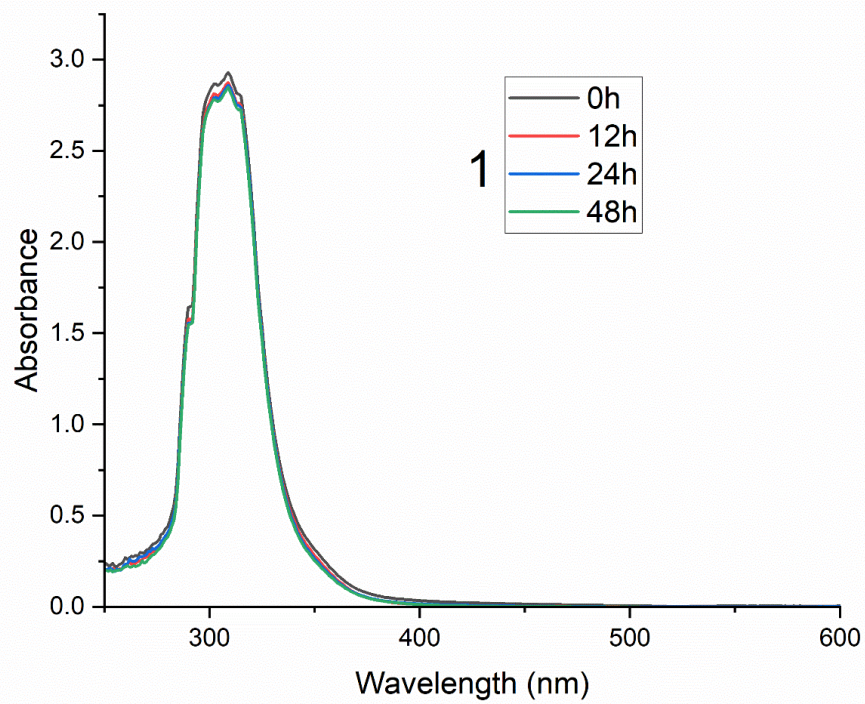
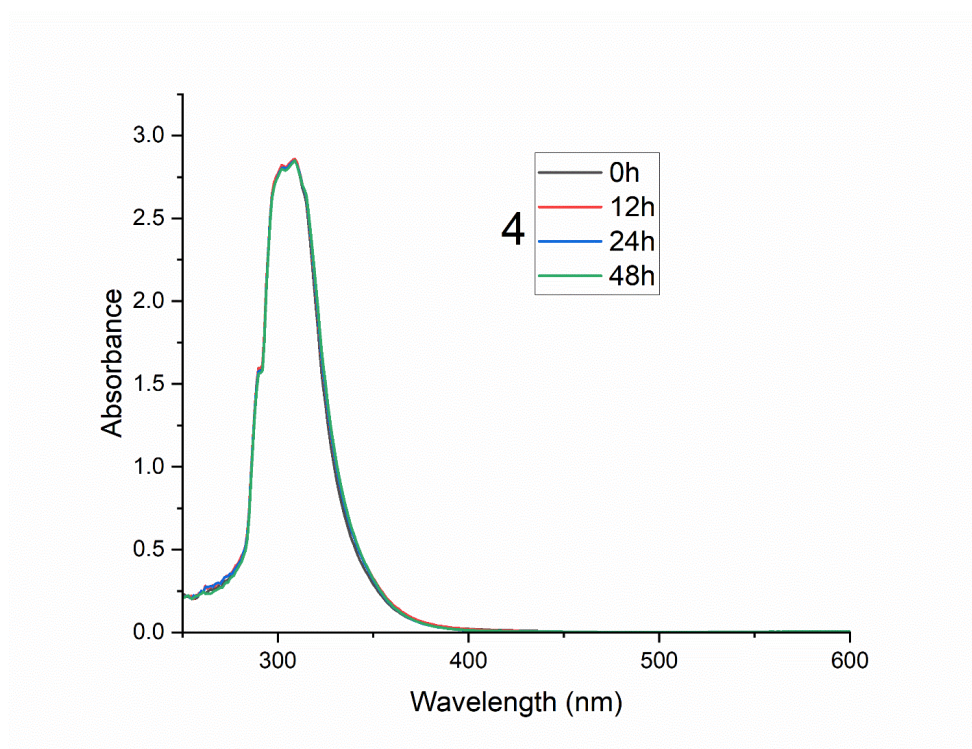
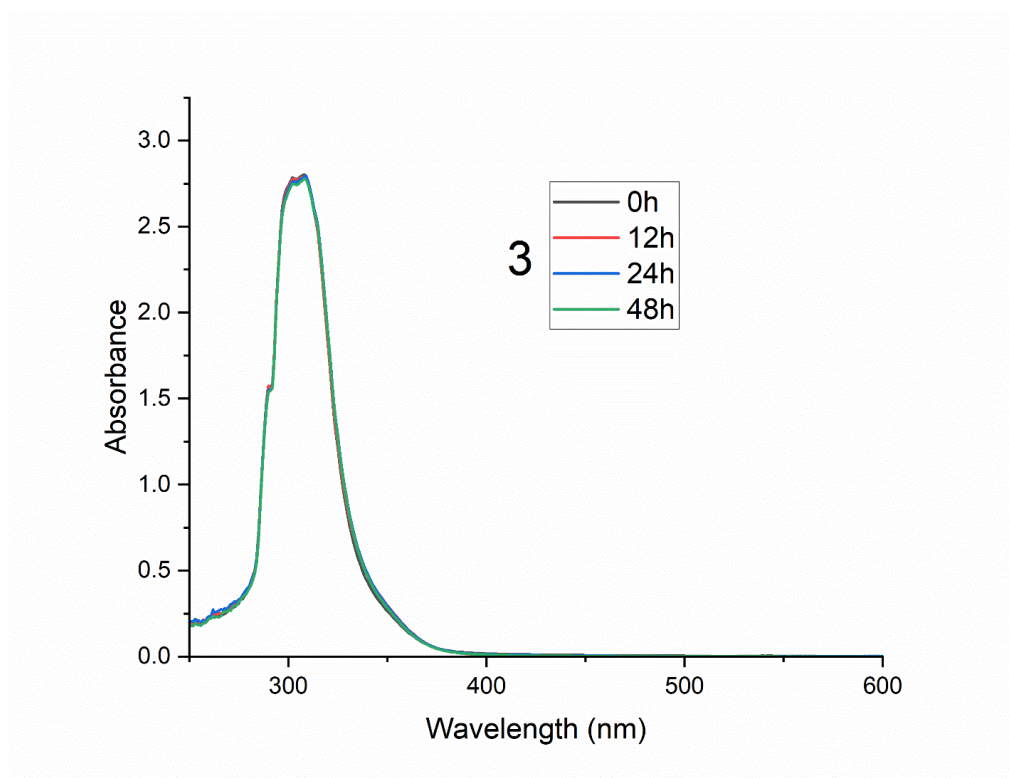
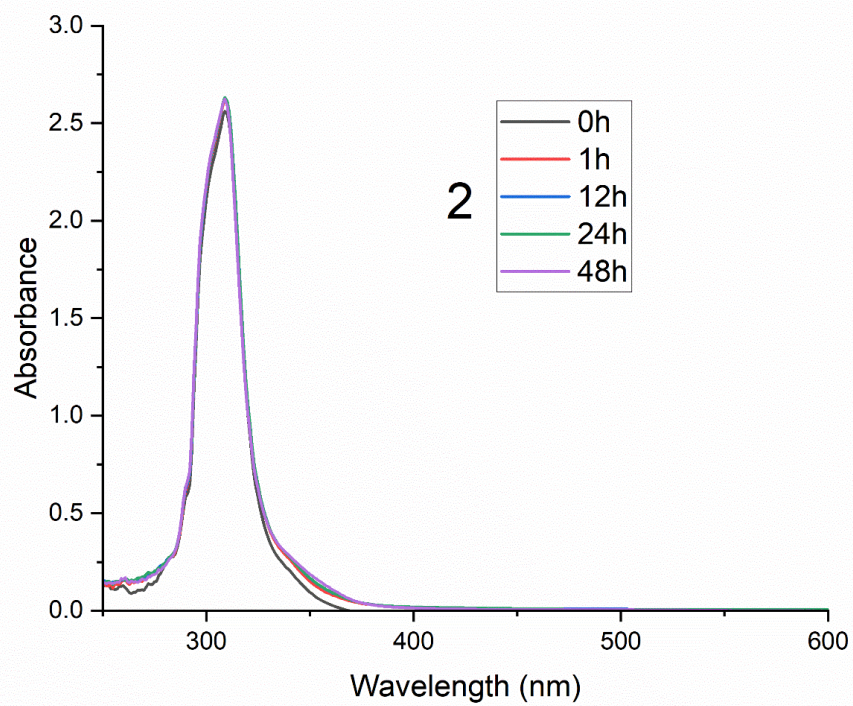
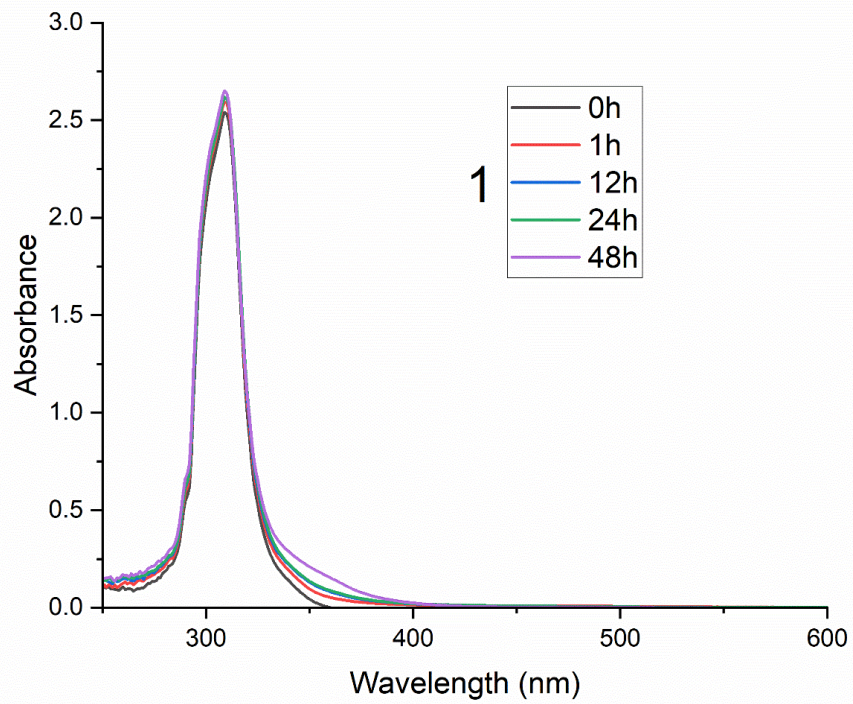


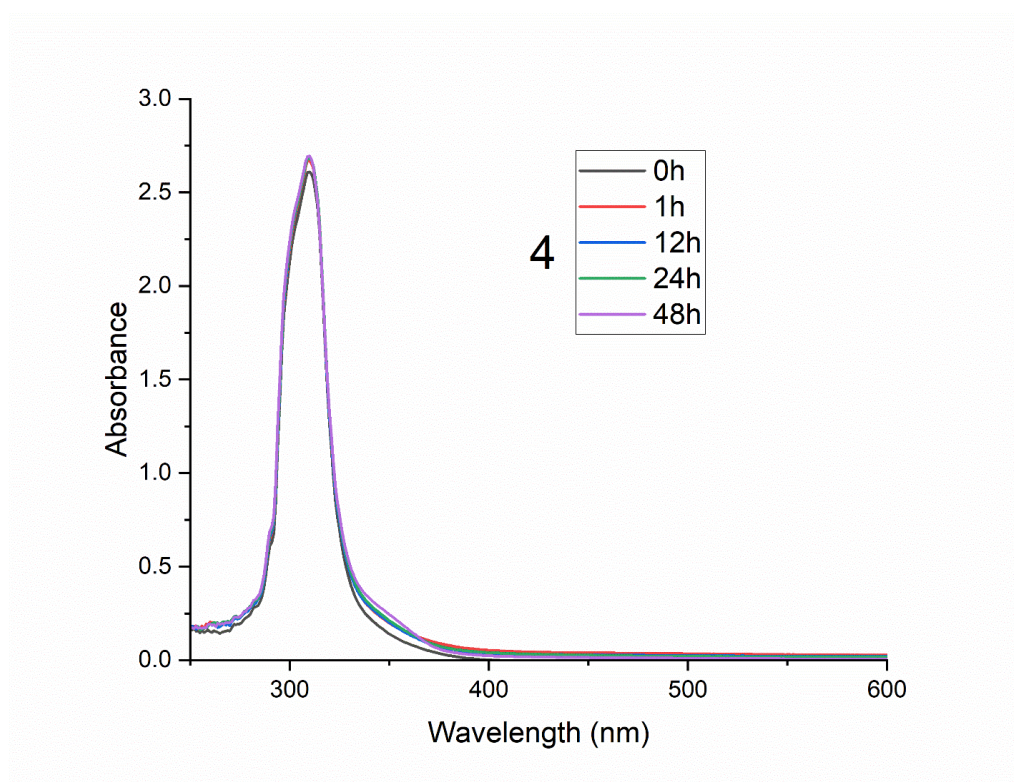
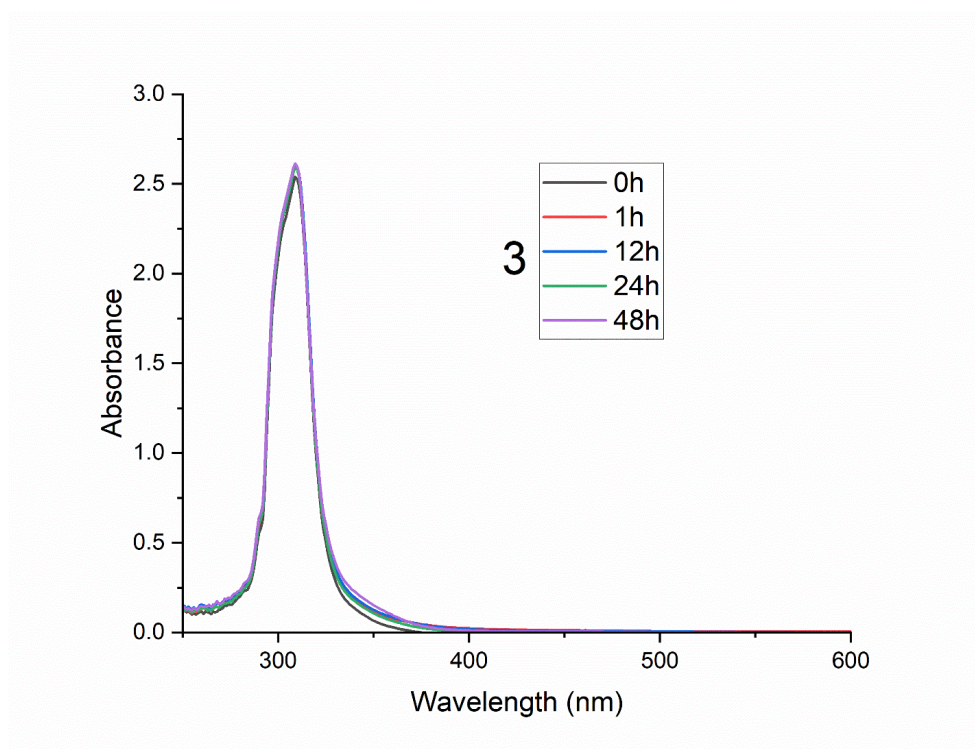
Figure S19: ^{31}P NMR spectrum of complex **4** in DMSO-d_6





Figures S20: UV-Vis spectra of (0.25 mM, 10 mL) complexes stability (1-4) at the different timing in the solution of DMSO.





Figures S21: UV-Vis spectra of (0.25 mM, 10 mL) complexes stability (1-4) at the different timing in the solution of EtOH:H₂O (1:1).