Supplementary Information (SI) for RSC Advances.
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Supplementary data

Synthesis and antitumor activity of mono and digold(I) alkynyl complexes with oligo(ethylene glycol)methylether

Yanyan Zeng[b,c,#], Fei Zheng[a,#] Lingyu Jin[b,#], Qiu Mei Chen[a], Ping Zhou[b], Xiaoqing Mou[b], Xiang Hua Wu[a,*], Jun Feng Zhang[a,*], and Wen Xiu Ren[b,d*]

[a]Yunnan Key Laboratory of Modern Separation Analysis and Substance Transformation, College of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming 650500, China

[b]Department of Radiology, the Affiliated Hospital of Southwest Medical University, Luzhou 646000, China

[c]The Affiliated Dazu's Hospital of Chongqing Medical University,Chongqing 402360, China

[d]Precision Imaging and Intelligent Analysis Key Laboratory of Luzhou, Southwest Medical University, Luzhou, 646000, Sichuan, China

E-mail addresses: chxhwu@sina.com (X. H. Wu), junfengzhang@126.com (J. F. Zhang), xrenwenxiux@swmu.edu.cn (W. X. Ren)

Y. Zeng, F. Zheng and L. Jin contributed equally to this work.

Supplemental Materials

1. Crystallographic details

Table S1. Crystal data and structure refinement for complexes **1b** and **1c**

Complex	**1b**	**1c**
Formula	$C_{54}H_{44}Au_2O_2P_2$	$C_{58}H_{52}Au_2O_4P_2$
Fw	1180.76	1268.87
Temp(K)	293(2)	293(2)
Wavelength(Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	P1	P1
a(Å)	10.033	10.434(2)
b(Å)	10.151	10.785(2)
c(Å)	13.402	13.251(3)
α(°)	102.15	92.47(3)
β(°)	106.83	110.71(3)
γ(°)	111.15	110.25(3)
V(Å^3)	1140.0	1285.2(6)
Z	1	1
Density (calculated)(Mg/m^3)	1.720	1.639
Absorption coefficient(mm^{-1})	6.538	5.809
F(000)	572	620
θ Range(°)	3.061-24.999	6.394-49.994
Index ranges	-11<=h<=11 -11<=k<=12 -15<=l<=15	-12 <=h<=12 -11<=k<=12 -15<=l<=15
Reflections collected	8962	9554
Independent reflec.	3987 [R(int) = 0.0694]	4431 [R(int) = 0.0936]
Data / restraints / parameters	3987 / 0 / 272	
Goodness-of-fit on F^2	1.028	1.036
Final *R* indices [I>2sigma(I)]	R_1 = 0.0456,	R_1 = 0.0709, wR_2 =

	wR_2 = 0.1069	0.1812
R indices (all data)	R_1 = 0.0474, wR_2 = 0.1082	R_1 = 0.0992, wR_2 = 0.2190
Largest diff. peak and hole	2.56 and -2.30 e. Å^{-3}	1.28 and -2.07 e. Å^{-3}

Table S2. Selected bond lengths (Å) and angles (deg) for complexes **1b** and **1c**

complex **1b**		complex **1c**	
Au(1)-P(1)	2.2821(15)	Au(1)-P(1)	2.274(4)
Au(1)-C(1)	2.012(7)	Au(1)-C(1)	2.035(17)
C(1)-C(2)	1.191(9)	C(1)-C(2)	1.16(2)
C(9)-O(1)	1.408(11)	C(6)-O(1)	1.386(18)
C(1)-Au(1)-P(1)	173.22(18)	C(1)-Au(1)-P(1)	175.1(3)
C(2)-C(1)-Au(1)	174.1(6)	C(2)-C(1)-Au(1)	169.0(12)

2. NMR and MS spectra

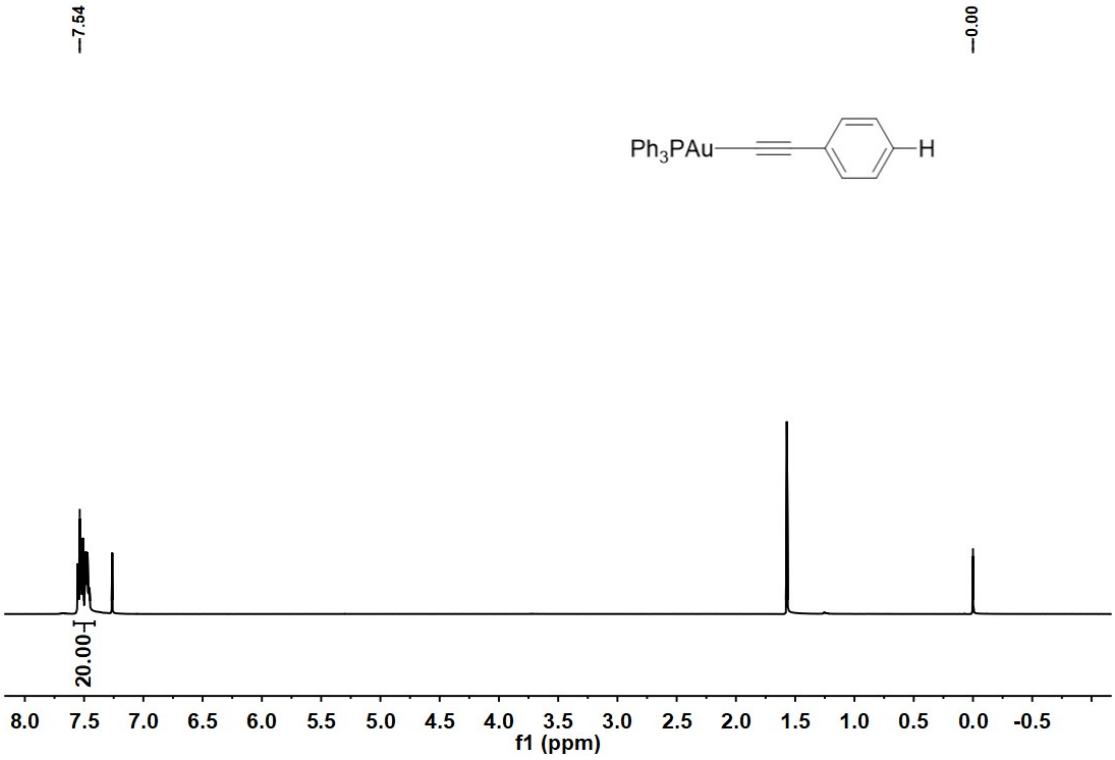


Fig. S1 ^{1}H NMR spectra of complex **1a** in $CDCl_3$

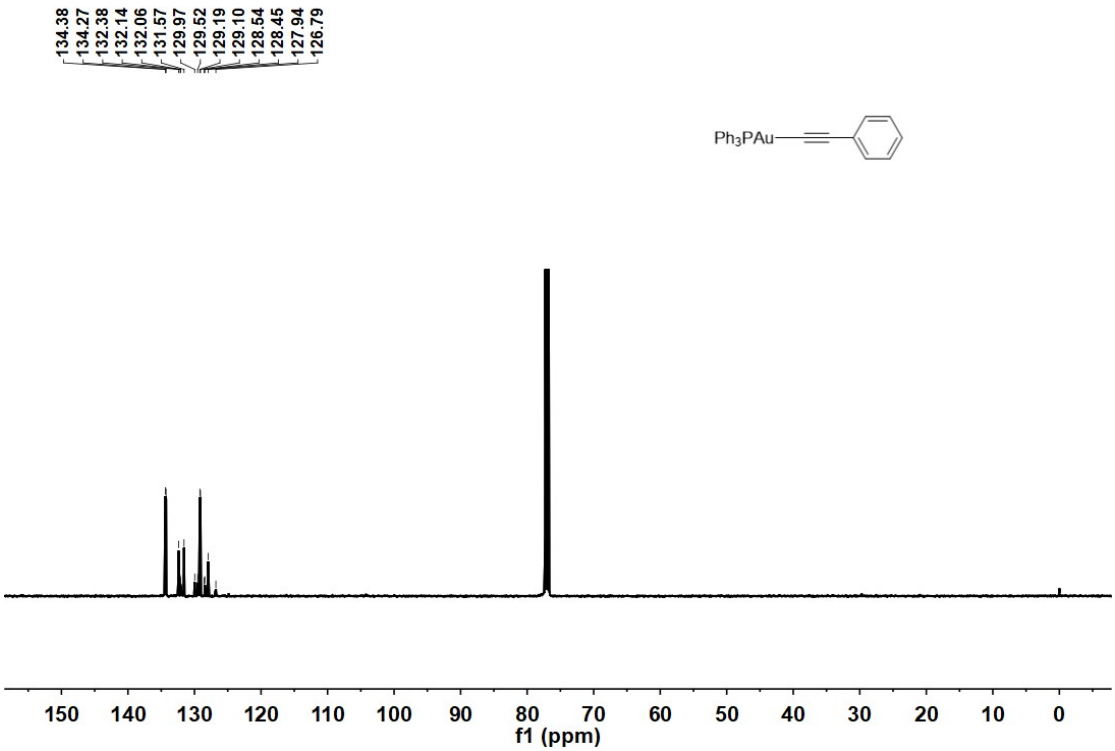


Fig. S2 ^{13}C NMR spectra of complex **1a** in $CDCl_3$

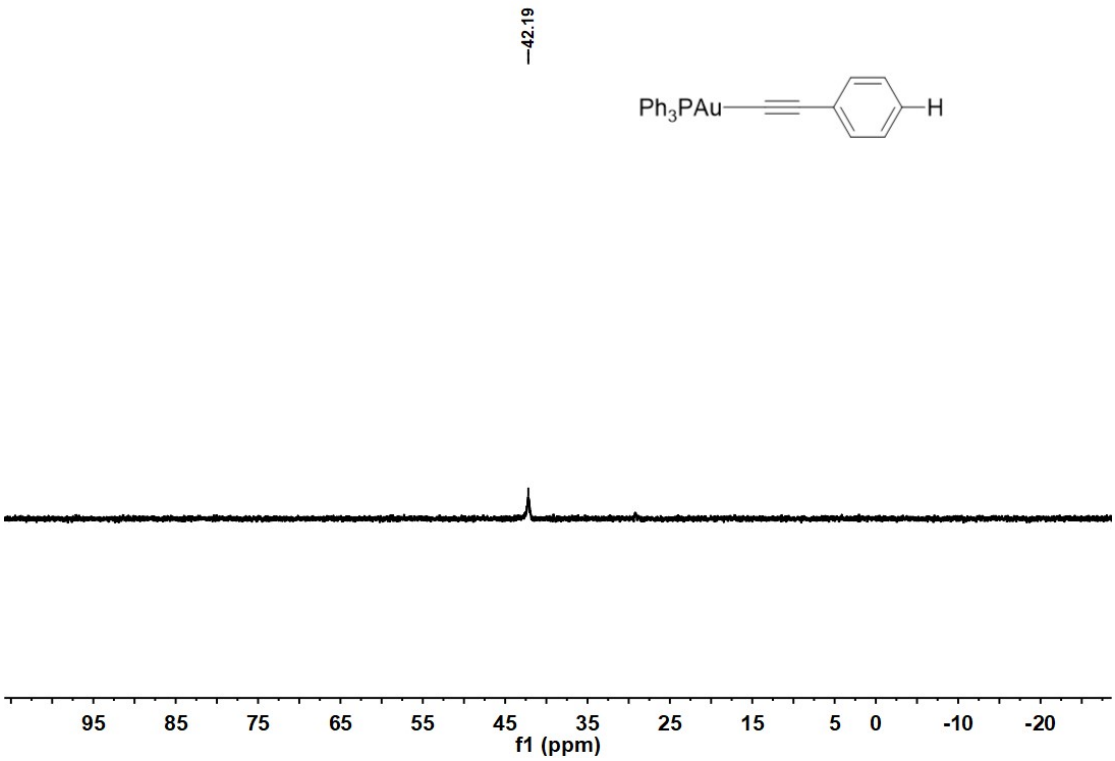


Fig. S3 ^{31}P NMR spectra of complex **1a** in $CDCl_3$

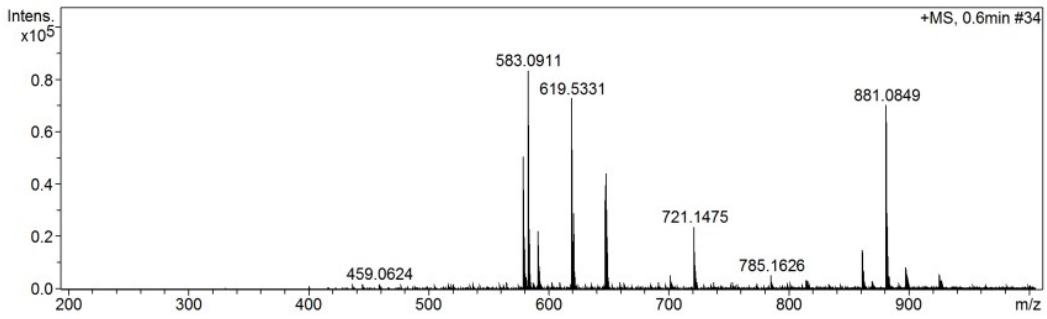


Fig. S4. MS spectra of complex **1a**.

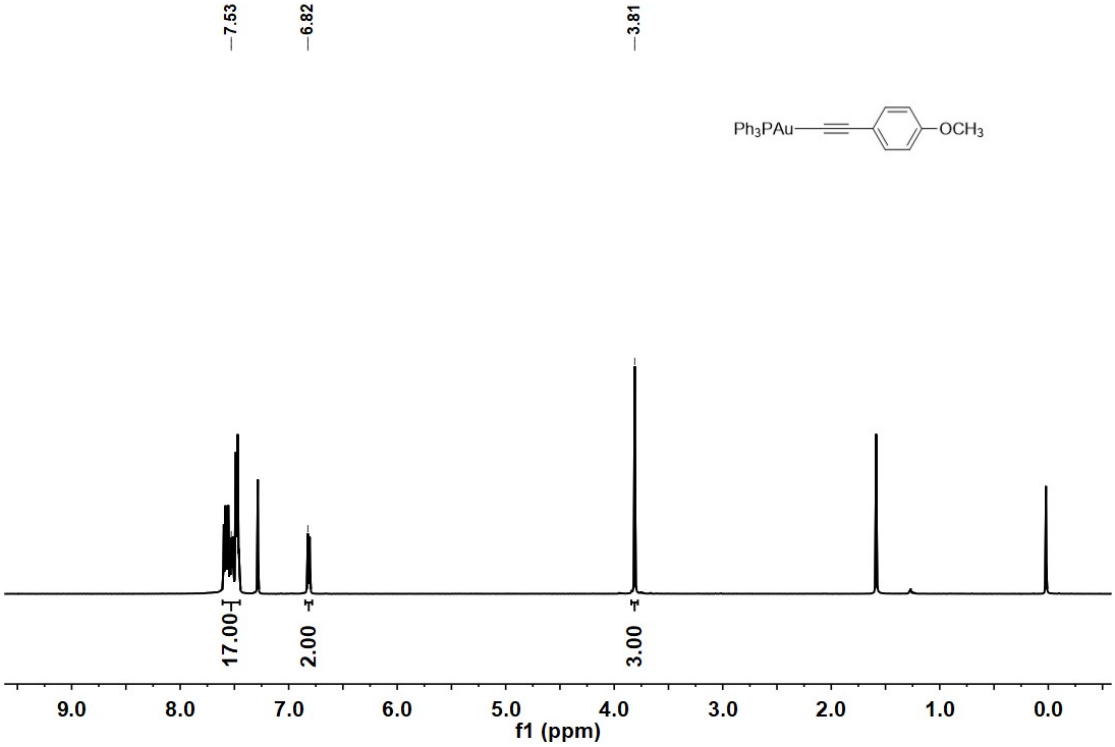


Fig. S5 ^{1}H NMR spectra of complex **1b** in $CDCl_3$

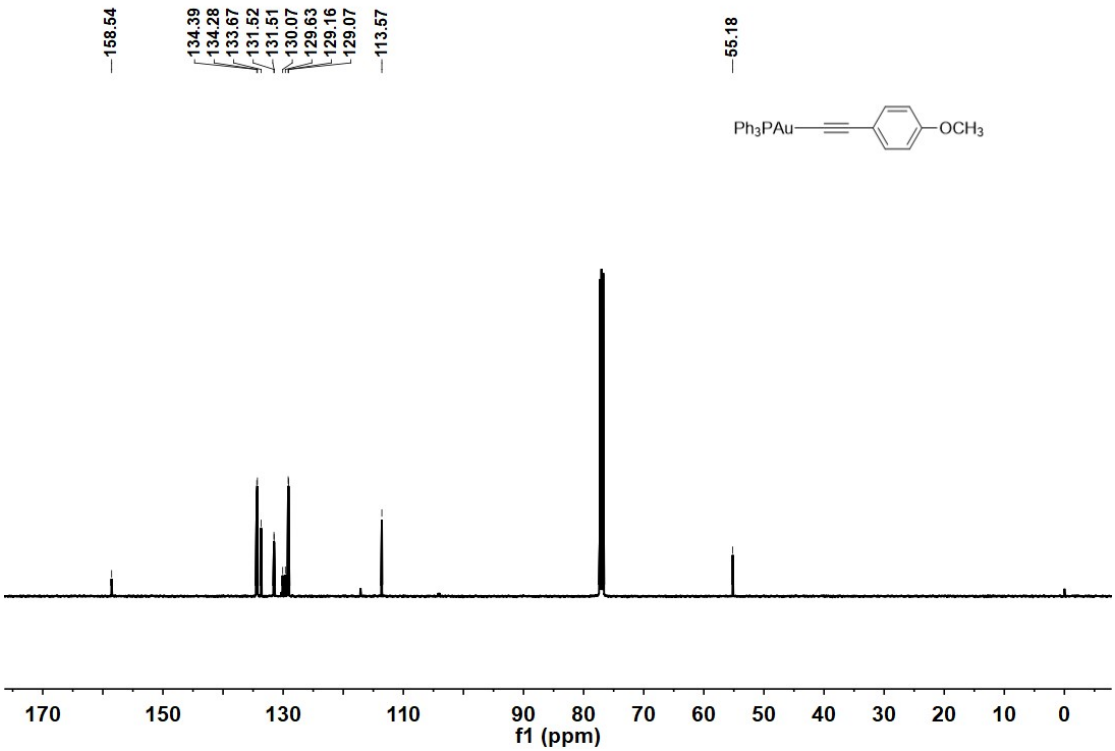


Fig. S6 ^{13}C NMR spectra of complex **1b** in $CDCl_3$

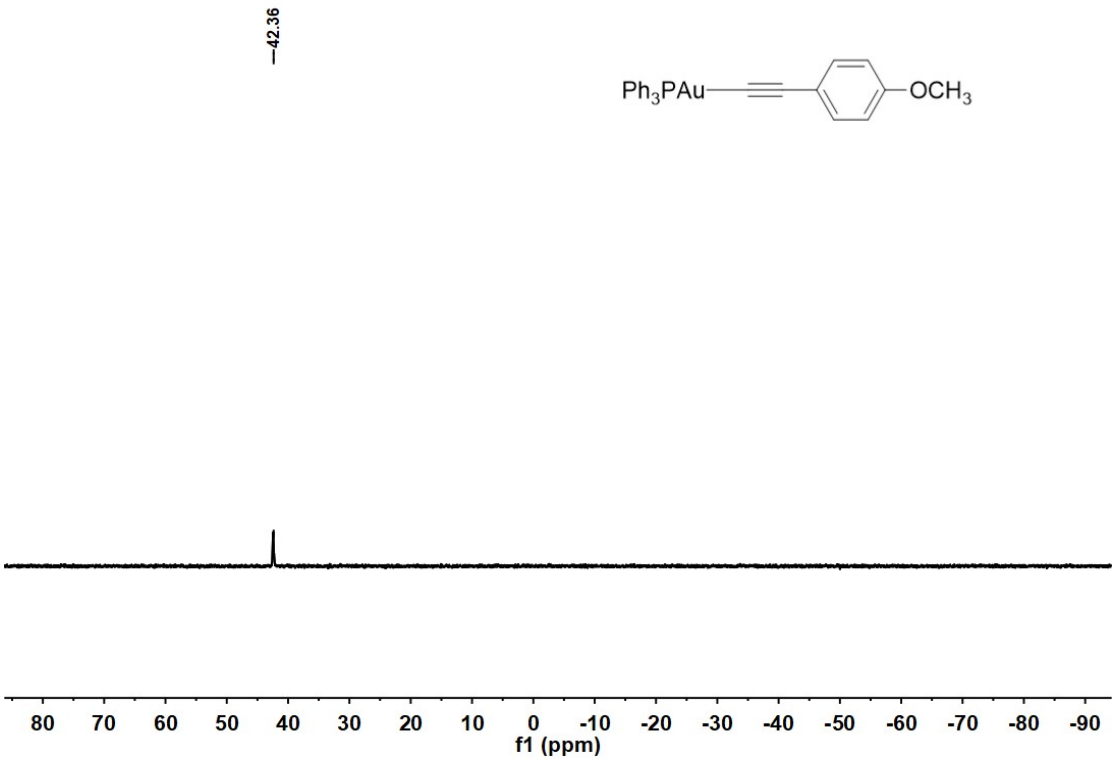


Fig. S7 ^{31}P NMR spectra of complex **1b** in $CDCl_3$

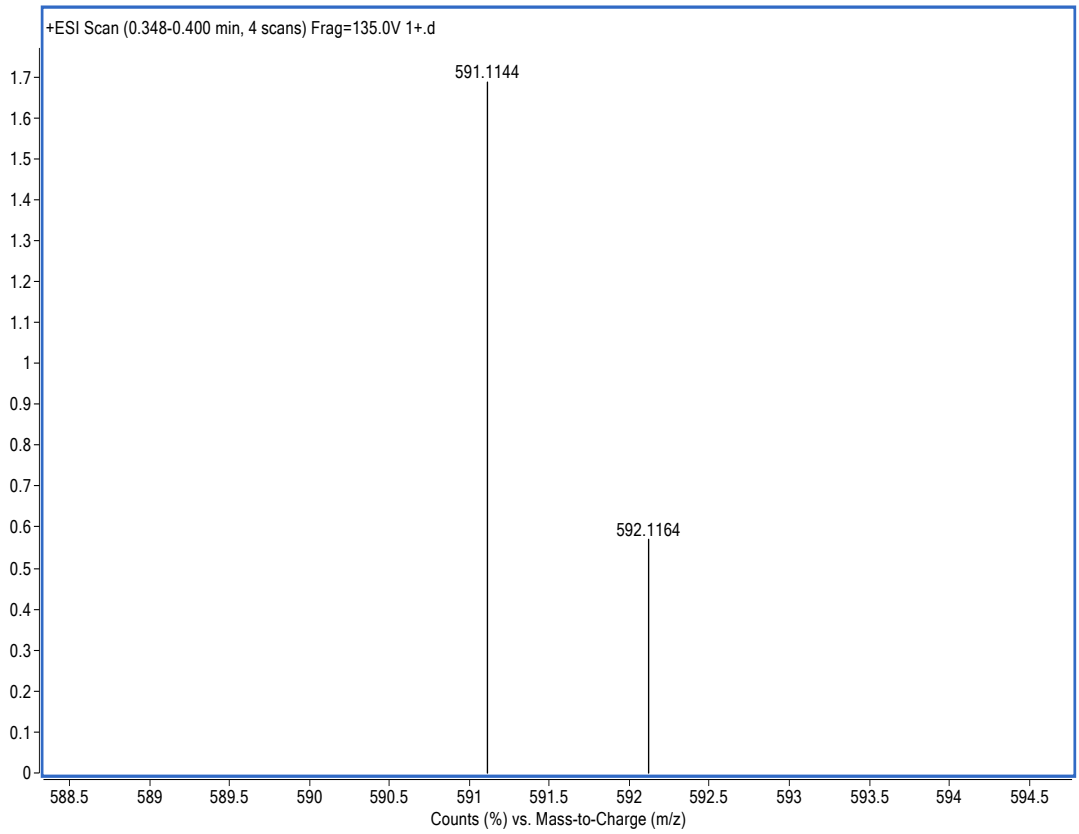


Fig. S8. MS spectra of complex **1b**.

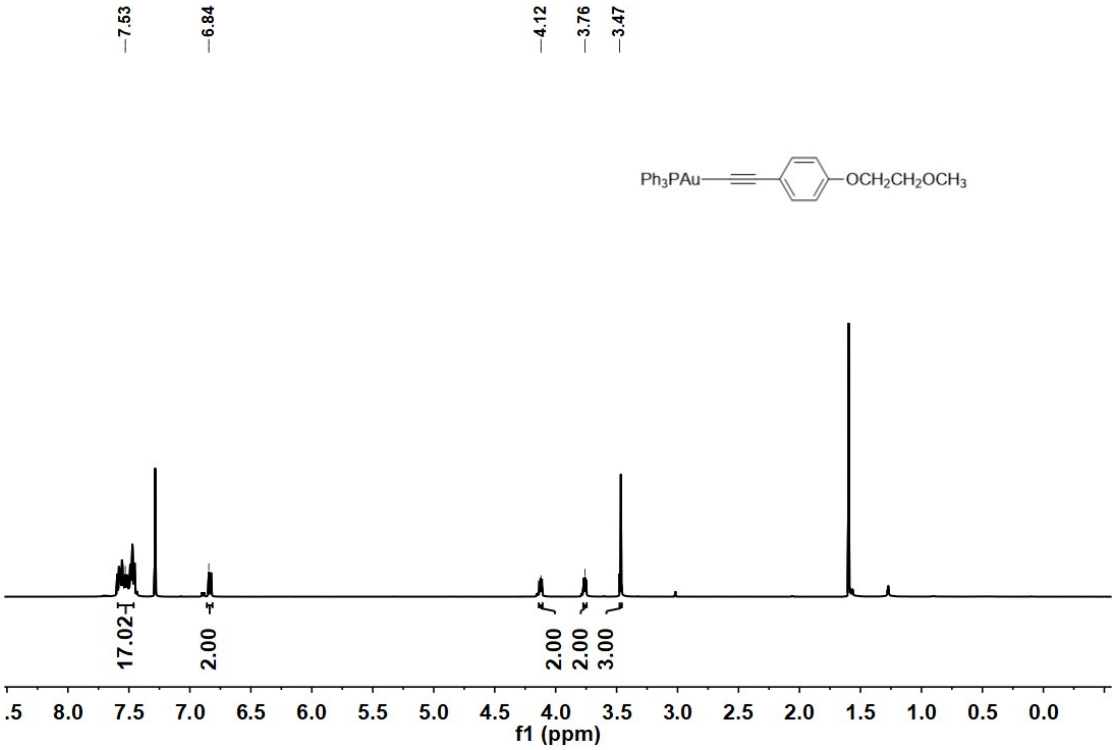


Fig. S9 ^{1}H NMR spectra of complex **1c** in $CDCl_3$

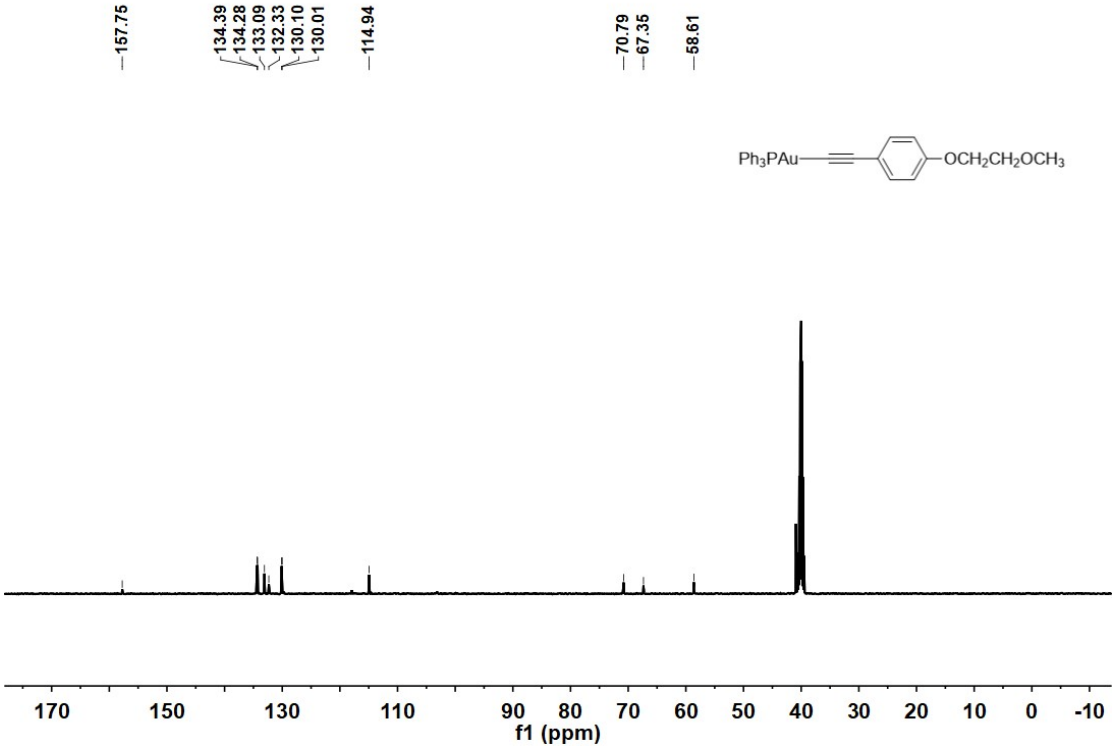


Fig. S10 ^{13}C NMR spectra of complex **1c** in DMSO

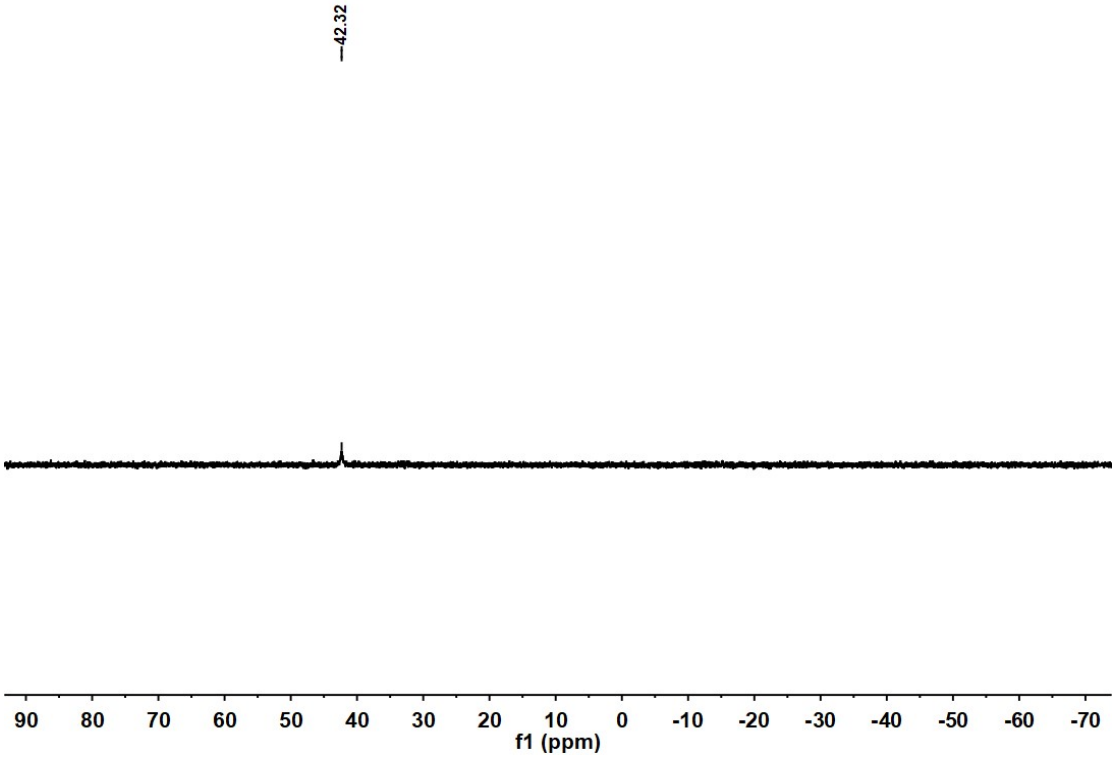


Fig. S11 ^{31}P NMR spectra of complex **1c** in $CDCl_3$

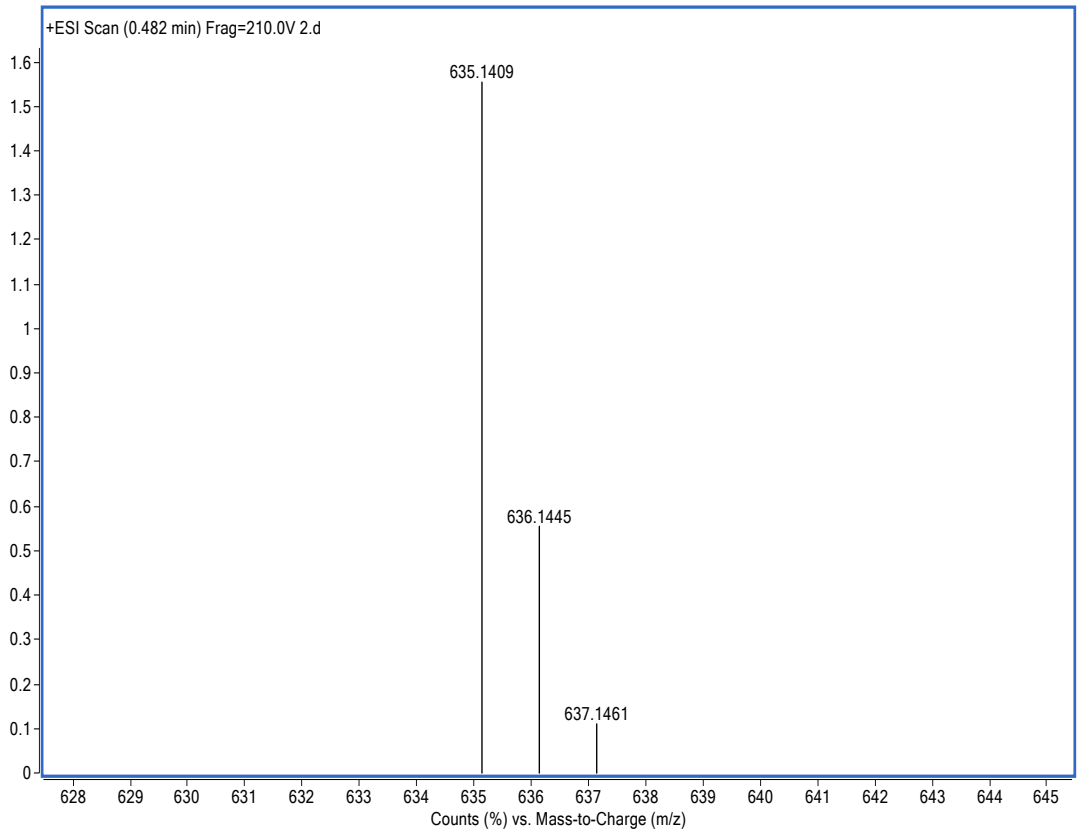


Fig. S12. MS spectra of complex **1c**.

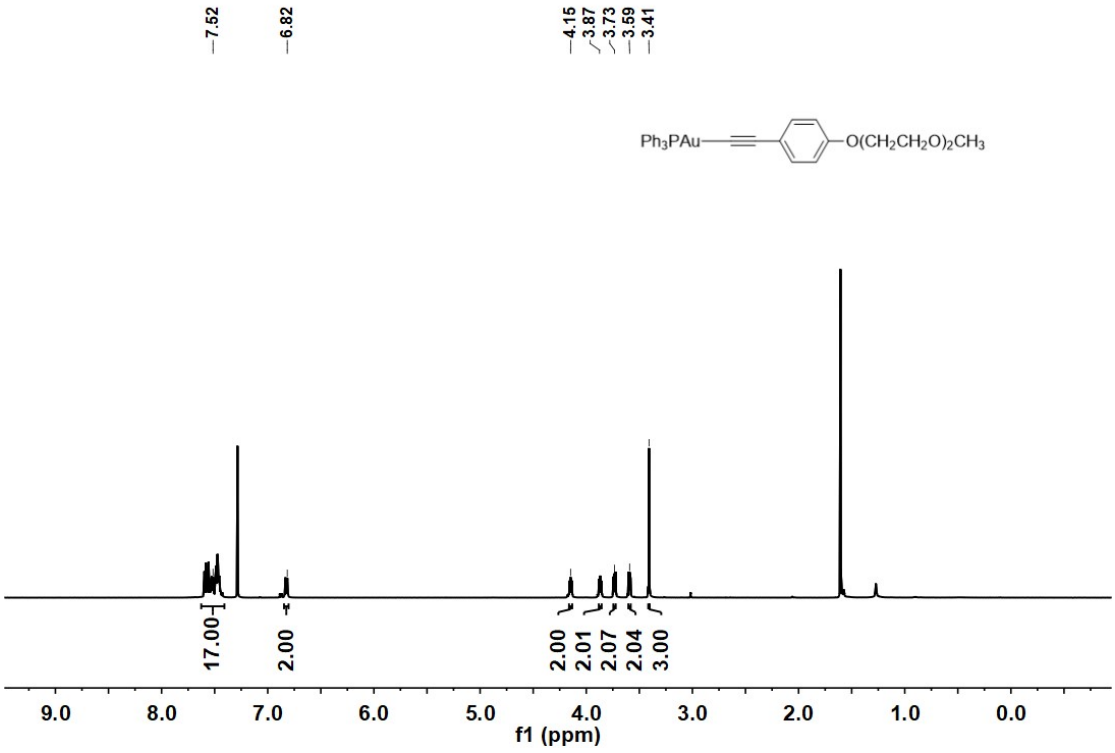


Fig. S13 ^{1}H NMR spectra of complex **1d** in $CDCl_3$

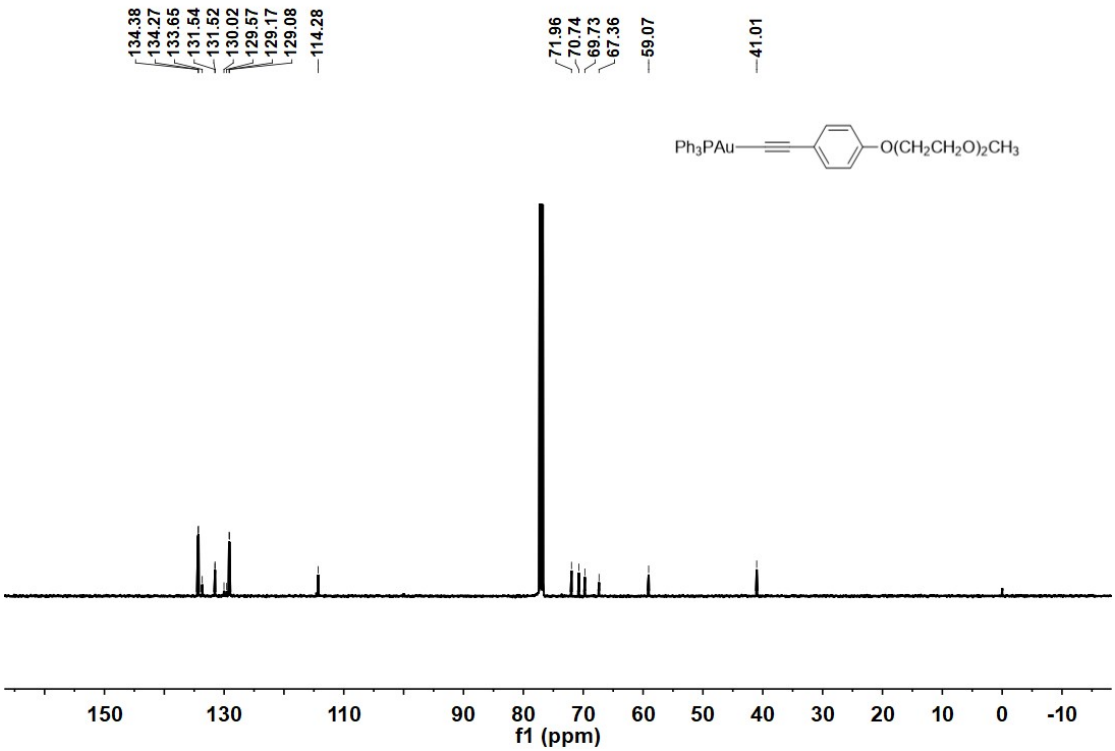


Fig. S14 ^{13}C NMR spectra of complex **1d** in $CDCl_3$

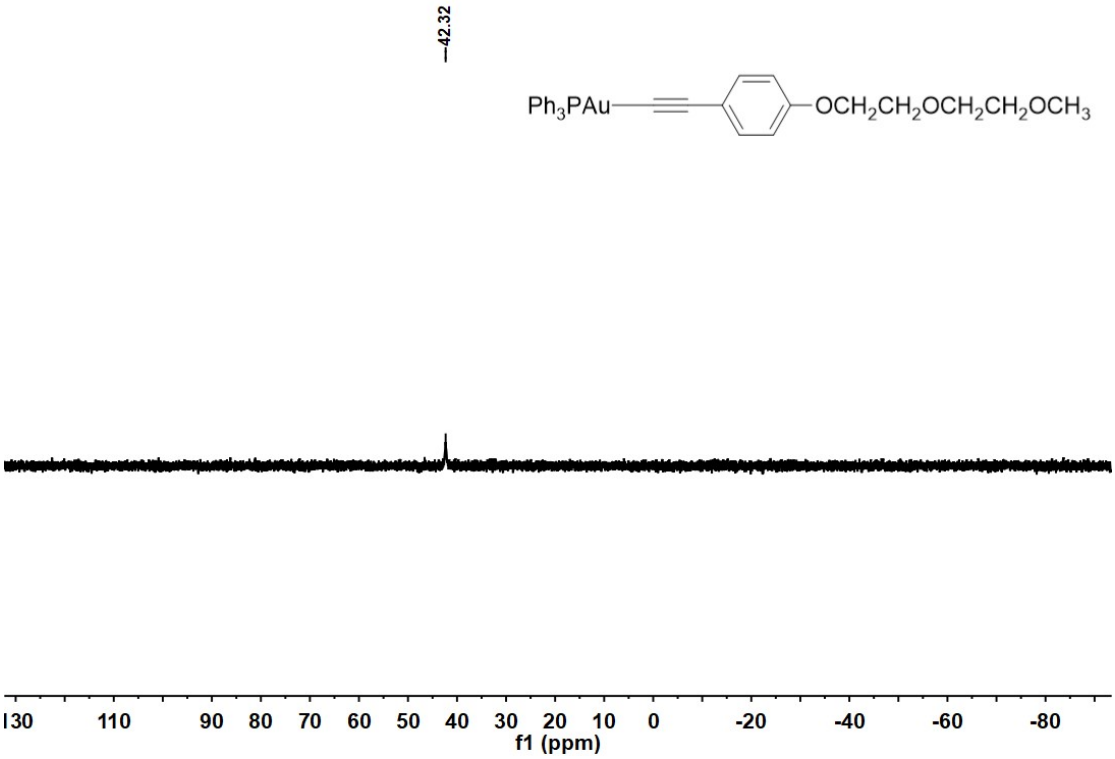


Fig. S15 ^{31}P NMR spectra of complex **1d** in $CDCl_3$

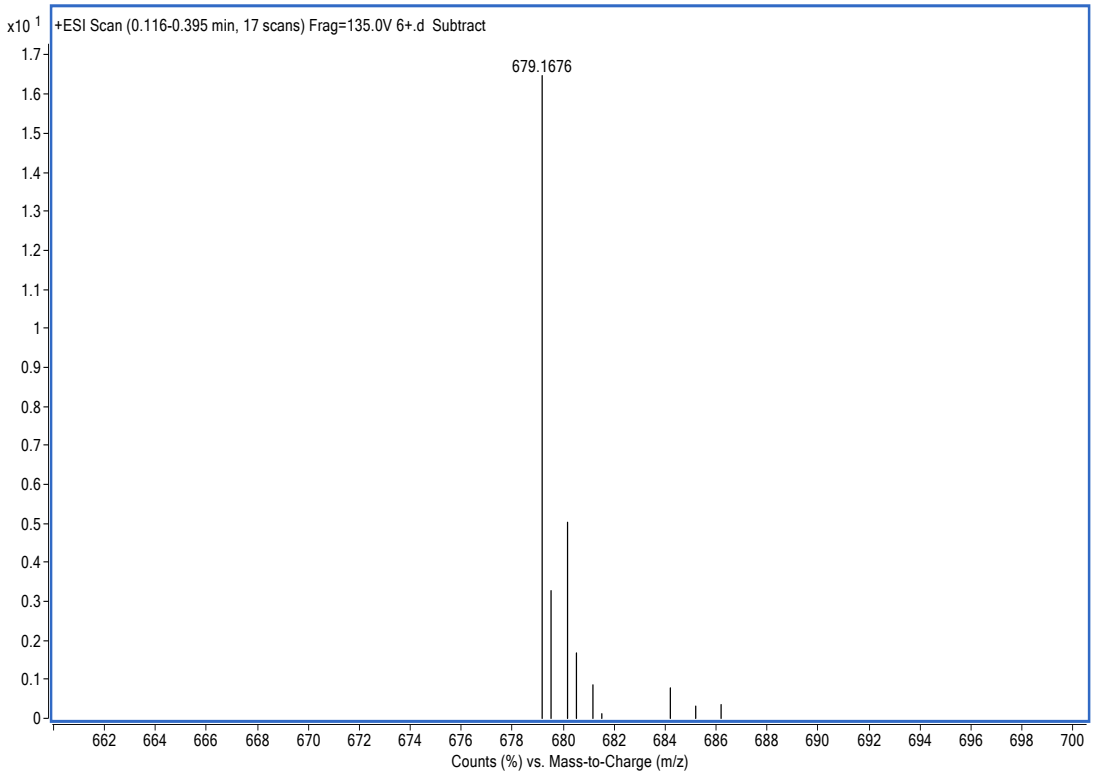


Fig. S16. MS spectra of complex **1d**.

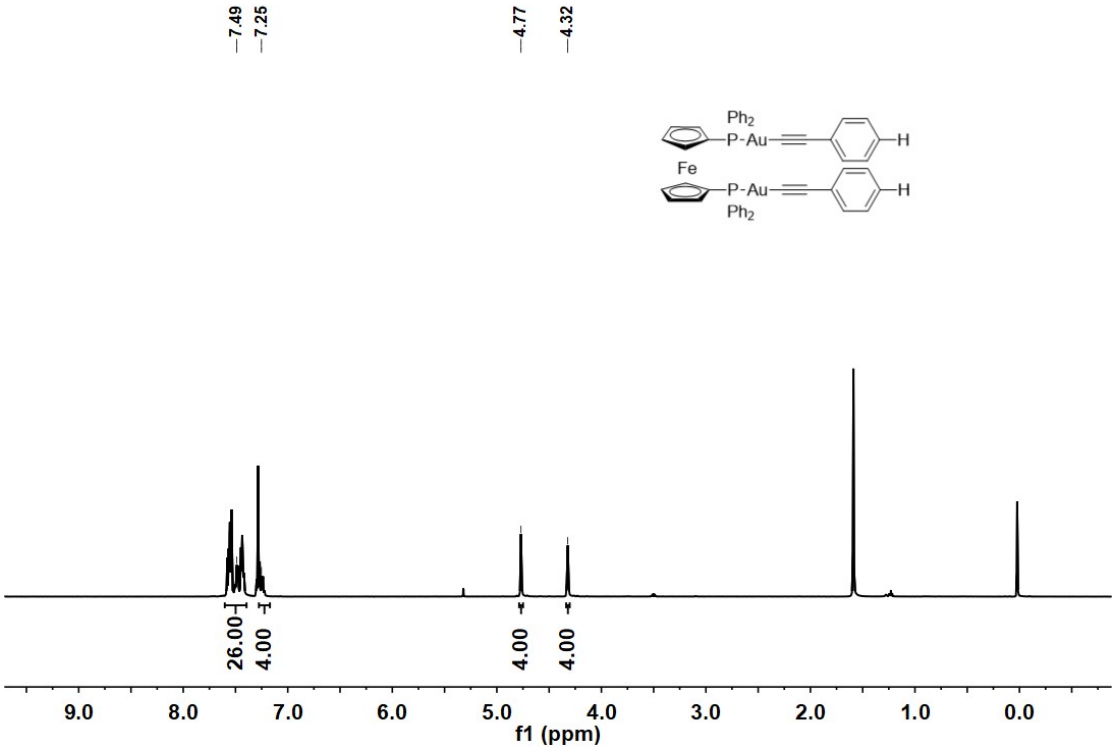


Fig. S17 ^{1}H NMR spectra of complex **2a** in $CDCl_3$

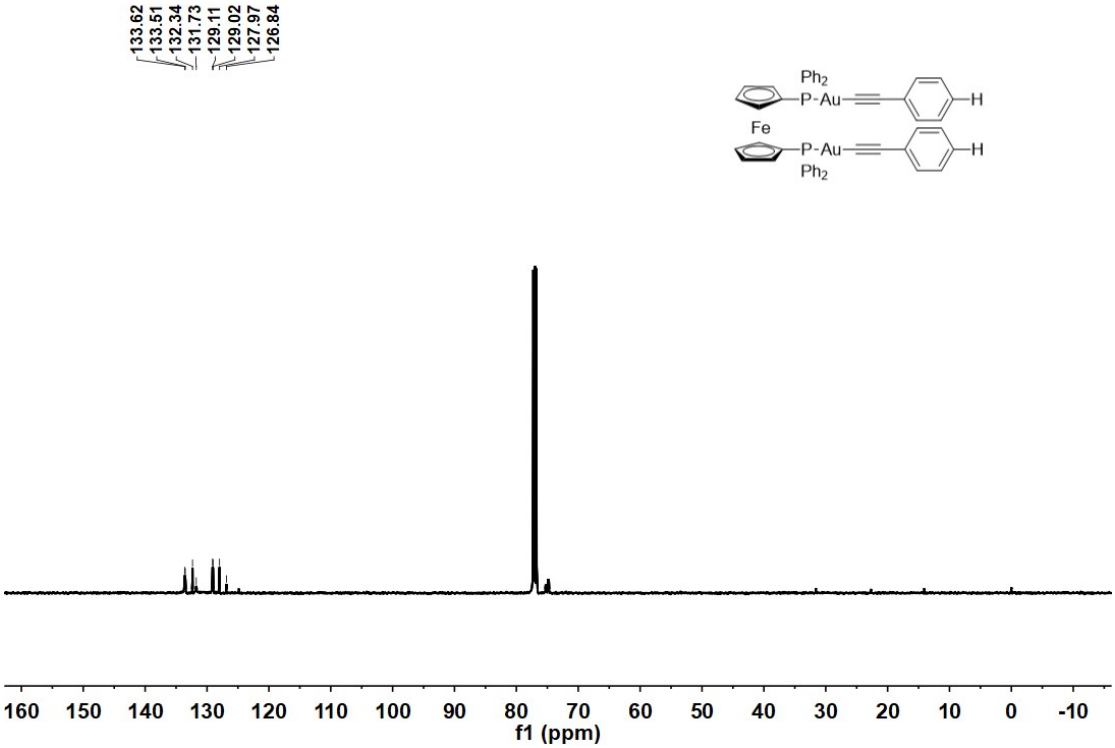


Fig. S18 ^{13}C NMR spectra of complex **2a** in $CDCl_3$

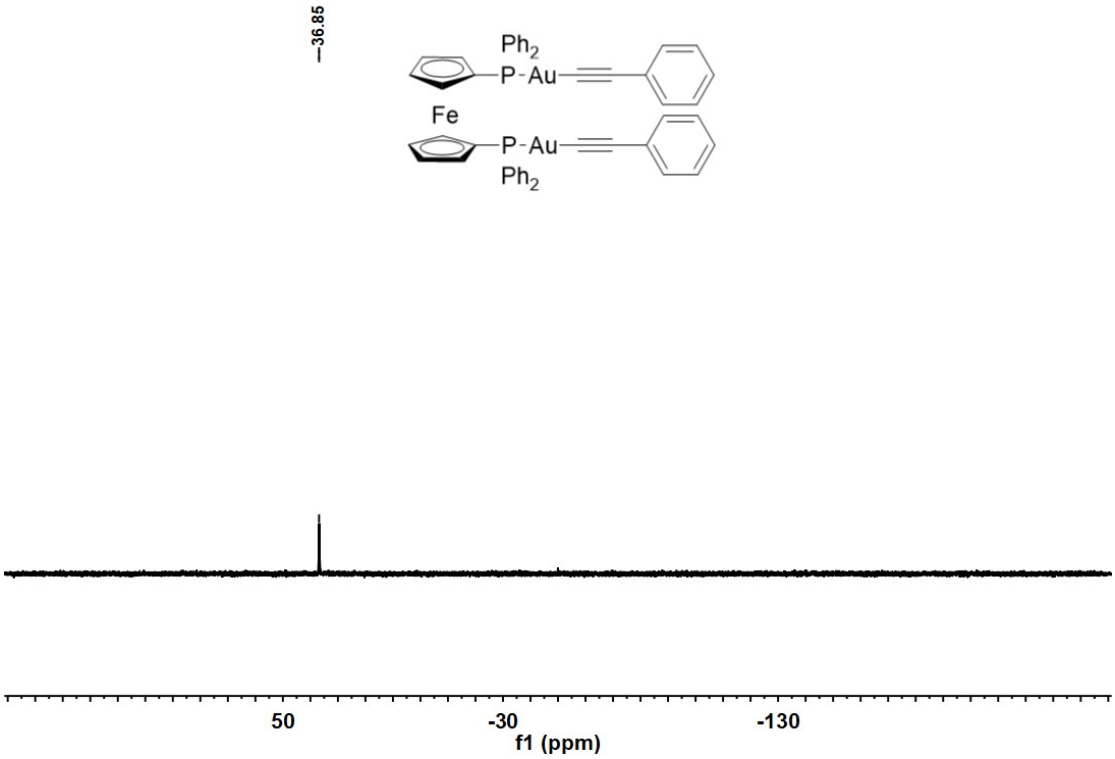


Fig. S19 ^{31}P NMR spectra of complex **2a** in $CDCl_3$

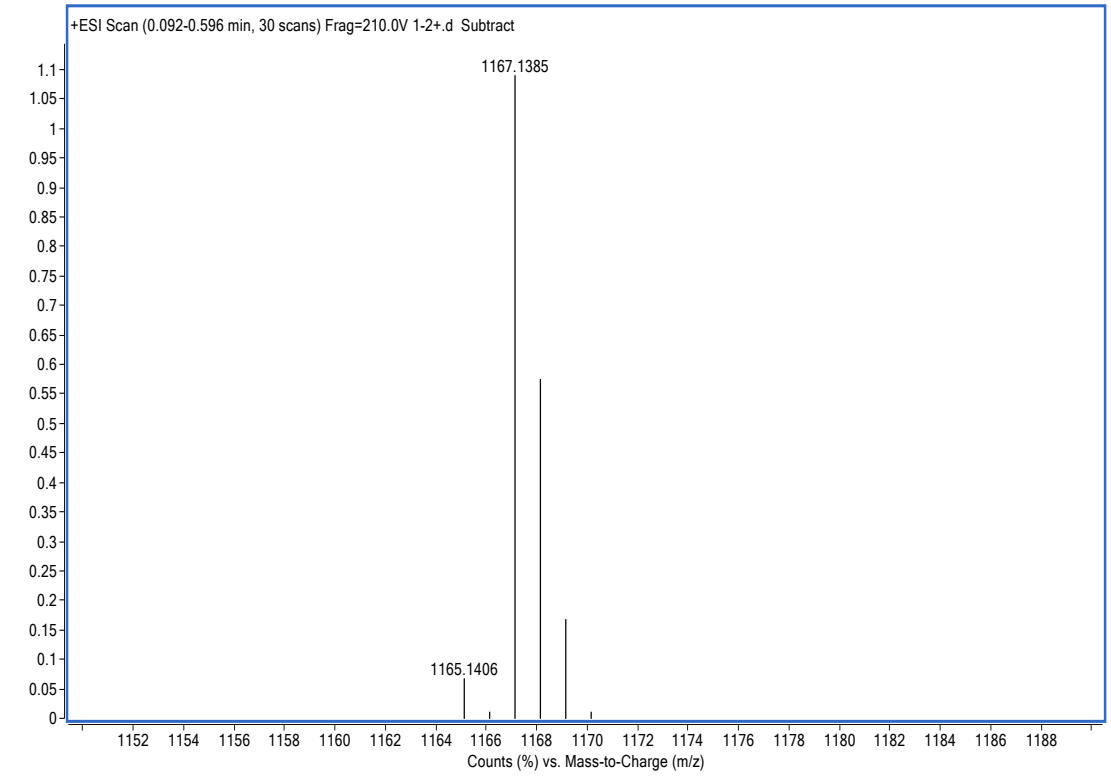


Fig. S20. MS spectra of complex **2a**.

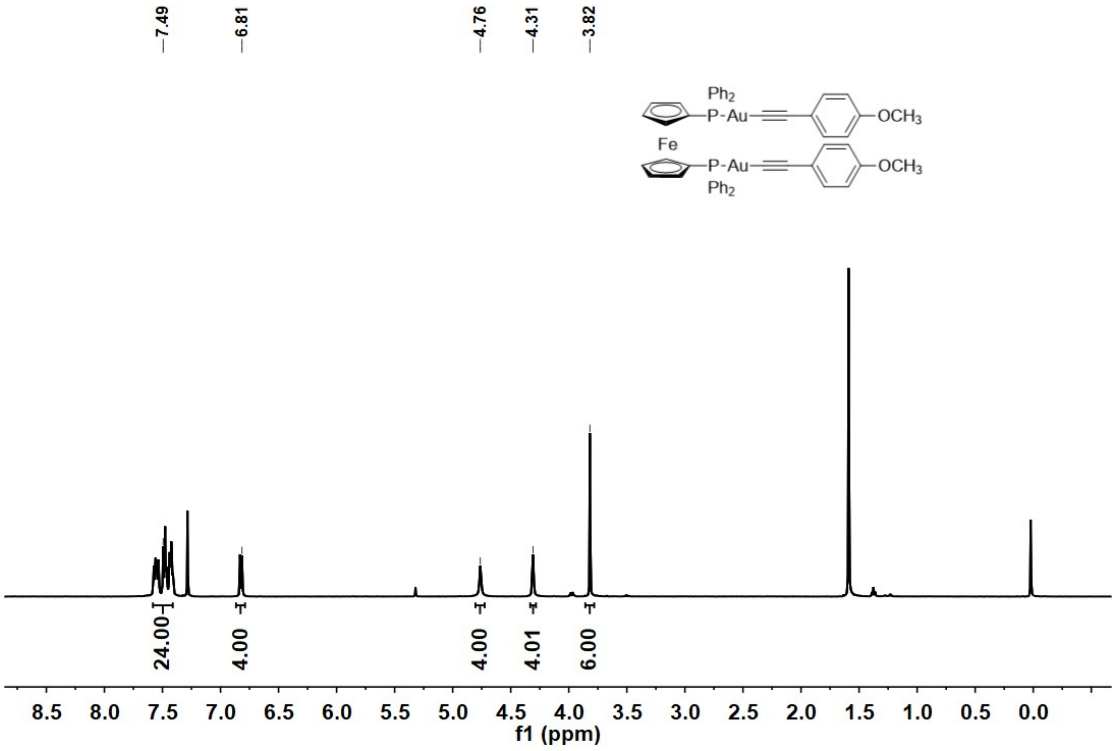


Fig. S21 ^{1}H NMR spectra of complex **2b** in $CDCl_3$

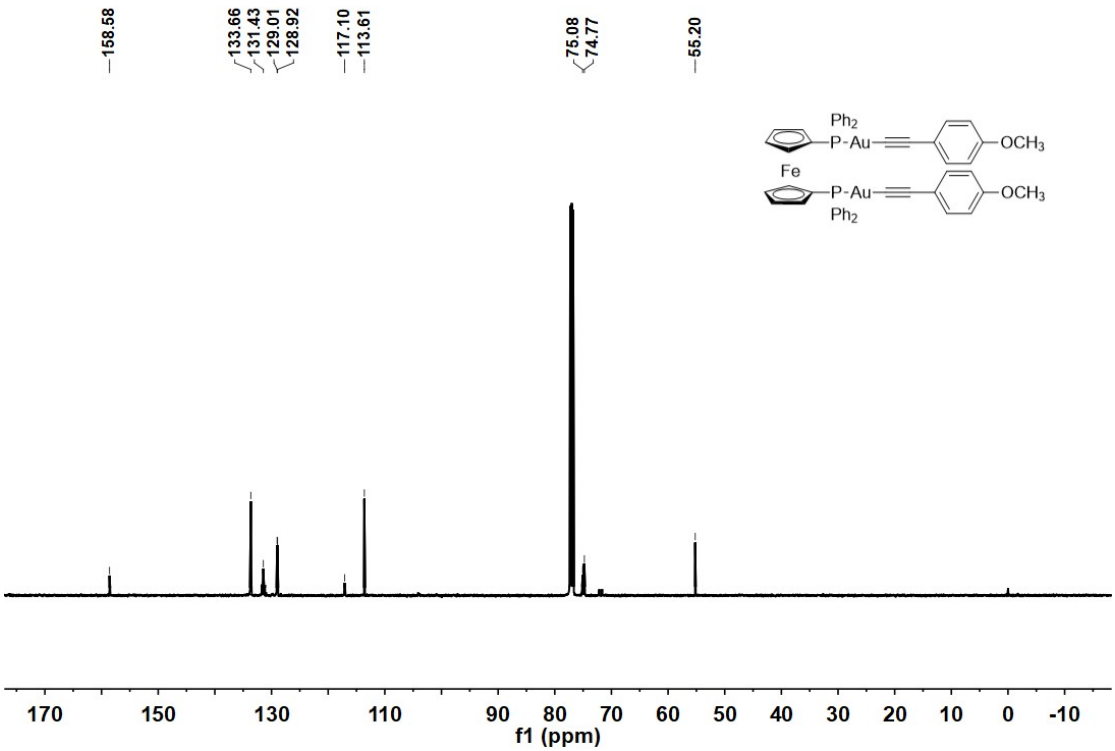


Fig. S22 ^{13}C NMR spectra of complex **2b** in $CDCl_3$

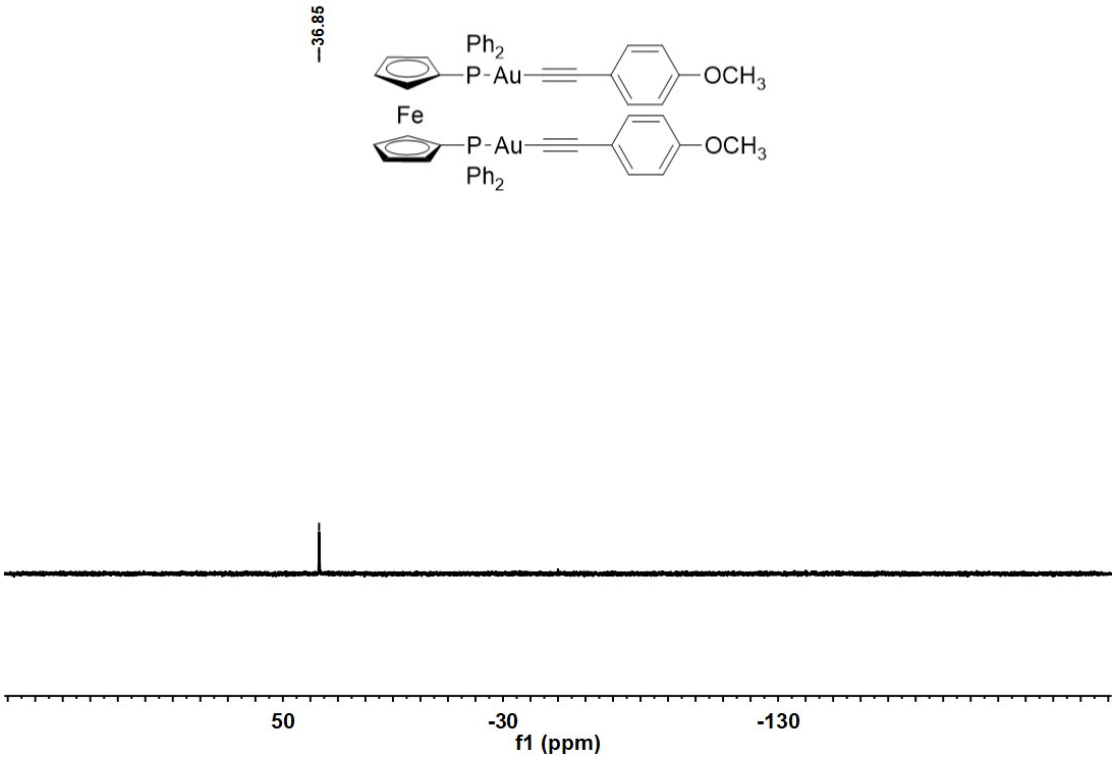


Fig. S23 ^{31}P NMR spectra of complex **2b** in $CDCl_3$

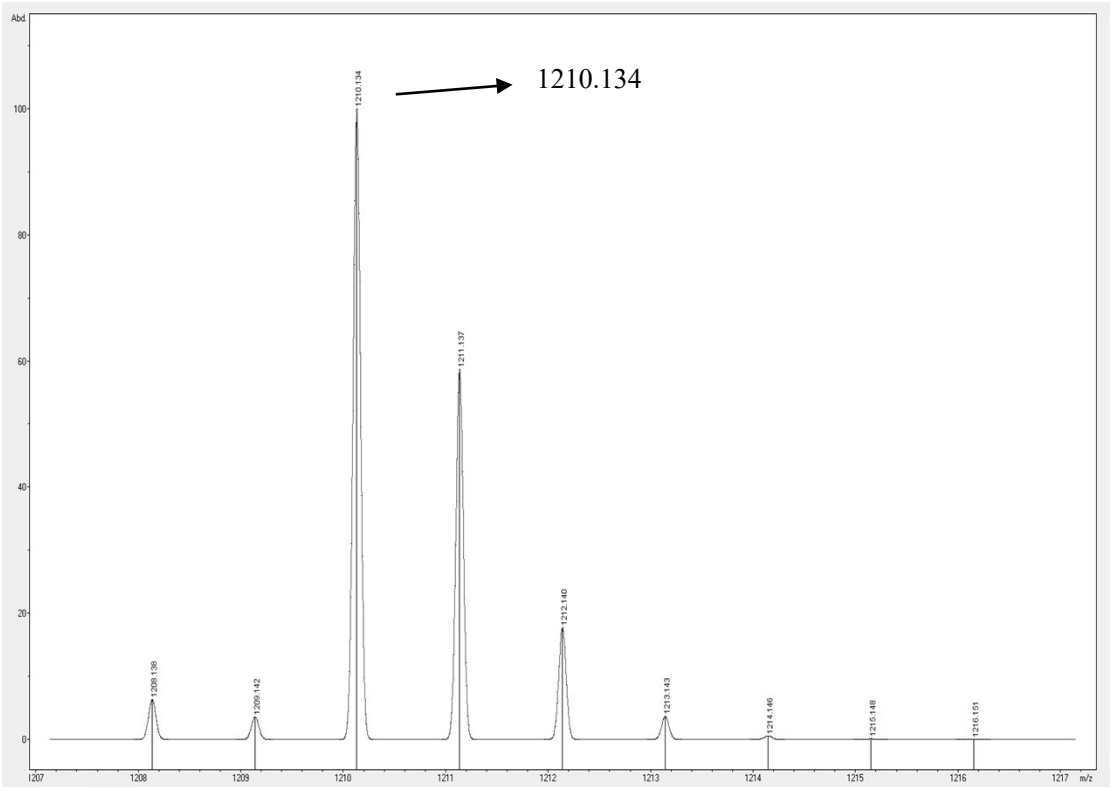


Fig. S24. MS spectra of complex **2b**.

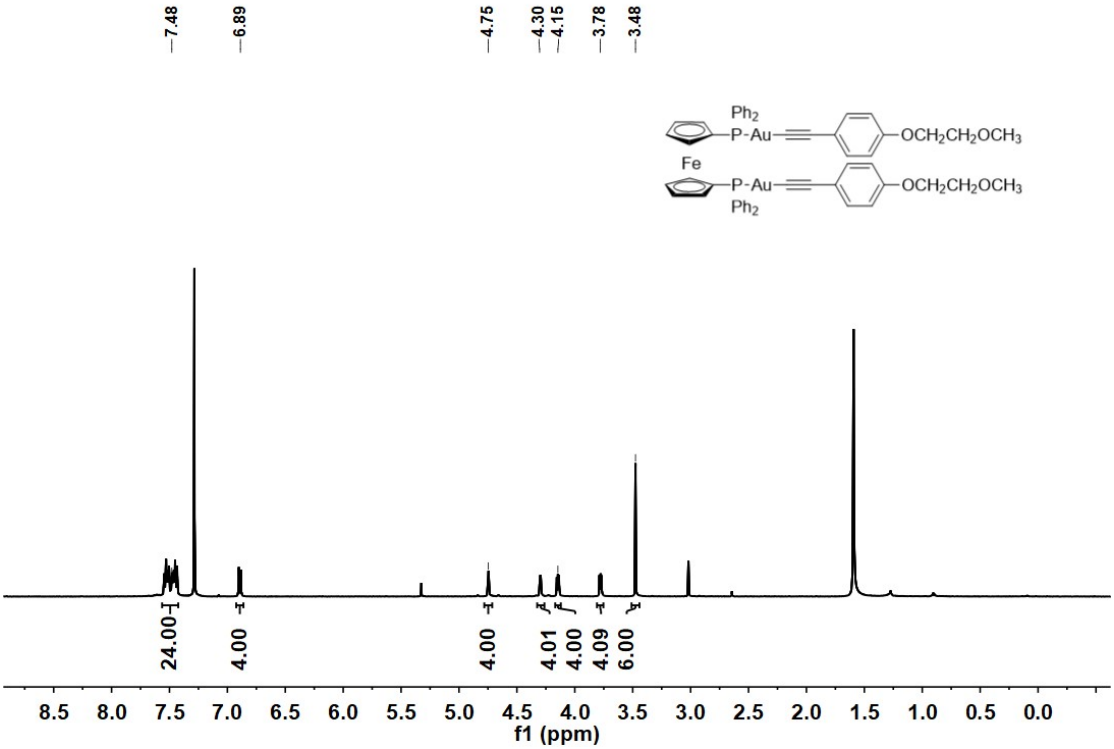


Fig. S25 ^{1}H NMR spectra of complex **2c** in $CDCl_3$

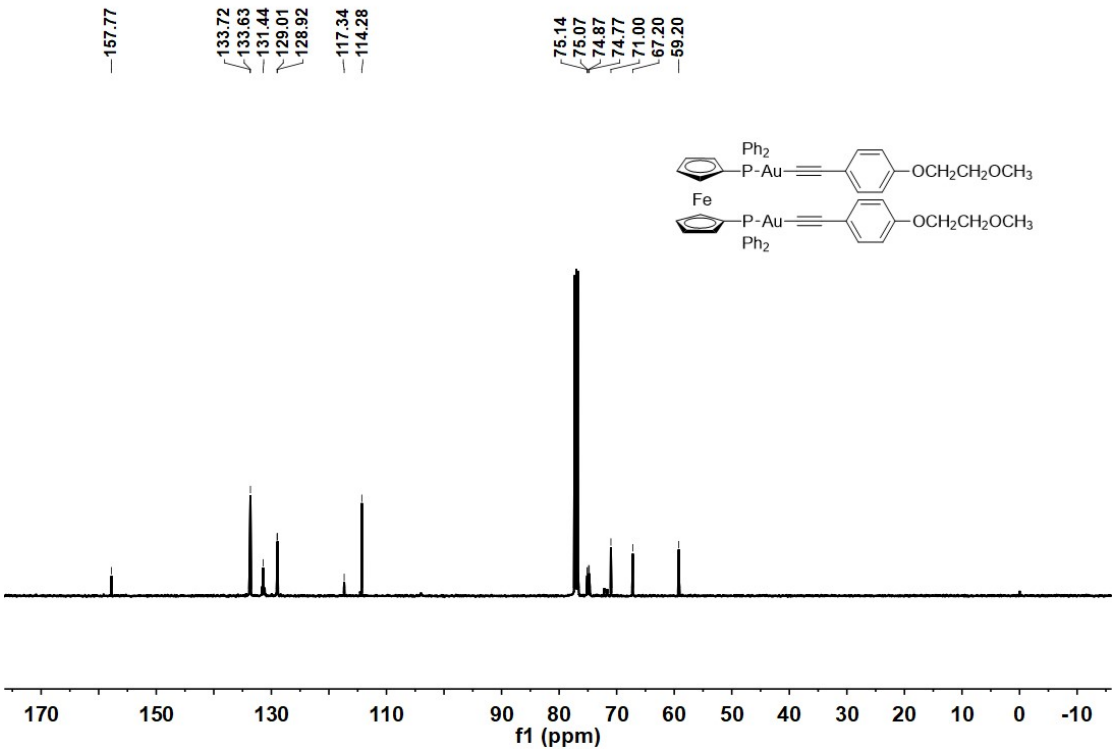


Fig. S26 ^{13}C NMR spectra of complex **2c** in $CDCl_3$

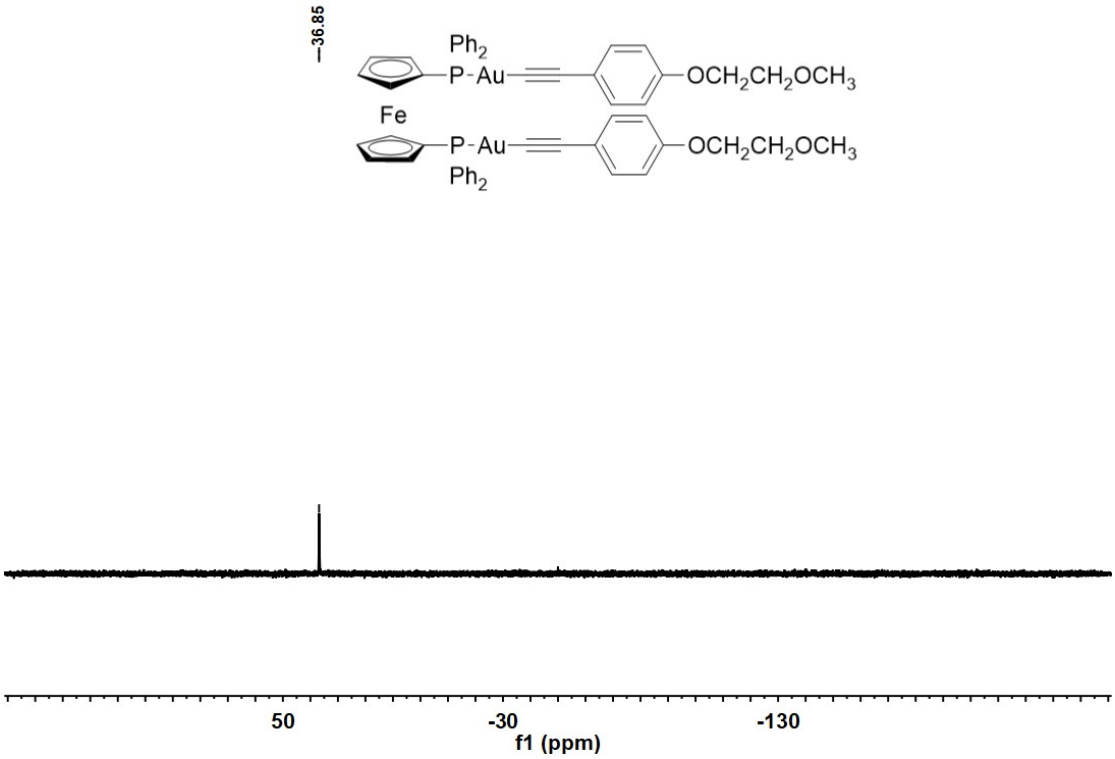


Fig. S27 ^{31}P NMR spectra of complex **2c** in $CDCl_3$

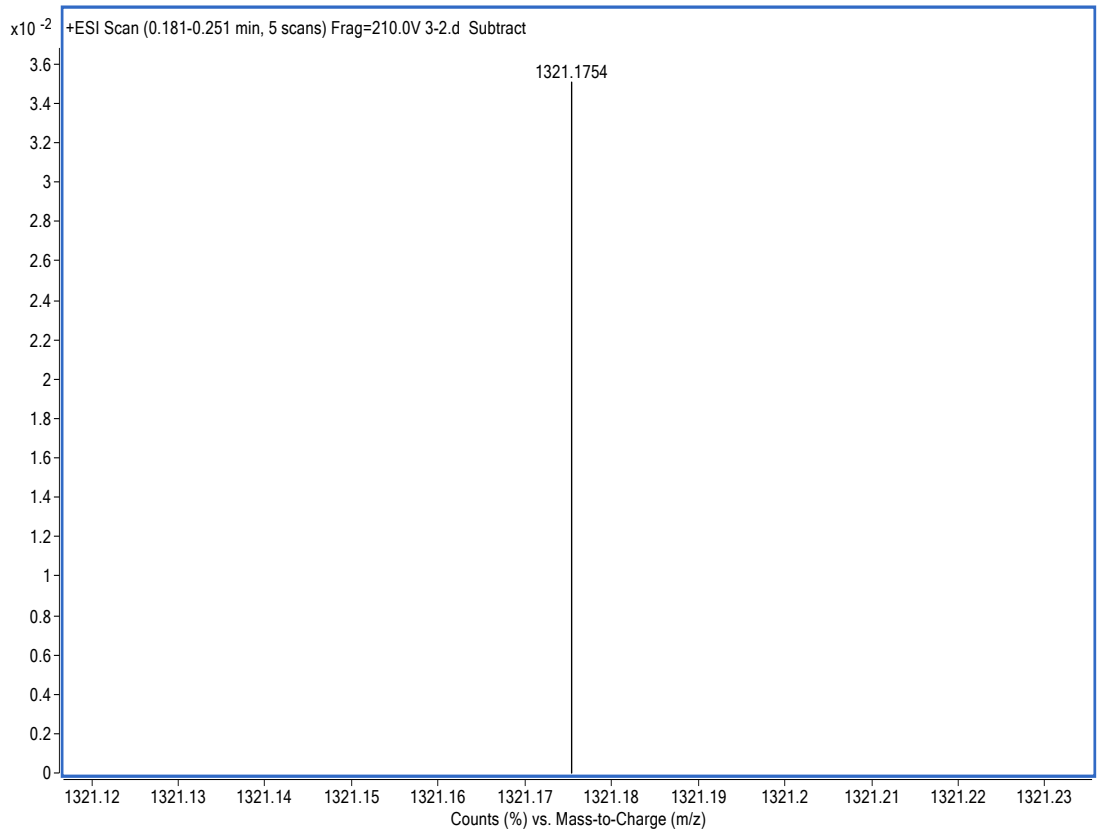


Fig. S28. MS spectra of complex **2b**.

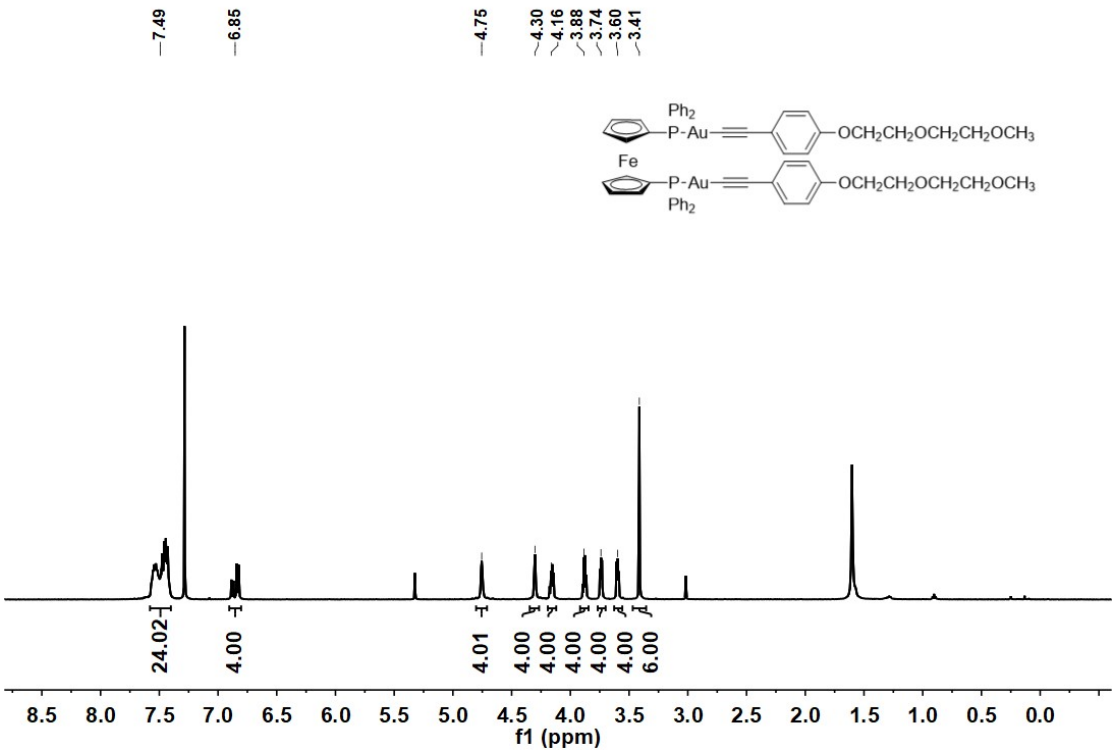


Fig. S29 ^{1}H NMR spectra of complex **2d** in $CDCl_3$

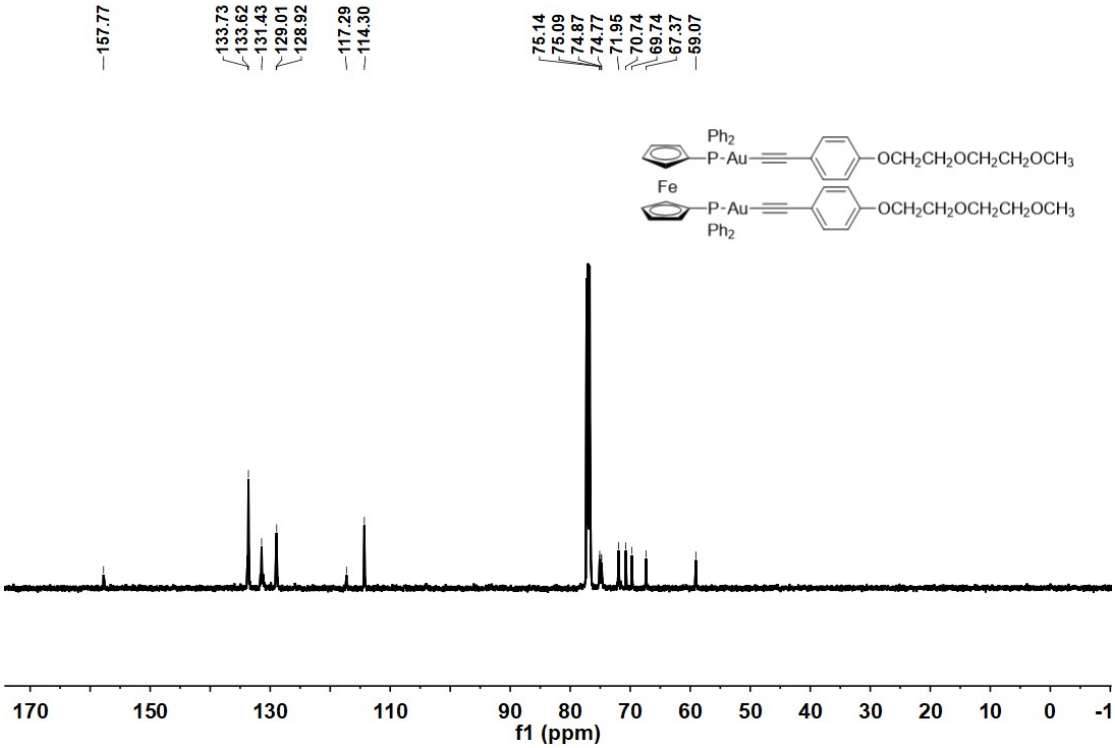


Fig. S30 ^{13}C NMR spectra of complex **2d** in $CDCl_3$

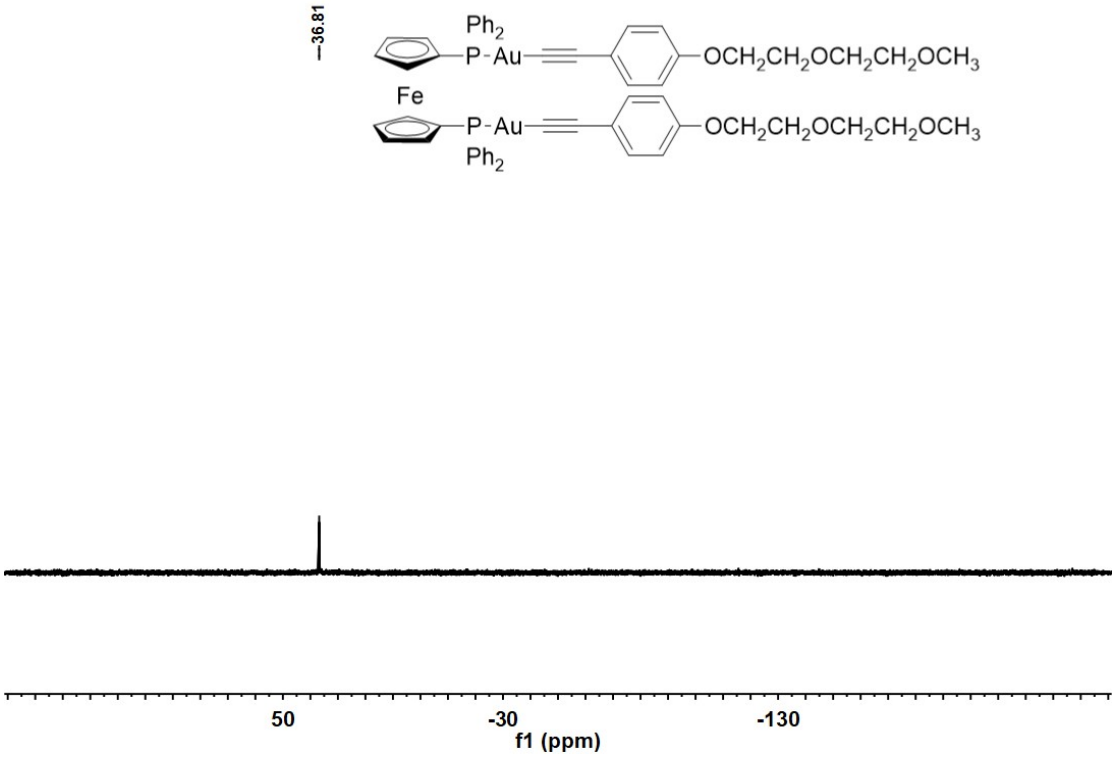


Fig. S31 ^{31}P NMR spectra of complex **2d** in $CDCl_3$

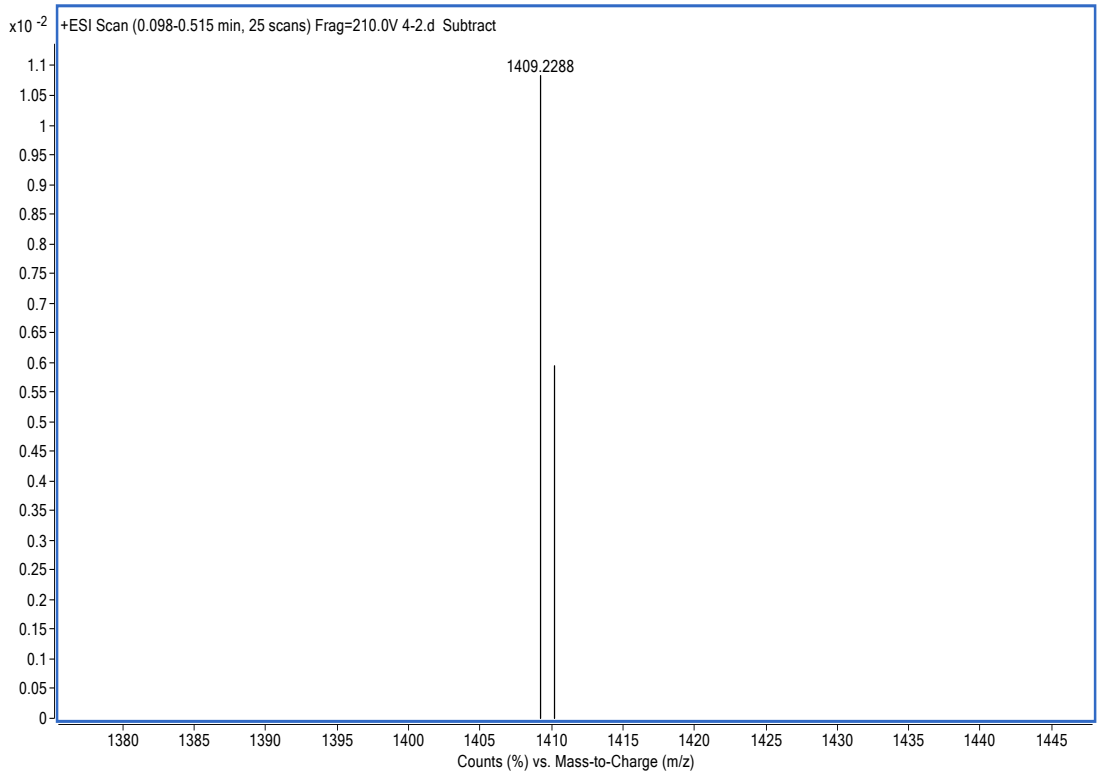
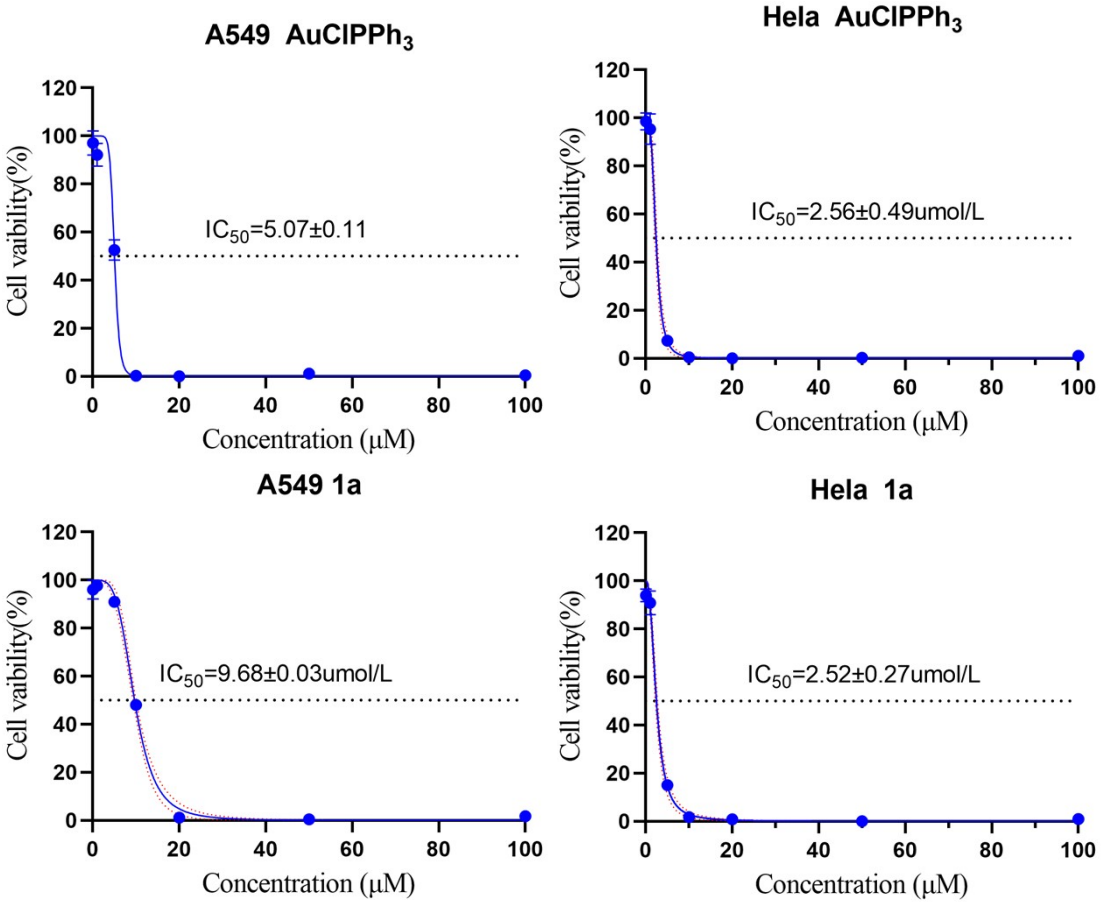
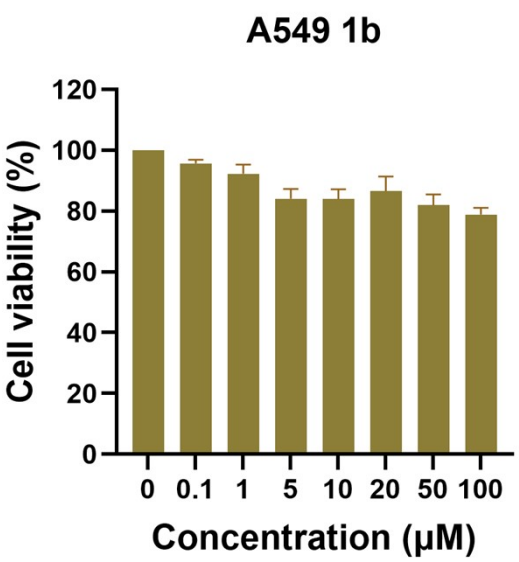
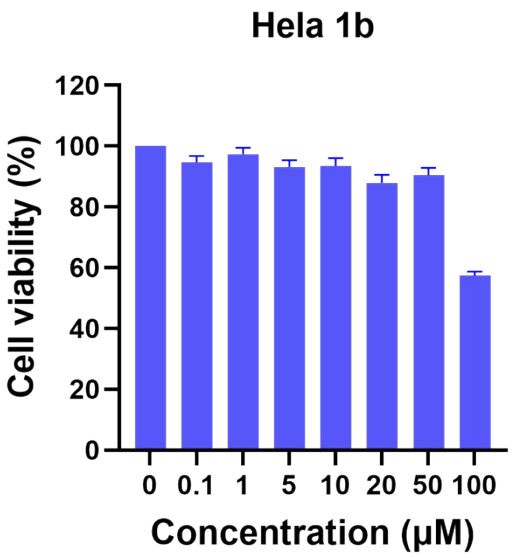


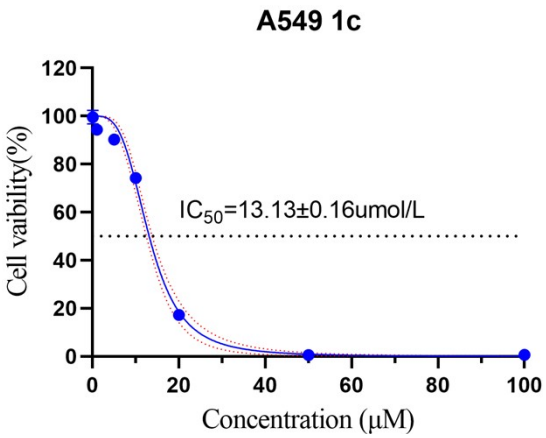
Fig. S32 MS spectra of complex **2d**.

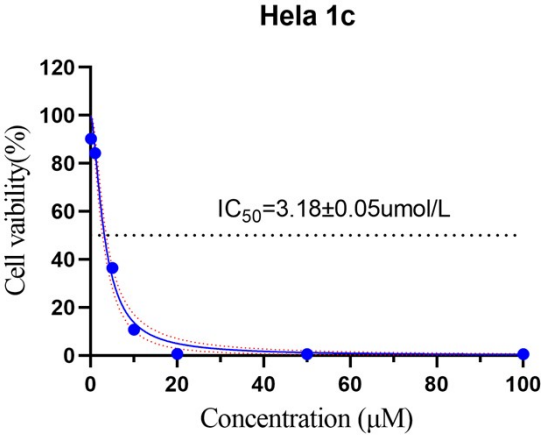
3. Antiproliferative activity




A549 1b
Cell viability (%)
120
100
80
60
40
20
0
0 0.1 1 5 10 20 50 100
Concentration (μM)


Hela 1b
Cell viability (%)
120
100
80
60
40
20
0
0 0.1 1 5 10 20 50 100
Concentration (μM)


A549 1c
Cell vaibility(%)
IC50=13.13±0.16umol/L
0 20 40 60 80 100
Concentration (μM)


Hela 1c
Cell vaibility(%)
IC50=3.18±0.05umol/L
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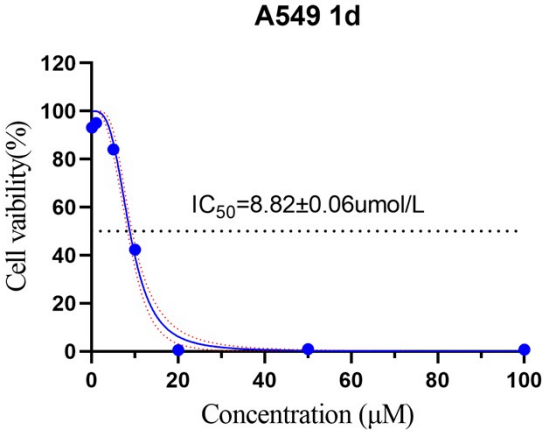
Concentration (μM)


A549 1d
Cell vaibility(%)
IC50=8.82±0.06umol/L
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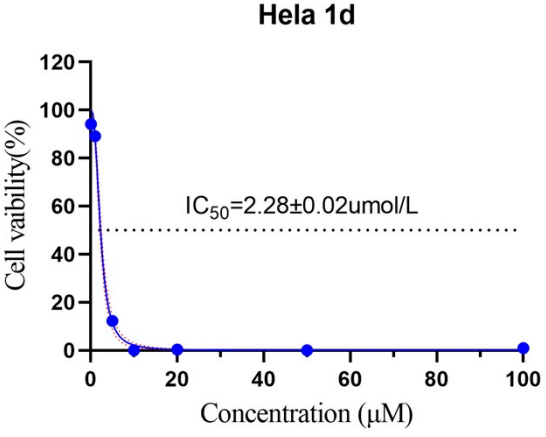
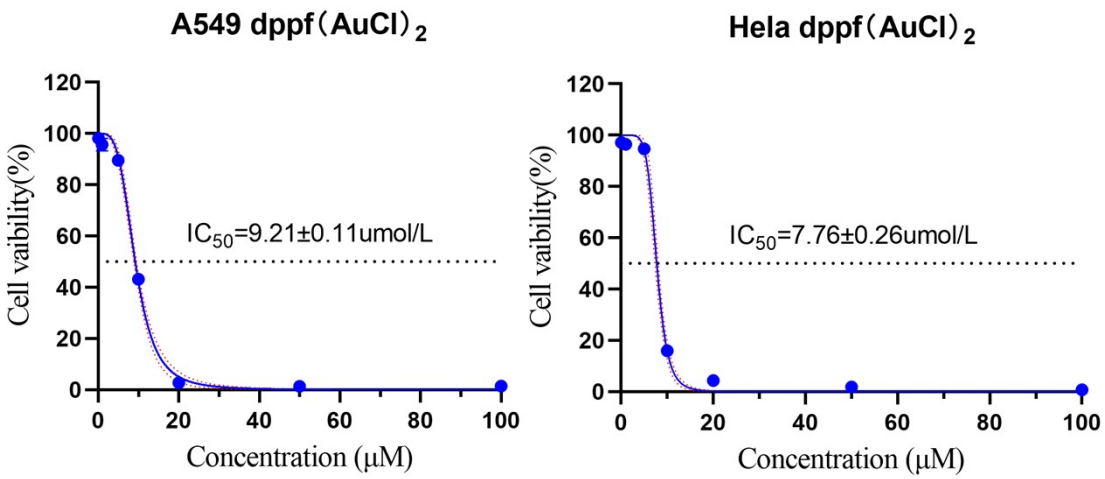
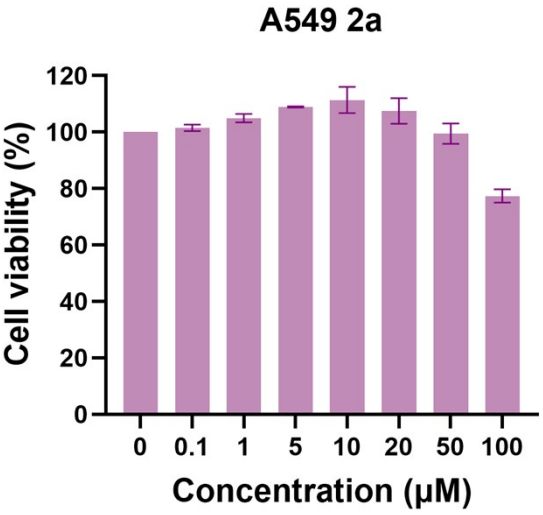
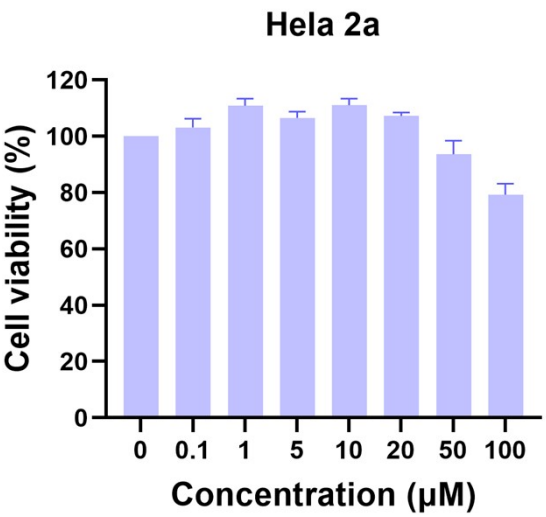
Concentration (μM)

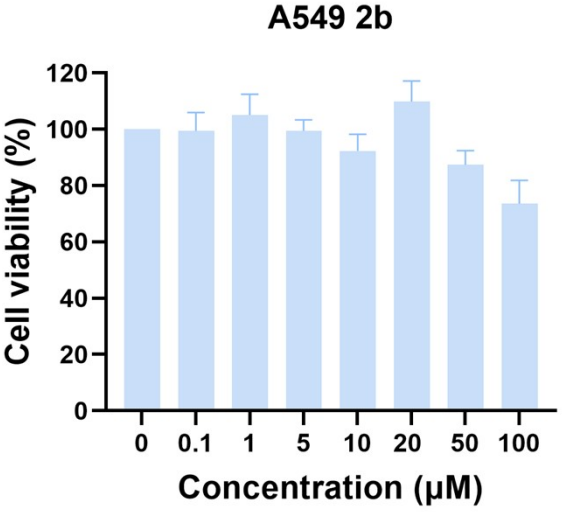

Hela 1d
Cell vaibility(%)
IC50=2.28±0.02umol/L
0 20 40 60 80 100
Concentration (μM)

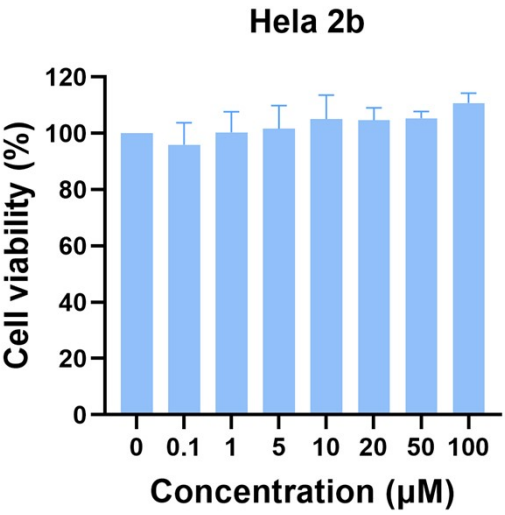

A549 dppf(AuCl)2
Cell vaibility(%)
IC50=9.21±0.11umol/L
Concentration (μM)

Hela dppf(AuCl)2
Cell vaibility(%)
IC50=7.76±0.26umol/L
Concentration (μM)


A549 2a
Cell viability (%)
Concentration (μM)


Hela 2a
Cell viability (%)
Concentration (μM)


A549 2b
Cell viability (%)
Concentration (μM)


Hela 2b
Cell viability (%)
Concentration (μM)

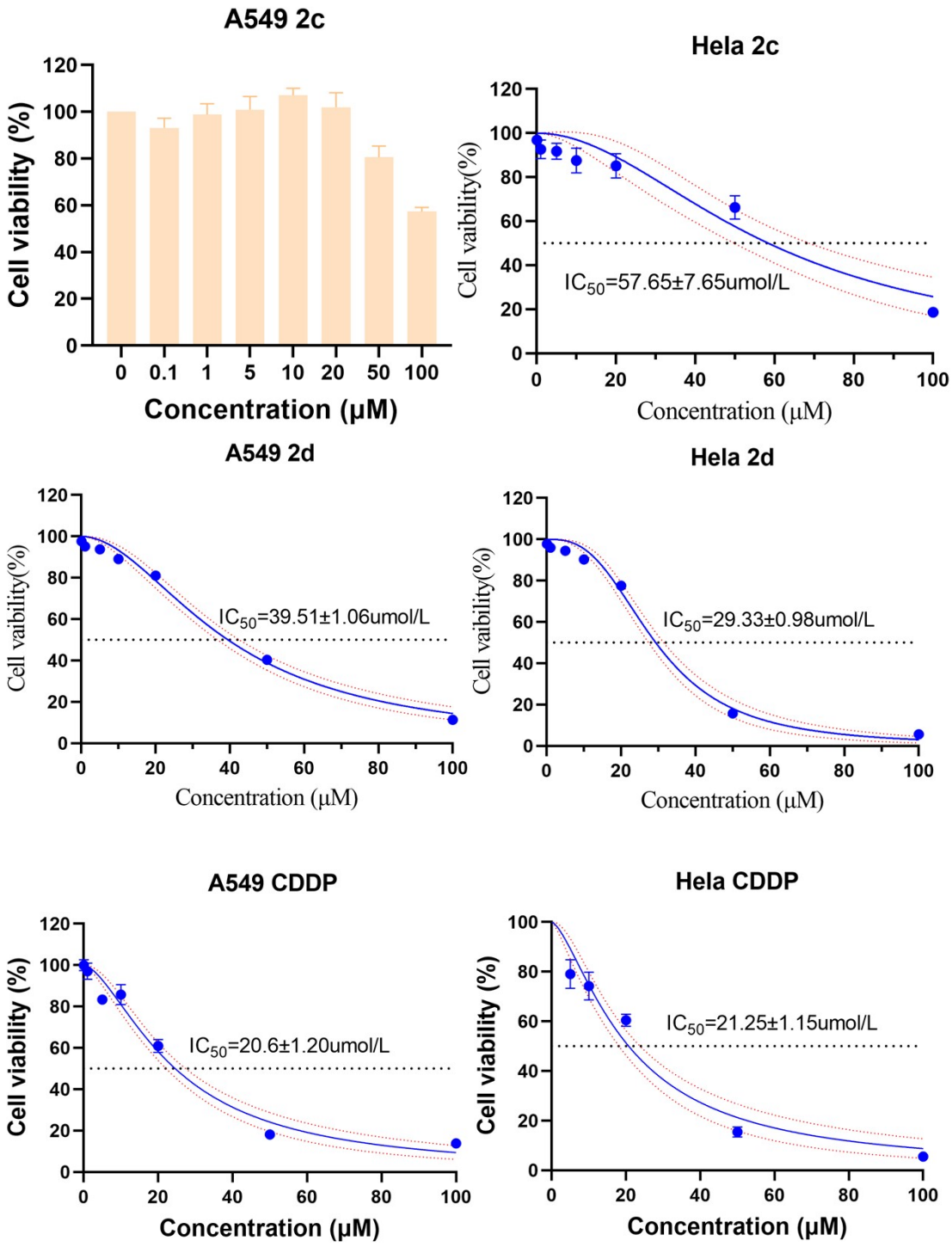


Fig. S33 Antiproliferative activity of **PPh_3AuCl**, mono gold(I) complexes **1a~1d**, **dppf$(AuCl)_2$**, digold(I) complexes **2a~2d**, and cisplatin against A549 and Hela (24 h, CCK-8 assays, IC_{50}, mean ± SD [μM]).

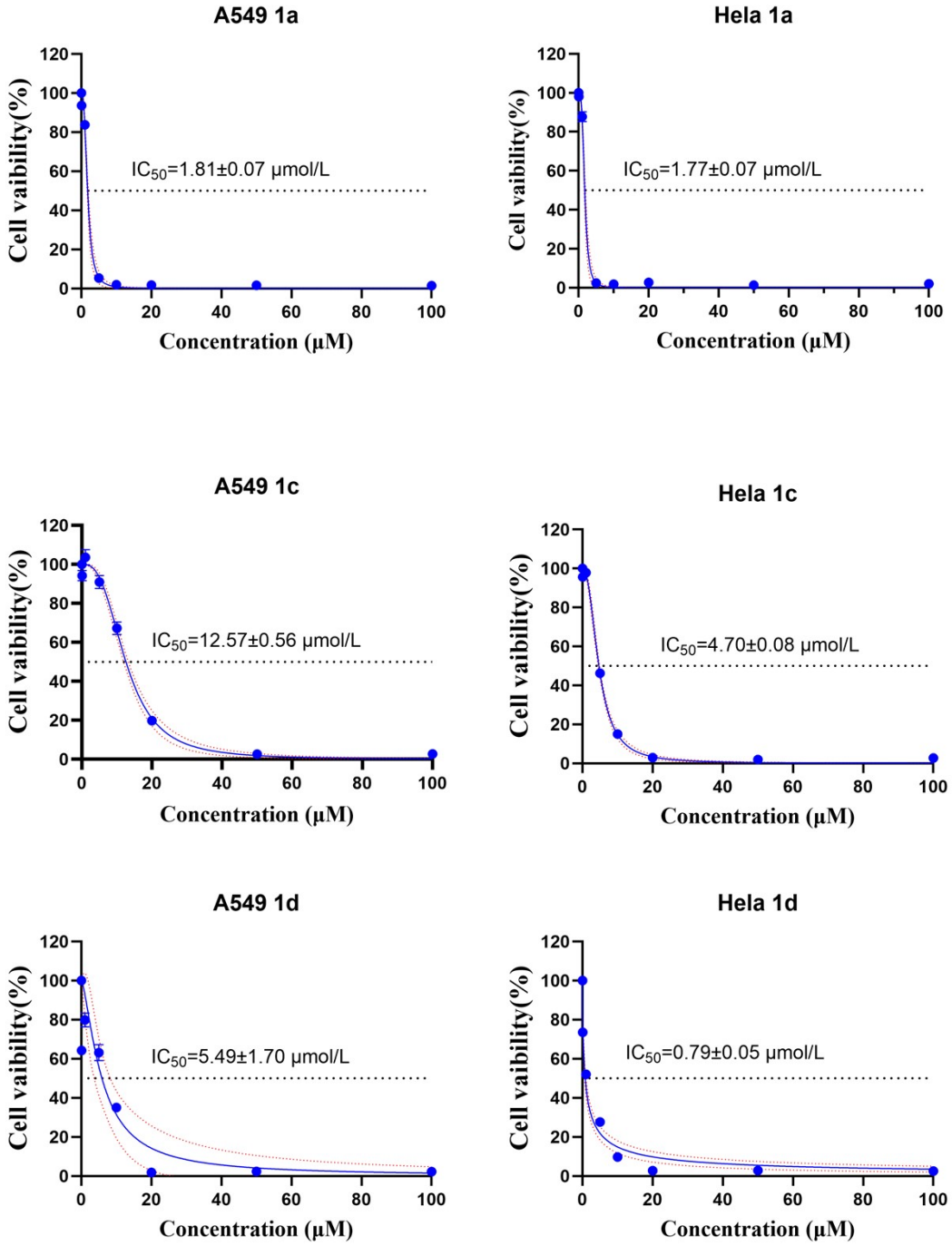


Fig. S34 Antiproliferative activity of **1a**, **1c**, and **1d** against A549 and Hela (48 h, CCK-8 assays, IC_{50}, mean ± SD [μM]).

4. Inhibition of TrxR

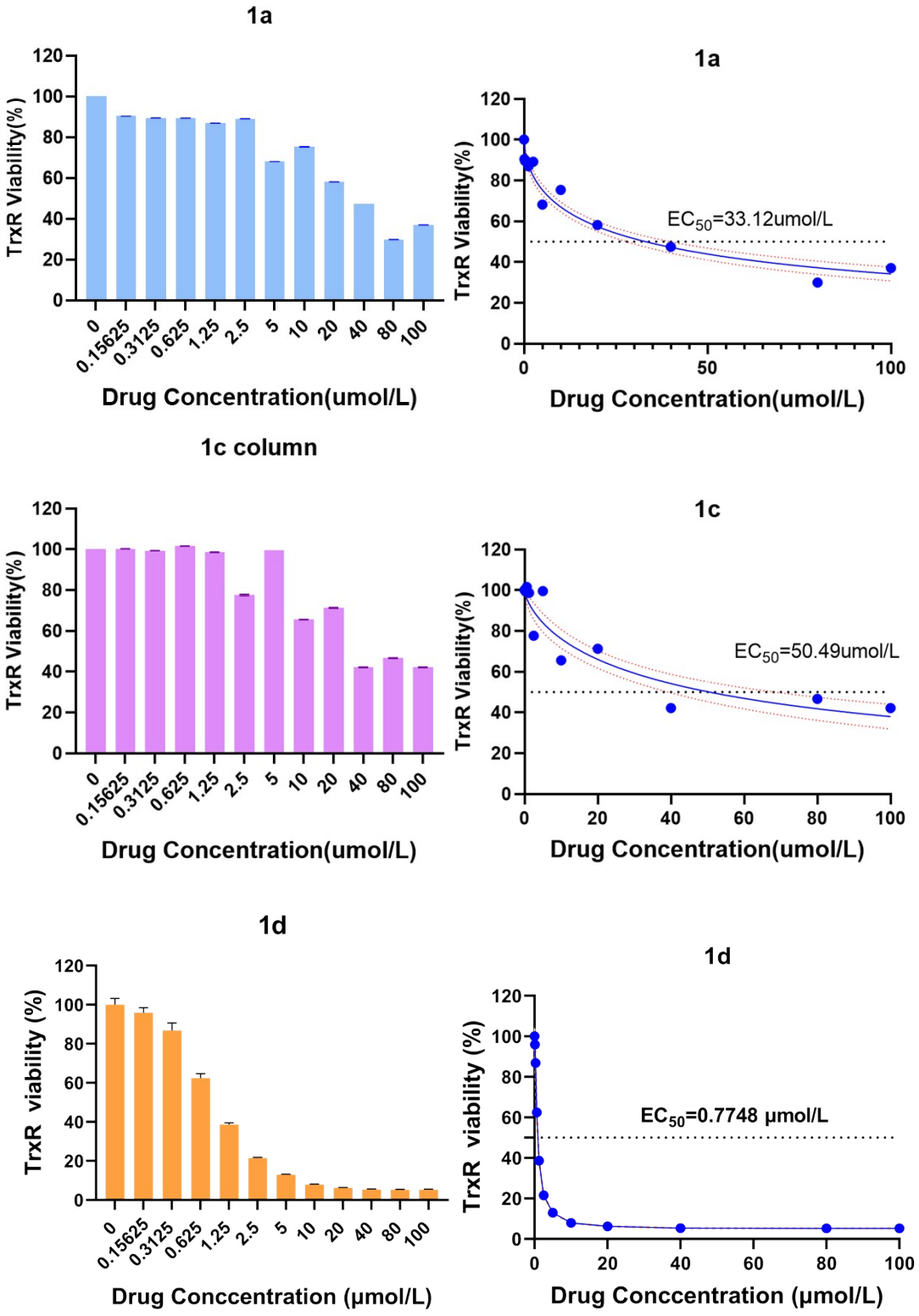


Fig. S35 Inhibition to the activity of purified TrxR by complexes **1a**, **1c** and **1d**