Dinuclear NHC-gold(I)-thiolato and -alkynyl complexes: synthesis, anticancer activity, and catalytic activity in lactonization reactions

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X-ray Crystallography

The crystal that was of suitable quality for single crystal X-ray diffraction analysis were obtained by slow vapor diffusion of the antisolvent (pentane) into saturated solutions of the complexes (in dichloromethane) at 4 °C. CCDC 2341052 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

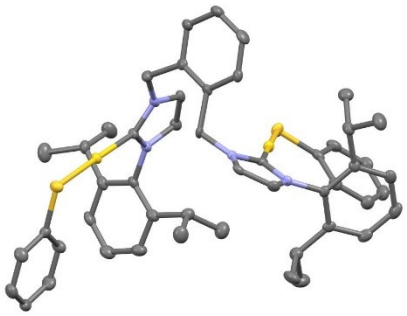


Figure S1 X-ray molecular structure of **2a**, showing thermal displacement ellipsoids at the 50% probability level and hydrogen atoms omitted for clarity.

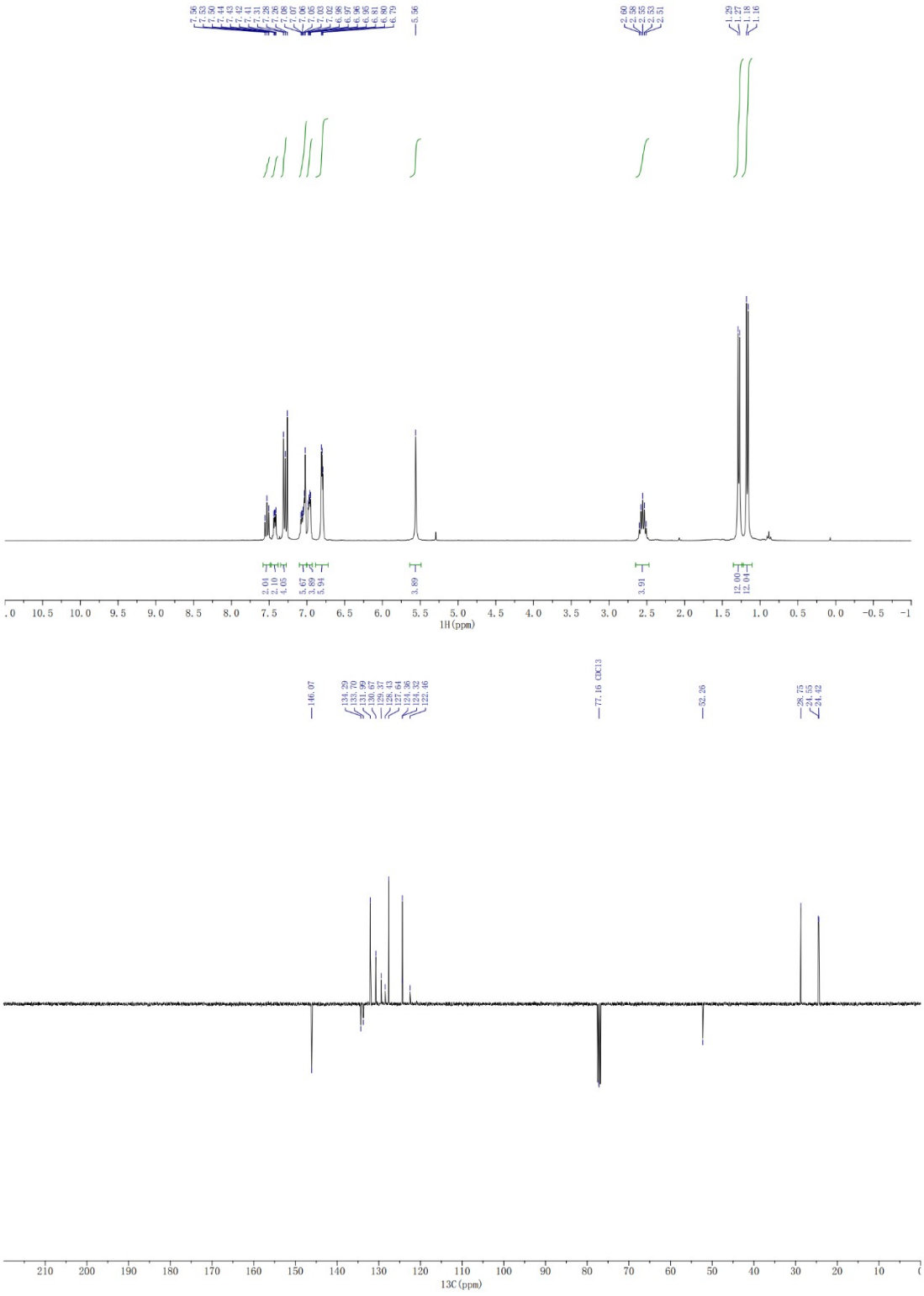
Table S1 Crystal data and structure refinement for **2a**

Identification code	**2a**
Empirical formula	$C_{50}H_{56}Au_2N_4S_2$
Formula weight	1171.04
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.7037(2)
b/Å	14.9460(4)
c/Å	16.9881(5)
α/°	110.305(2)
β/°	101.236(2)
γ/°	92.613(2)
Volume/Å	3 2249.19(11)
Z	2
ρcalcg/cm^3	1.729
μ/mm^{-1}	6.647
F(000)	1148.0

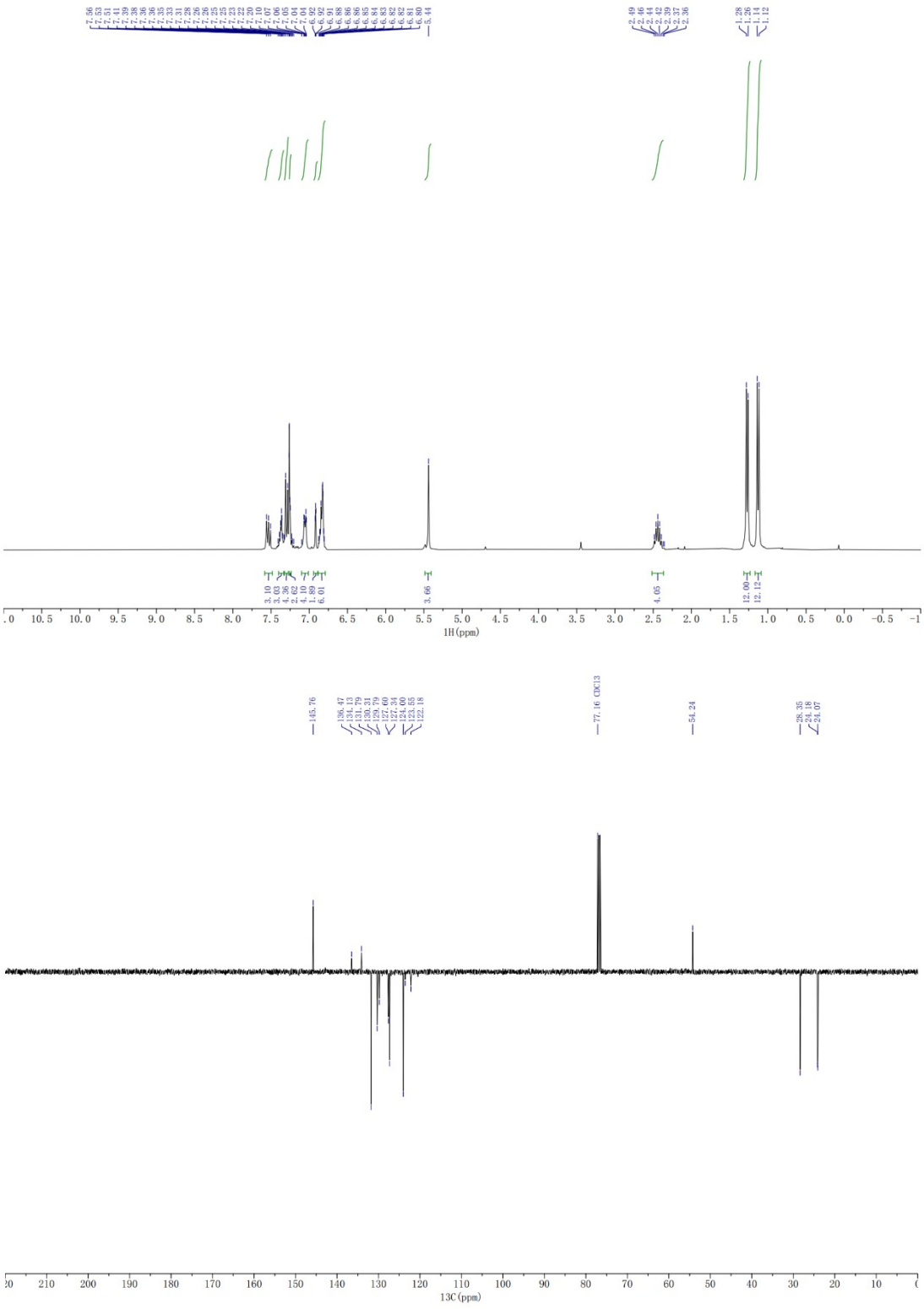
Crystal size/mm^3	0.35 × 0.26 × 0.07
Radiation	Mo Kα(λ = 0.71073)
2Θ range for data collection/°	5.148 to 57.522
Index ranges	-13 ≤ h ≤ 12, -19 ≤ k ≤ 20, -20 ≤ l ≤ 22
Reflections collected	44349
Independent reflections	10251 [Rint = 0.0727, Rsigma = 0.0691]
Data/restraints/parameters	10251/6/531
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.0683
Final R indexes [all data]	R_1 = 0.0592, wR_2 = 0.0767
Largest diff. peak/hole / e Å-3 2.00/-1.43	

NMR spectra

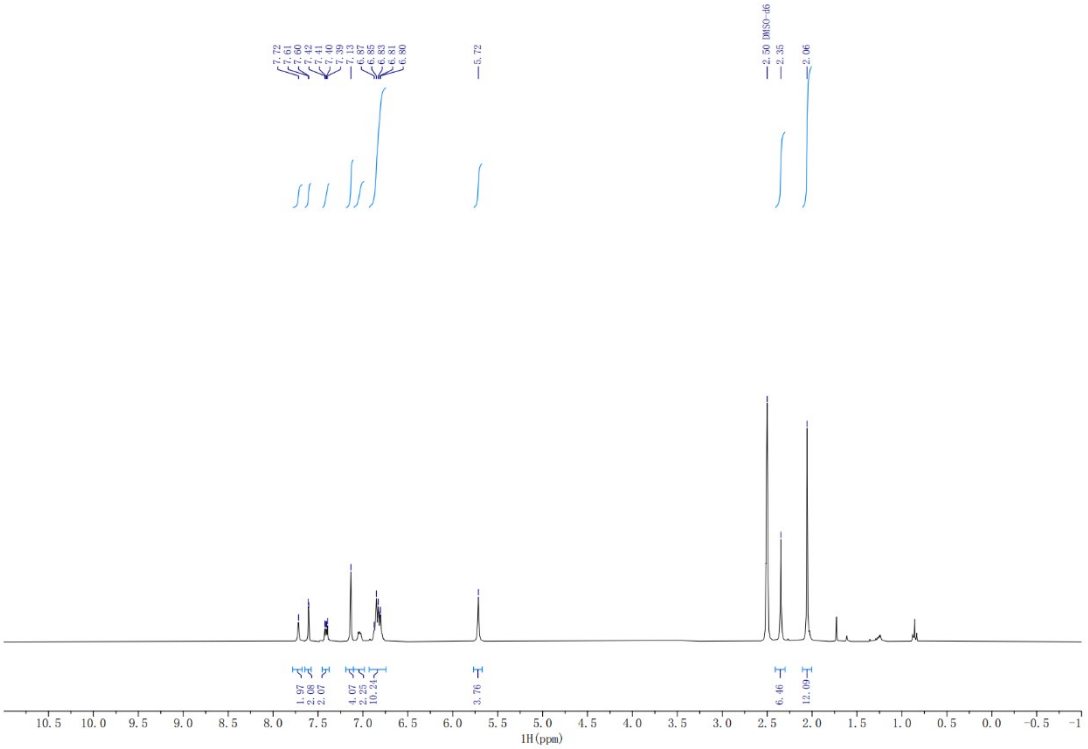
^{1}H, ^{13}C {1H} apt of [(IPr)$^{o\text{-xylene}}$(AuSPh)$_2$] (2a)

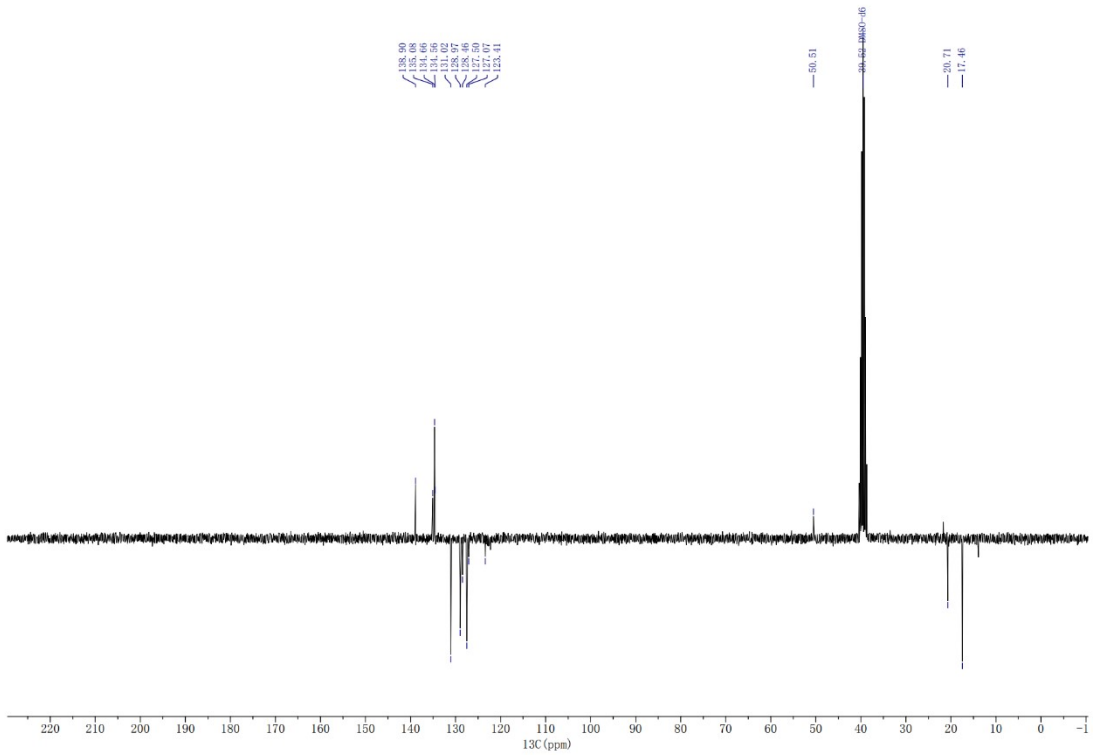


^{1}H, ^{13}C {1H} apt of [(IPr)$^{m\text{-xylene}}$(AuSPh)$_2$] (2b)

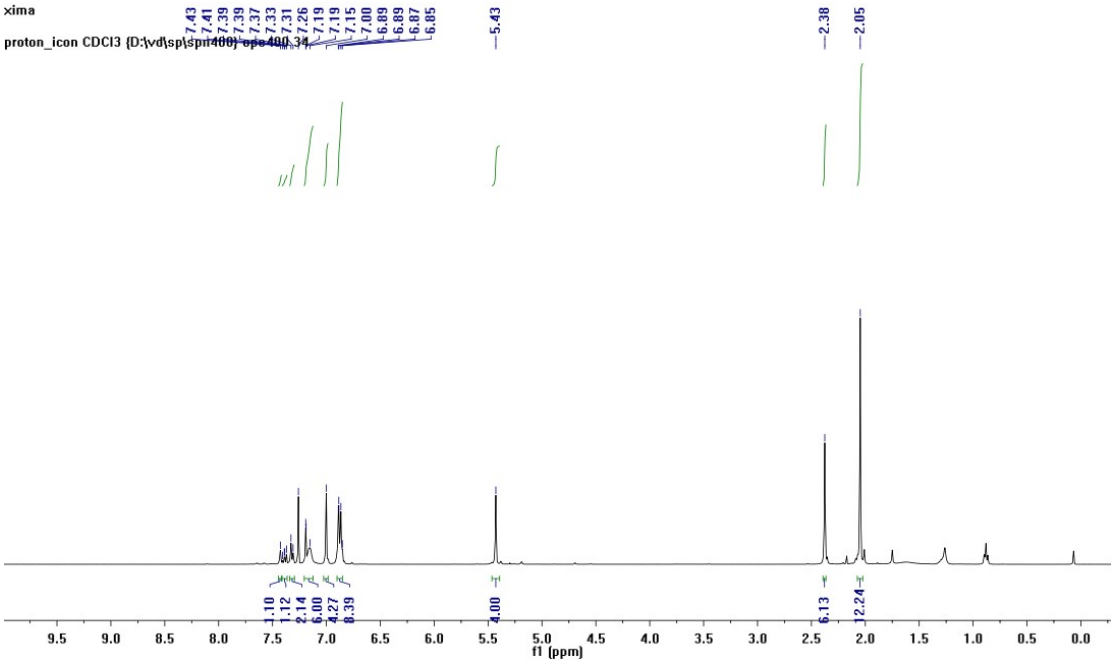


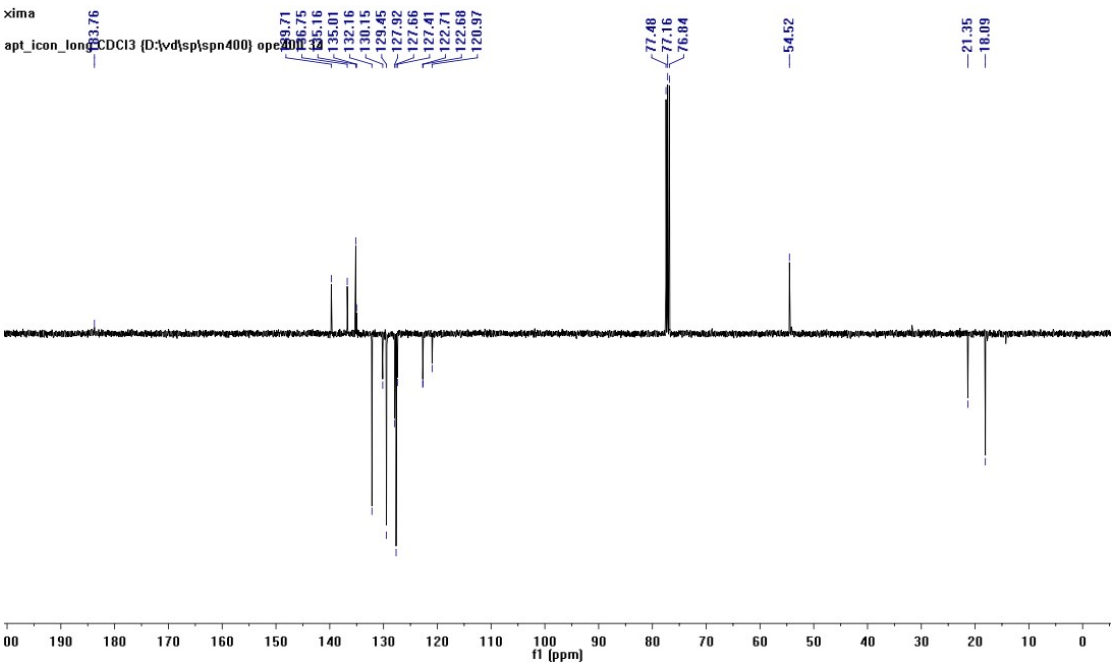
^{1}H, ^{13}C {1H} apt and 2D NMR of [(IMes)$^{o\text{-xylene}}$(AuSPh)$_2$] (2c)

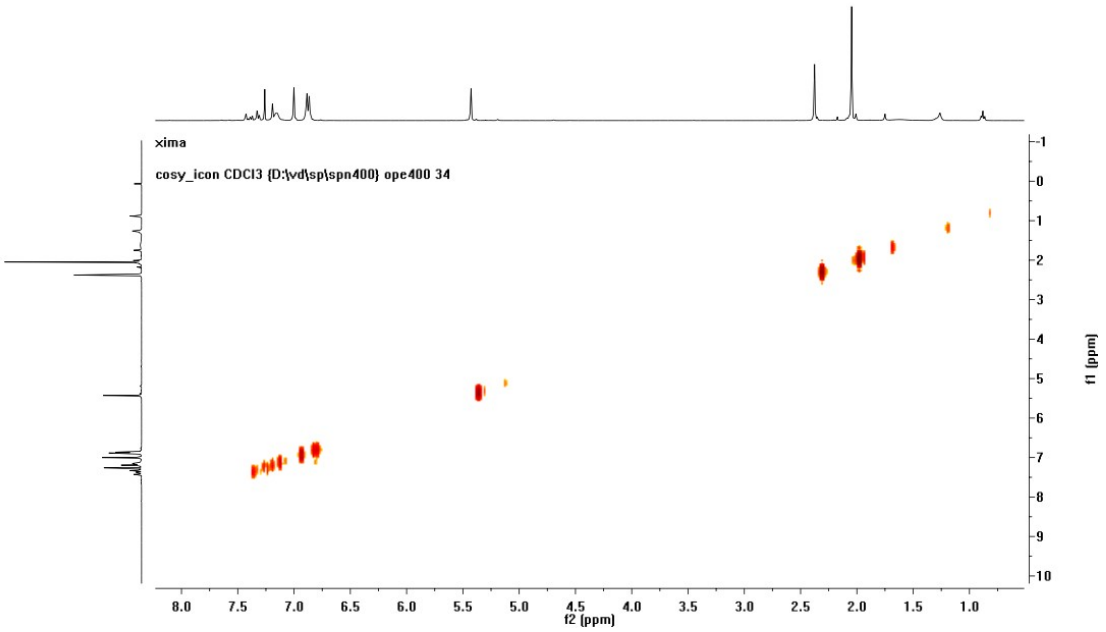




^{1}H, ^{13}C {1H} apt and 2D NMR of [(IMes)$^{m\text{-xylene}}$(AuSPh)$_2$] (2d)



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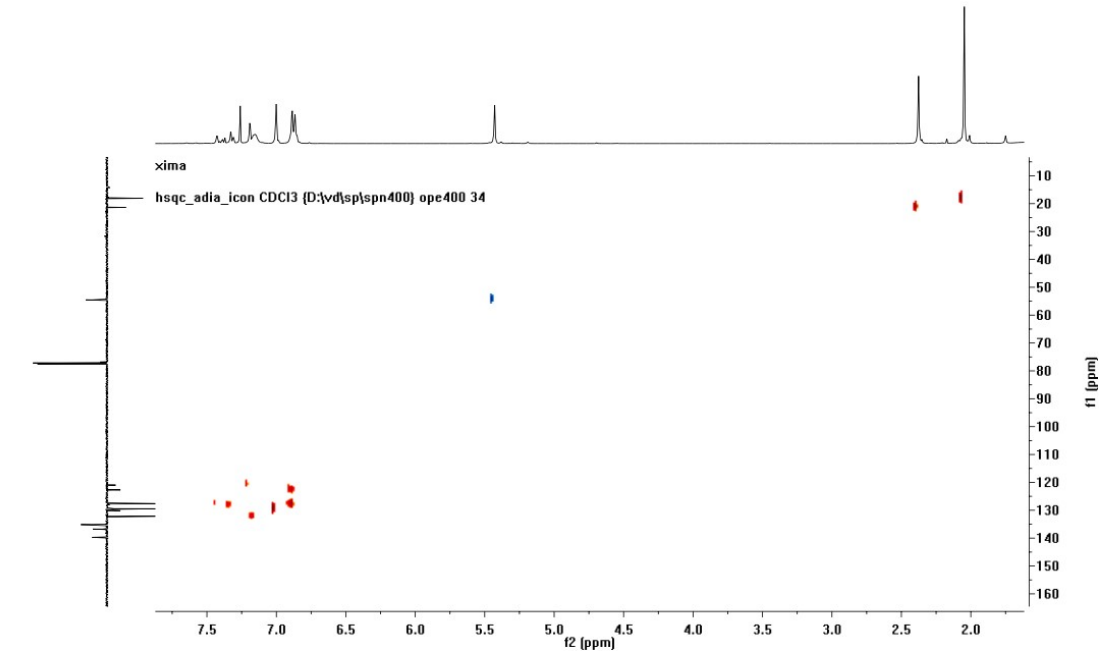
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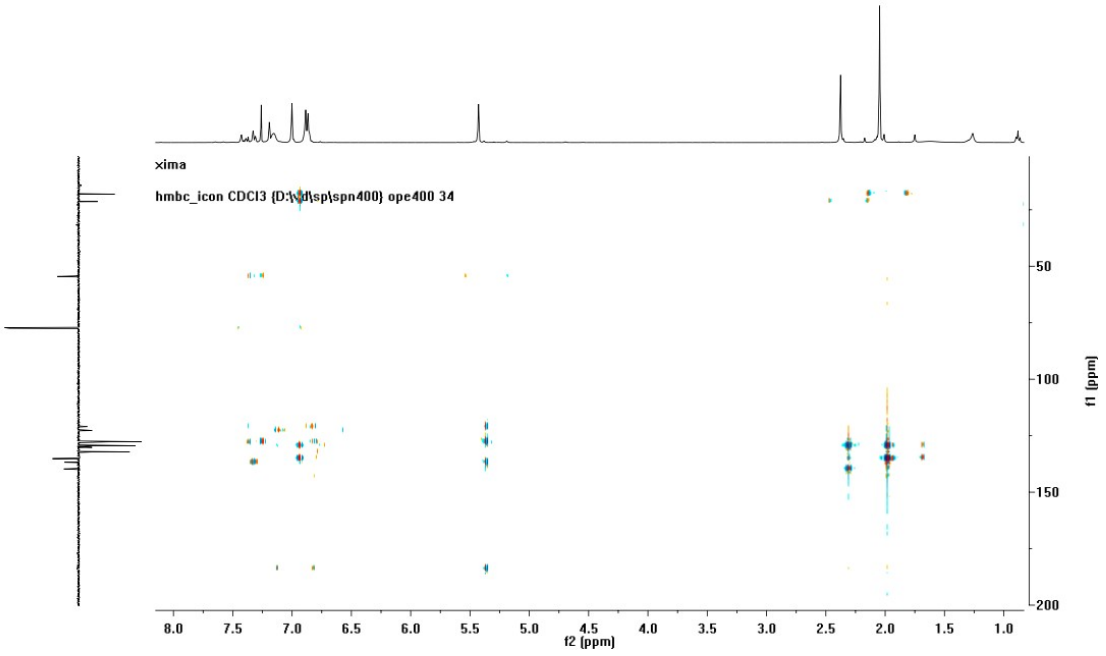
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2.0
1.5
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f2 (ppm)

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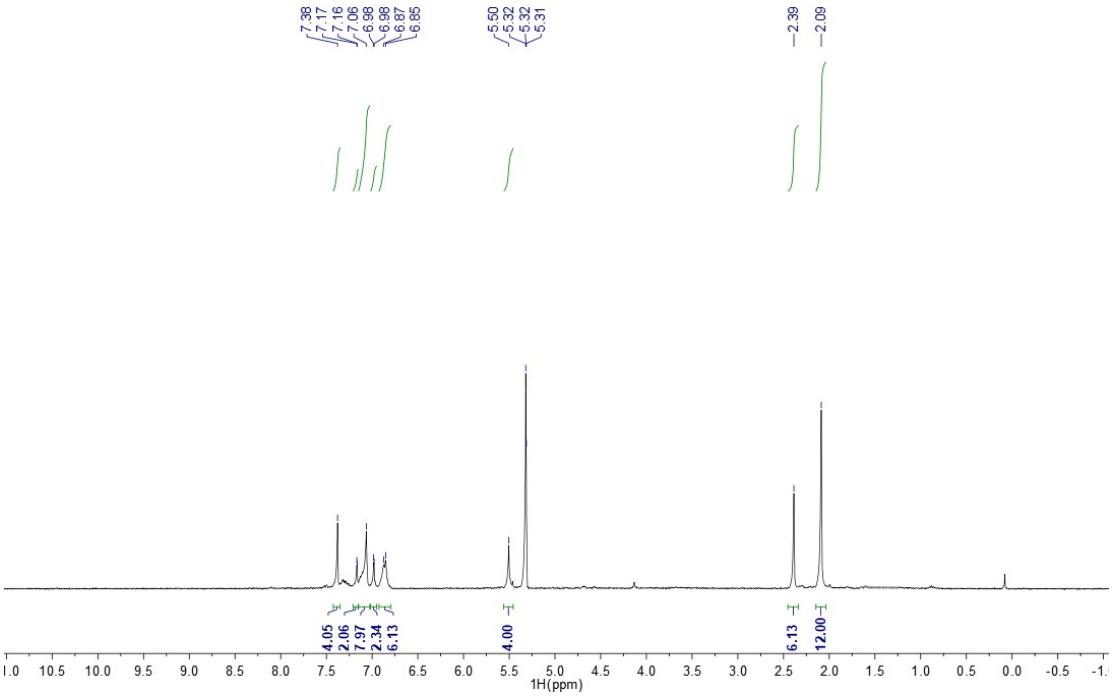
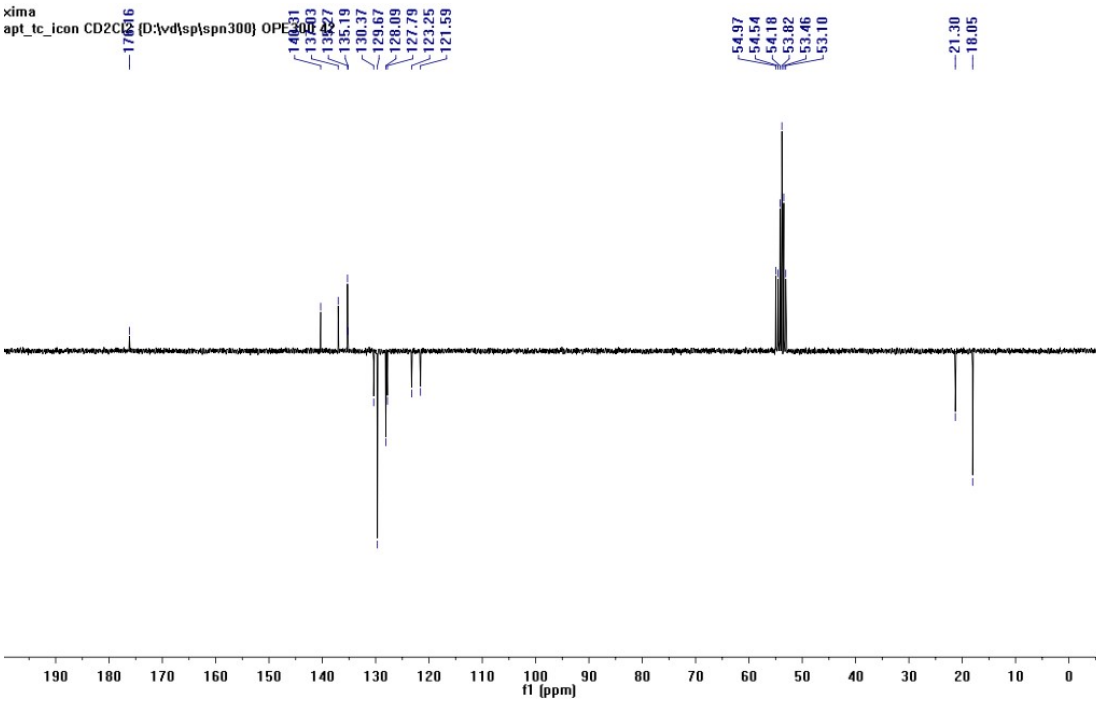
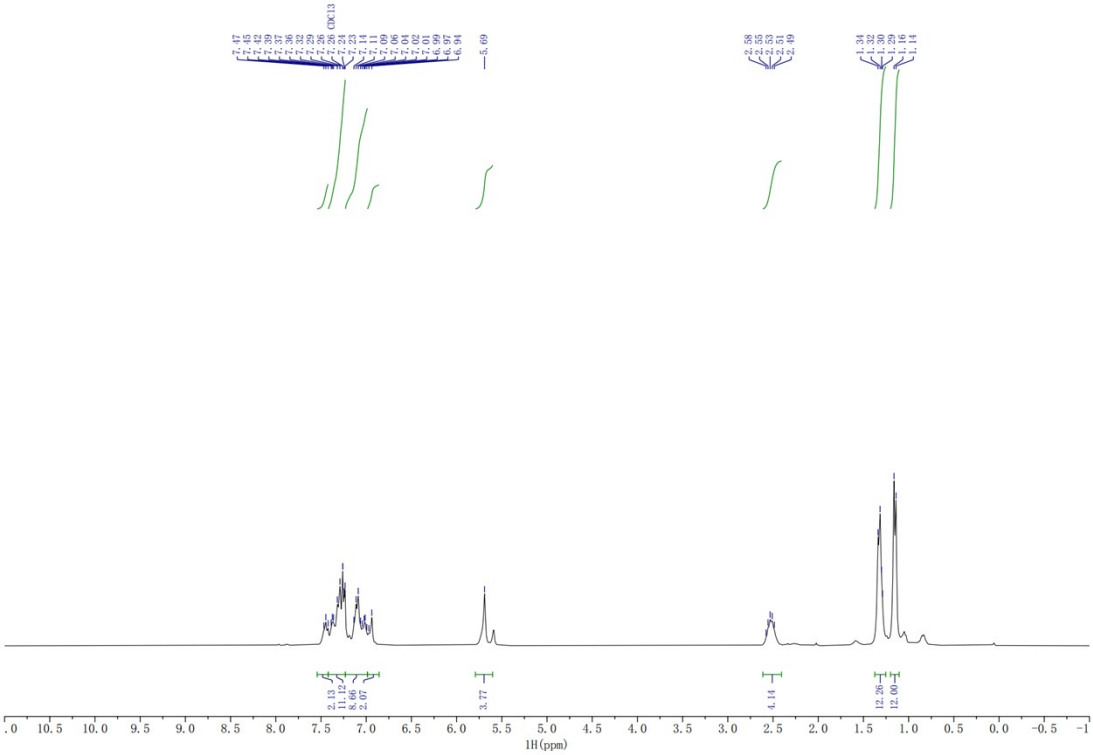
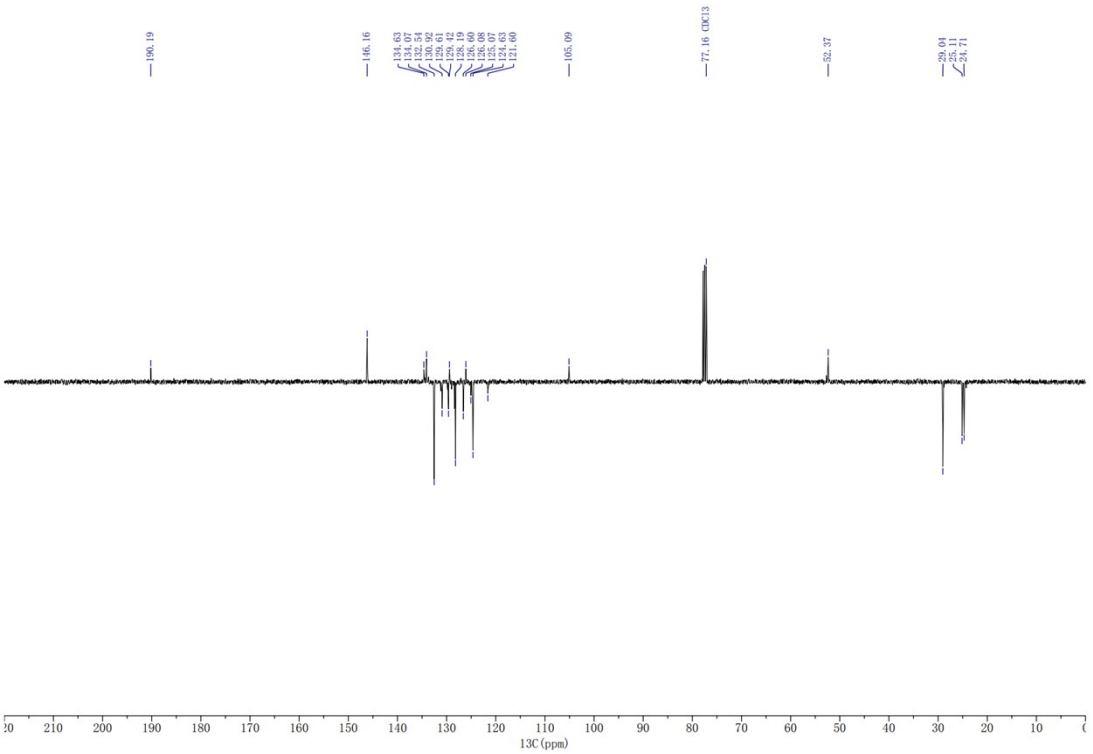


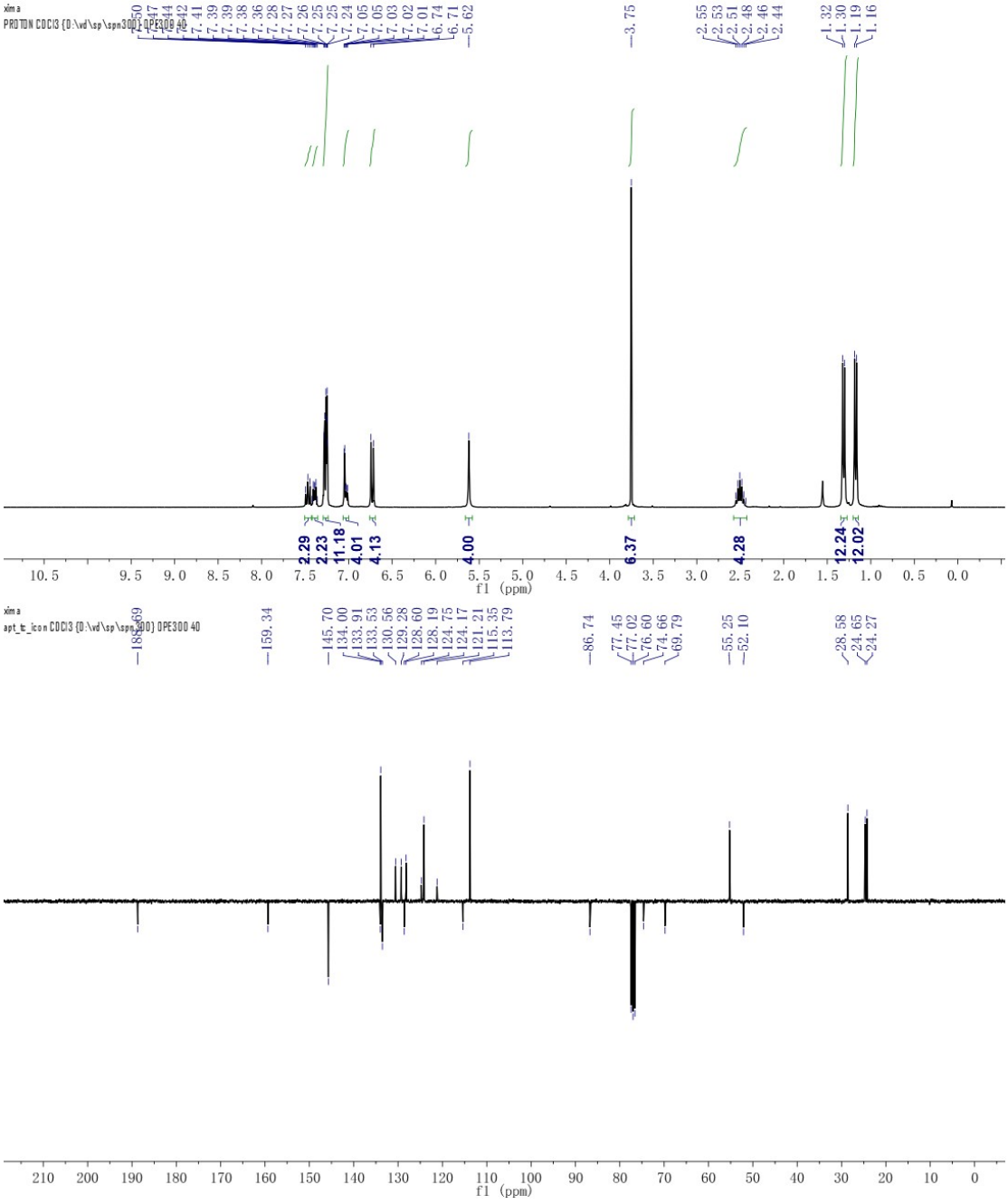


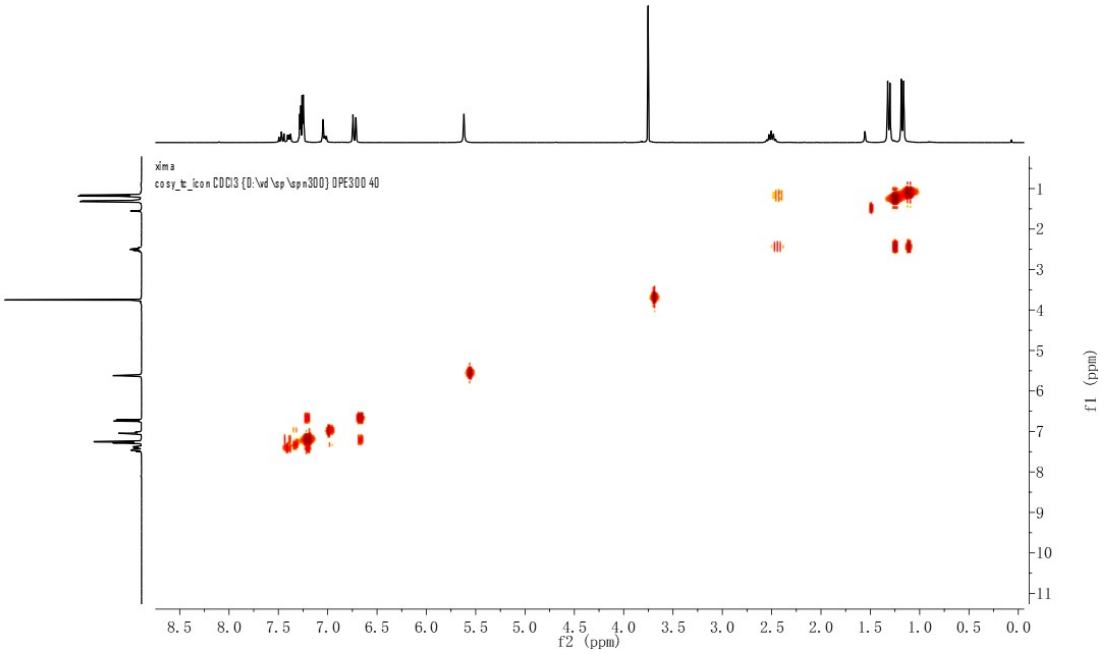
^{1}H, ^{13}C {^{1}H} apt of [(IPr)$^{o\text{-xylene}}${Au((phenylethynyl)}$_2$] (3a)





^{1}H, ^{13}C {^{1}H} apt and 2D NMR of [(IPr)$^{o\text{-xylene}}${Au(4-methoxyphenyl)buta-1,3-diyn-1-yl)}$_2$] (3b)

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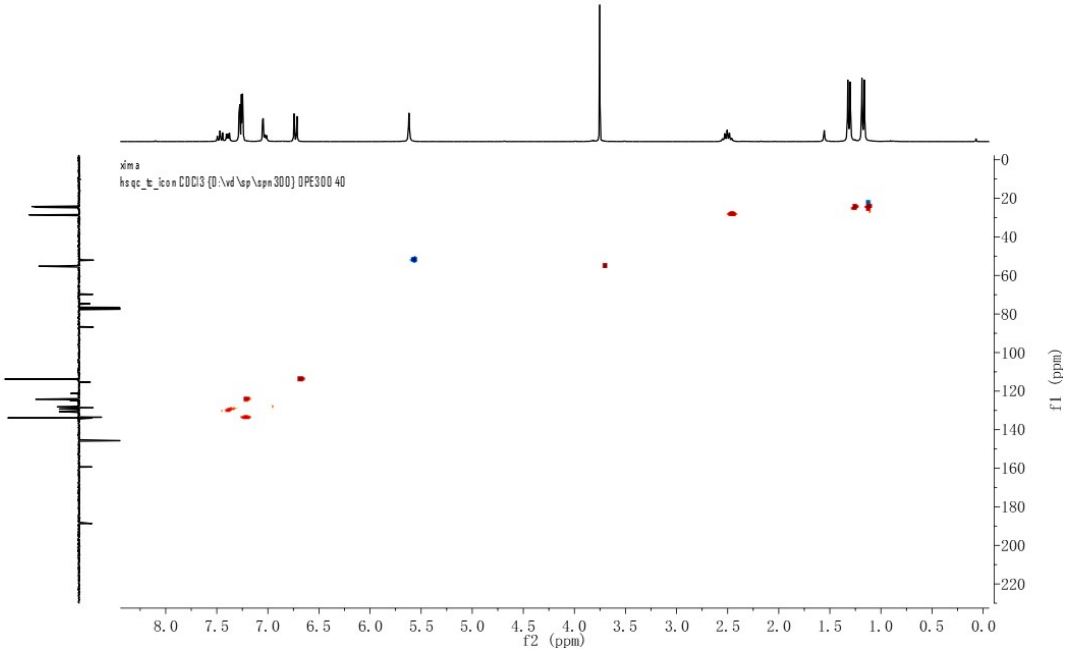
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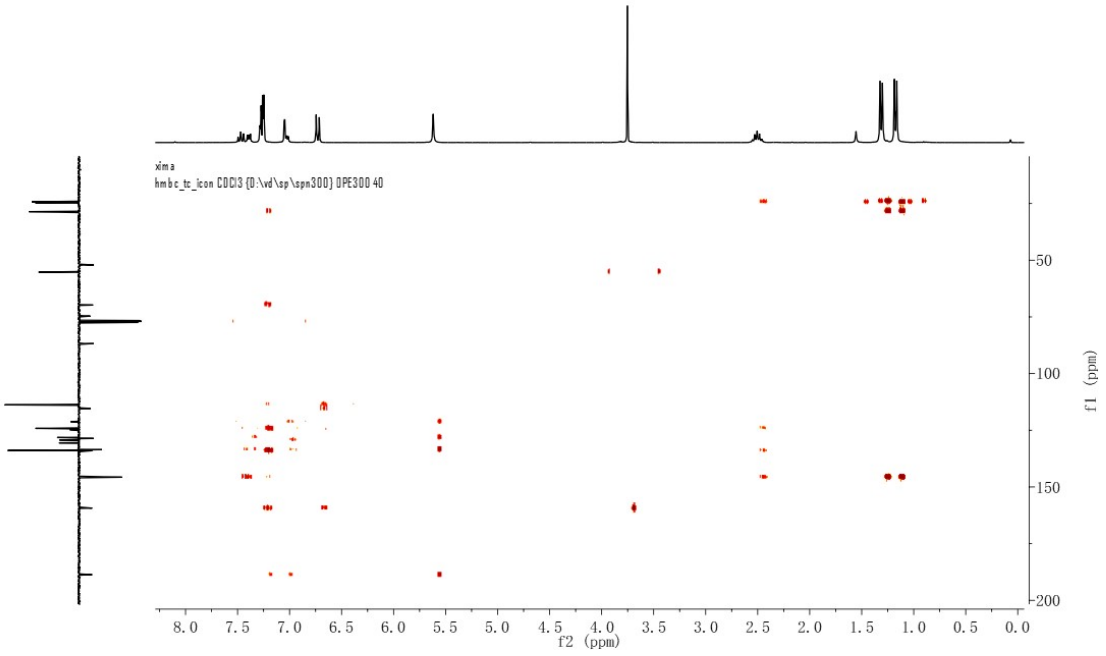
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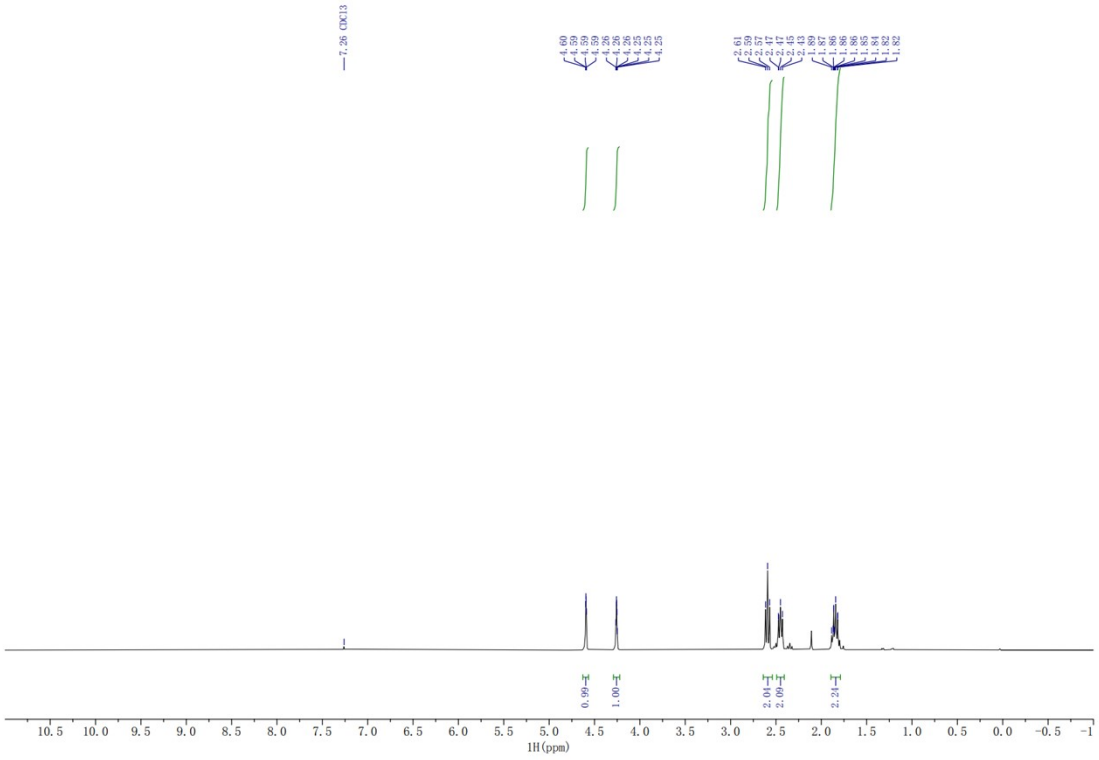
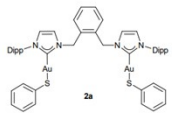
f2 (ppm)

^{1}H NMR of alkynoic acid (4)[1]

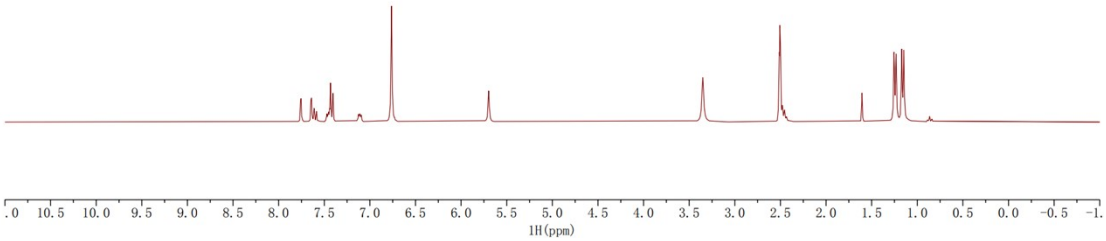


Stability studies of complexes 2a-e in DMSO-d_6

2a, ^{1}H NMR (300 MHz, DMSO-d_6)
Time = 0h



2a, ^{1}H NMR (300 MHz, DMSO-d_6)
Time = 24h



2b, ^{1}H NMR (300 MHz, DMSO-d_6)
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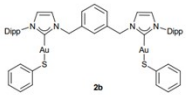

2b, ^{1}H NMR (300 MHz, DMSO-d_6)
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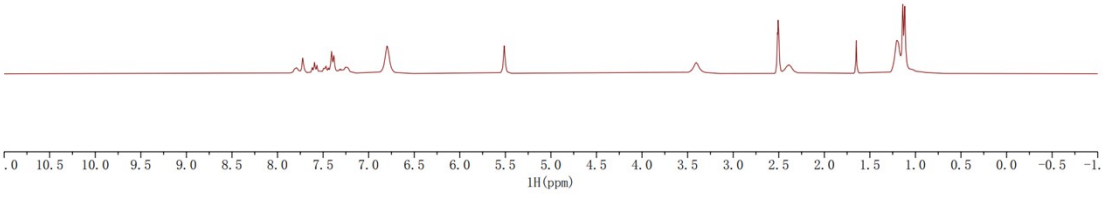

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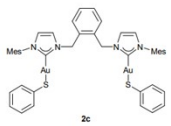

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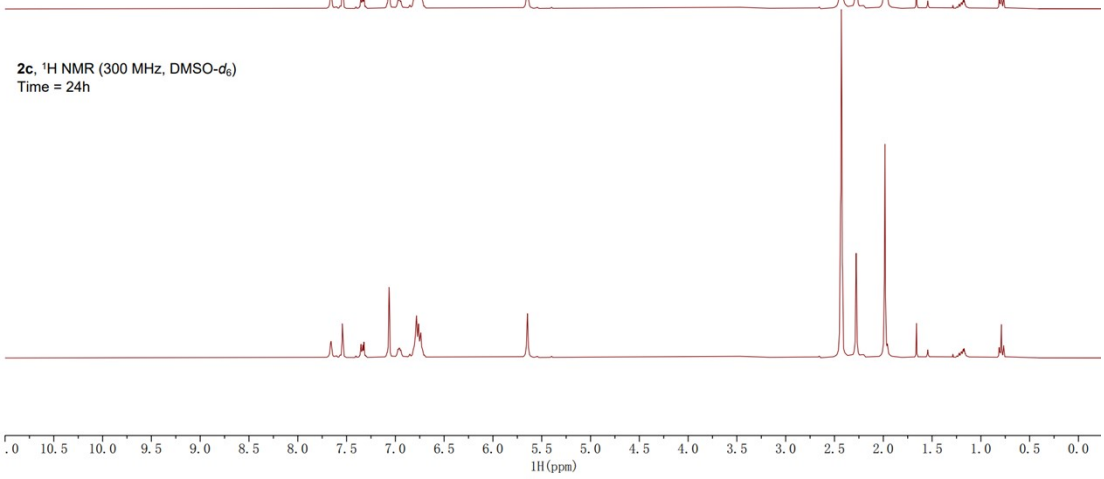

2d, ^{1}H NMR (300 MHz, DMSO-d_6)
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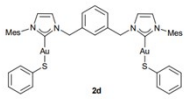

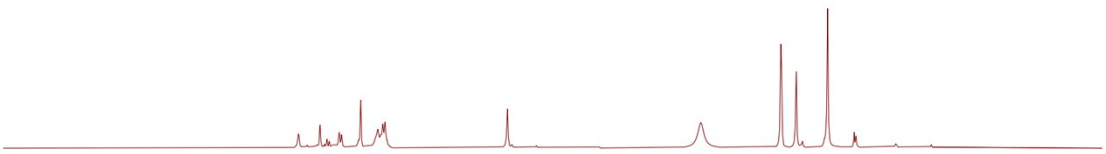

2d, ^{1}H NMR (300 MHz, DMSO-d_6)
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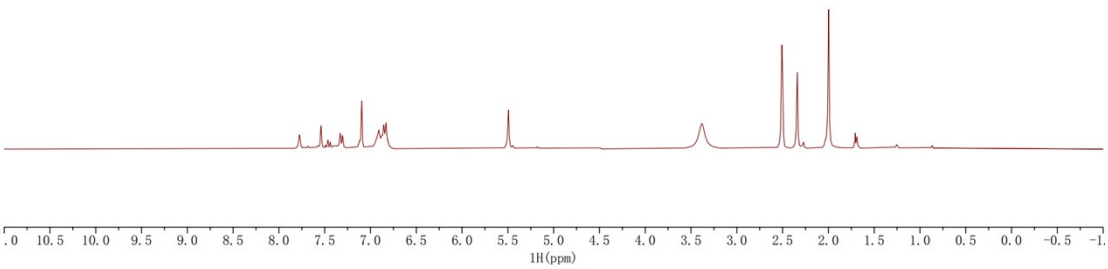

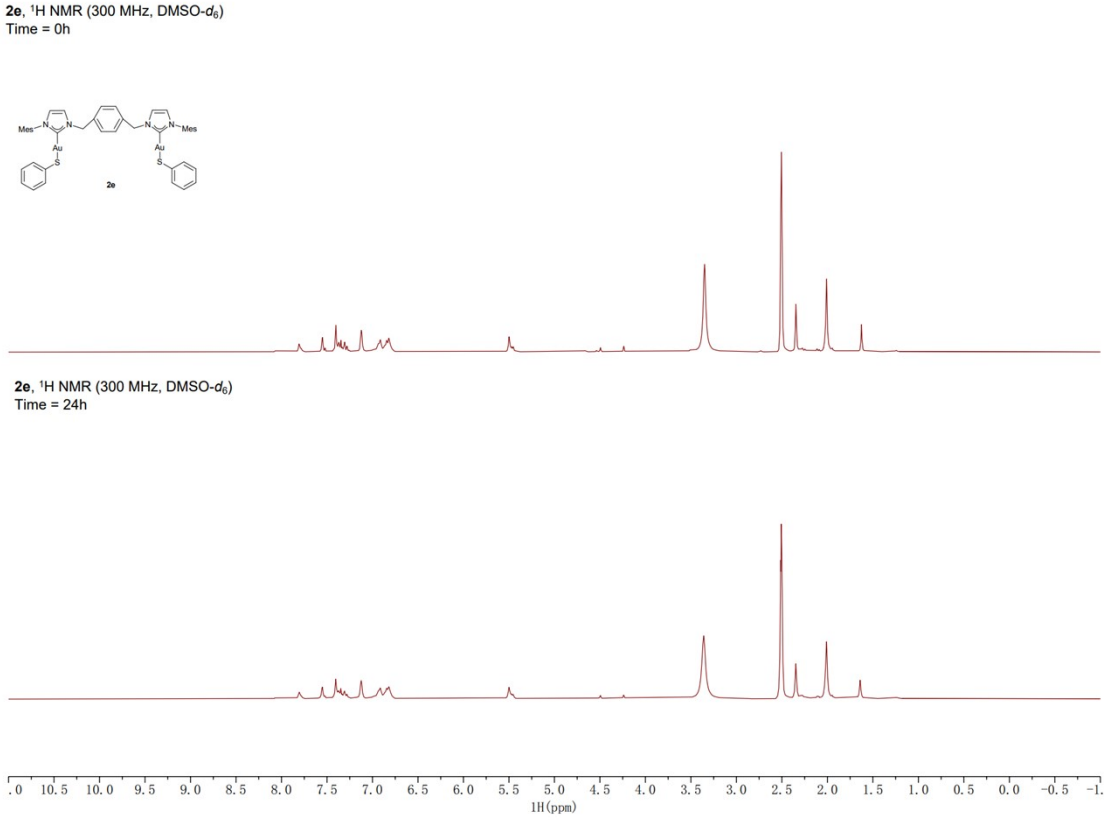

References

1. D. Gasperini, L. Maggi, S. Dupuy, R. M. P. Veenboer, D. B. Cordes, A. M. Z. Slawin and S. P. Nolan, *Adv. Synth. Catal.*, **2016**, *358*, 3857–3862.