Electronic Supplementary Information

Acridine based (S,N,S) pincer ligand: designing of silver(I) complexes for efficient activation of A^3(aldehyde, alkyne and amine) coupling

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Table S1 Crystal Data and Structural Refinements for 1 and 2

Structural Parameters	1	2
Empirical formula	$C_{29}H_{24}N_3O_3AgS_2$	$C_{54}H_{42}N_4O_6Ag_2S_4.CH_3CN$
Formula wt.	634.52	1227.99
Crystal size [mm]	0.42 × 0.22 × 0.18	0.40 × 0.16 × 0.12
Crystal system	Monoclinic	Monoclinic
Space group	*P* 2*(1)n*	*P* 21
Unit Cell dimension	*a* = 9.7209(4) Å	*a* = 8.4602(17)Å
	b = 16.6776(7) Å	*b* = 18.321(4)Å
	c = 17.4452(7) Å	*c* = 16.881(4)Å
	α = 90.00°	α = 90.00°
	β = 105.202(2)°	β = 93.979(4)°
	γ = 90.00°	γ = 90.00°
Volume [Å3]	2729.27(19)	2610.2(10)
Z	4	2
Density (Calc.) [Mg.m-3]	1.544	1.562
Absorption coeff. [mm-1]	0.928	0.966
F(000)	1288	1244.0
θ range [°]	1.92–25.00	1.21–25.00
Index ranges	$-11 \le h \le 11$	$-10 \le h \le 10$
	$-19 \le k \le 19$	$-21 \le k \le 21$
	$-20 \le l \le 20$	$-20 \le l \le 20$
Reflections collected	32540	25052
Independent reflections (*R*int.)	4693(0.0352)	9168(0.0535)
Max./min. Transmission	0.849 / 0.780	0.894/ 0.828
Data/restraints/ parameters	4693 / 0 / 344	9168/ 0 / 659
Goodness-of-fit on *F*2	1.040	1.001
Final R indices [$I > 2\sigma(I)$]	*R1* = 0.0414	*R1* = 0.0404
	wR2 = 0.1016	*wR2* = 0.0800
R indices (all data)	*R1* = 0.0619	*R1* = 0.0543
	wR2 = 0.1115	*wR2* = 0.0845
Largest diff. peak/hole [e.Å^{-3}]	0.882/ -0.266	0.730/ -0.257

Table S2 Bond Lengths and Bond Angles of 1 and 2

Complex	Bond Length[Å]		Bond Angle[°]	
1	Ag(1) — S(1)	2.5682(11)	N(2) — Ag(1) — S(1)	123.43(11)
	Ag(1) — S(2)	2.5017(11)	N(2) — Ag(1) — O(1)	92.86(15)
	N(2) — Ag(1)	2.329(4)	N(2) — Ag(1) — S(2)	105.79(11)
	O(1) — Ag(1)	2.499(4)	O(1) — Ag(1) — S(1)	107.27(10)
	C(19) — N(1)	1.350(5)	O(1) — Ag(1) — S(2)	94.96(12)
	C(7) — S(1)	1.831(4)	S(1) — Ag(1) —S(2)	123.59(4)
	C(21) — S(2)	1.839(4)	C(7) — S(1) — Ag(1)	103.31(13)
	N(3) — O(1)	1.198(5)	C(21) — S(1) — Ag(1)	106.54(14)
	N(3) — O(2)	1.234(5)	O(1) — N(3) —O(2)	120.1(4)
	N(3) — O(3)	1.185(6)	O(2) — N(3) —O(3)	120.5(5)
			O(3) — N(3) —O(1)	119.3(5)
			C(28) — N(2) —Ag(1)	157.8(4)
2	Ag(1) — S(1)	2.4894(15)	N(1) — Ag(1) — S(1)	88.81(10)
	Ag(1) — S(2)	2.4834(15)	N(1) — Ag(1) — O(1)	88.90(15)
	N(1) — Ag(1)	2.660(4)	N(1) — Ag(1) — O(2)	137.60(13)
	O(1) — Ag(1)	2.384(4)	N(1) — Ag(1) — S(2)	86.76(11)
	O(2) — Ag(1)	2.690(5)	O(1) — Ag(1) — S(1)	120.13(11)
	C(19) — N(1)	1.350(5)	O(1) — Ag(1) — S(2)	113.76(11)
	C(7) — S(1)	1.838(5)	S(1) — Ag(1) —S(2)	125.79(5)
	C(21) — S(2)	1.848(5)	O(2) — Ag(1) — S(1)	108.82(12)
	N(2) — O(1)	1.230(6)	O(2) — Ag(1) — S(2)	110.28(12)
	N(2) — O(2)	1.242(6)	O(1) — Ag(1) — O(2)	48.77(14)
	N(2) — O(3)	1.230(6)	O(1) — N(2) —O(2)	117.5(5)

Table S3 Non-covalent interactions C–H···O distances in (Å) found in the crystal lattice of complex 1 and 2

1		2	
C(16)–H(16)···O(2)	2.629(4)	C(2)–H(2)···O(1)	2.553(4)
C(17)–H(17)···O(1)	2.819(4)	C(6)–H(6)···O(4)	2.834(7)
C(18)–H(18)···O(1)	2.580(4)	C(9)–H(9)···O(6)	3.018(7)
C(21)–H(21B)···O(3)	2.650(4)	C(11)–H(11)···O(2)	2.789(7)
C(23)–H(23)···O(1)	2.737(4)	C(14)–H(14)···O(2)	2.482(6)
C(24)–H(24)···O(1)	2.800(5)	C(17)–H(17)···O(3)	2.802(6)
C(25)–H(25)···O(1)	2.869(3)	C(44)–H(44)···O(5)	2.654(7)
C(27)–H(27)···O(3)	2.437(4)	C(56)–H(56C)···O(3)	2.697(5)

NMR Spectra:

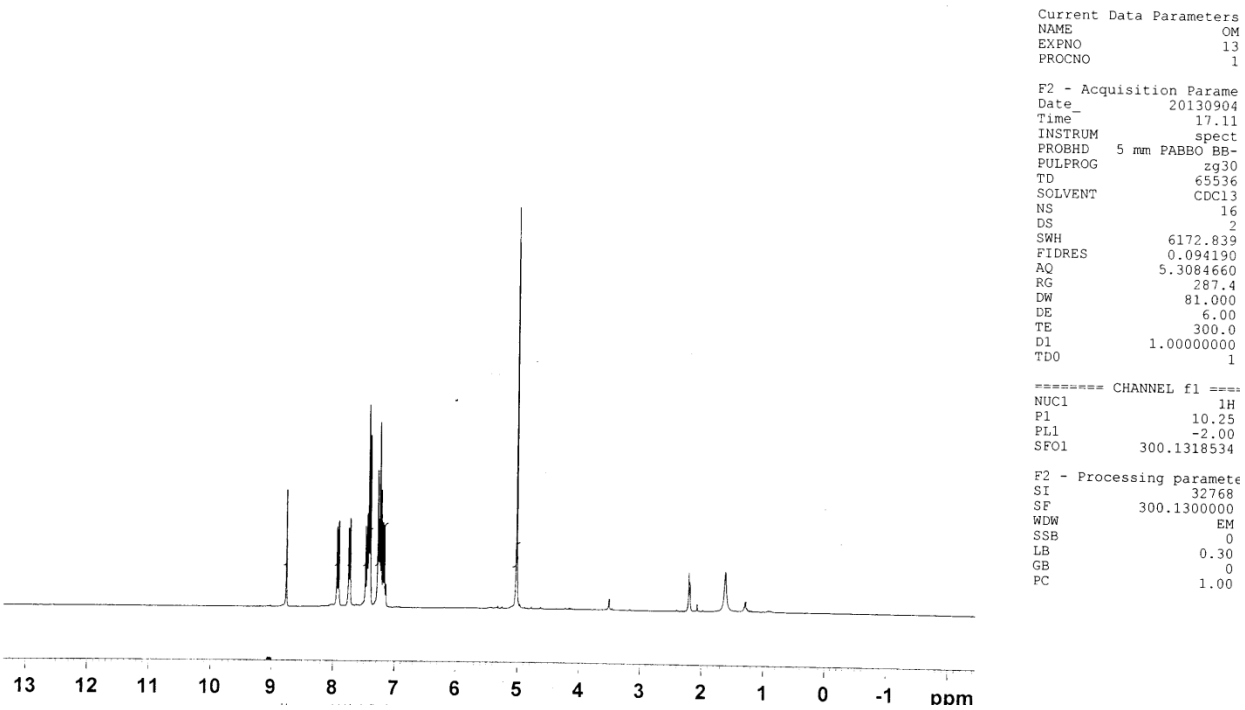

Figure S1. ^{1}H NMR spectra of SNS Pincer Ligand **L**

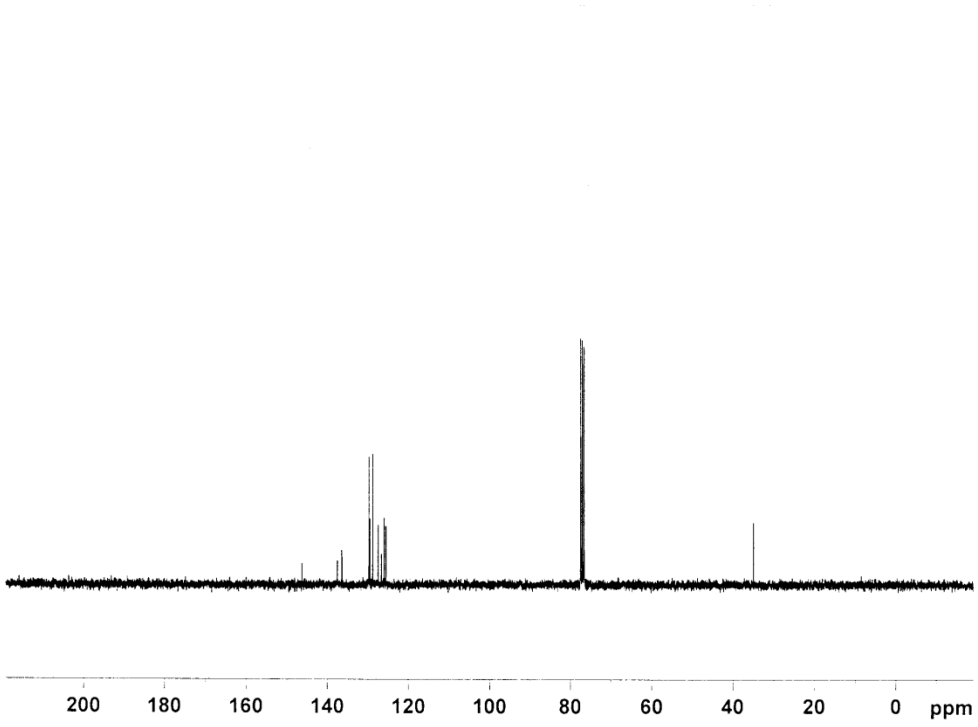


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Figure S2. $^{13}C\{^{1}H\}$ NMR spectra of SNS Pincer Ligand **L**

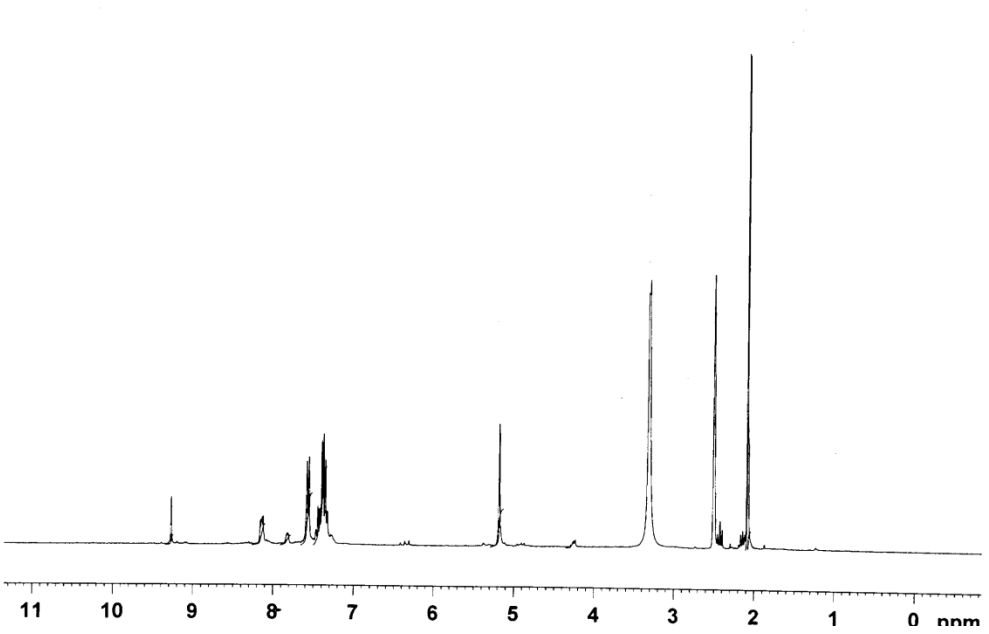


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Figure S3. ^{1}H NMR spectra of Complex **1**

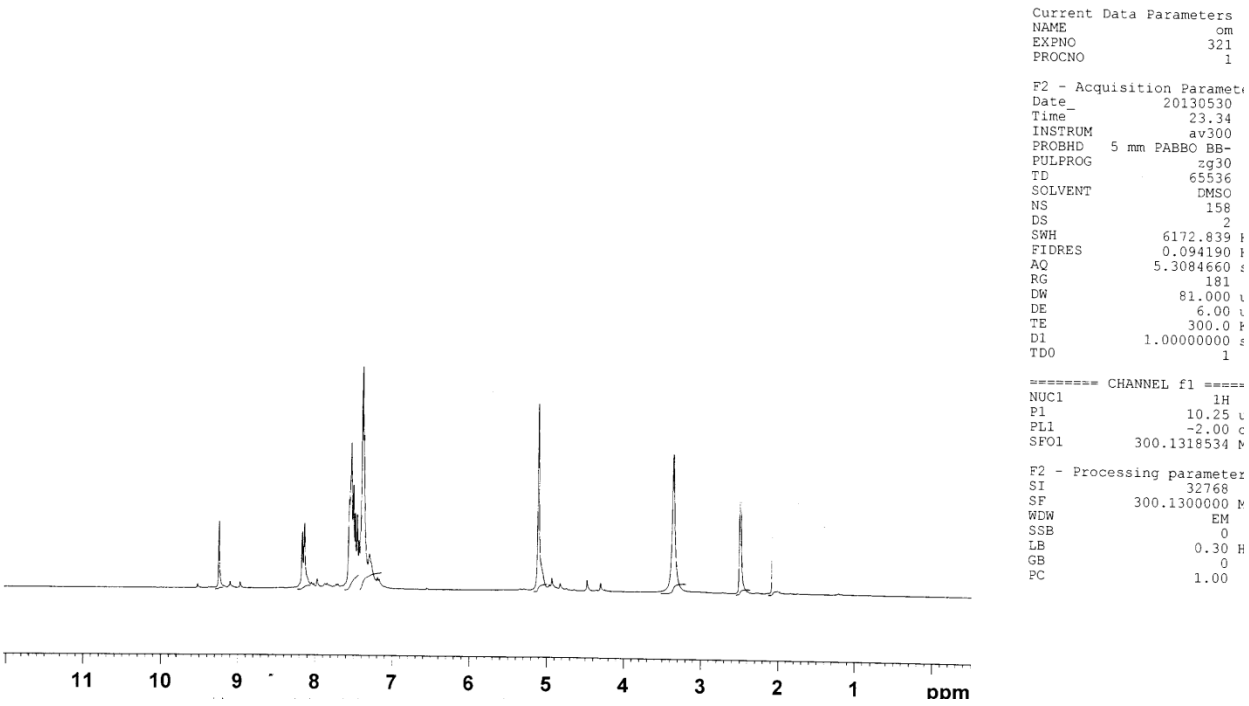


Figure S4. ^{1}H NMR spectra of Complex **2**

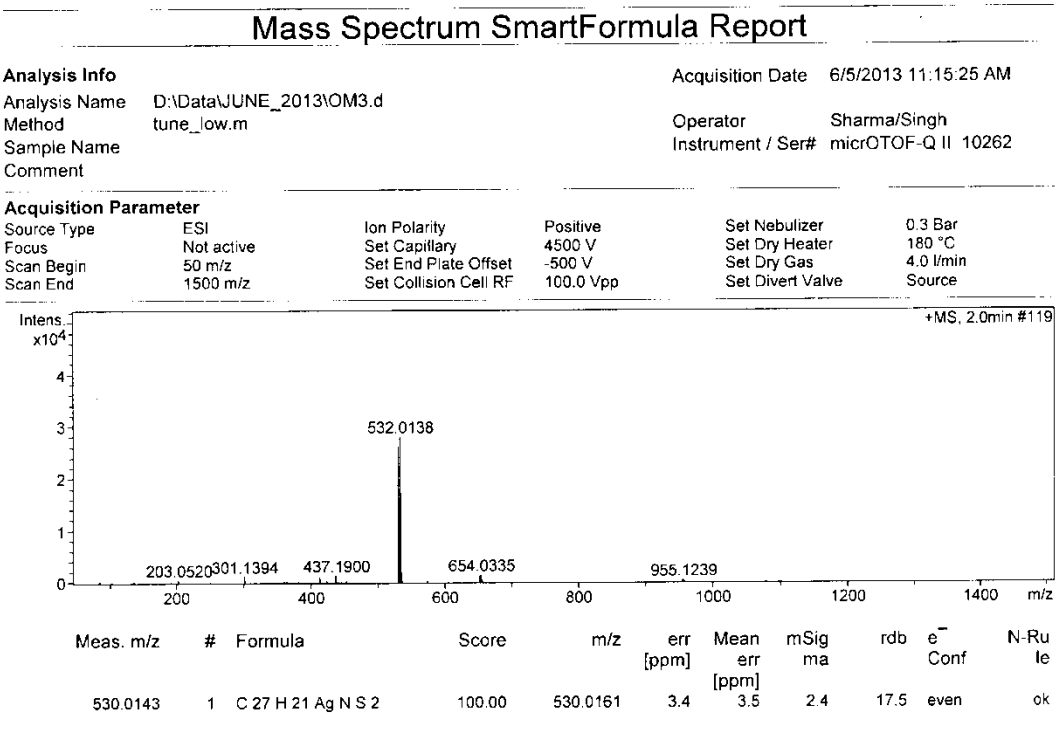


Figure S5. Mass spectra of Complex **1**

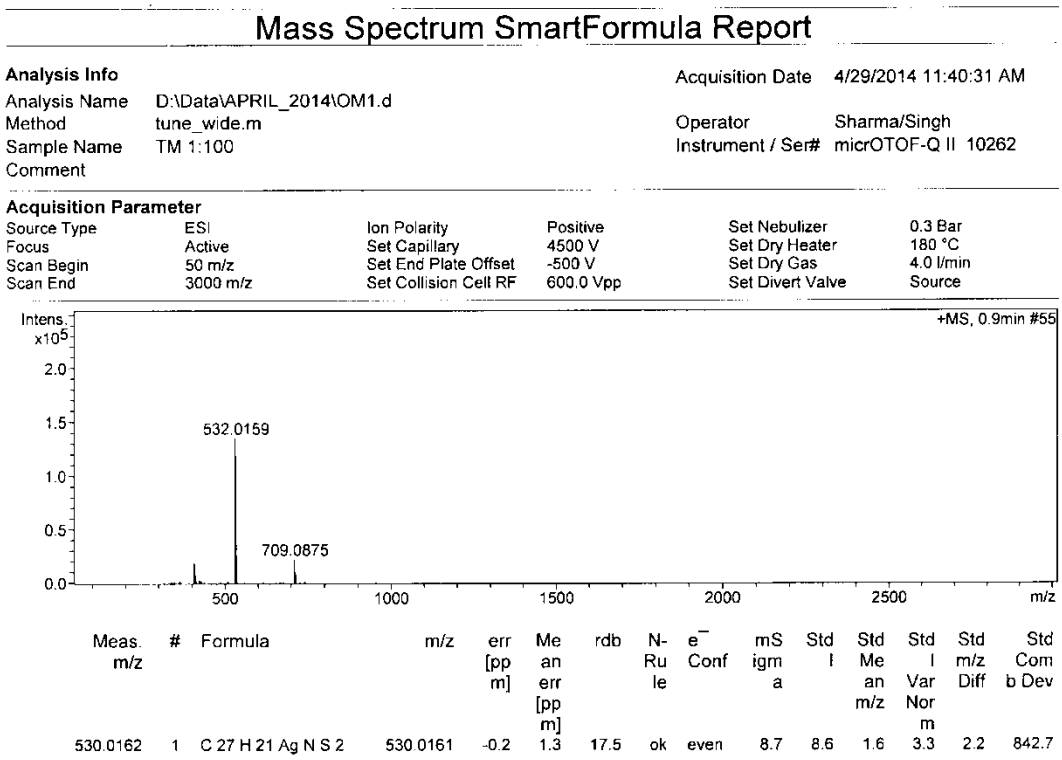
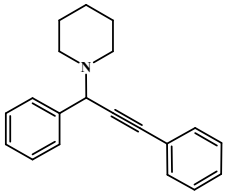
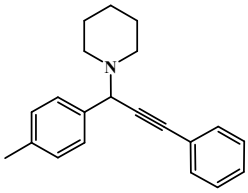


Figure S6. Mass spectra of Complex **2**

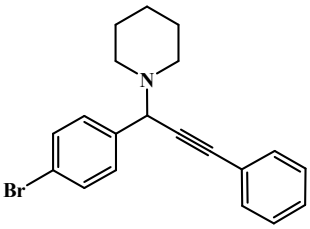
NMR Data of Catalysis Products[1]:



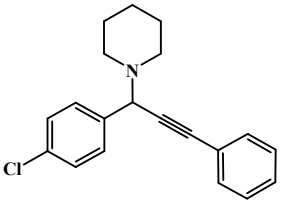
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.42−1.51 (m, 2H), 1.52-170 (m, 4H), 2.51-2.62 (m, 4H), 4.80 (s, 1H), 7.25−7.40 (m, 5H), 7.42−7.54 (m, 3H), 7.61−7.65 (m, 2H).



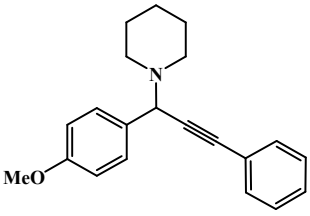
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.43−1.56 (m, 2H), 1.56-178 (m, 4H), 2.40 (s, 3H), 2.55-2.69 (m, 4H), 4.84 (s, 1H), 7.22−7.44 (m, 5H), 7.49−7.55 (m, 2H), 7.57−7.61 (m, 2H).



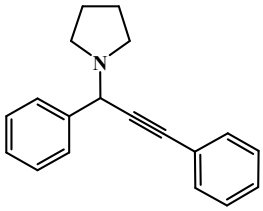
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.47−1.56 (m, 2H), 1.58-174 (m, 4H), 2.55-2.66 (m, 4H), 4.81 (s, 1H), 7.32−7.53 (m, 5H), 7.57−7.60 (m, 2H), 7.61−7.64 (m, 2H).



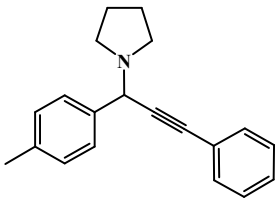
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.45−1.55 (m, 2H), 1.56-171 (m, 4H), 2.54-2.62 (m, 4H), 4.80 (s, 1H), 7.34−7.48 (m, 5H), 7.54−7.58 (m, 2H), 7.60−7.65 (m, 2H).



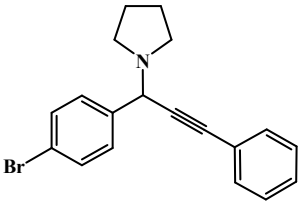
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.41−1.53 (m, 2H), 1.54-170 (m, 4H), 2.52-2.65 (m, 4H), 3.82 (s, 3H), 4.78 (s, 1H), 6.94−7.38 (m, 5H), 7.54−7.62 (m, 4H).



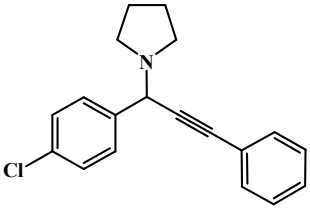
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.78−1.91 (m, 4H), 2.69−2.82 (m, 4H), 4.92 (s, 1H), 7.28−7.38 (m, 4H), 7.39−7.43 (m, 2H), 7.53−7.68 (m, 4H).



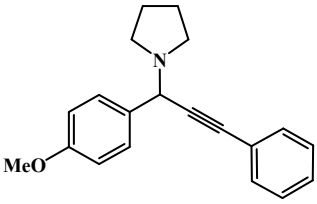
^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.80−1.88 (m, 4H), 2.42 (s, 3H), 2.72−2.80 (m, 4H), 4.90 (s, 1H), 7.21−7.25 (m, 2H), 7.32−7.40 (m, 3H), 7.52−7.59 (m, 4H).



^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.81−1.85 (m, 4H), 2.66−2.70 (m, 4H), 4.91 (s, 1H), 7.35−7.42 (m, 5H), 7.52−7.58 (m, 2H), 7.58−7.62 (m, 2H).



^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.80−1.84 (m, 4H), 2.65−2.68 (m, 4H), 4.89 (s, 1H), 7.33−7.39 (m, 5H), 7.50−7.55 (m, 2H), 7.56−7.60 (m, 2H).



^{1}H NMR ($CDCl_3$, 25 °C vs Me_4Si) δ (ppm): 1.82−1.85 (m, 4H), 2.68−2.75 (m, 4H), 2.82 (s, 3H), 4.88 (s, 1H), 6.92−6.94 (m, 2H), 7.32−7.36 (m, 3H), 7.50−7.58 (m, 4H).

1. (a) C. Wei, Z. Li and C.-J. Li, *Org. Lett.,* 2003, **23**, 4473. (b) X. Yao and C.-J. Li, *Org. Lett*., 2005, **20**, 4395. (c) Y. Zhao, X. Zhou, T. Okamura, M. Chen, Y. Lu, W.-Y. Sun and J.-Q. Yu, *Dalton Trans*., 2012, **41**, 5889. (d) M.-T. Chen, B. Landers and O. Navarro, *Org. Biomol. Chem*. 2012, **10**, 2206. (e) Y. Li, X. Chen, Y. Song, L. Fang, G. Zou, *Dalton Trans*., 2011, **40**, 2046.