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Supporting Information

Copper-based catalysts derived from salen-type ligands: Synthesis of 5substituted-1H-tetrazoles *via* [3+2] cycloaddition and propargylamines *via* A³coupling reactions

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Table of contents

Figure S1	¹ H NMR spectrum of L ¹ H taking CDCl₃ as solvent.		
Figure S2	D ₂ O exchange of ¹ H NMR spectrum of L ¹ H taking CDCl₃ as solvent.		
Figure S3	¹³ C NMR spectrum of L ¹ H taking CDCl₃ as solvent.		
Figure S4	¹ H NMR spectrum of L ² H taking CDCl₃ as solvent.		
Figure S5	¹³ C NMR spectrum of L ² H taking CDCl₃ as solvent.		
Figure S6	¹ H NMR spectrum of L ³ H taking CDCl₃ as solvent.		
Figure S7	¹³ C NMR spectrum of L ³ H taking CDCl₃ as solvent.		
Figure S8	¹ H NMR spectrum of L ⁴ H taking CDCl₃ as solvent.		
Figure S9	¹³ C NMR spectrum of L ⁴ H taking CDCl₃ as solvent.		
Figure S10	ESI-MS Spectrum of L ¹ H using acetonitrile as solvent.		
Figure S11	ESI-MS Spectrum of L ² H using acetonitrile as solvent.		
Figure S12	ESI-MS Spectrum of L ³ H using acetonitrile as solvent.		
Figure S13	ESI-MS Spectrum of L ⁴ H using acetonitrile as solvent.		
Figure S14	Electronic absorption spectra and spectral data of ligands L ¹ H-L ⁴ H in dichloromethane		
	solution.		
Figure S15	Electronic absorption spectra and spectral data of complexes 1-4 in dichlorometha		
	solution.		
Figure S16	FT-IR spectrum of free ligand L ¹ H.		
Figure S17	FT-IR spectrum of free ligand L ² H.		
Figure S18	FT-IR spectrum of free ligand L ³ H.		
Figure S19	FT-IR spectrum of free ligand L ^₄ H.		
Figure S20	FT-IR spectrum of complex 1.		
Figure S21	FT-IR spectrum of complex 2.		
Figure S22	FT-IR spectrum of complex 3 .		
Figure S23	FT-IR spectrum of complex 4.		
Figure S24	ESI-MS spectra of complex 1 using acetonitrile as solvent.		
Figure S25	ESI-MS spectra of complex 2 using acetonitrile as solvent.		
Figure S26	ESI-MS spectra of complex 3 using acetonitrile as solvent.		
Figure S27	ESI-MS spectra of complex 4 using acetonitrile as solvent.		
Table S1	Crystal data and structural refinement parameters for complex 1, 2 and 4.		
Table S2	Selected bond angles and bond distances of complex 1.		
Table S3	Selected bond angles and bond distances of complex 2.		
Table S4	Selected bond angles and bond distances of complex 4.		
Figure S28-S51	¹ H NMR and ¹³ C NMR spectrum of 3a-3I taking DMSO as solvent.		
Figure S52- S81	¹ H NMR and ¹³ C NMR spectrum of 7aa-7ao taking CDCl₃ as solvent.		
Figure S82- S109	¹ H NMR and ¹³ C NMR spectrum of 8aa-8an taking CDCl₃ as solvent.		
Figure S110- S139	¹ H NMR and ¹³ C NMR spectrum of 9aa-9ao taking CDCl₃ as solvent.		
Figure S140- S169	¹ H NMR and ¹³ C NMR spectrum of 10aa-10ao taking CDCl₃ as solvent.		

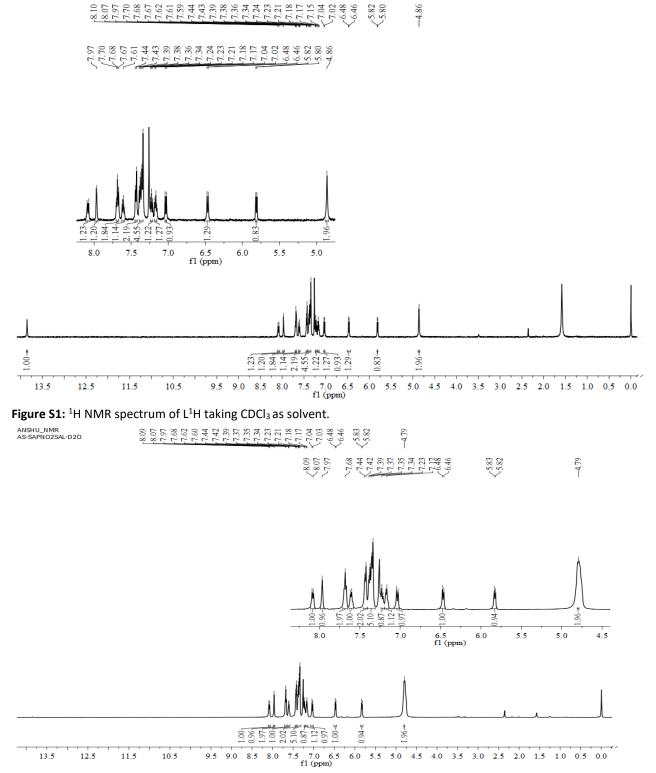


Figure S2: D₂O exchange of ¹H NMR spectrum of L¹H taking CDCl₃ as solvent.

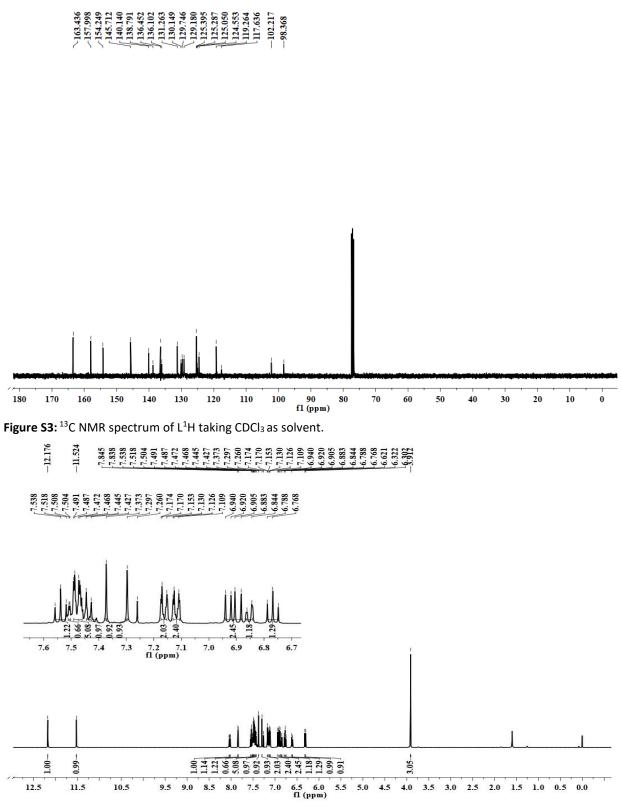


Figure S4: ¹H NMR spectrum of L²H taking CDCl₃ as solvent.

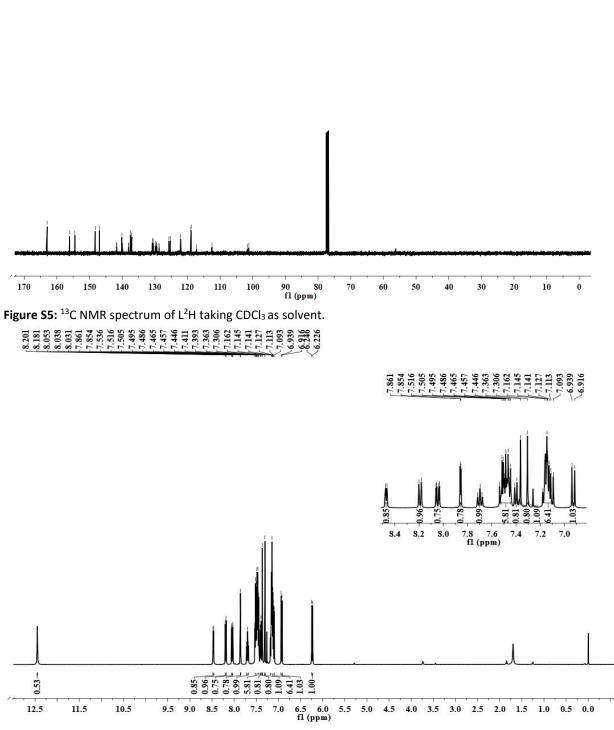


Figure S6: ¹H NMR spectrum of L³H taking CDCl₃ as solvent.

~156.084 ~154.498

-162.971

146.966 146.966 146.966 146.966 137.431 137.659 147.659 147.65

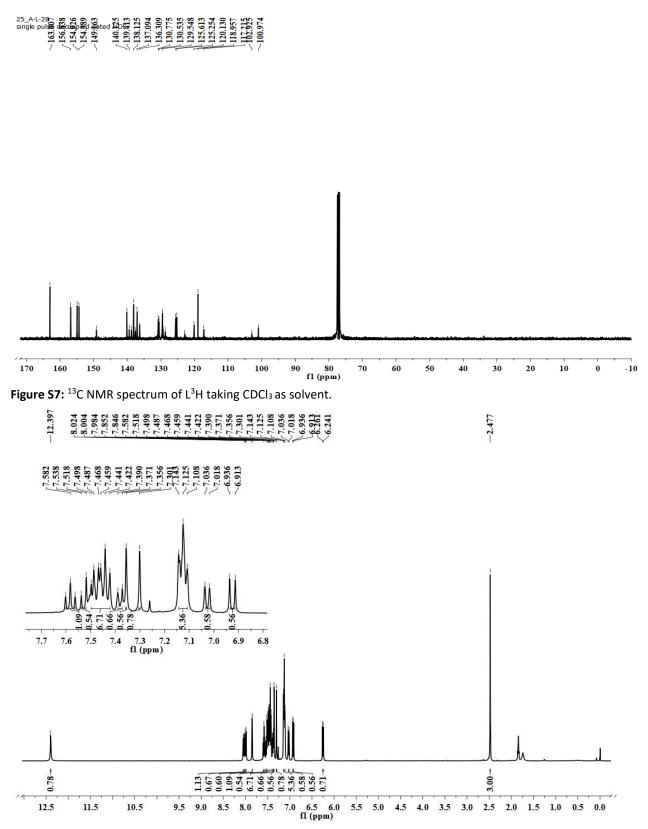
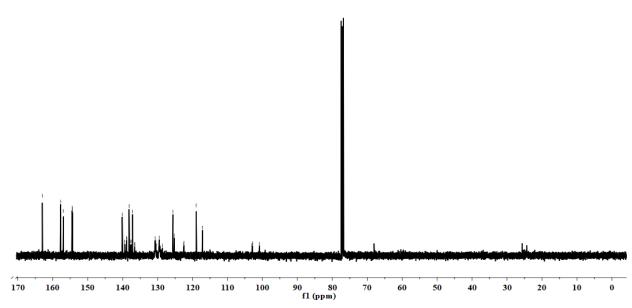
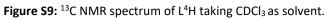


Figure S8: ¹H NMR spectrum of L⁴H taking CDCl₃ as solvent.

$\begin{array}{c} 140.125\\ -138.890\\ -138.890\\ -138.156\\ -137.657\\ -137.657\\ -137.558\\ -137.568\\ -137.19\\ -130.495\\ -130.495\\ -125.604\\ -125.560\\ -125.560\\ -125.560\\ -125.556\\ -$ -162.982 -157.731 -156.937 -154.446 -154.373





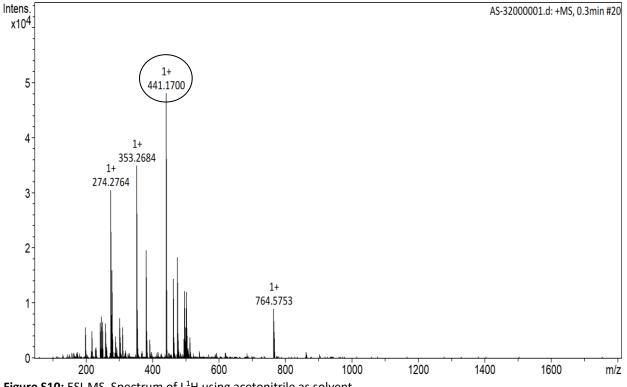
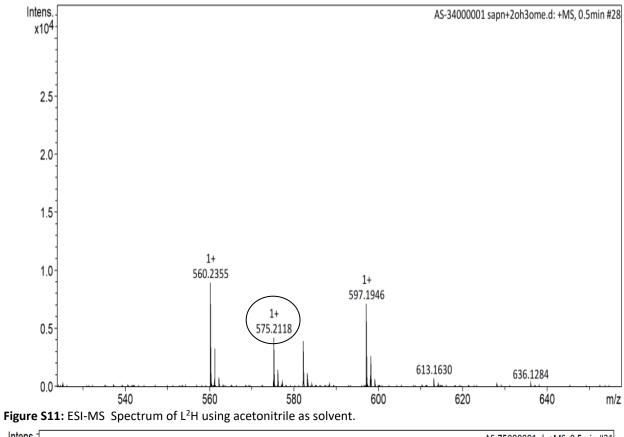


Figure S10: ESI-MS Spectrum of L¹H using acetonitrile as solvent.



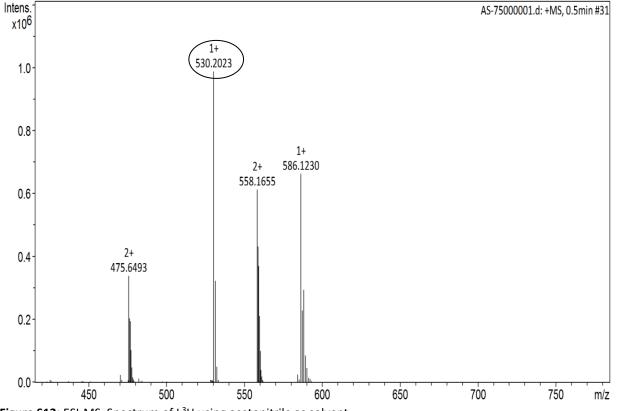


Figure S12: ESI-MS Spectrum of L³H using acetonitrile as solvent.

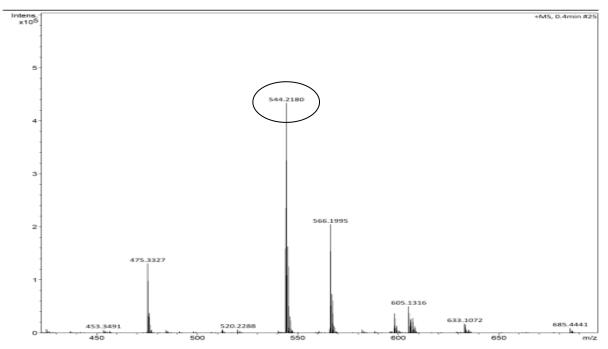
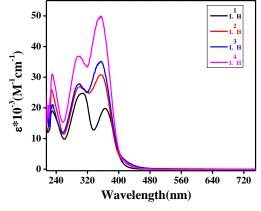
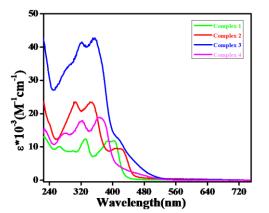


Figure S13: ESI-MS Spectrum of L⁴H using acetonitrile as solvent.



Molecule	λ _{max} (nm)	ε (M ⁻¹ cm ⁻¹)
L ¹ H	230, 307, 365	19130, 24920, 20160
L ² H	227, 298, 355	26130, 27020, 31020
L ³ H	231, 297, 355	21380, 28170, 35510
L ⁴ H	229, 297, 355	31230, 37010, 50180

Figure S14: Electronic absorption spectra and spectral data of ligands L¹H-L⁴H in dichloromethane solution.



Complex 1 264,331,386,404 10200,12560,11990,12000 Complex 2 304,344,406,422 23550,23670,9770,9650 Complex 3 282,320,351,418 33490,41720,42660,11950 Complex 4 280,321,364,456 14280,17990,19110,2420	Molecule	$\lambda_{\max}(\mathbf{nm})$	ε (M ⁻¹ cm ⁻¹)
Complex 3 282, 320, 351, 418 33490, 41720, 42660, 11950	Complex 1	264, 331, 386, 404	10200, 12560, 11990, 12000
	Complex 2	304, 344, 406, 422	23550, 23670, 9770, 9650
Complex 4 280,321,364,456 14280,17990,19110,2420	Complex 3	282, 320, 351, 418	33490, 41720, 42660, 11950
	Complex 4	280, 321, 364, 456	14280, 17990, 19110, 2420

Figure S15: Electronic absorption spectra and spectral data of complexes 1-4 in dichloromethane solution.

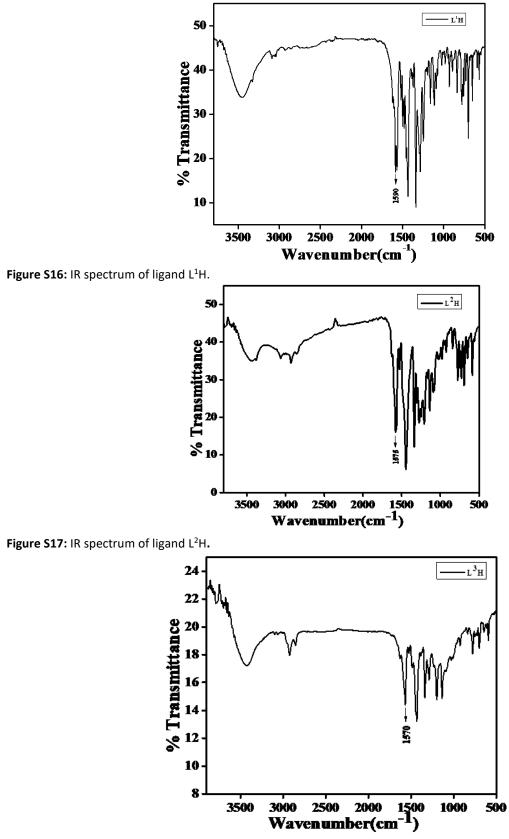


Figure S18: IR spectrum of ligand L³H.

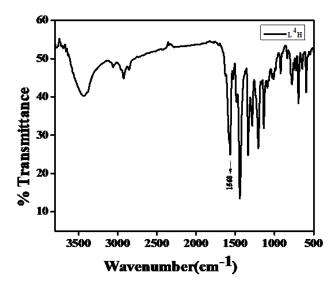


Figure S19: IR spectrum of ligand L⁴H.

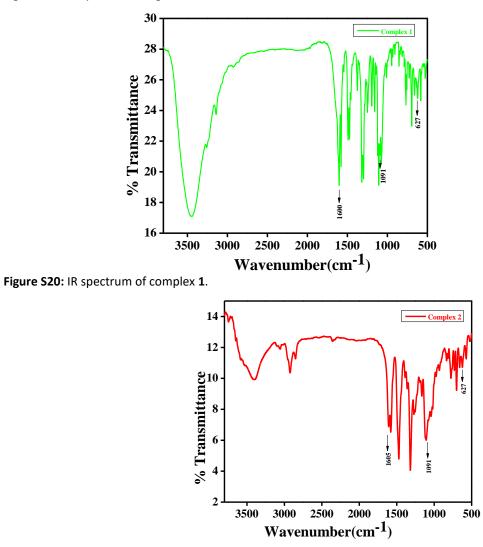


Figure S21: IR spectrum of complex 2.

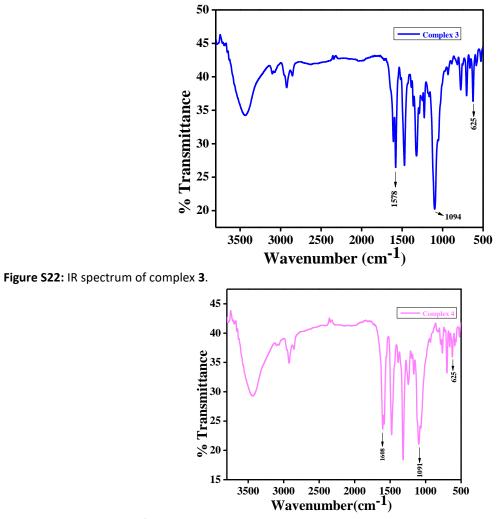


Figure S23: IR spectrum of complex 4.

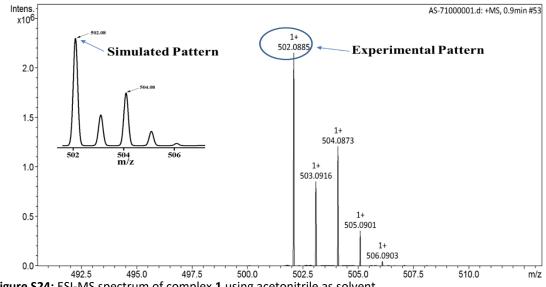
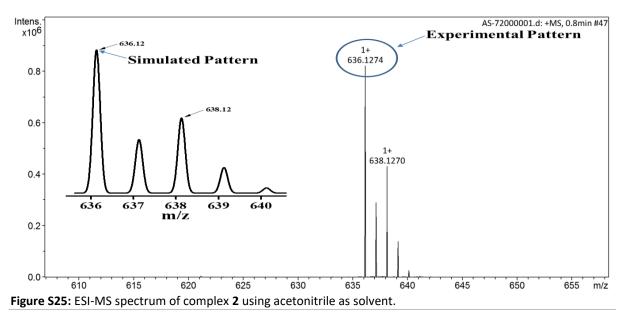


Figure S24: ESI-MS spectrum of complex 1 using acetonitrile as solvent.



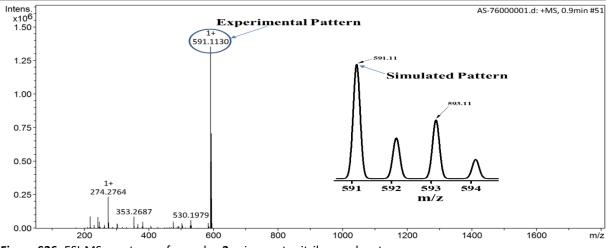


Figure S26: ESI-MS spectrum of complex 3 using acetonitrile as solvent.

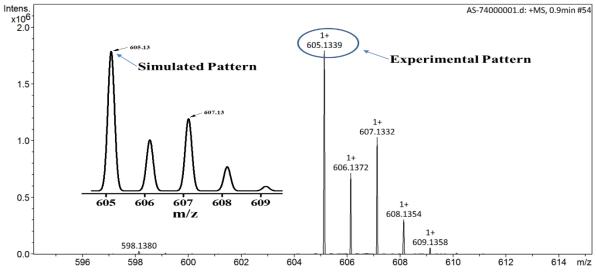


Figure S27: ESI-MS spectrum of complex 4 using acetonitrile as solvent.

nement parameters for comp	blexes 1 , 2 and 4.		
C24 H19 Cu N6 O3, Cl O4	C32 H25 Cl Cu N6 O9,	C31 H25 Cl2 Cu N7 O11	
	0.35(C7 H8), 0.15(C O)	[+ solvent]	
Green	Green	Green	
602.44	773.02	806.03	
293(2)	296(2)	293(2)	
0.71073	0.71073	0.71073	
monoclinic	triclinic	triclinic	
P 21/n	P -1	P -1	
12.216(3)	11.0303(12)	10.1909(4)	
15.250(4)	13.7093(13)	12.3887(5)	
13.903(4)	14.831(2)	15.5047(5)	
90	88.132(8)	77.781(2)	
111.406(12)	68.696(6)	77.754(2)	
90	70.091(6)	69.406(2)	
4	2	2	
1.659	1.314	1.512	
1228.0	793	822.0	
2.326-28.564	2.927-25.349	2.720-28.312	
-16 <h<16, -14<k<20<="" td=""><td>-13<h<13, -16<k<16<="" td=""><td>-13<h<13, -16<k<16<="" td=""></h<13,></td></h<13,></td></h<16,>	-13 <h<13, -16<k<16<="" td=""><td>-13<h<13, -16<k<16<="" td=""></h<13,></td></h<13,>	-13 <h<13, -16<k<16<="" td=""></h<13,>	
-18 <l<17< td=""><td>-17< <17</td><td>-20<l<20< td=""></l<20<></td></l<17<>	-17< <17	-20 <l<20< td=""></l<20<>	
Full matrix least-squares	Full matrix least-squares	Full matrix least-	
on F ²	on F ²	squares on F ²	
6016/13/ 350	7079/1/464	8667/0/470	
1.051	1.066	1.046	
0.0434	0.0729	0.0597	
0.0551	0.1163	0.1114	
0.1266	0.2135	0.1623	
0.1363	0.2476	0.1893	
$GOF = [\Sigma[w(Fo^2 - Fc^2)^2] / M - N)]^{1/2} (M = number of reflections, N = number of parameters refined). BR1 = \Sigma Fo - Fc / \Sigma Fo ,$			
	C24 H19 Cu N6 O3, Cl O4 Green 602.44 293(2) 0.71073 monoclinic <i>P 21/n</i> 12.216(3) 15.250(4) 13.903(4) 90 111.406(12) 90 4 1.659 1228.0 2.326-28.564 -16 <h<16, -14<k<20<br="">-18< <17 Full matrix least-squares on F² 6016/13/350 1.051 0.0434 0.0551 0.1266 0.1363</h<16,>	Green $0.35(C7 H8), 0.15(C O)$ GreenGreen 602.44 773.02 $293(2)$ $296(2)$ 0.71073 0.71073 monoclinictriclinic $P 21/n$ $P -1$ $12.216(3)$ $11.0303(12)$ $15.250(4)$ $13.7093(13)$ $13.903(4)$ $14.831(2)$ 90 $88.132(8)$ $111.406(12)$ $68.696(6)$ 90 $70.091(6)$ 4 2 1.659 1.314 1228.0 793 $2.326-28.564$ $2.927-25.349$ $-16-13-18< <17-17< <17Full matrix least-squareson F20.16^{1}3.507079/1/4641.0511.0660.04340.07290.05510.11630.12660.21350.13630.2476$	

 c wR₂ = [Σ [w(Fo²-Fc²)₂]/ Σ [w(Fo₂)₂]]^{1/2}

 Table S2: Selected bond angles and bond distances of complex 1.

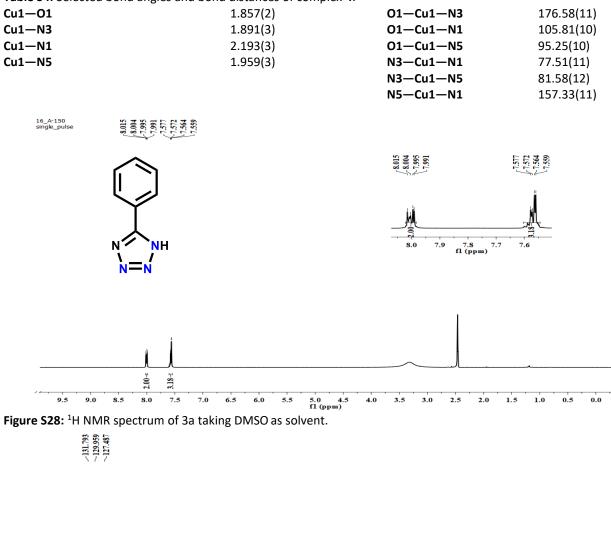
	Bond Lengths (Å)	Во	nd Angles(°)
Cu1—01	1.8552(18)	O1—Cu1—N3	174.73(8)
Cu1—N3	1.883(2)	O1—Cu1—N1	103.20(8)
Cu1—N1	2.075(2)	O1—Cu1—N5	94.91(8)
Cu1—N5	1.974(2)	N3—Cu1—N1	81.00(9)
		N3—Cu1—N5	80.72(8)
		N5—Cu1—N1	161.53(8)

 Table S3: Selected bond angles and bond distances of complex 2.

 Bond Lengths (Å)

Table 33. Selected bolid ang	ies and bond distances of compl	CA Z .	
Bond Lengths (Å)		Bond Angles(°)	
Cu1—O1	1.854(3)	O1—Cu1—N3	168.85(18)
Cu1—N3	1.887(4)	O1—Cu1—N1	104.67(15)
Cu1—N1	2.090(4)	O1—Cu1—N5	94.97(15)
Cu1—N5	1.973(4)	N3—Cu1—N1	79.93(17)
		N3—Cu1—N5	80.09(17)
		N5—Cu1—N1	160.02(17)

 Table S4: Selected bond angles and bond distances of complex 4.



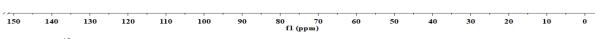


Figure S29: ¹³C NMR spectrum of taking 3a DMSO as solvent.

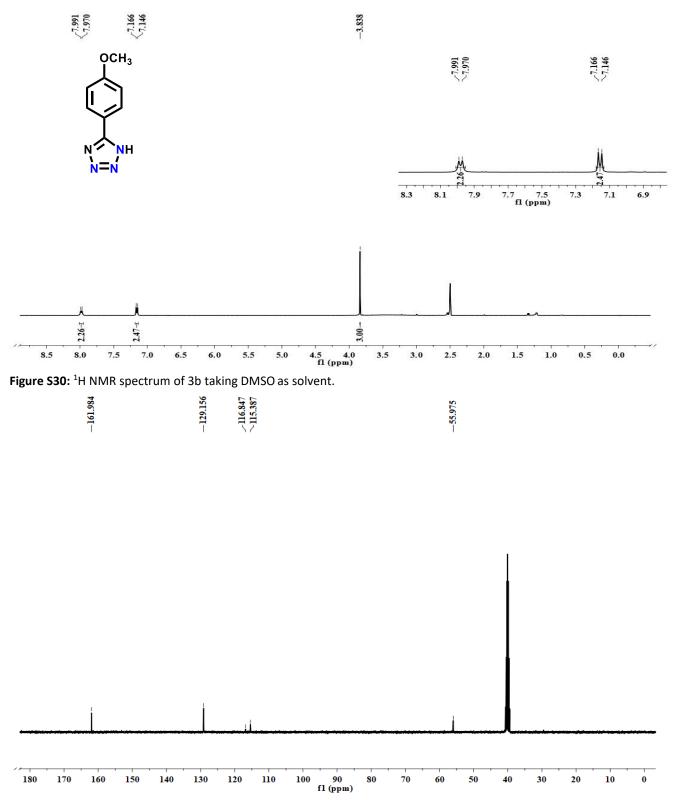


Figure S31: ¹³C NMR spectrum of 3b taking DMSO as solvent.

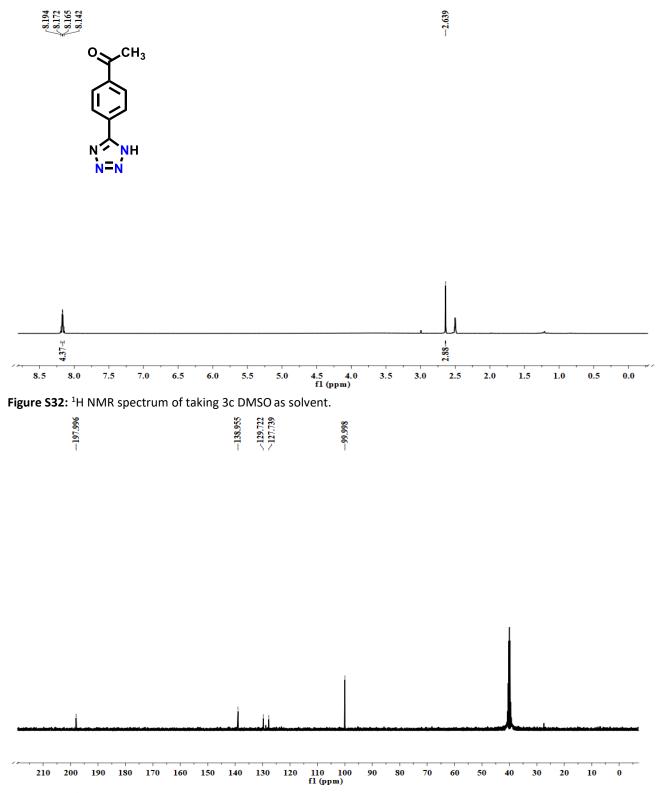


Figure S33: ¹³C NMR spectrum of 3c taking DMSO as solvent.

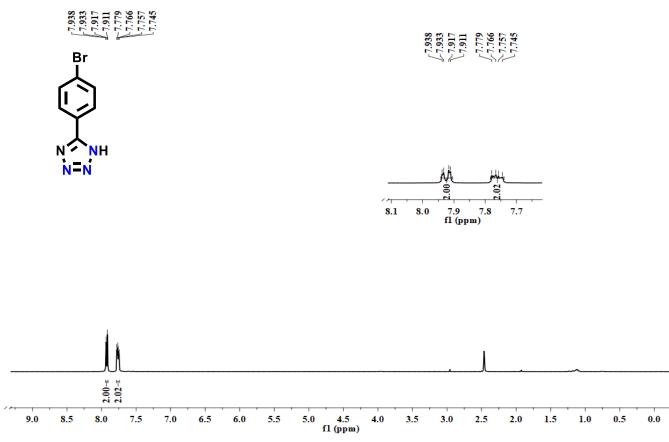


Figure S34: ¹H NMR spectrum of 3d taking DMSO as solvent.



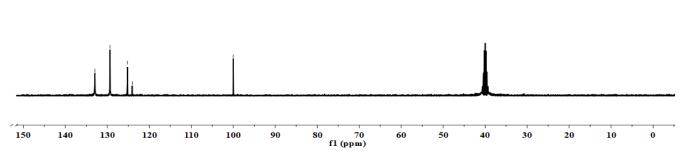


Figure S35: ¹³C NMR spectrum of 3d taking DMSO as solvent.

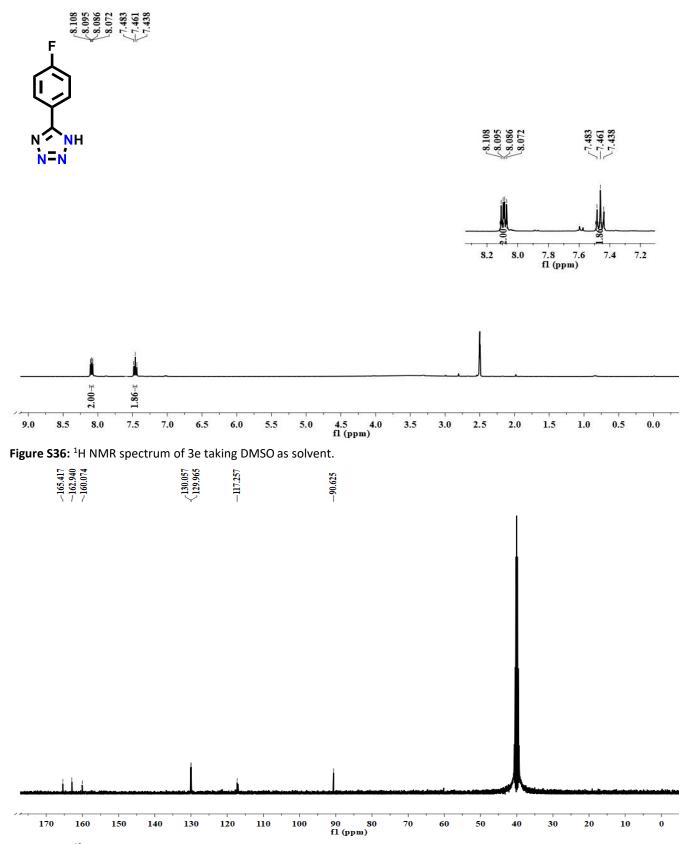
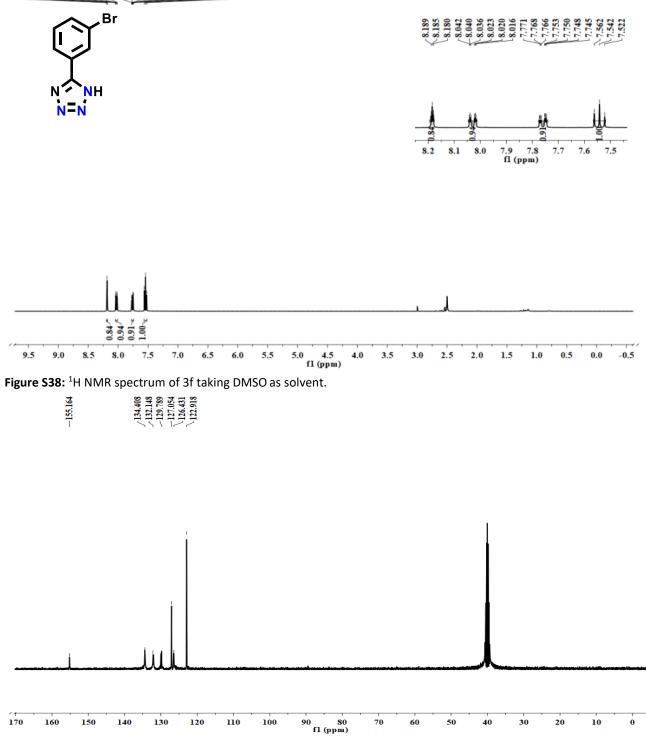
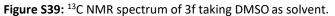


Figure S37: ¹³C NMR spectrum of 3e taking DMSO as solvent.

8.189 8.185 8.185 8.185 8.042 8.040 8.040 8.036 8.0376 8.036





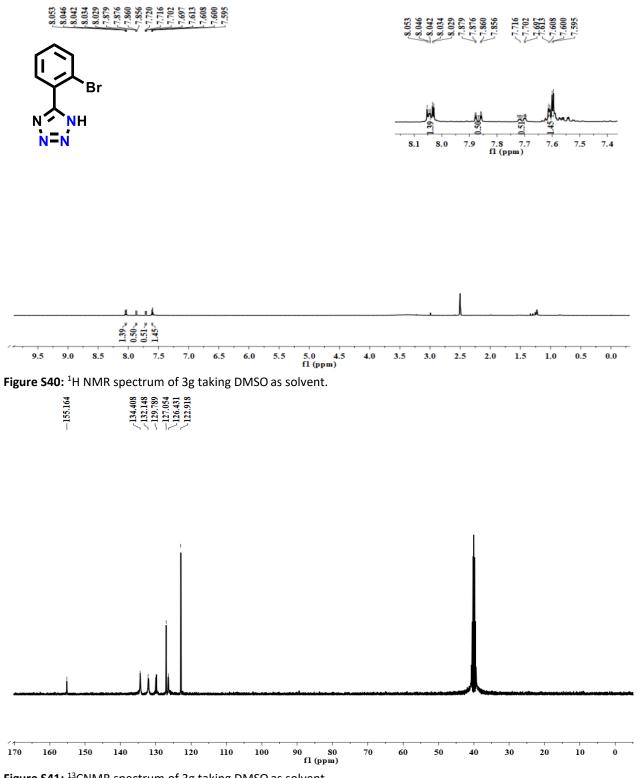


Figure S41: ¹³CNMR spectrum of 3g taking DMSO as solvent.

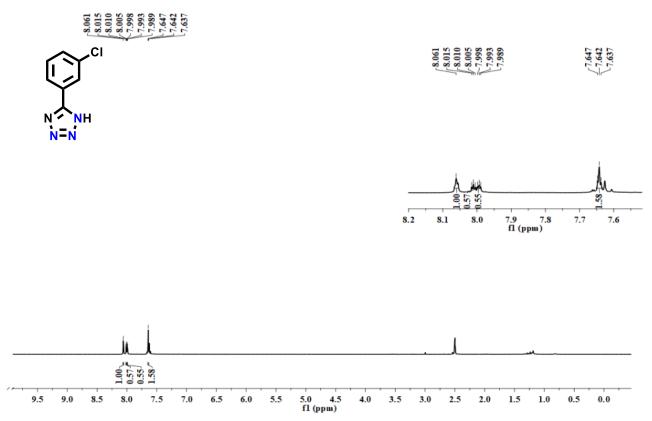


Figure S42: ¹H NMR spectrum of 3h taking DMSO as solvent



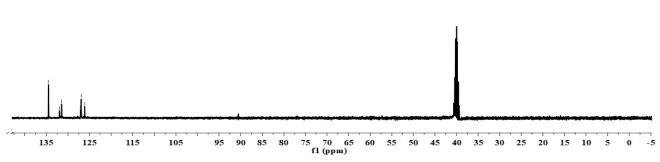
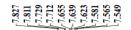
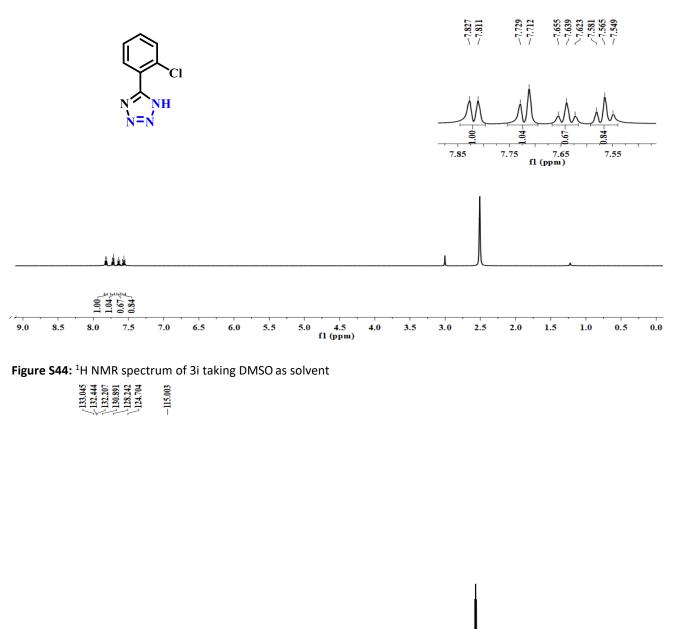
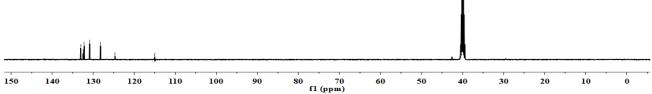
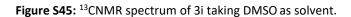


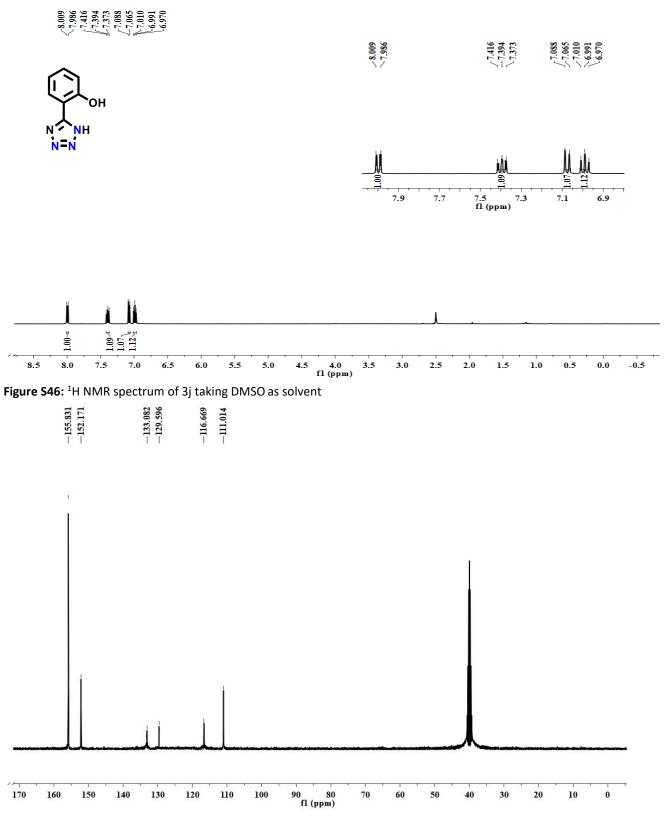
Figure S43: ¹³CNMR spectrum of 3h taking DMSO as solvent.

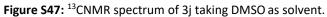












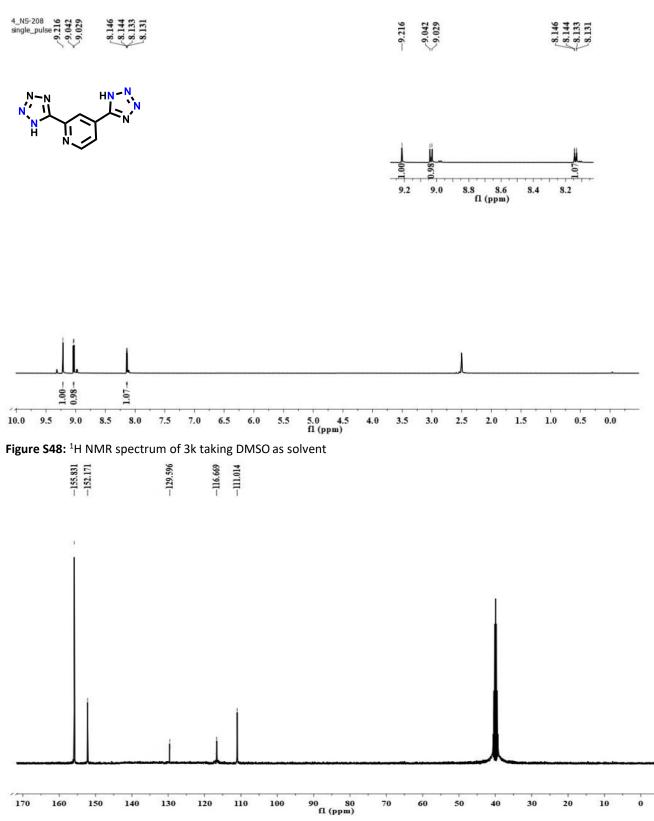


Figure S49: ¹³CNMR spectrum of 3k taking DMSO as solvent.





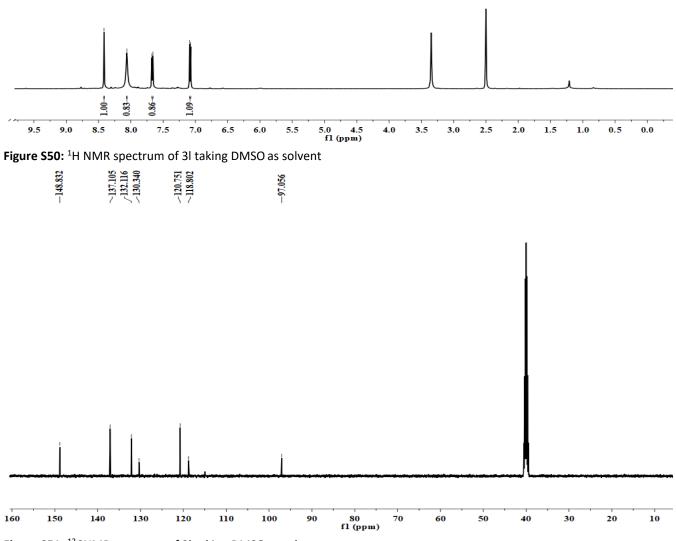


Figure S51: ¹³CNMR spectrum of 3I taking DMSO as solvent.

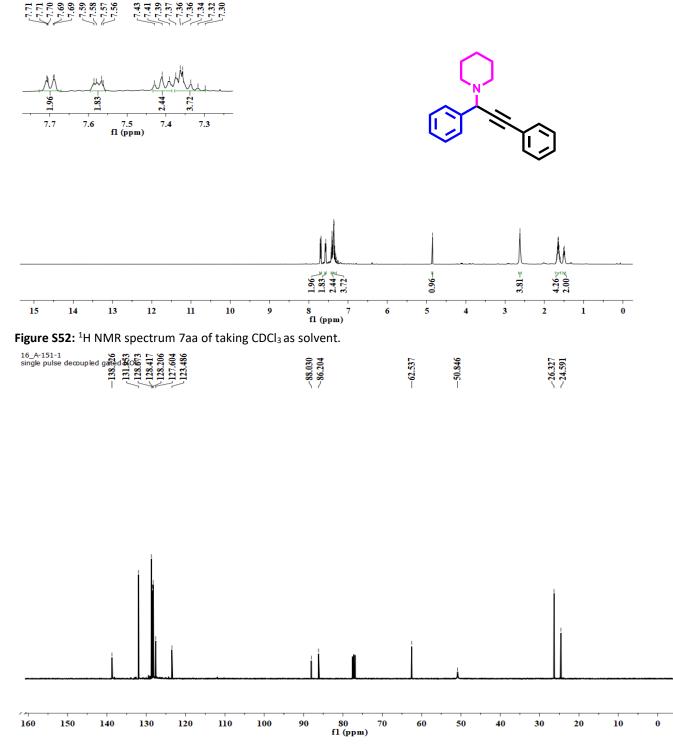


Figure S53: ¹³C NMR spectrum of 7aa taking CDCl₃as solvent.

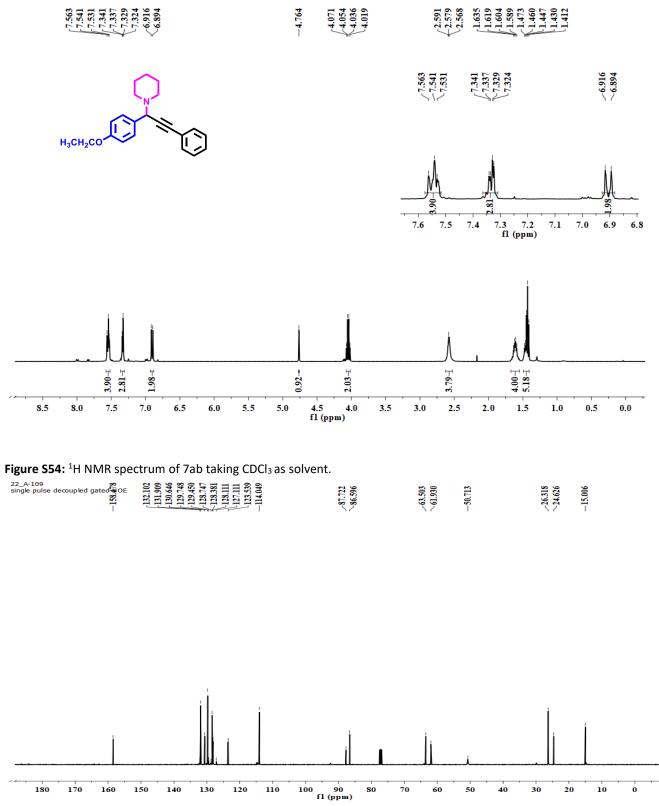


Figure S55: ¹³C NMR spectrum of 7ab taking CDCl₃ as solvent.

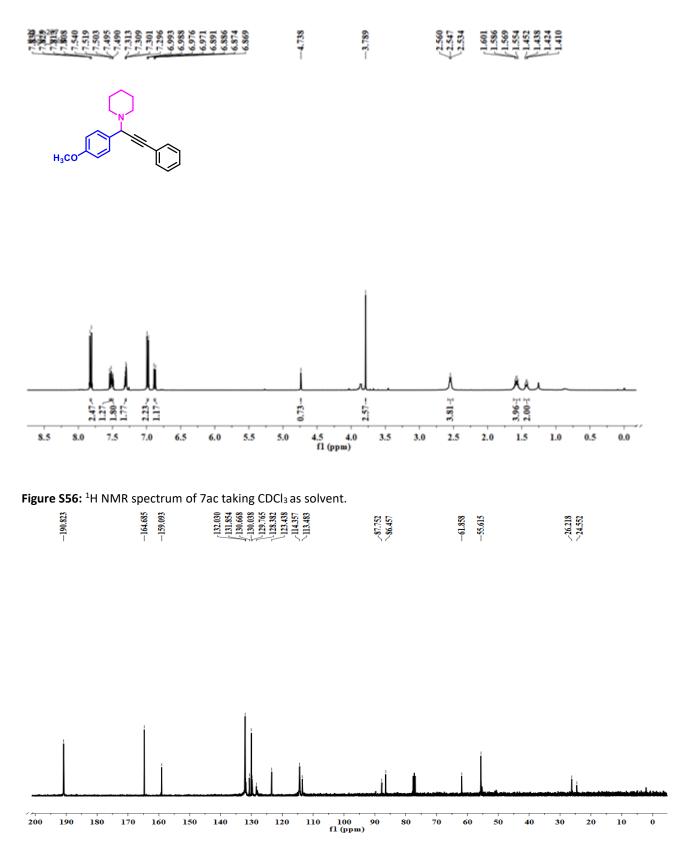
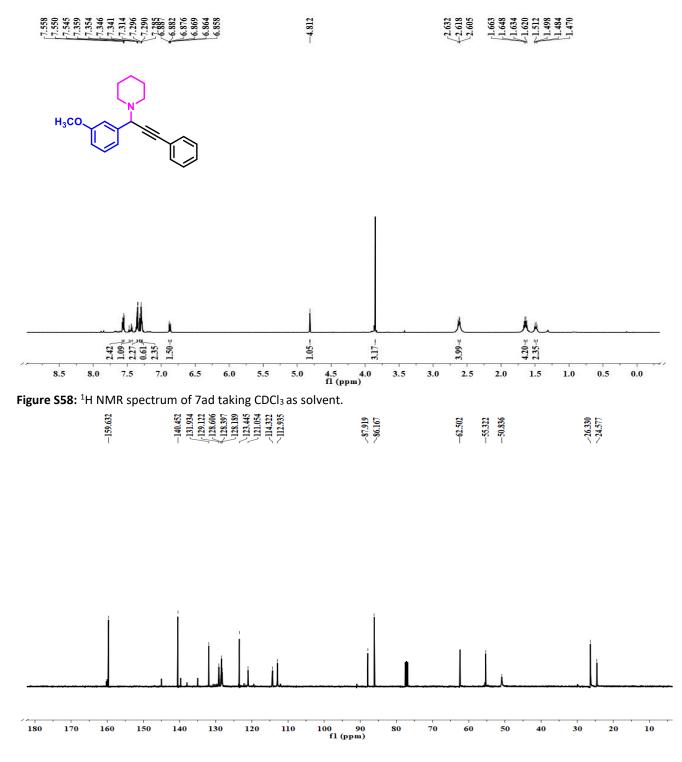
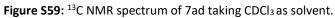
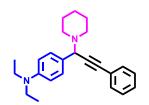


Figure S57: ¹³C NMR spectrum of 7ac taking CDCl₃ as solvent.





7.52 7.52 7.50 7.51 7.52 7.50 7.51 7.52 7.52 7.52 7.52 7.52 7.52 7.52 7.53 7.54 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55 7.55



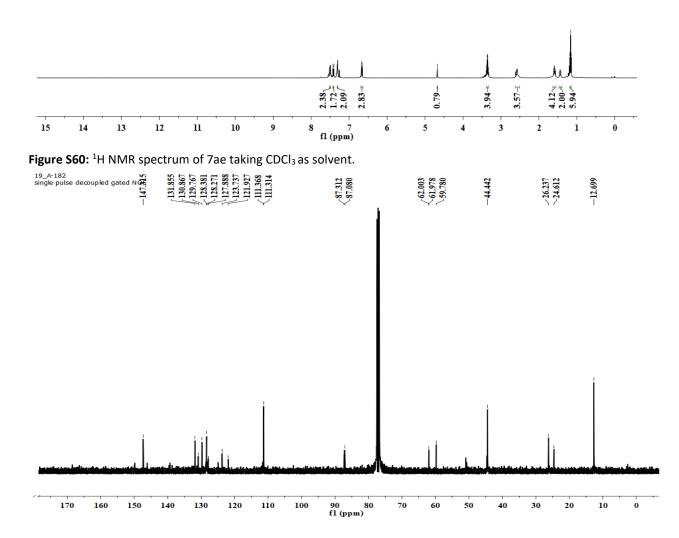


Figure S61: ¹³C NMR spectrum of 7ae taking CDCl₃ as solvent.

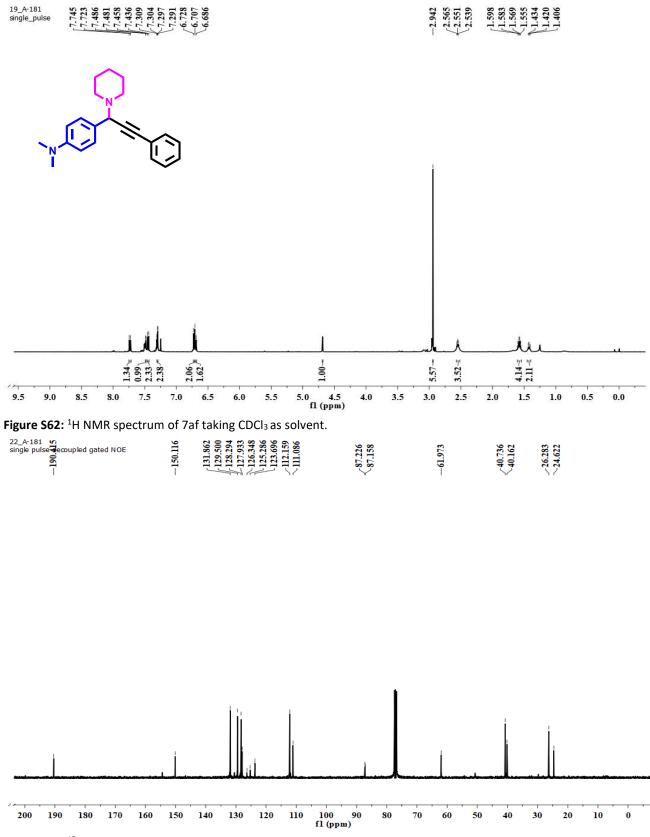


Figure S63: ¹³C NMR spectrum of 7af taking CDCl₃ as solvent.

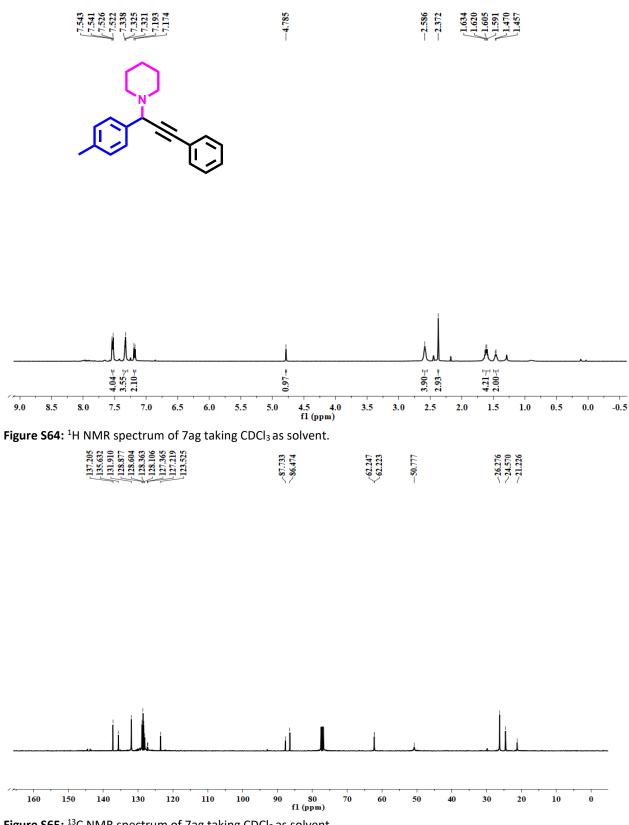


Figure S65: ¹³C NMR spectrum of 7ag taking CDCl₃ as solvent.

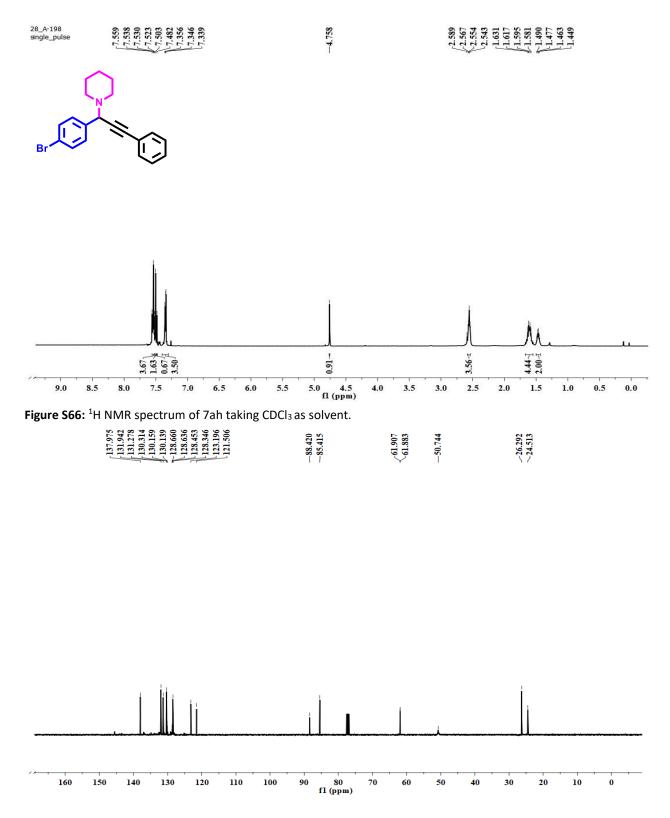


Figure S67: $^{\rm 13}{\rm C}$ NMR spectrum of 7ah taking CDCl3 as solvent

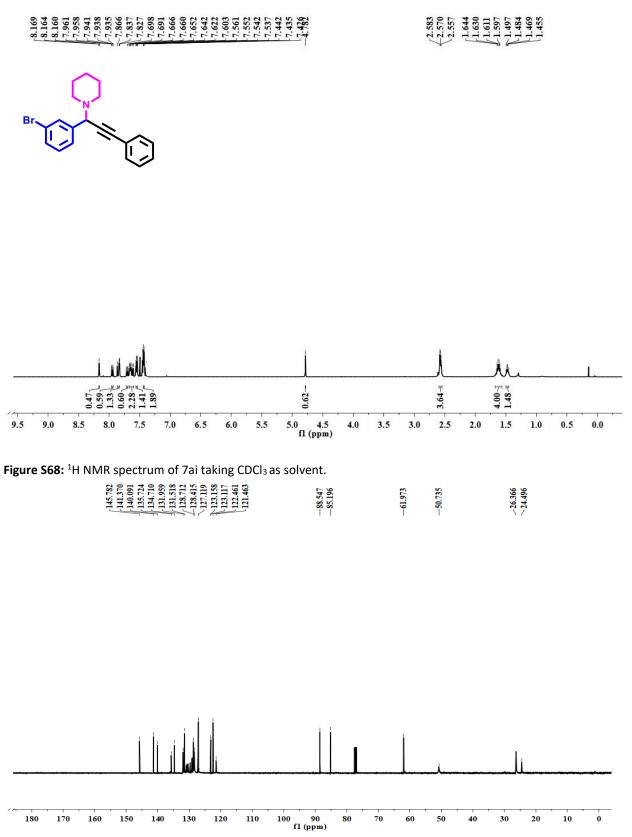


Figure S69: ¹³C NMR spectrum of 7ai taking CDCl₃ as solvent

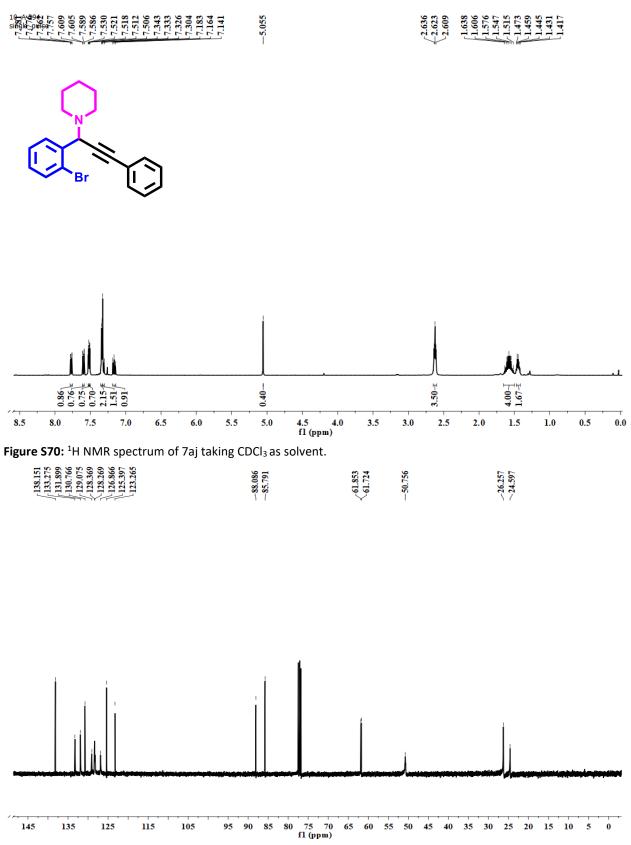


Figure S71: ¹³C NMR spectrum of 7aj taking CDCl₃ as solvent

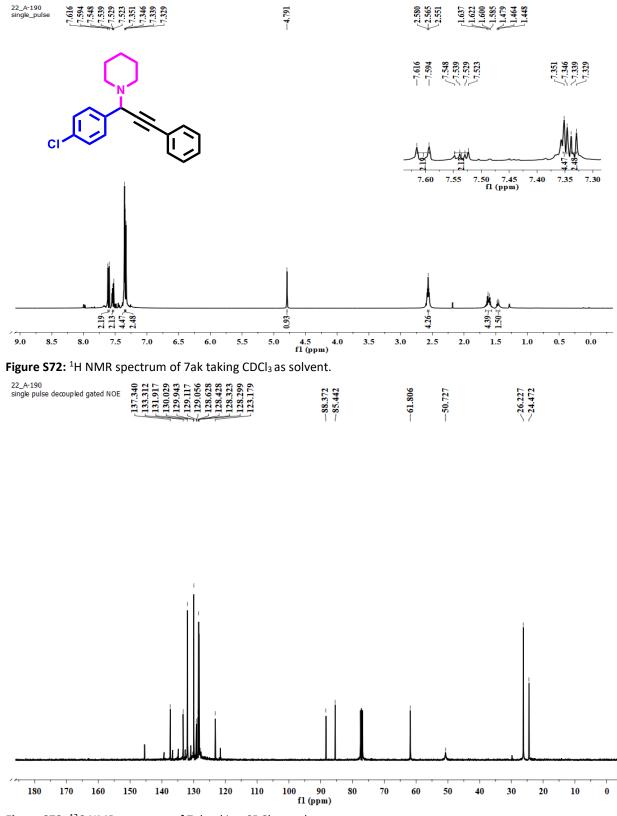


Figure S73: ¹³C NMR spectrum of 7ak taking CDCl₃ as solvent

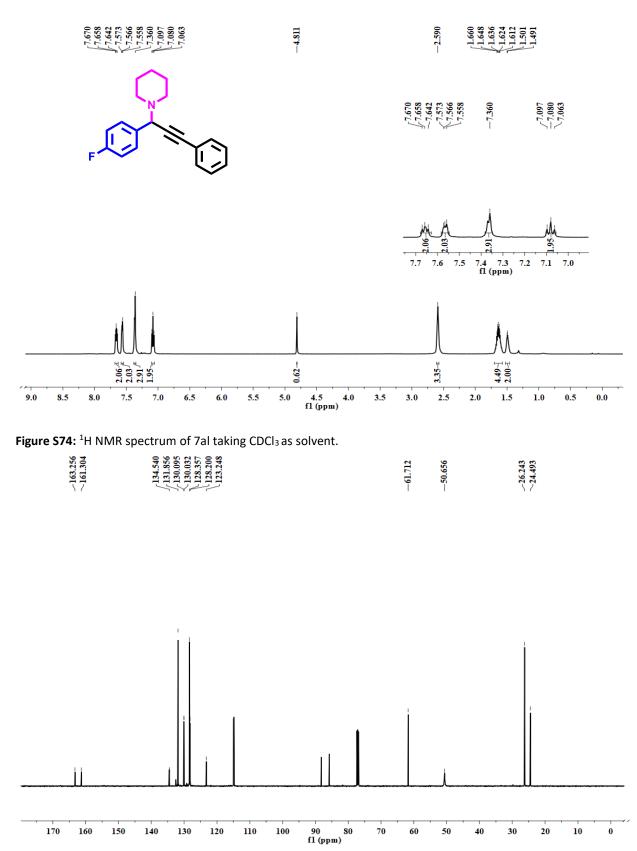


Figure S75: ¹³C NMR spectrum of 7al taking CDCl₃ as solvent

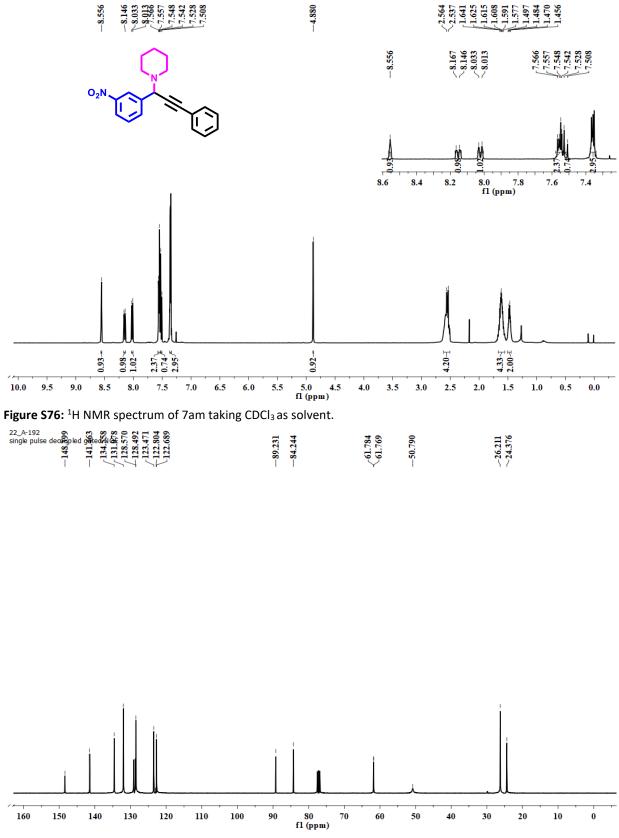


Figure S77: ¹³C NMR spectrum of 7am taking CDCl₃ as solvent

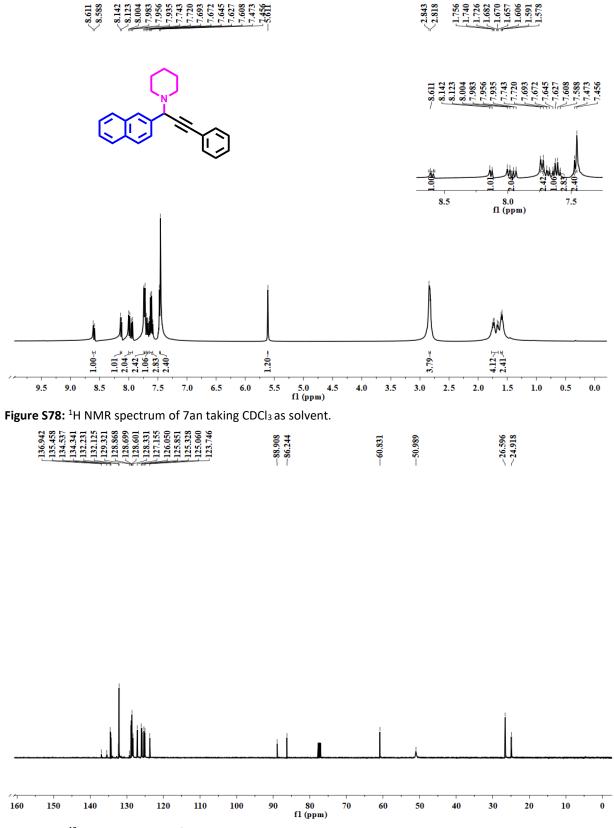


Figure S79: ¹³C NMR spectrum of taking CDCl₃ as solvent

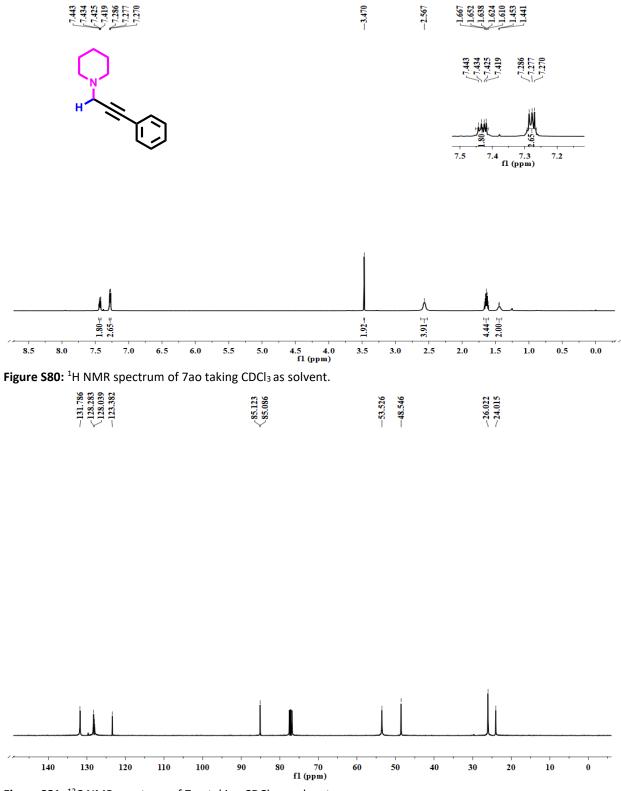
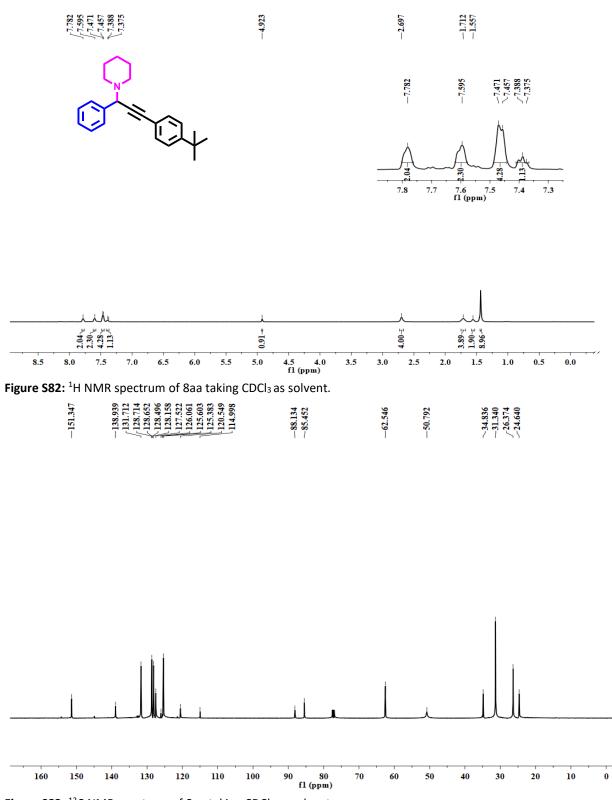
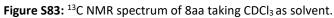


Figure S81: ¹³C NMR spectrum of 7ao taking CDCl₃ as solvent.





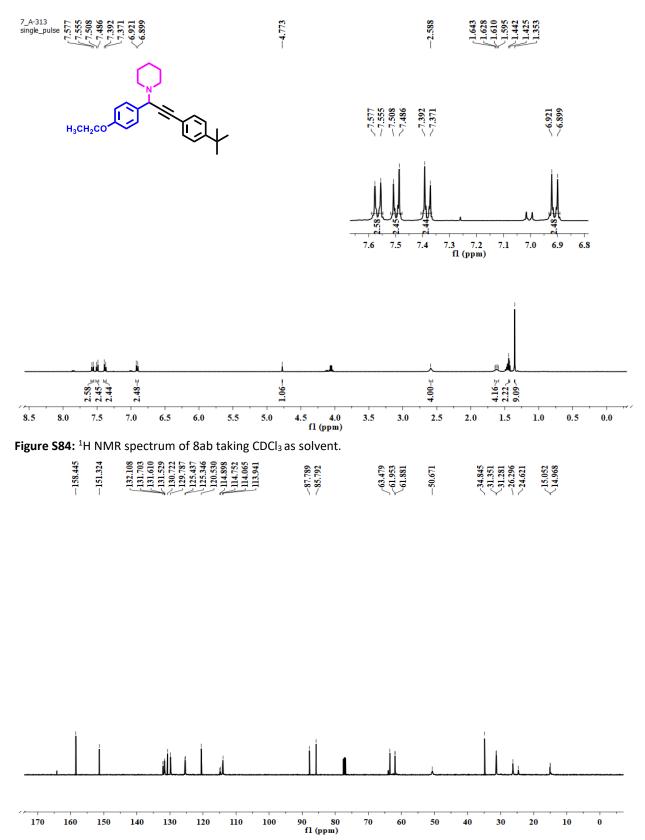


Figure S85: ¹³C NMR spectrum of 8ab taking CDCl₃ as solvent.

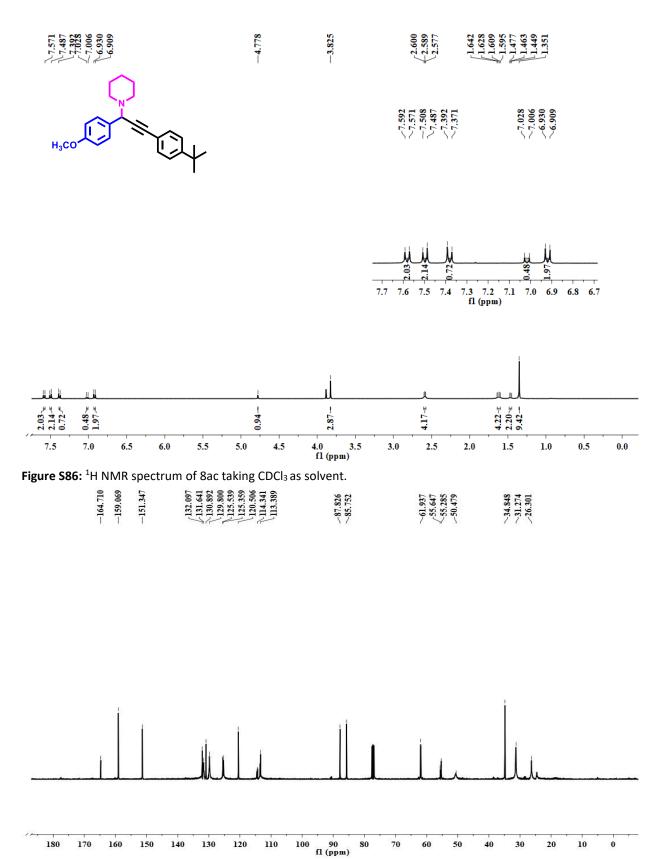


Figure S87: ¹³C NMR spectrum of 8ac taking CDCl₃ as solvent.

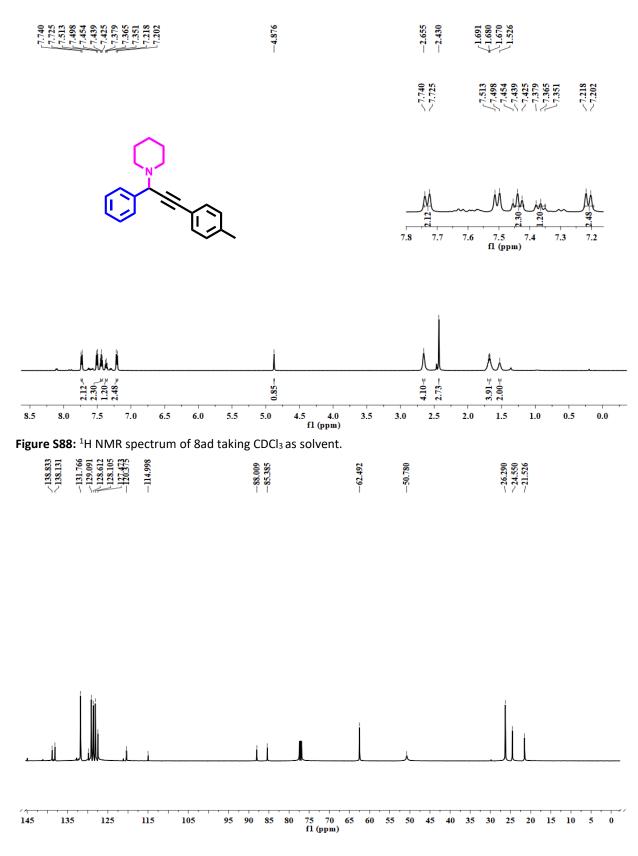


Figure S89: ¹³C NMR spectrum of 8ad taking CDCl₃ as solvent.

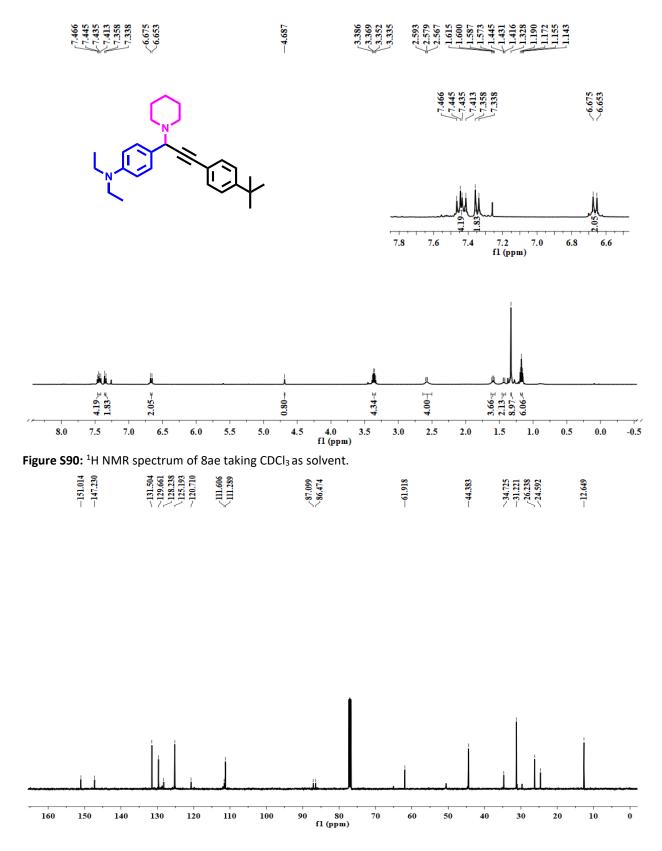


Figure S91: ¹³C NMR spectrum of 8ae taking CDCl₃ as solvent.

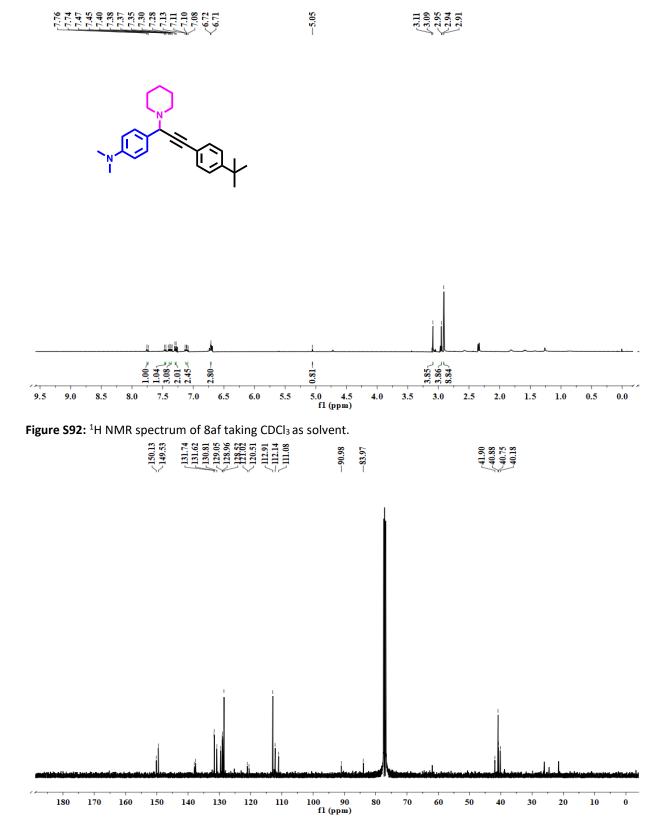


Figure S93: ¹³C NMR spectrum of 8af taking CDCl₃ as solvent.

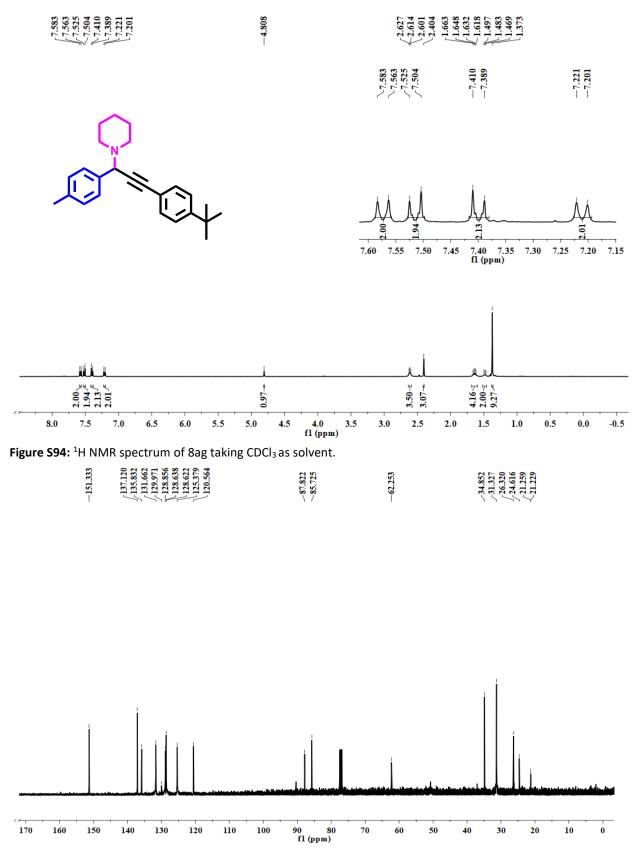


Figure S95: $^{\rm 13}{\rm C}$ NMR spectrum of 8ag taking CDCl3 as solvent.

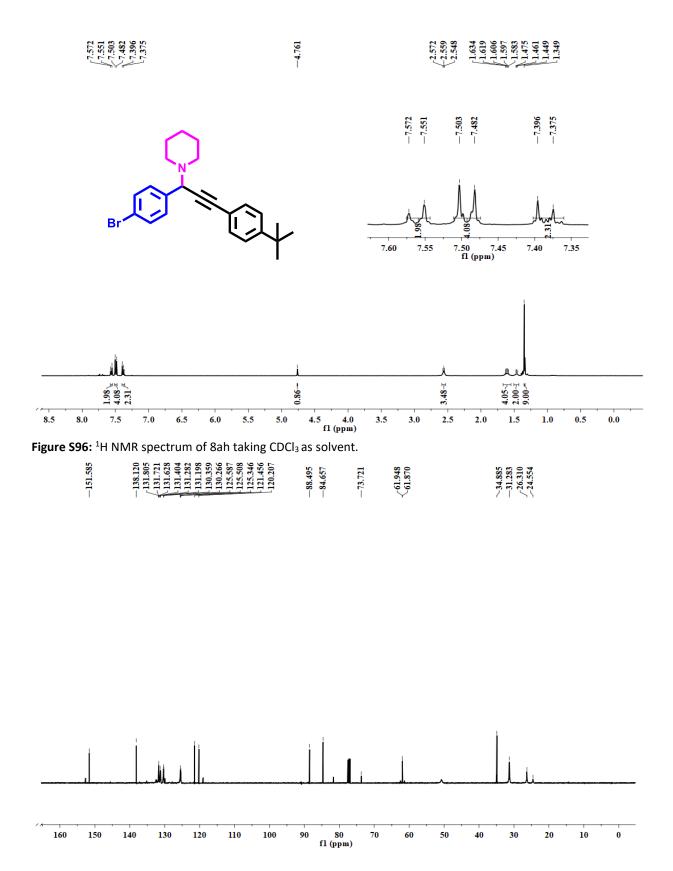


Figure S97: ¹³C NMR spectrum of 8ah taking CDCl₃ as solvent.

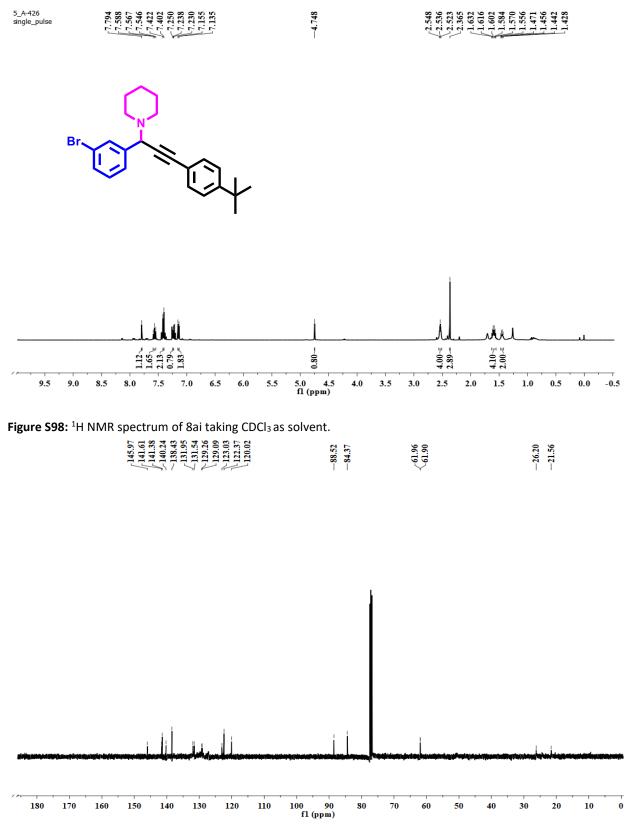


Figure S99: ¹³C NMR spectrum of 8ai taking CDCl₃ as solvent.

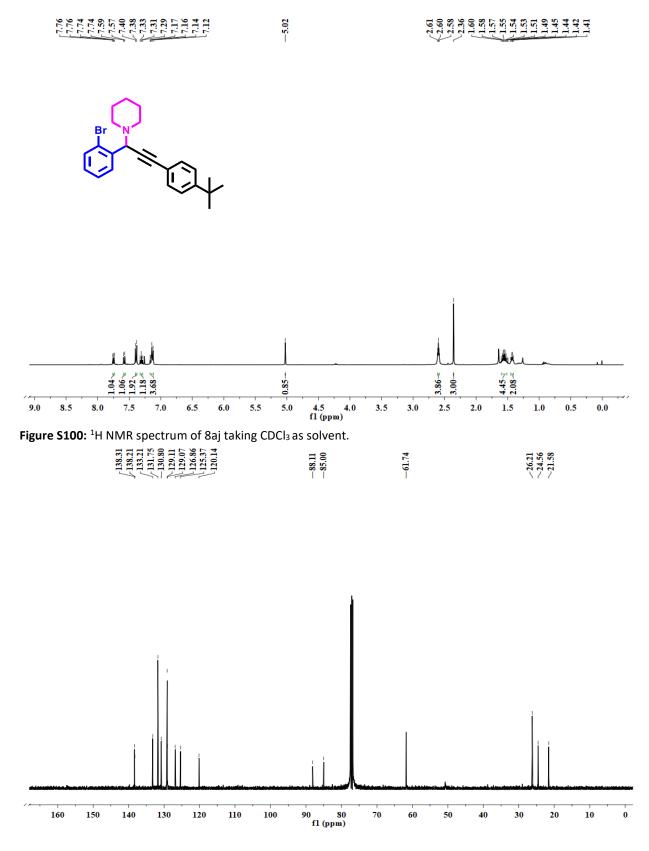
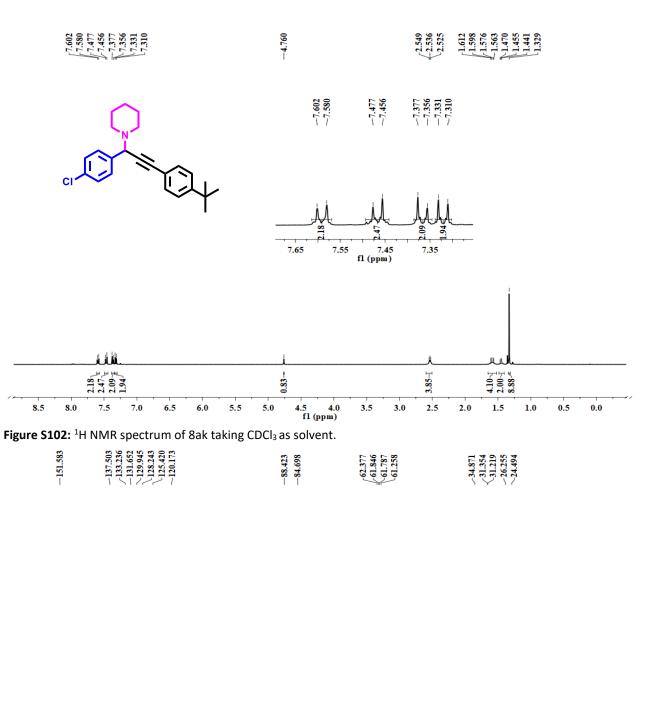


Figure S101: ¹³C NMR spectrum of 8aj taking CDCl₃ as solvent.



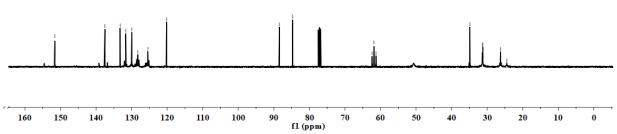
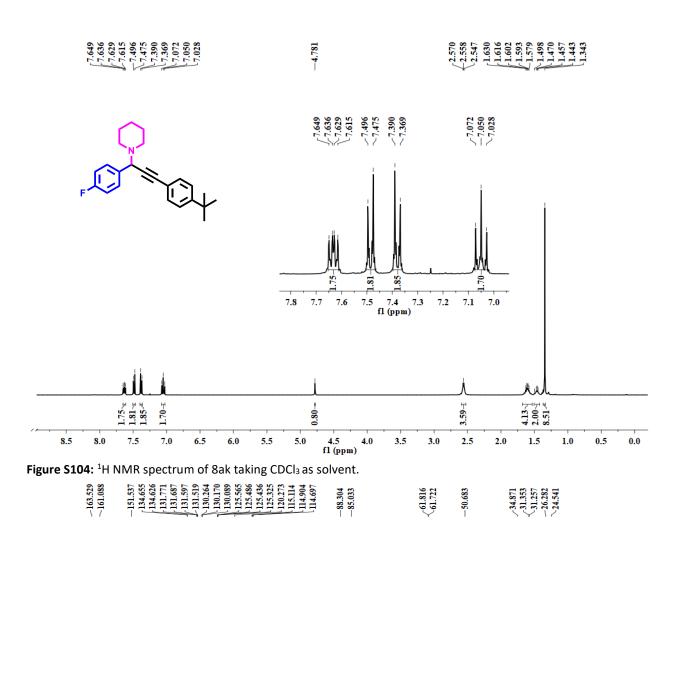


Figure S103: ¹³C NMR spectrum of 8ak taking CDCl₃ as solvent.



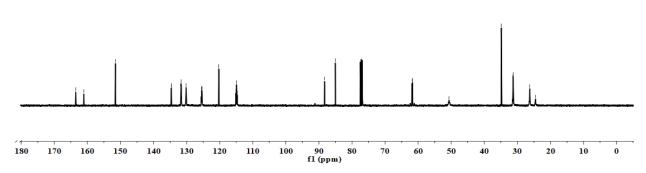


Figure S105: ¹³C NMR spectrum of 8ak taking CDCl₃ as solvent.

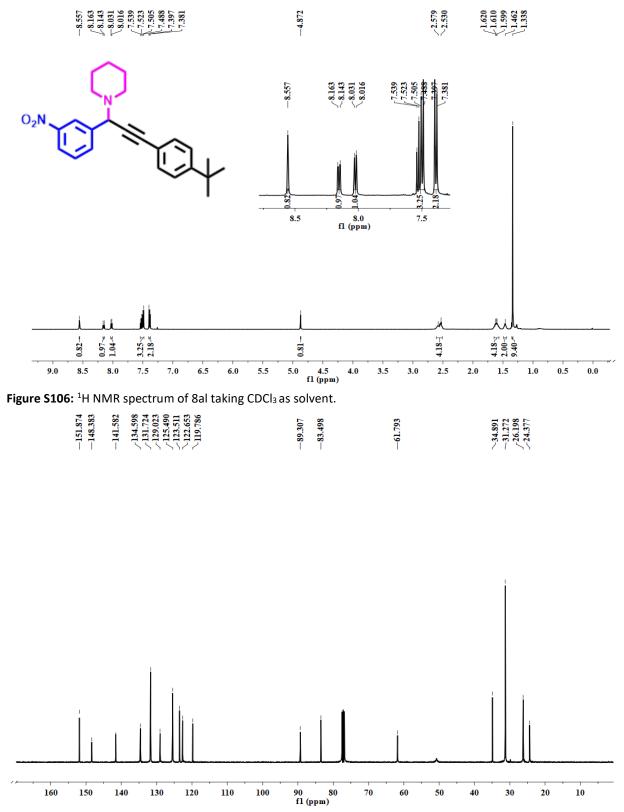


Figure S107: ¹³C NMR spectrum of 8al taking CDCl₃ as solvent.

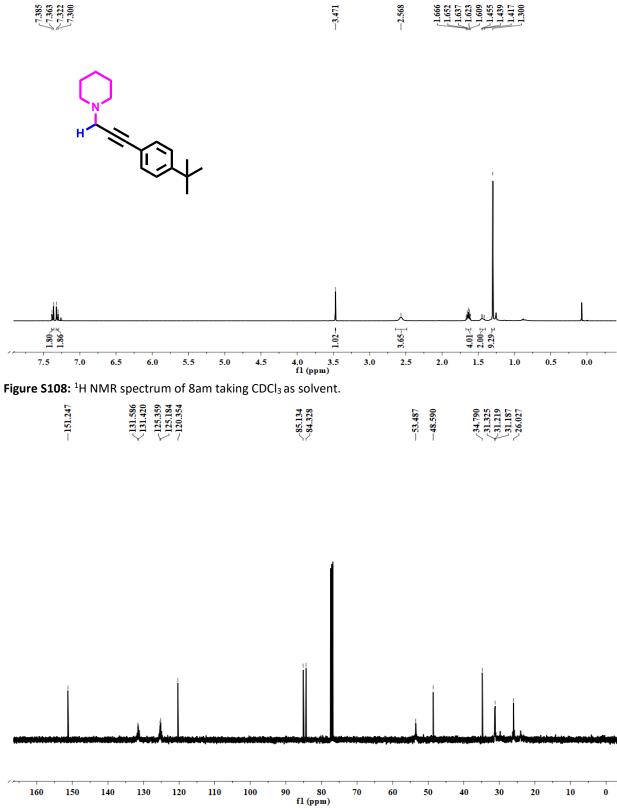


Figure S109: $^{\rm 13}{\rm C}$ NMR spectrum of 8am taking CDCl3 as solvent.

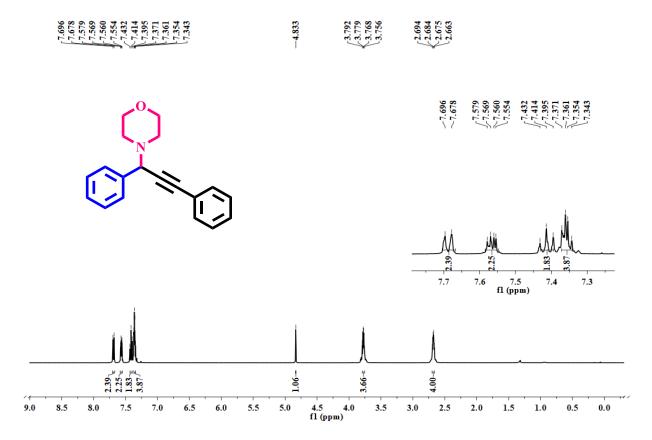


Figure S110: ¹H NMR spectrum of 9aa taking CDCl₃ as solvent.

-137.958 -137.958 -128.724 -128.460 -128.461 -127.93 -123.121 -123.121		-67.281 62.182 £62.164
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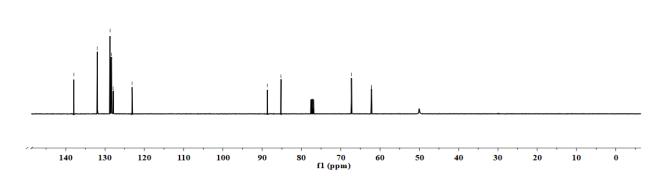
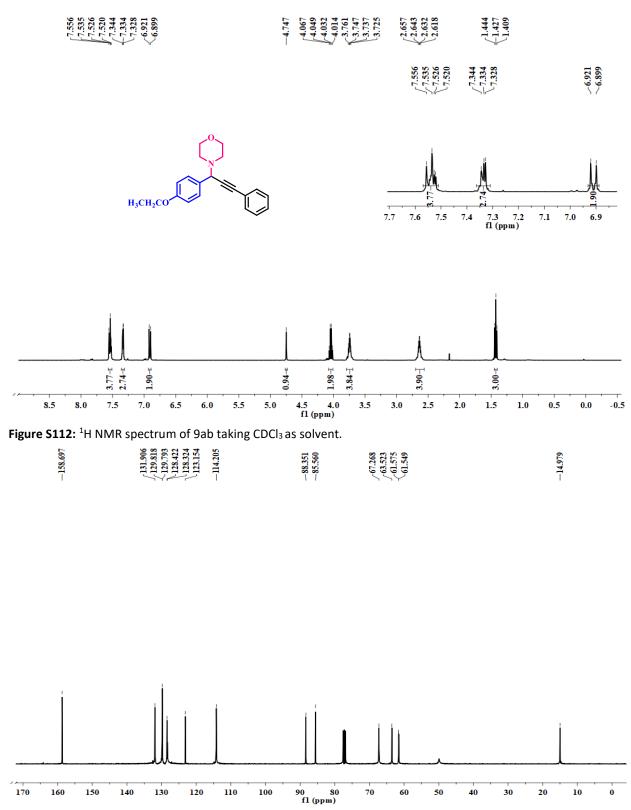
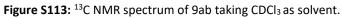


Figure S111: ¹³C NMR spectrum of 9aa taking CDCl₃ as solvent.





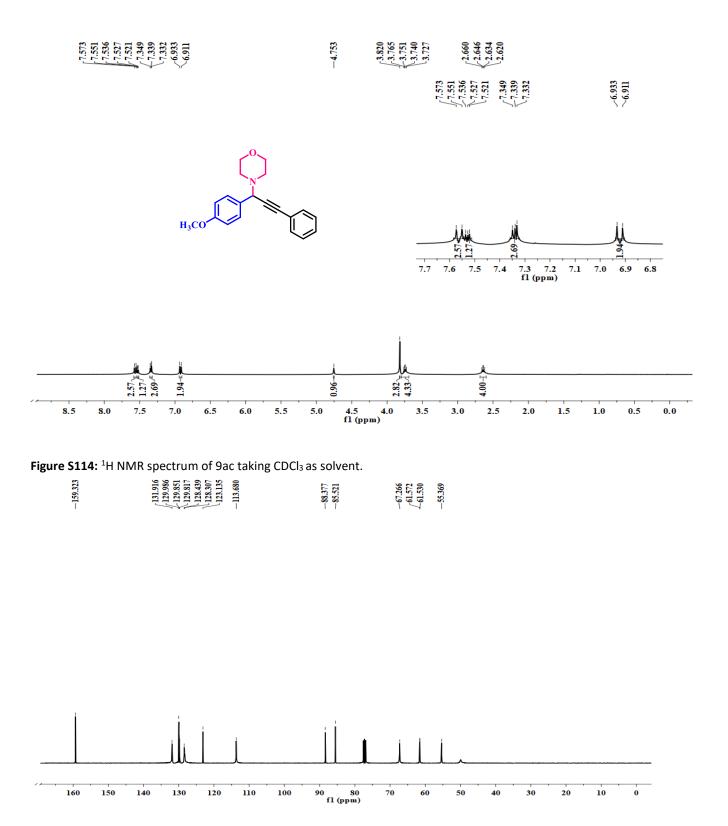
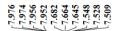


Figure S115: ¹³C NMR spectrum of 9ac taking CDCl₃ as solvent.



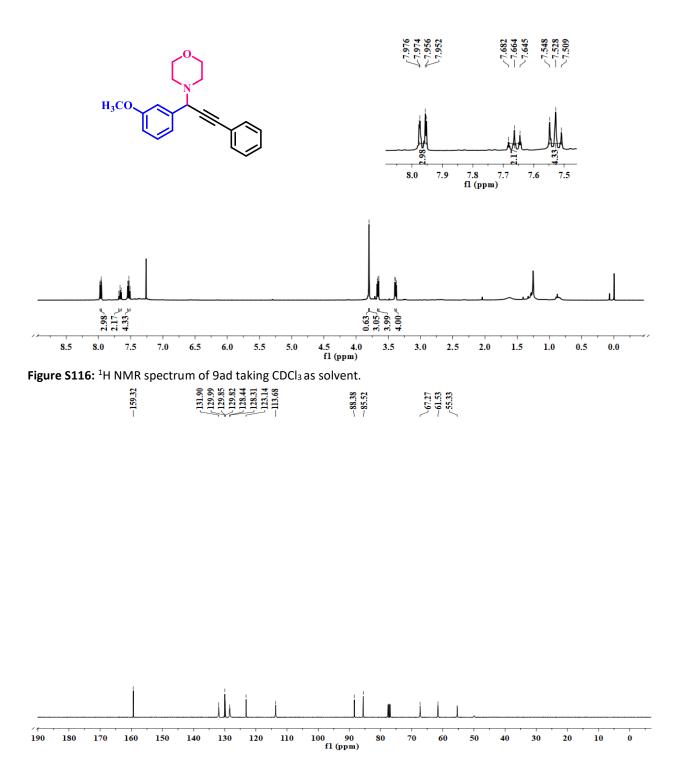
 3.809
 3.809

 3.672
 3.672

 3.648
 3.648

 3.400
 3.337

 3.375
 3.375





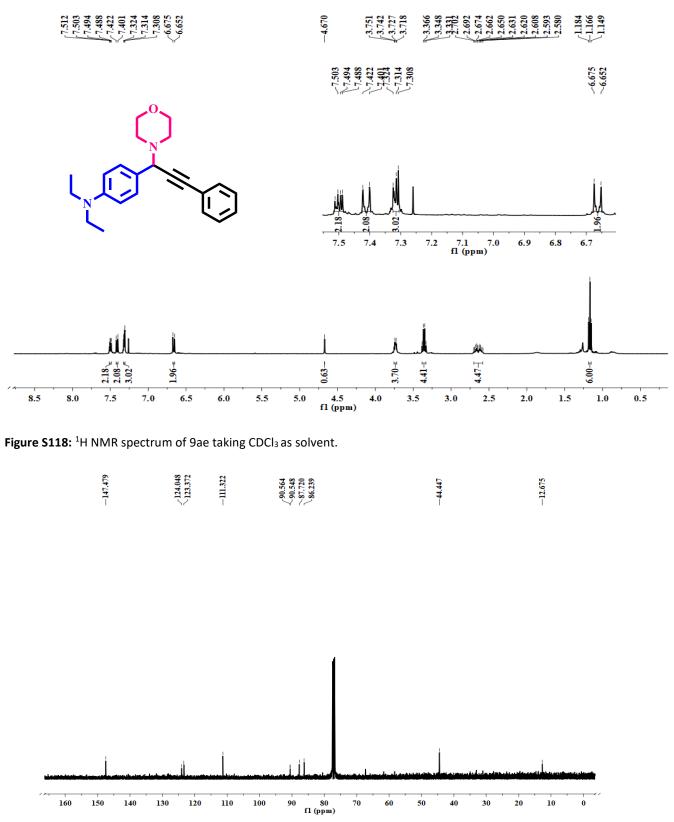


Figure S119: $^{\rm 13}{\rm C}$ NMR spectrum of 9ae taking CDCl3 as solvent.

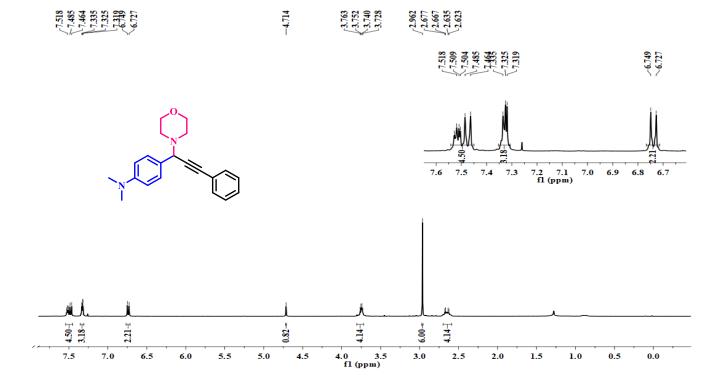
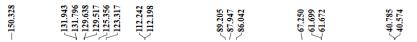


Figure S120: ¹H NMR spectrum of 9af taking CDCl₃ as solvent.



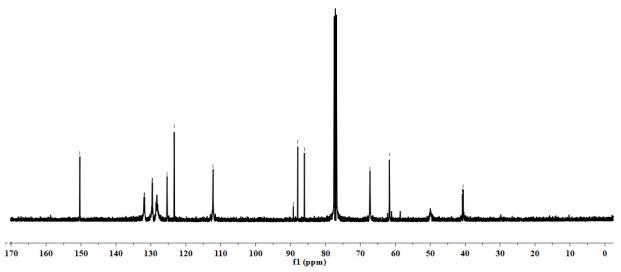
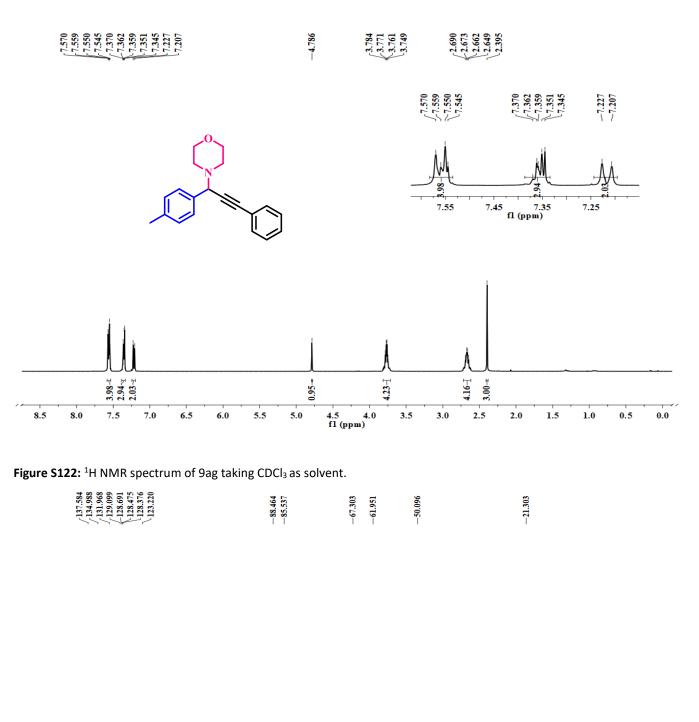


Figure S121: ¹³C NMR spectrum of 9af taking CDCl₃ as solvent.



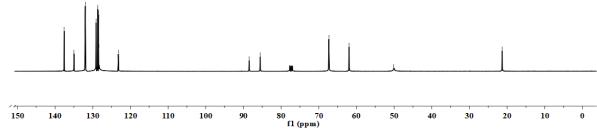


Figure S123: ¹³C NMR spectrum of 9ag taking CDCl₃ as solvent.

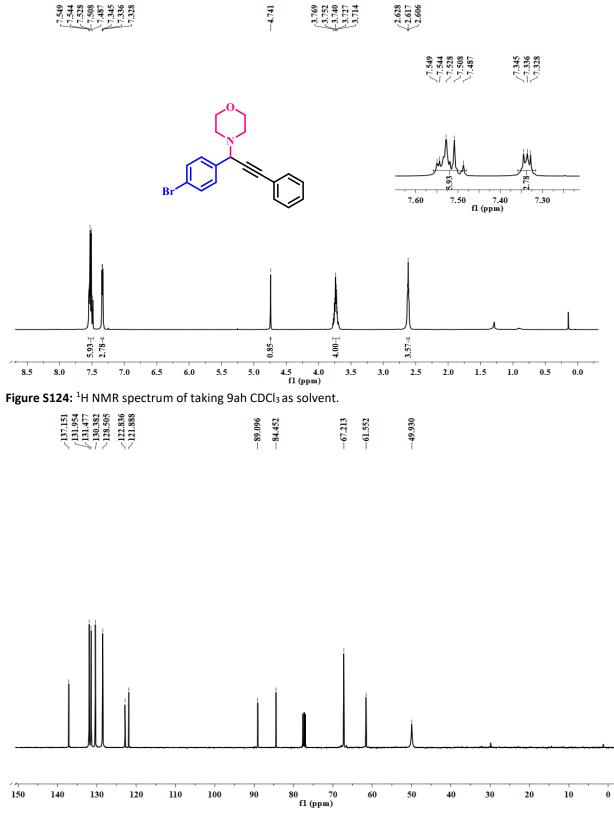
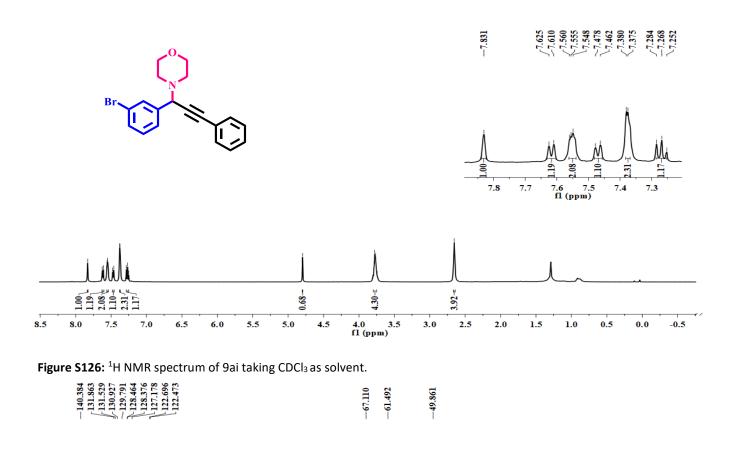


Figure S125: ¹³C NMR spectrum of 9ah taking CDCl₃ as solvent.

-2.654



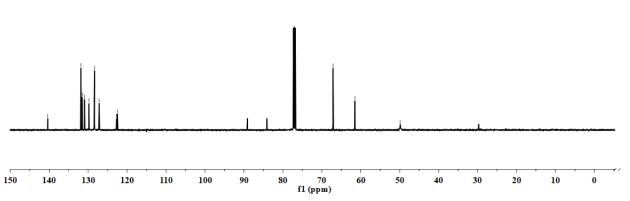
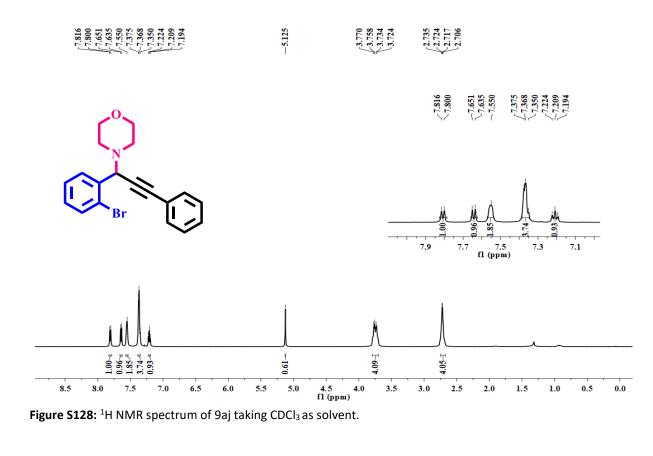
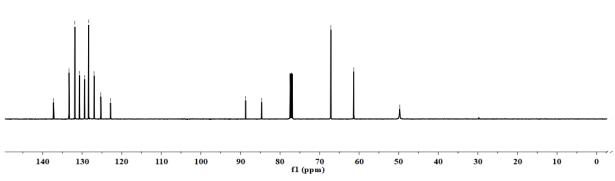
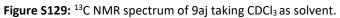


Figure S127: ¹³C NMR spectrum of 9ai taking CDCl₃ as solvent.









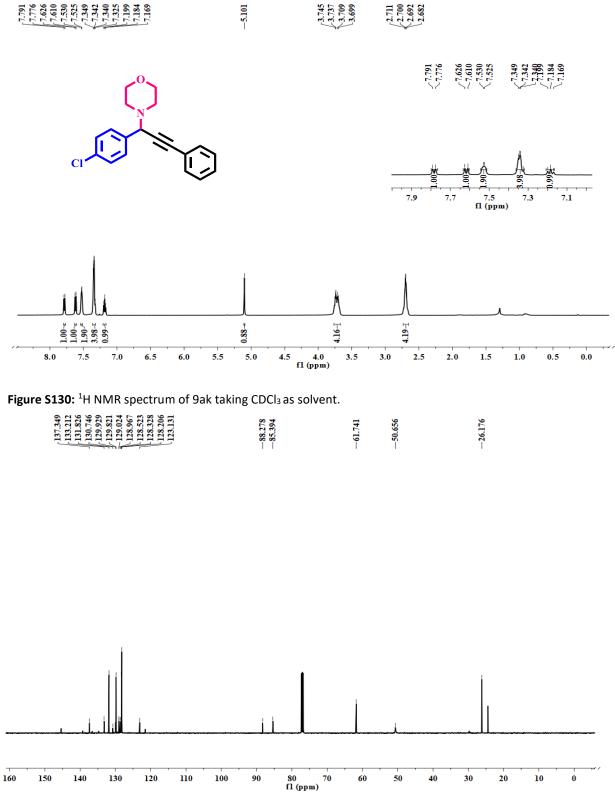
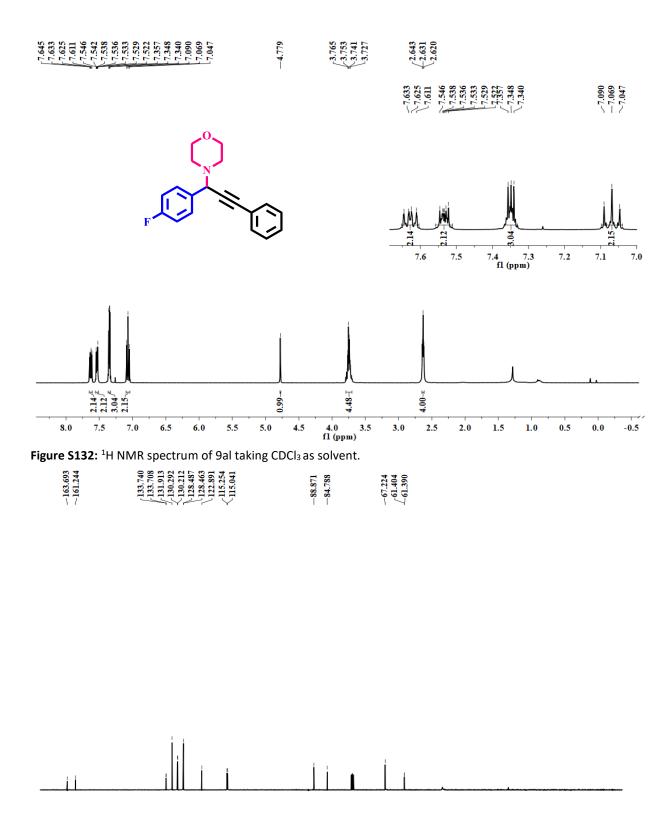


Figure S131: ¹³C NMR spectrum of 9ak taking CDCl₃ as solvent.



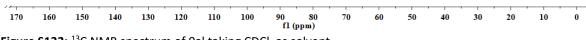


Figure S133: ¹³C NMR spectrum of 9al taking CDCl₃ as solvent.

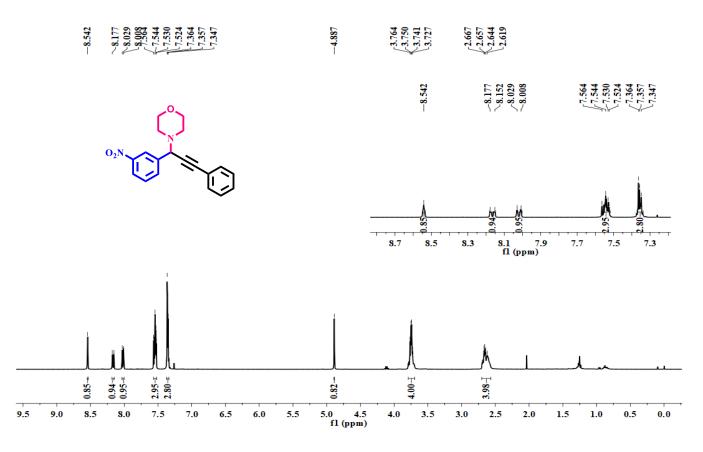


Figure S134: ¹H NMR spectrum of 9am taking CDCl₃ as solvent.

-148.454 -140.503 -140.503 -134.629 -131.976 -129.260 -129.260 -128.552 -128.552 -128.552 -128.552 -128.552 -122.599 -122.599	-89.905 -83.263	-67.103 -61.412

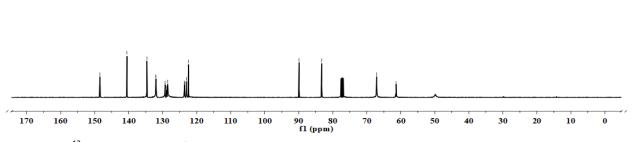


Figure S135: ¹³C NMR spectrum of 9am taking CDCl₃ as solvent.

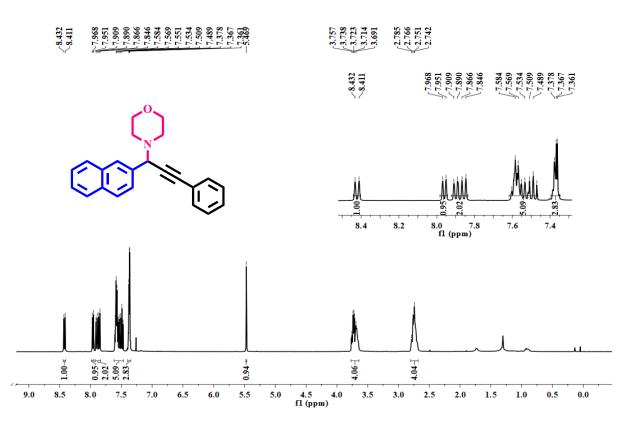


Figure S136: ¹H NMR spectrum of 9an taking CDCl₃ as solvent.



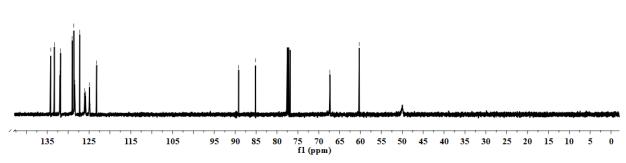
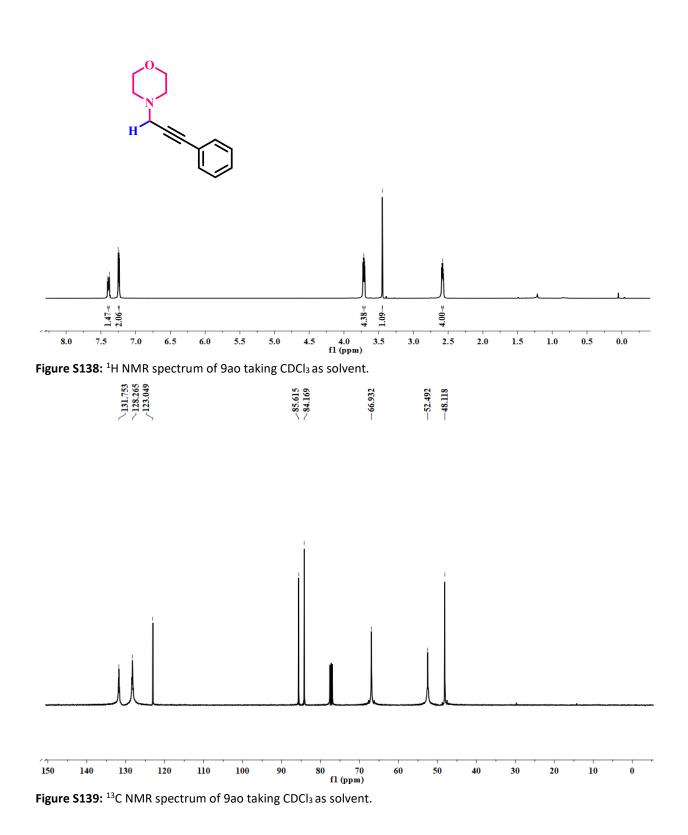


Figure S137: ¹³C NMR spectrum of 9an taking CDCl₃ as solvent.



3.724 3.713 3.701 3.447 2.592 2.592 2.569



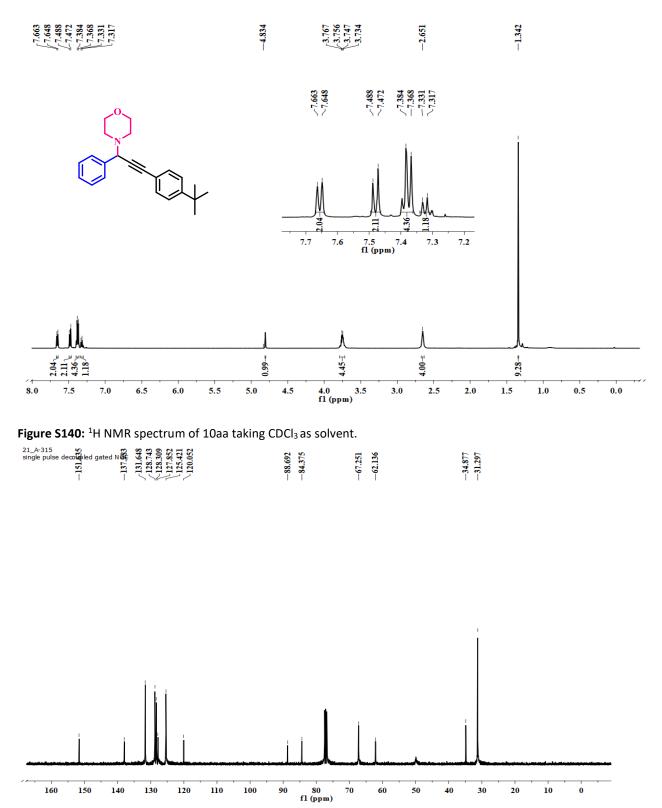
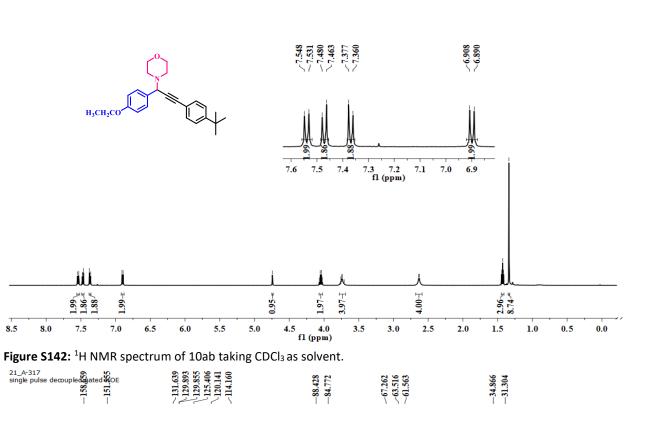


Figure S141: ¹³C NMR spectrum of 10aa taking CDCl₃ as solvent.





 $<^{2.637}_{2.629}$

-1.444 -1.430 -1.416 -1.338

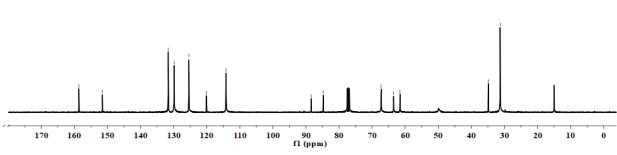


Figure S143: ¹³C NMR spectrum of 10ab taking CDCl₃ as solvent.

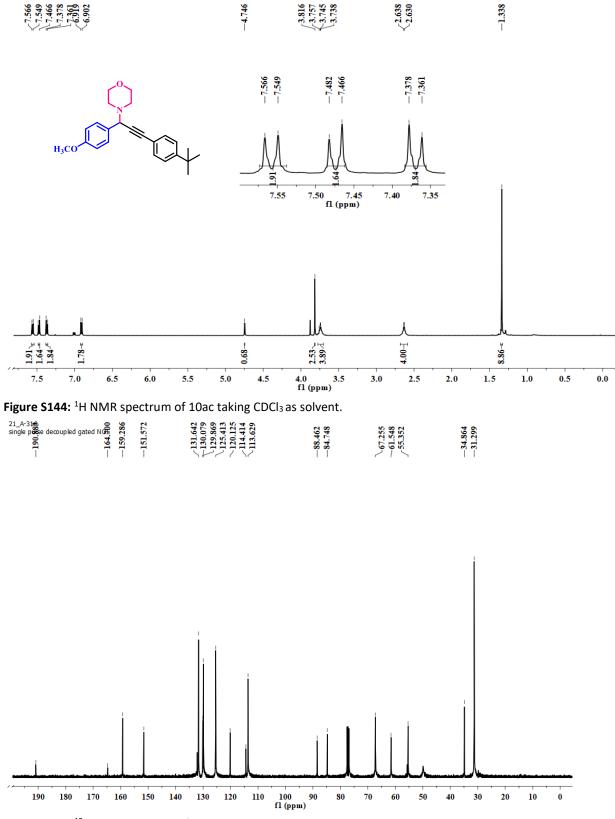


Figure S145: $^{\rm 13}{\rm C}$ NMR spectrum of 10ac taking CDCl3 as solvent.

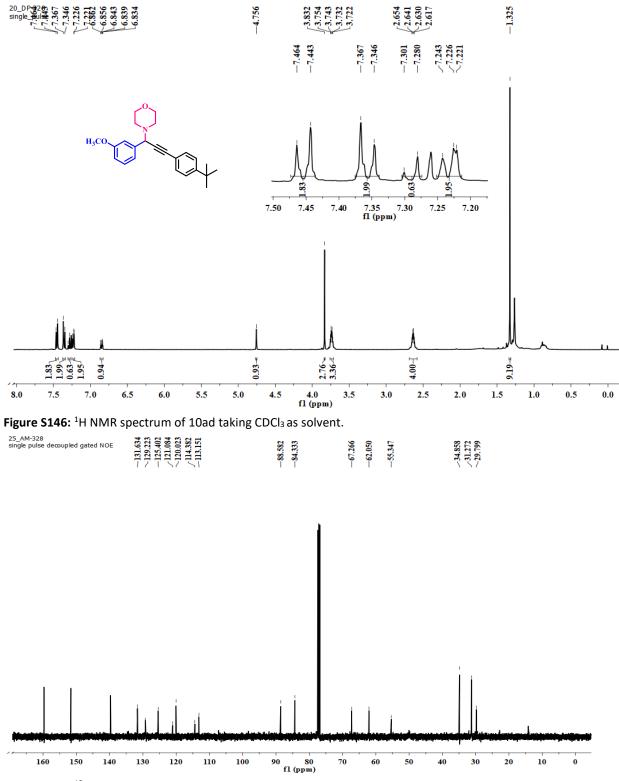
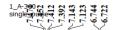


Figure S147: ¹³C NMR spectrum of 10ad taking CDCl₃ as solvent.



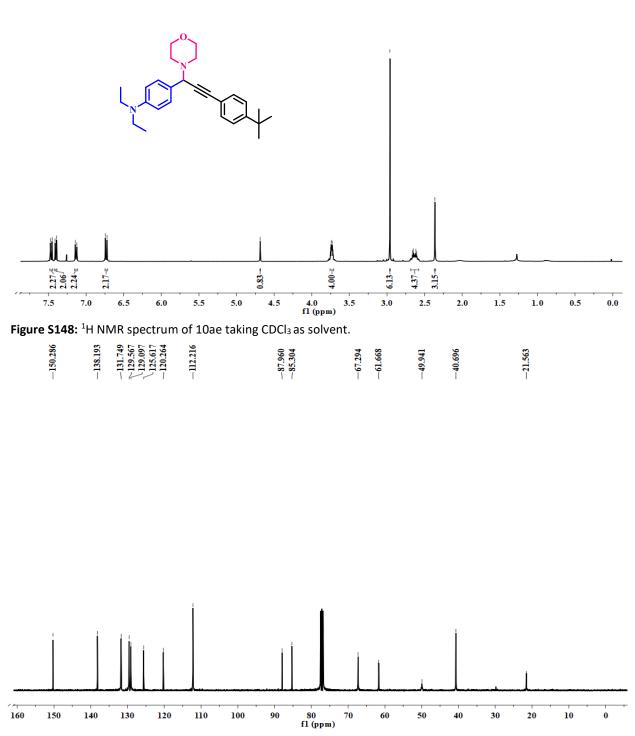
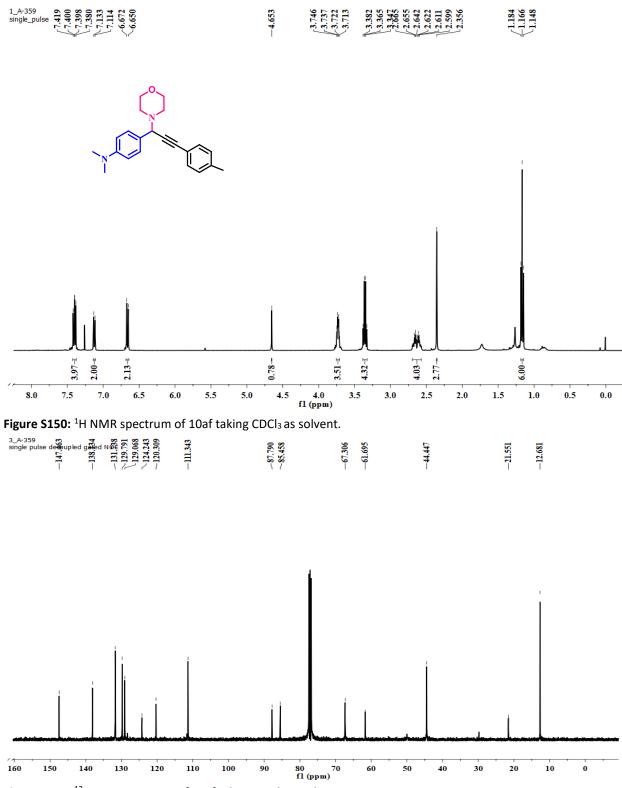
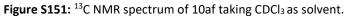


Figure S149: ¹³C NMR spectrum of 10ae taking CDCl₃ as solvent.





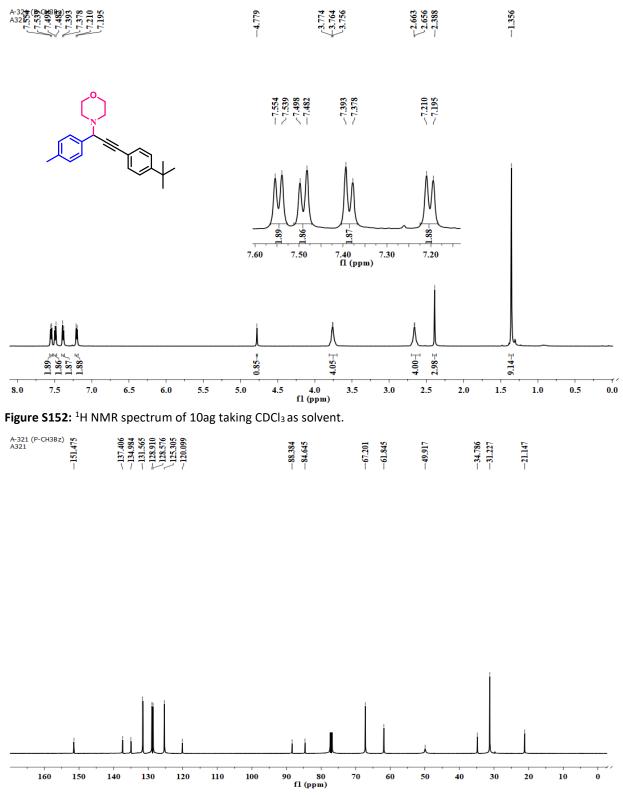
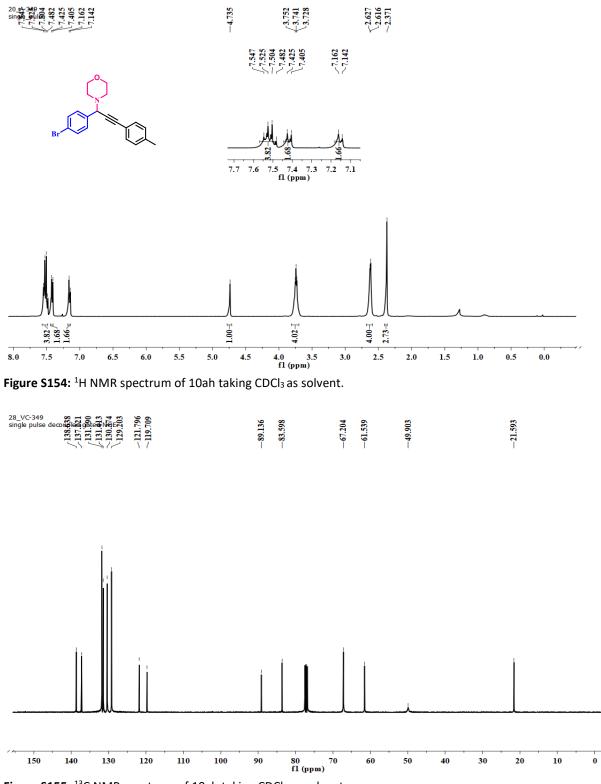
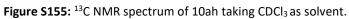
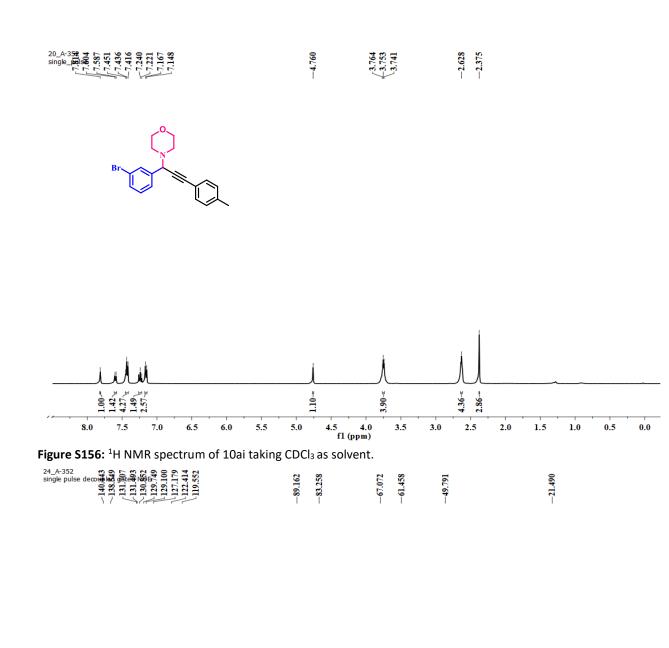


Figure S153: ¹³C NMR spectrum of 10ag taking CDCl₃ as solvent.







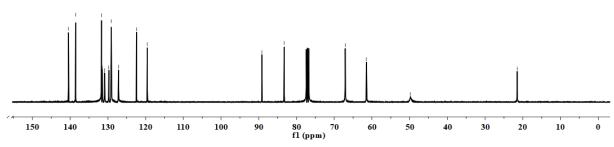


Figure S157: ¹³C NMR spectrum of 10ai taking CDCl₃ as solvent.

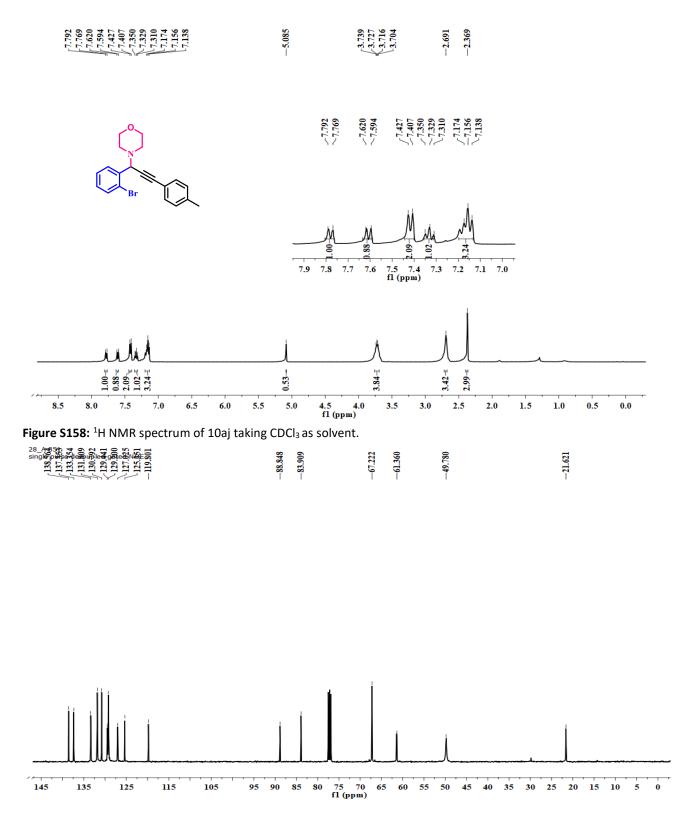


Figure S159: ¹³C NMR spectrum of 10aj taking CDCl₃ as solvent.

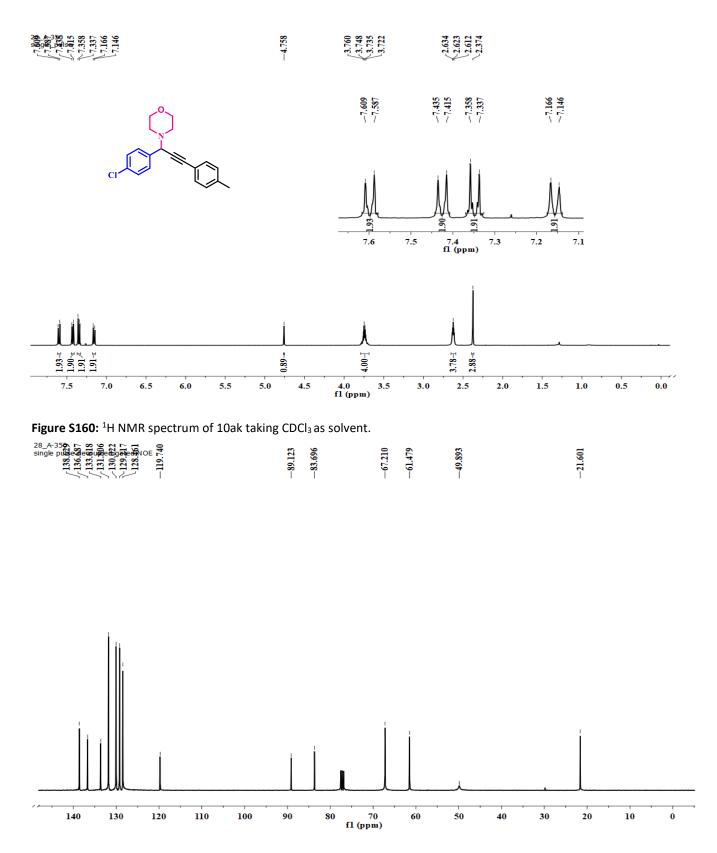


Figure S161: ¹³C NMR spectrum of 10ak taking CDCl₃ as solvent.

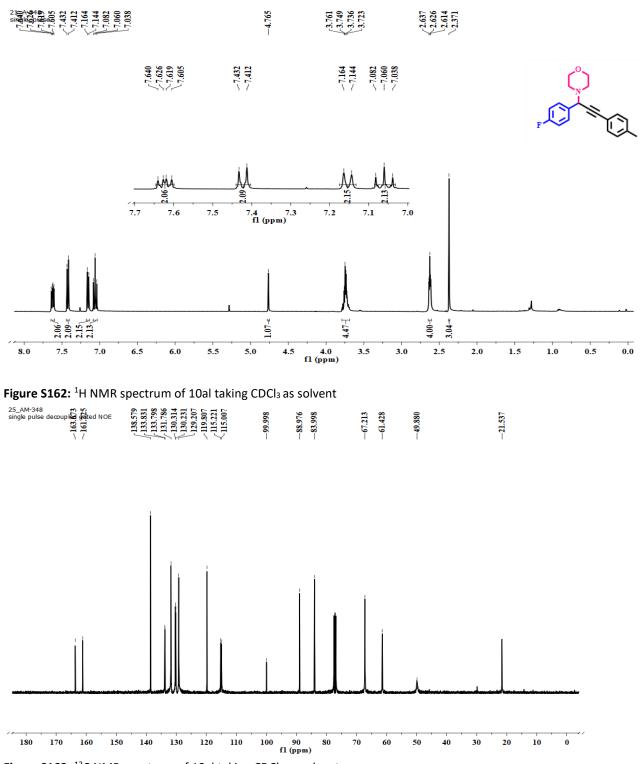


Figure S163: ¹³C NMR spectrum of 10al taking CDCl₃ as solvent.

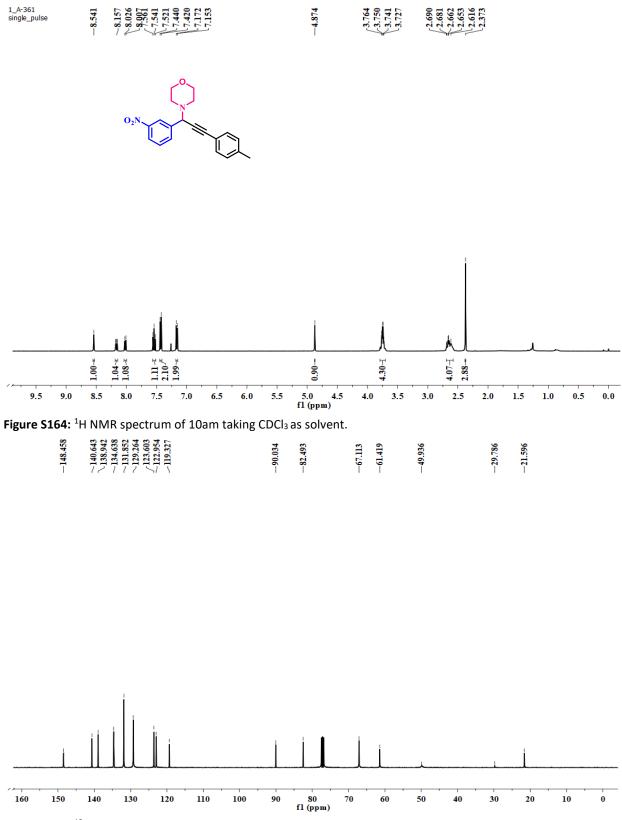
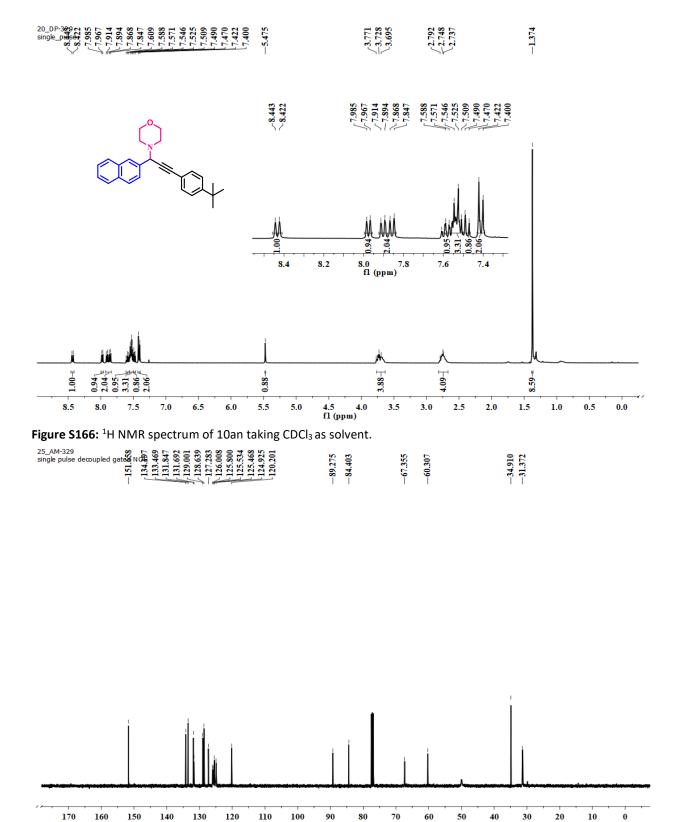
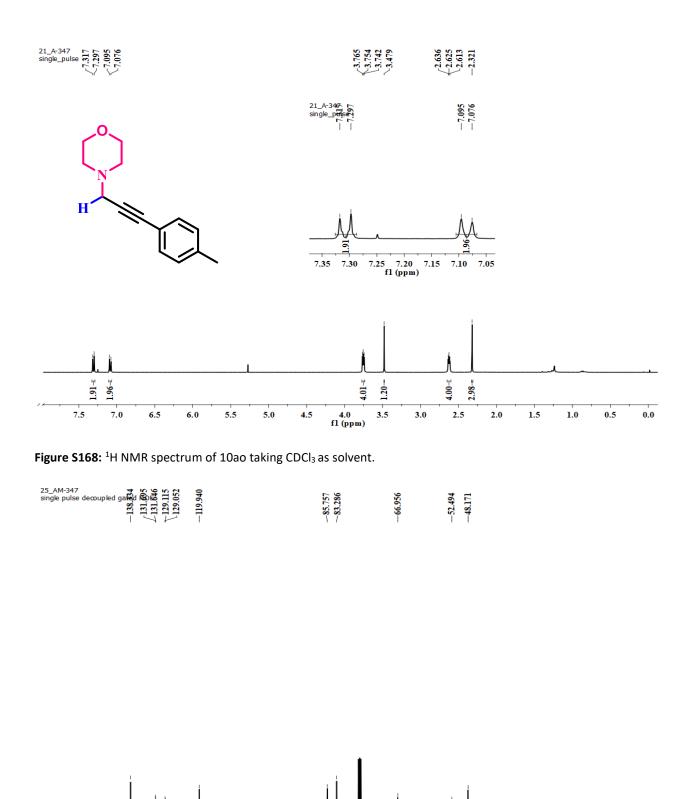


Figure S165: ¹³C NMR spectrum of 10am taking CDCl₃ as solvent.



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 fl (ppm)

Figure S167: ¹³C NMR spectrum of 10an taking CDCl₃ as solvent.



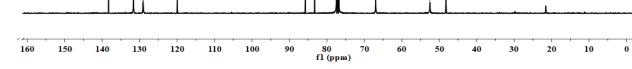


Figure S169: ¹³C NMR spectrum of 10ao taking CDCl₃ as solvent.