

Electronic Supporting Information for

Polymerization of 1-chloro-2-phenylacetylene derivatives by using Brookhart-type catalyst

Fulin Yang,^a Shuangjie Zhang,^a Tanxiao Shen,^a Juechen Ni,^a Jie Zhang,^a Xiao Cheng,^a Jing Zhi Sun,^{*a}
Zhisheng Fu,^{*a} Ben Zhong Tang^{*a,b,c}

^a MOE Key Laboratory of Macromolecules Synthesis of Functionalization, Department of Polymer Science and Engineering, Zhejiang University, Hangzhou 310027, China.

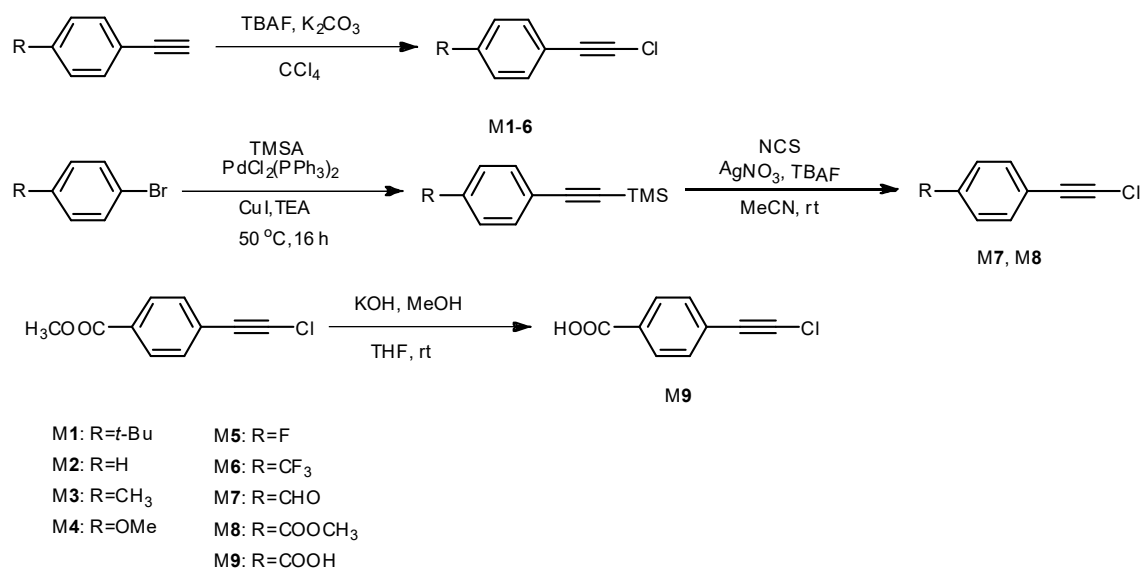
^b State Key Laboratory of Luminescent Materials and Devices, Center for Aggregation-Induced Emission, South China University of Technology, Guangzhou 510640, China.

^c Department of Chemistry, Hong Kong Branch of Chinese National Engineering Research Center for Tissue Restoration and Reconstruction, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong, China.

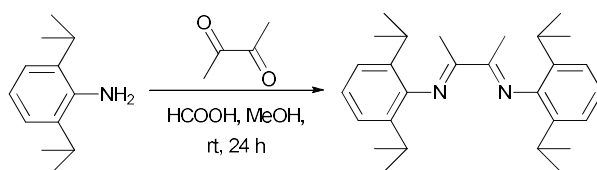
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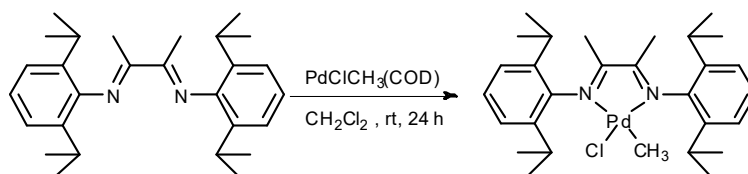
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Scheme S1. Synthetic route to 1-chloro-2-[(para-substituted)-phenyl] acetylene monomers.



Scheme S2. Synthetic route to α -diimine ligand.



Scheme S3. Synthetic route to (α -diimine)PdMeCl complex.

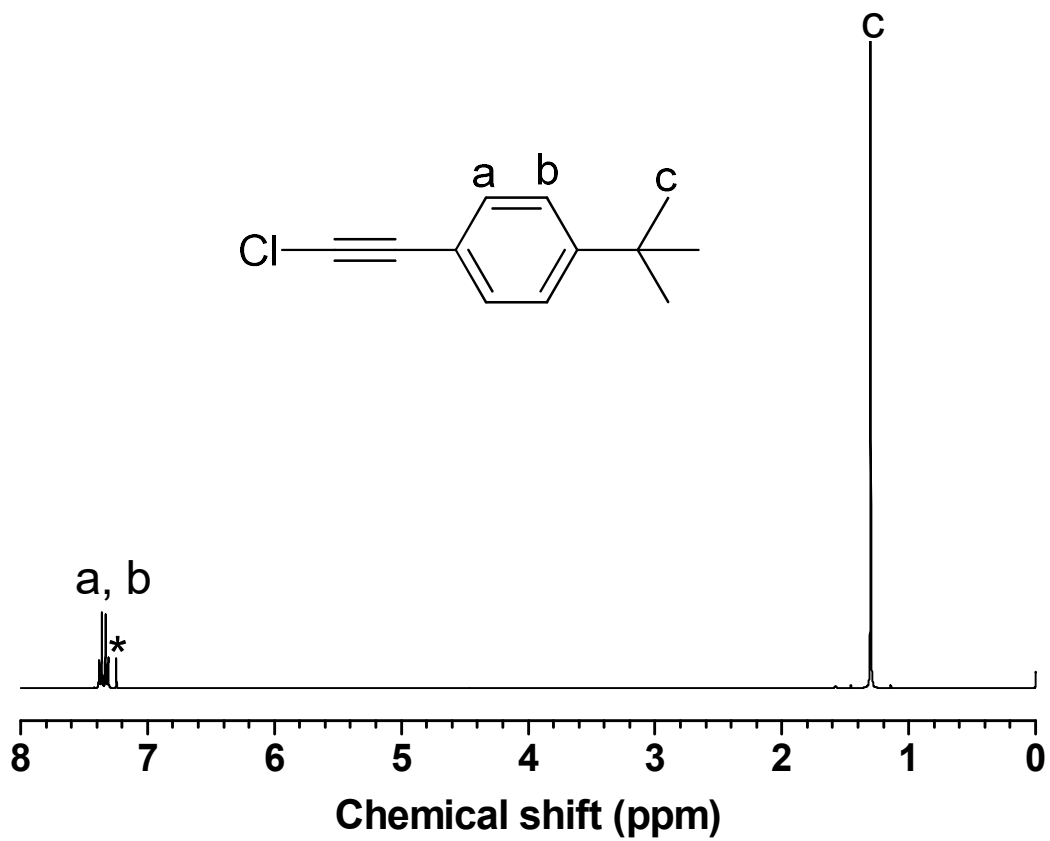


Figure S1. ¹H NMR spectrum of M1 in CDCl₃.

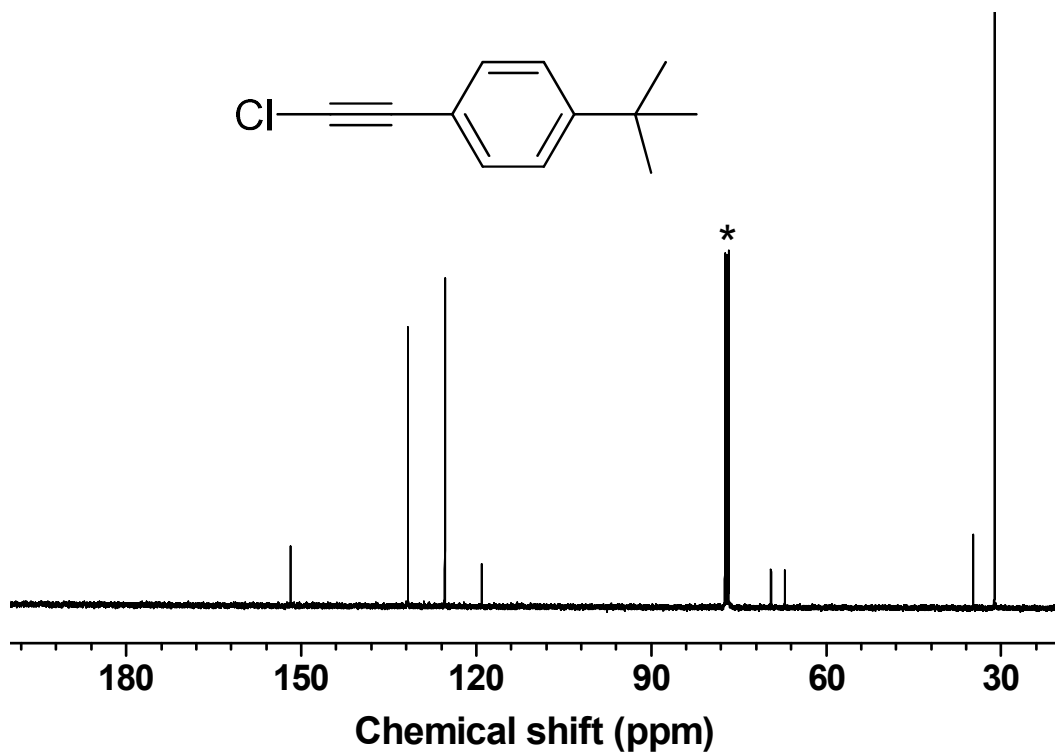


Figure S2. ¹³C NMR spectrum of M1 in CDCl₃.

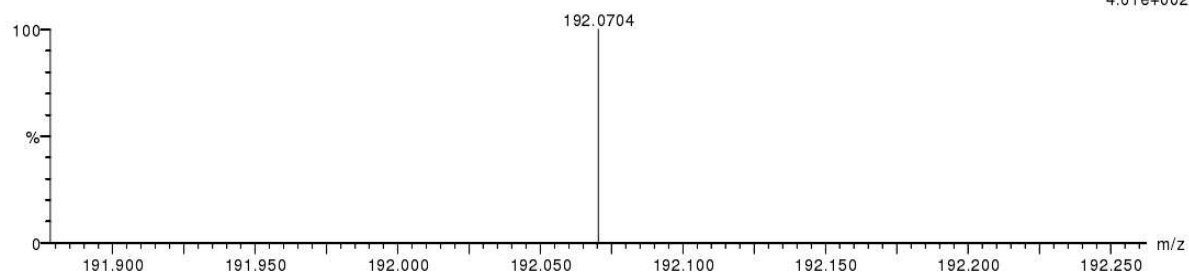
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
46 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 O: 0-10 Cl: 0-1
GCT Premier ZJU
TOF MS EI+

05-Jun-2018

yfl-nbu 977 (4.036)

4.61e+002



Minimum: -1.5
Maximum: 1.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
192.0704	192.0706	-0.2	-1.0	6.0	5546248.5	C12 H13 Cl

Figure S3. High resolution mass spectrum of M1.

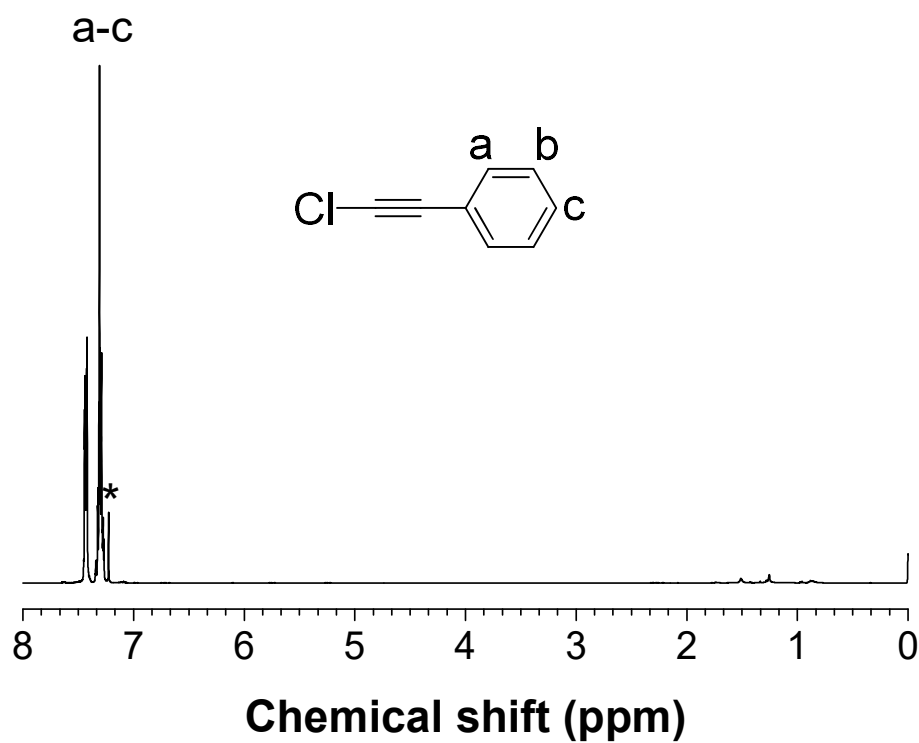


Figure S4. ¹H NMR spectrum of M2 in CDCl₃.

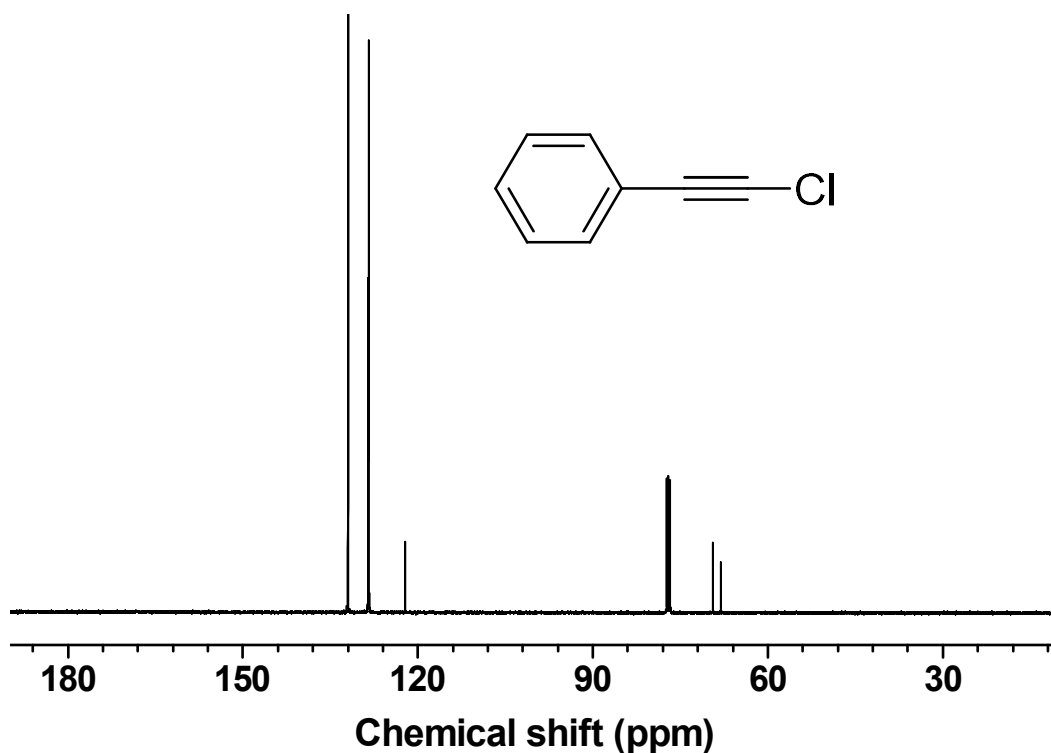


Figure S5. ^{13}C NMR spectrum of M2 in CDCl_3 .

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-200 Cl: 0-1

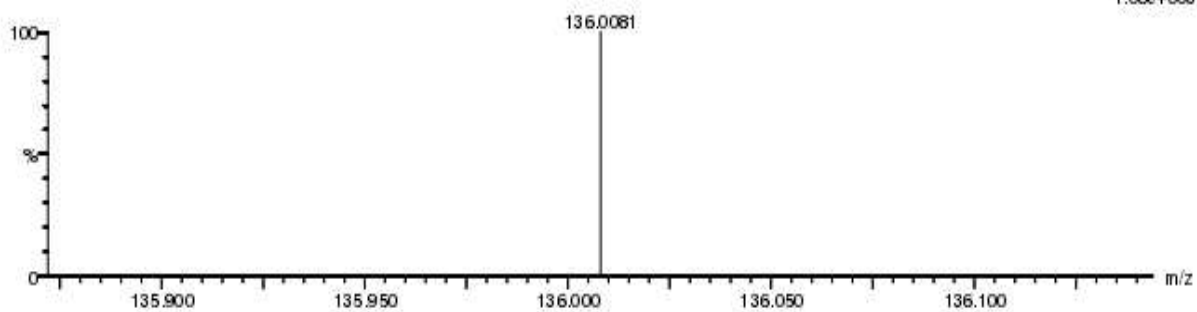
GCT Premier ZJU

TOF MS EI+

08-May-2018

y10508-1 423 (3.504)

1.08e+003



Minimum: -1.5

Maximum: 1.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
136.0081	136.0080	0.1	0.7	6.0	55.6554.5	C8 H5 Cl

Figure S6. High resolution mass spectrum of M2.

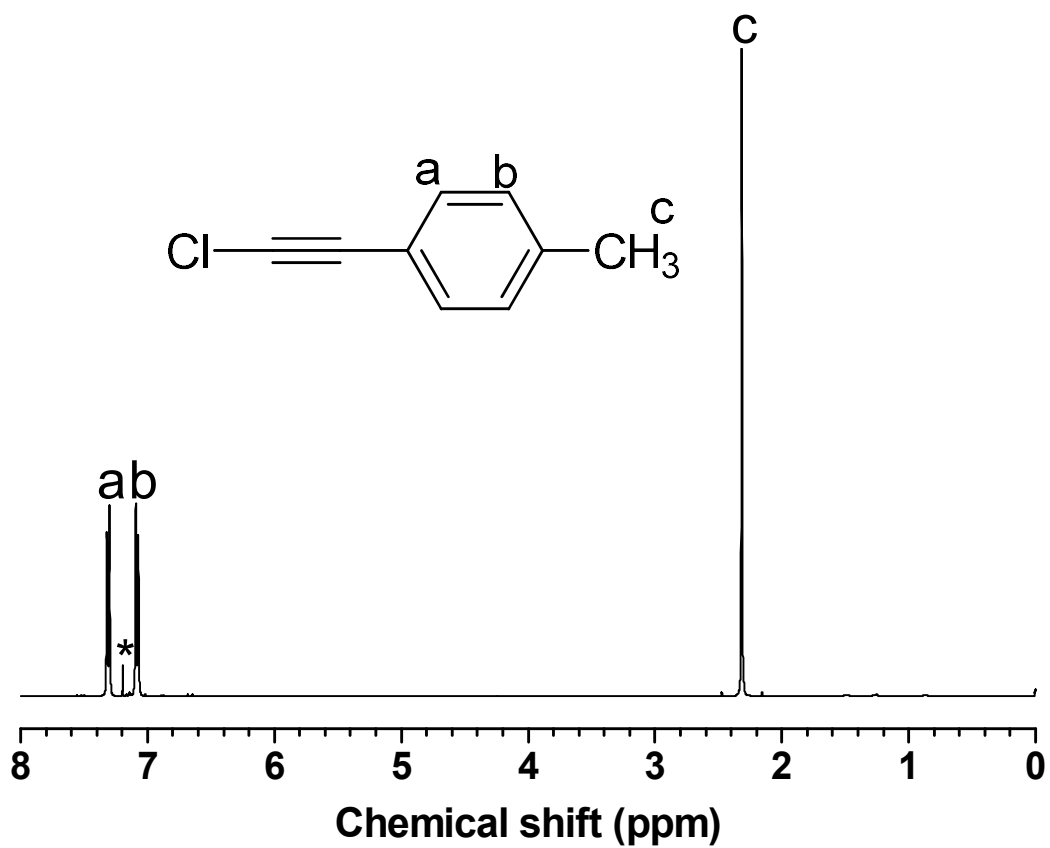


Figure S7. ¹H NMR spectrum of M3 in CDCl₃.

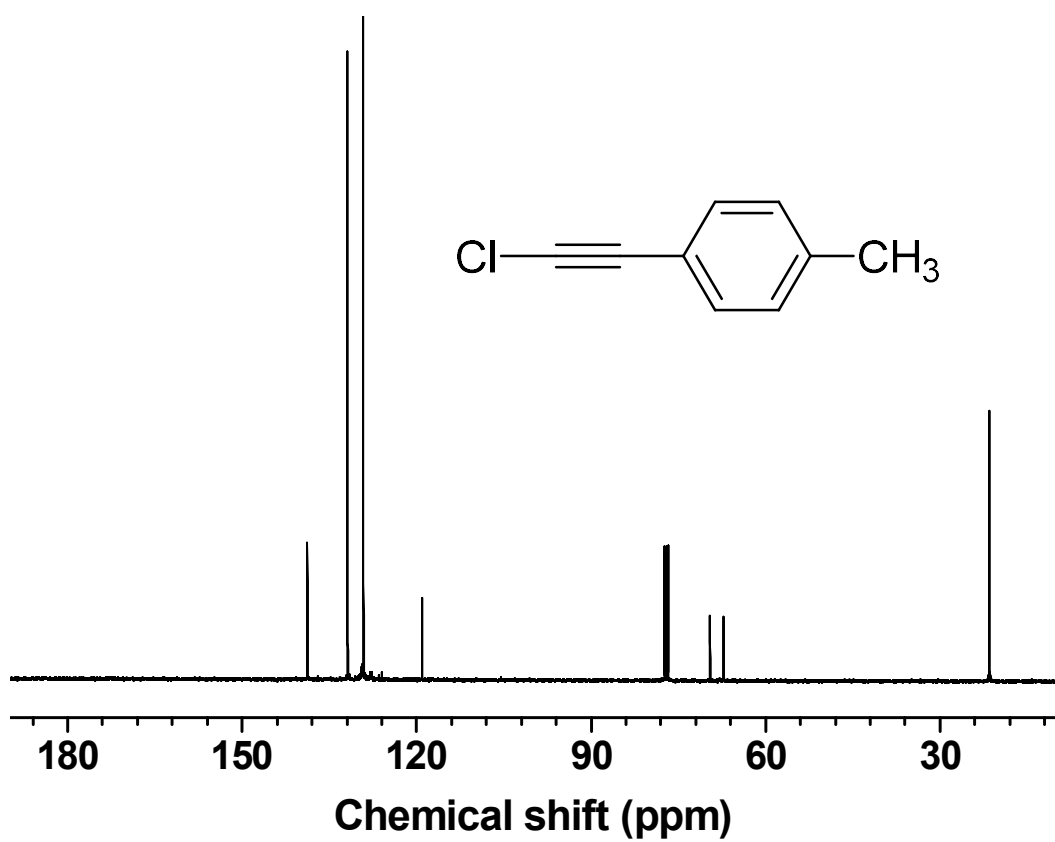


Figure S8. ¹³C NMR spectrum of M3 in CDCl₃.

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-200 Cl: 0-1

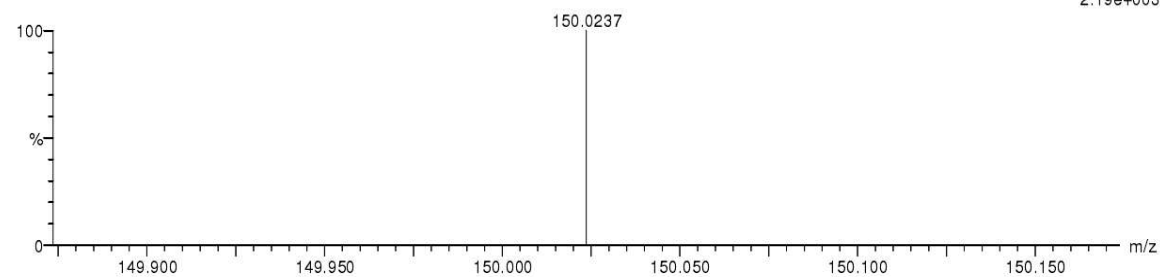
GCT Premier ZJU

TOF MS EI+

08-May-2018

yf10508-2 456 (3.625)

2.19e+003



Minimum:				-1.5		
Maximum:	1.0	10.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-RIT	Formula
150.0237	150.0236	0.1	0.7	6.0	5547112.0	C9 H7 Cl

Figure S9. High resolution mass spectrum of M3.

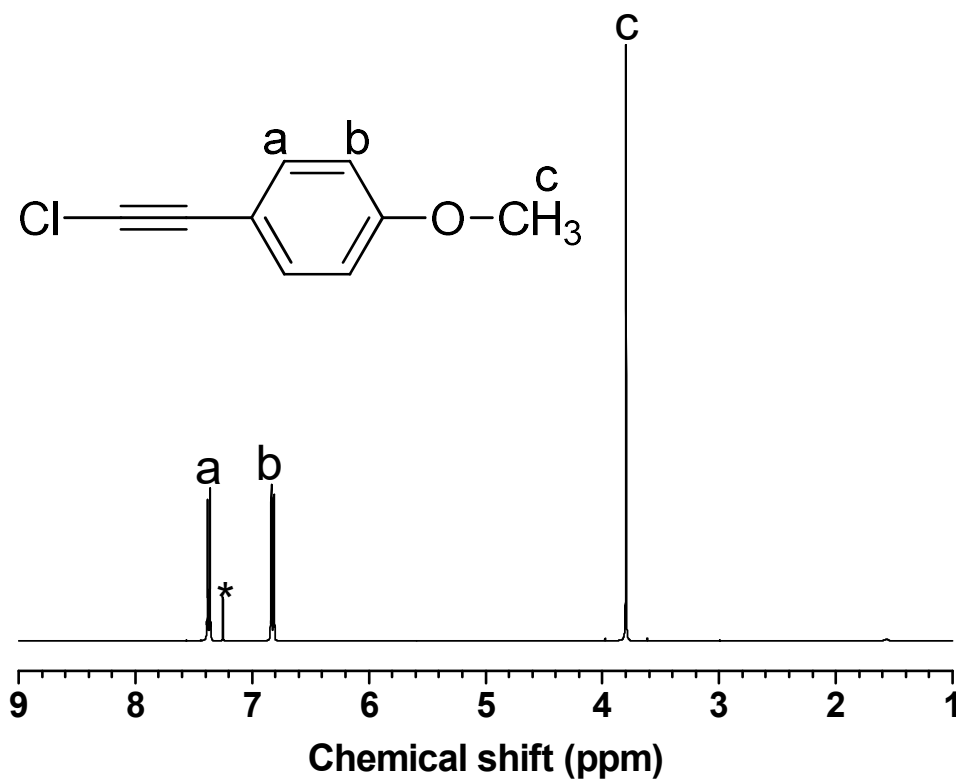


Figure S10. ¹H NMR spectrum of M4 in CDCl₃.

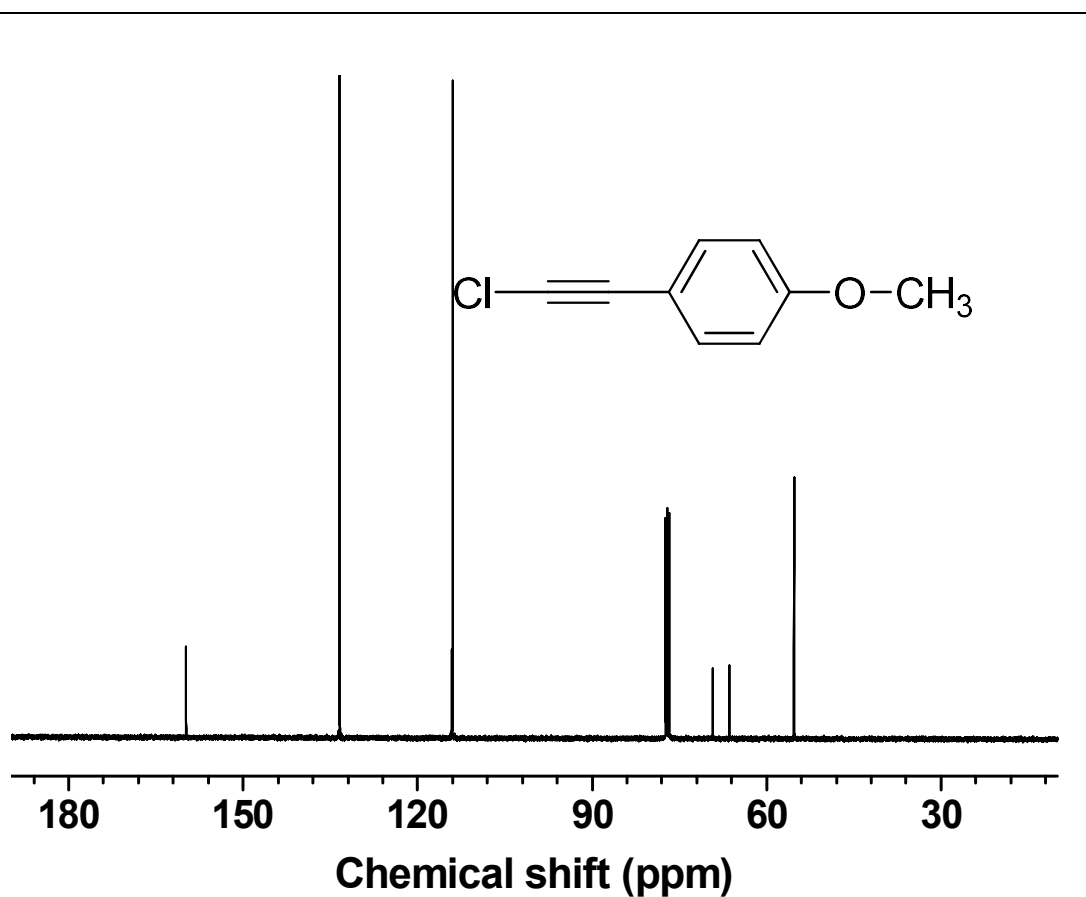


Figure S11. ^{13}C NMR spectrum of M4 in CDCl_3 .

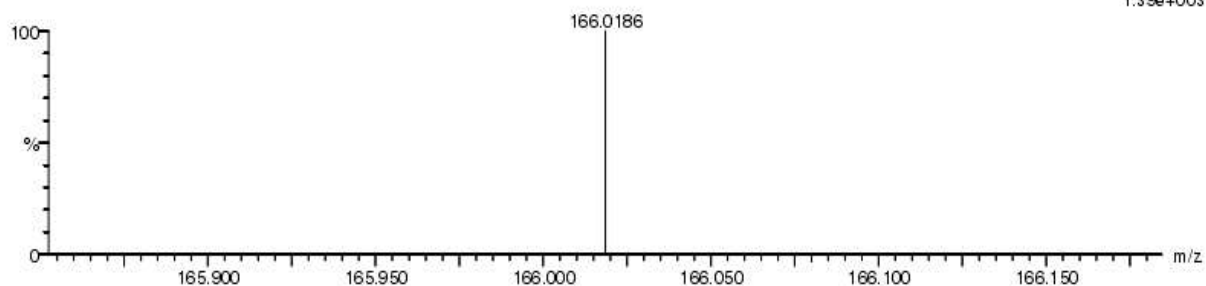
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
 72 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)
 Elements Used:
 C: 0-100 H: 0-200 N: 0-3 O: 0-4 S: 0-1 Cl: 1-1
 GCT Premier ZJU
 TOF MS EI+

12-Apr-2018

yfID412-1 615 (4.208)

1.39e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
166.0186	166.0185	0.1	0.6	6.0	5546710.0	C9 H7 O Cl

Figure S12. High resolution mass spectrum of M4.

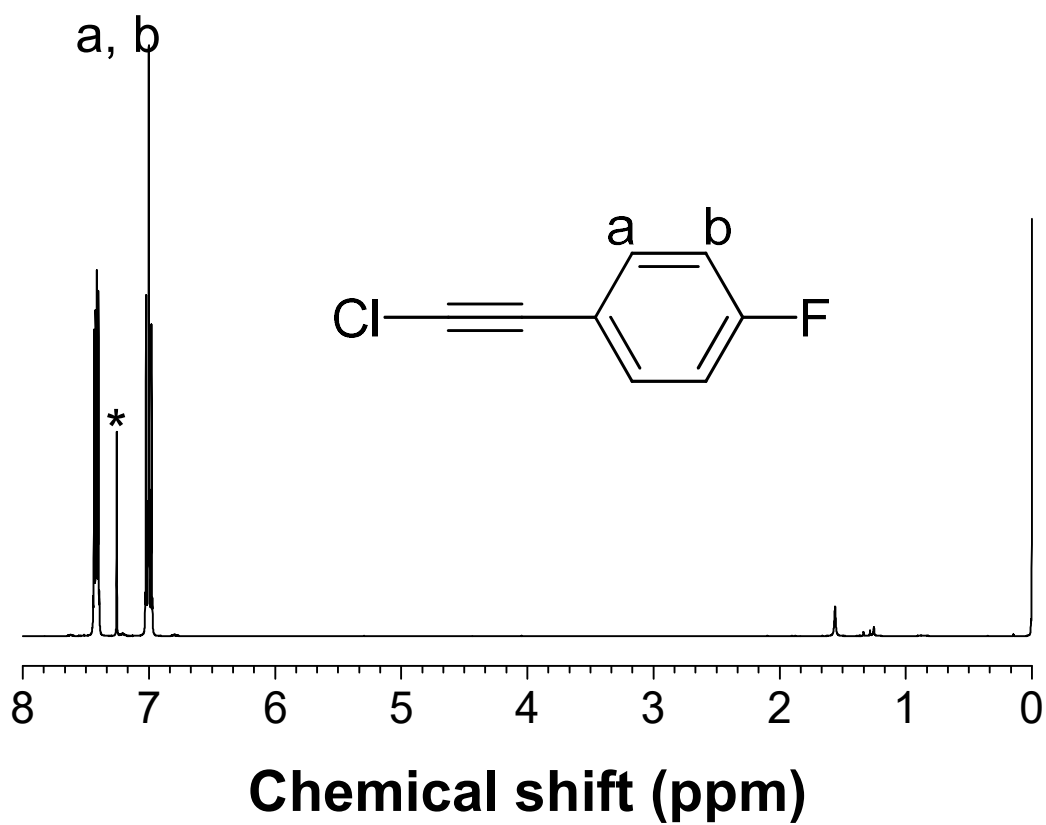


Figure S13. ^1H NMR spectrum of M5 in CDCl_3 .

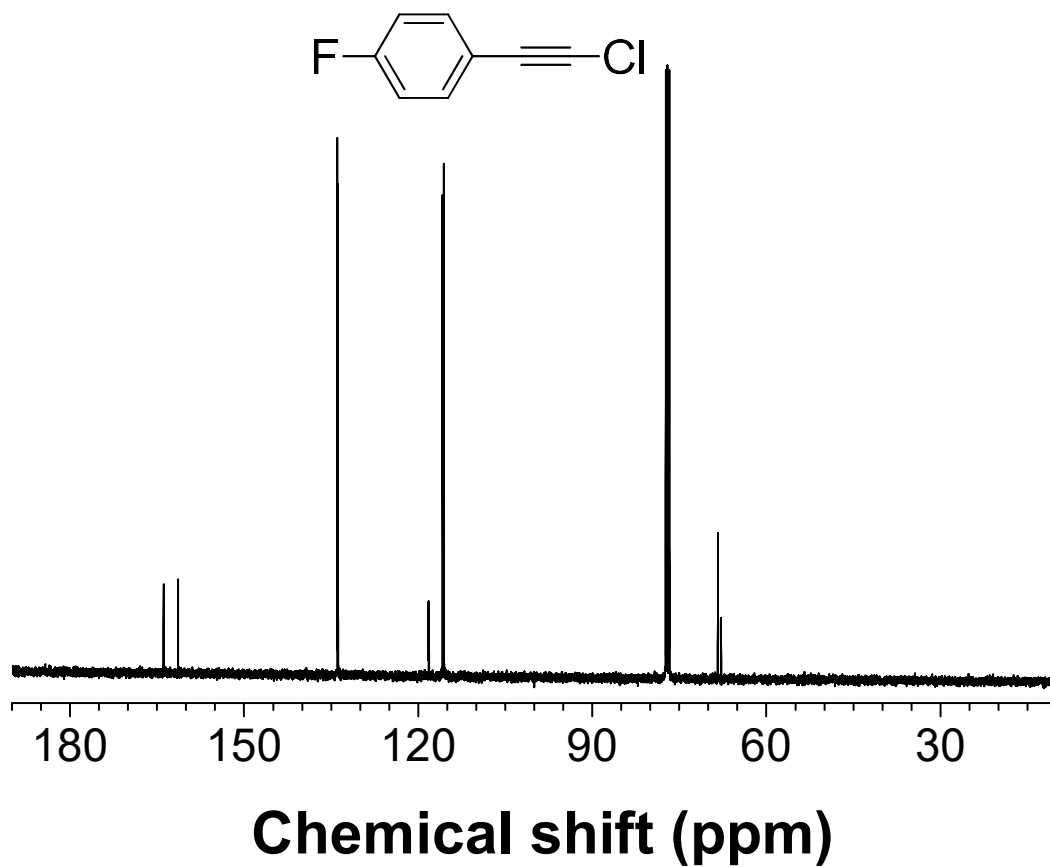


Figure S14. ^{13}C NMR spectrum of M5 in CDCl_3 .

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

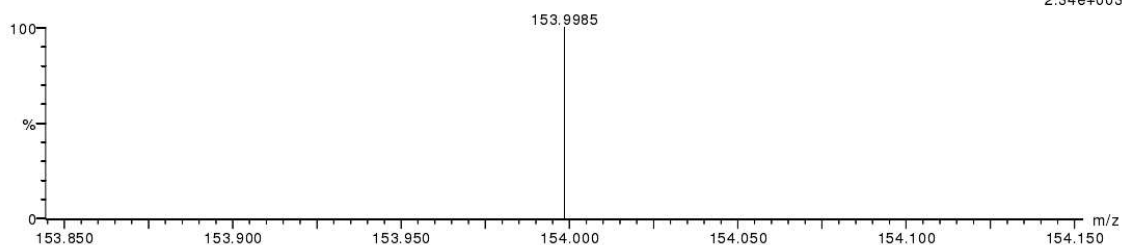
Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-200 Cl: 0-1 F: 0-1

GCT Premier ZJU
TOF MS EI+

08-May-2018

yfl0508-4 345 (3.218)

2.34e+003



Minimum:
Maximum:

1.0 10.0 -1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
153.9985	153.9986	-0.1	-0.6	6.0	5547185.0	C8 H4 Cl F

Figure S15. High resolution mass spectrum of M5.

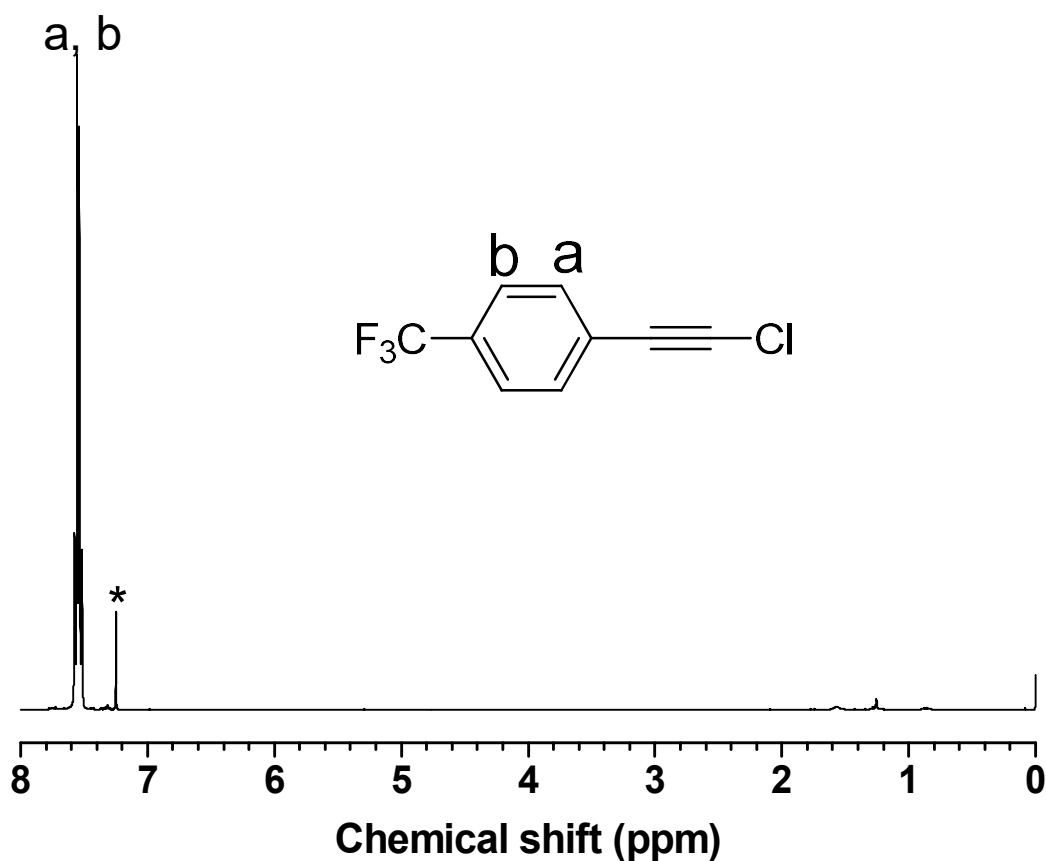


Figure S16. ^1H NMR spectrum of M6 in CDCl_3 .

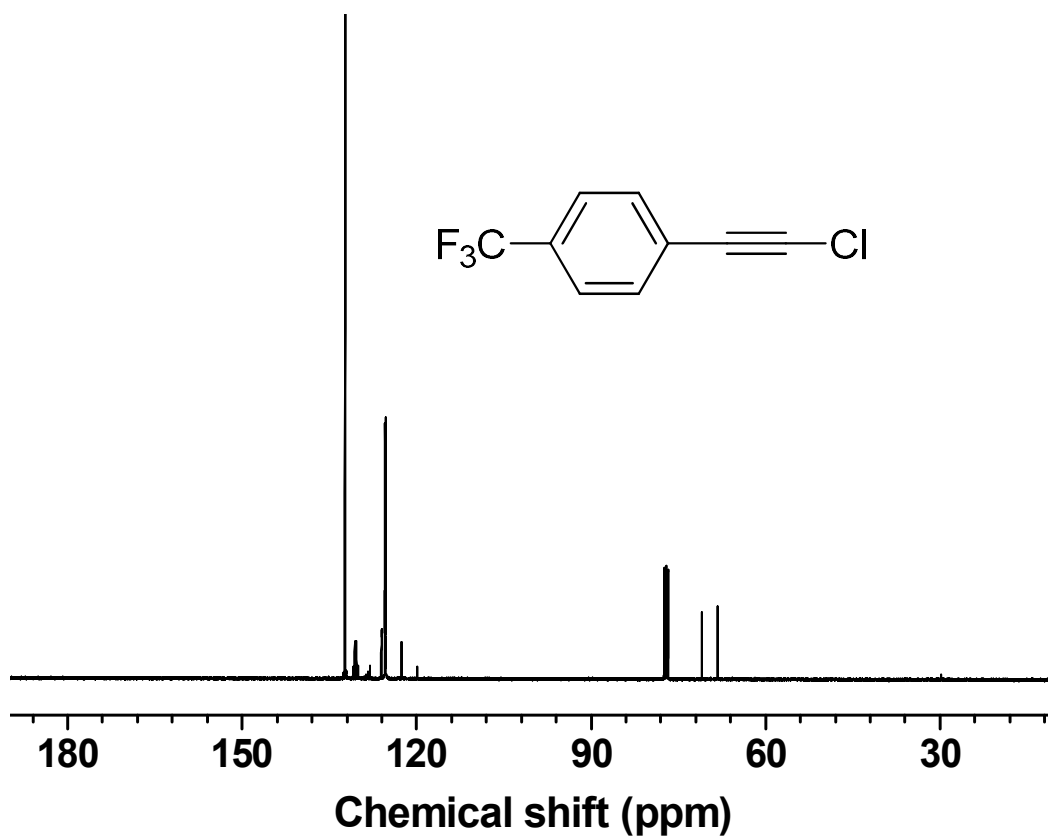


Figure S17. ^{13}C NMR spectrum of M6 in CDCl_3 .

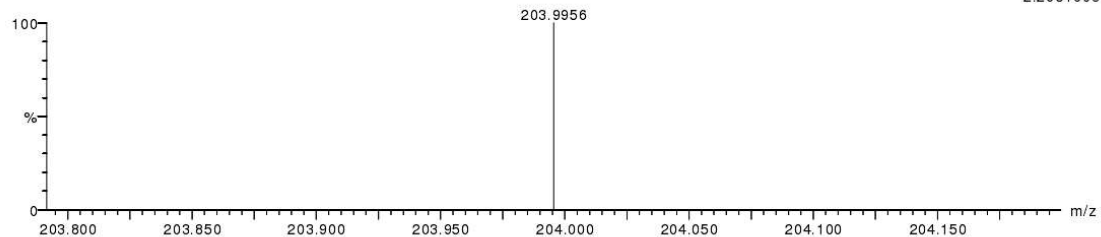
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-200 F: 0-3 Cl: 0-1
GCT Premier ZJU
TOF MS EI+

08-May-2018

yfl0508-5 370 (3.309)

2.26e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
203.9956	203.9954	0.2	1.0	6.0	5547147.0	C9 H4 F3 Cl

Figure S18. High resolution mass spectrum of M6.

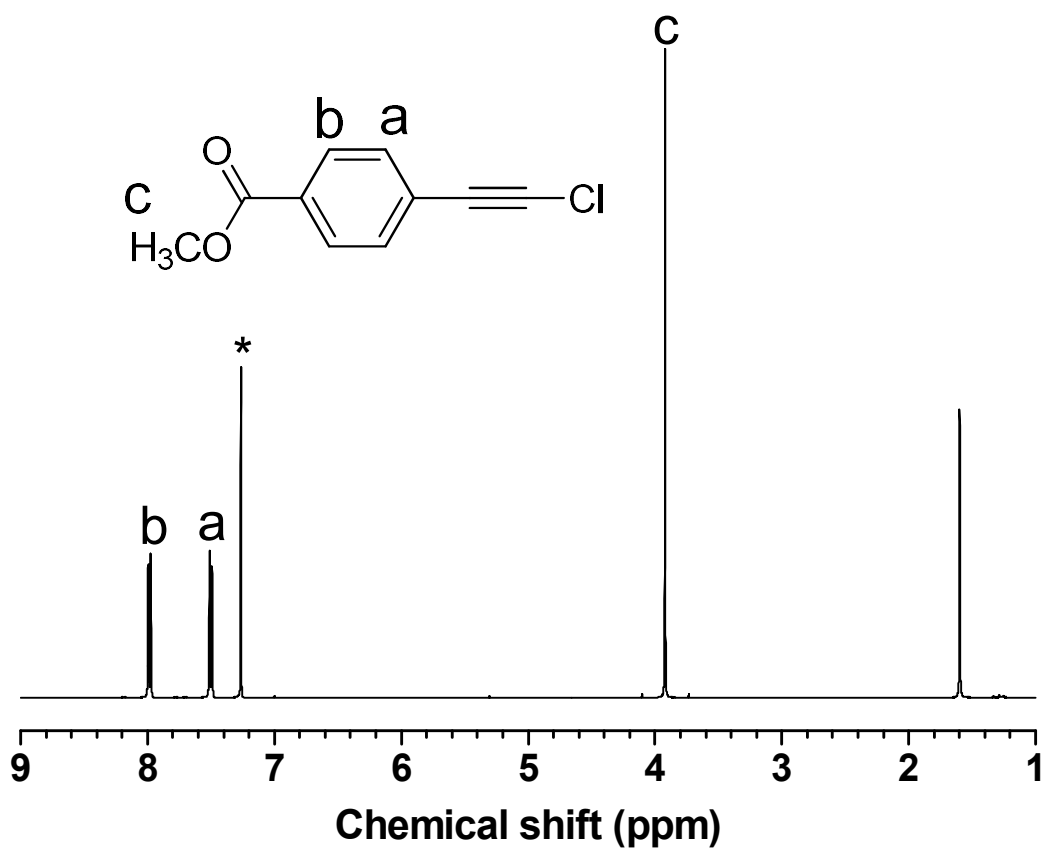


Figure S19. ^1H NMR spectrum of M7 in CDCl_3 .

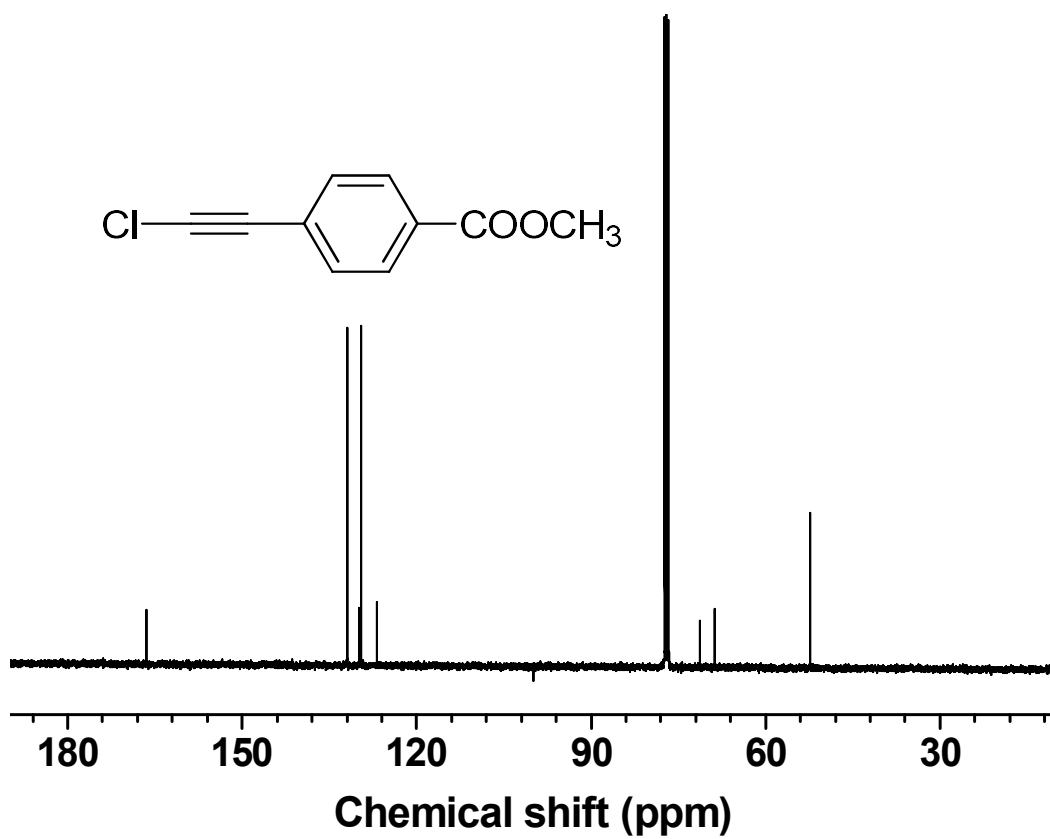


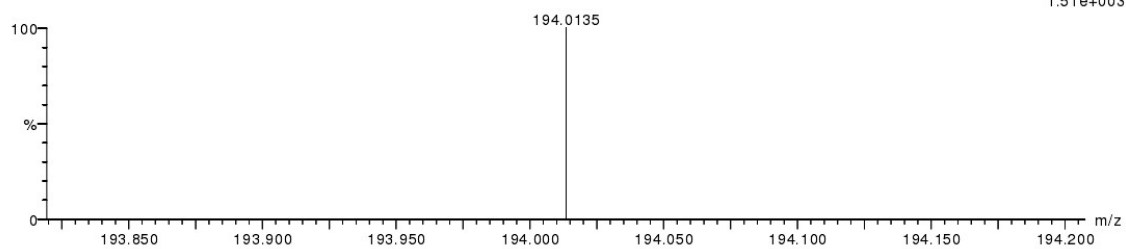
Figure S20. ^{13}C NMR spectrum of M7 in CDCl_3 .

Monoisotopic Mass, Odd and Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 O: 0-10 Cl: 0-1
GCT Premier ZJU
TOF MS EI+

05-Jun-2018

yfl-cooc 452 (2.110)

1.51e+003



Minimum: -1.5
Maximum: 1.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
194.0135	194.0135	0.0	0.0	7.0	5546774.0	C10 H7 O2 Cl

Figure S21. High resolution mass spectrum of M7.

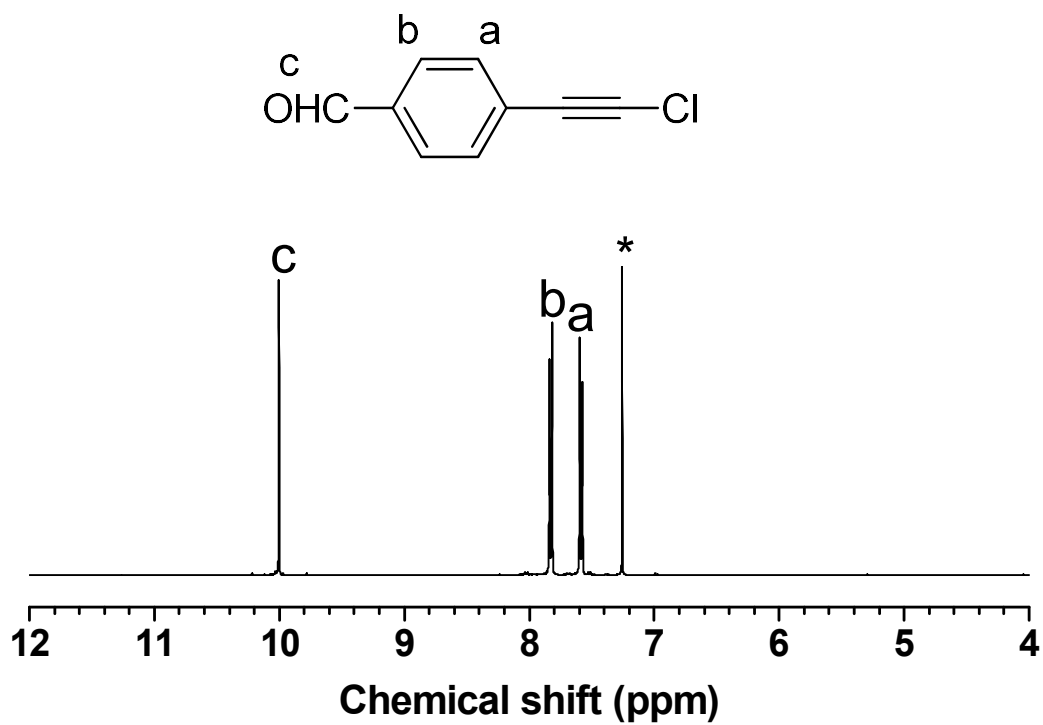


Figure S22. ¹H NMR spectrum of M8 in CDCl₃.

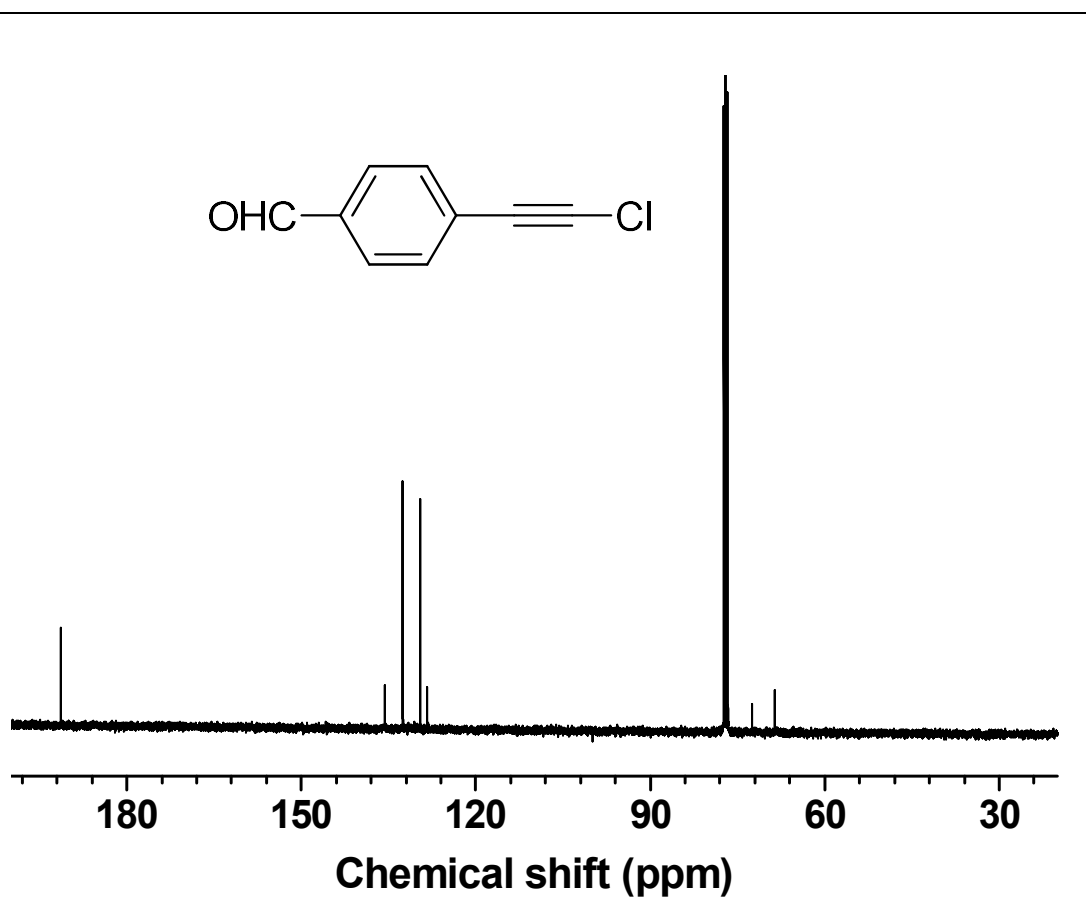


Figure S23. ^{13}C NMR spectrum of M8 in CDCl_3 .

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

73 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 0-3 O: 0-4 S: 0-1 Cl: 1-1

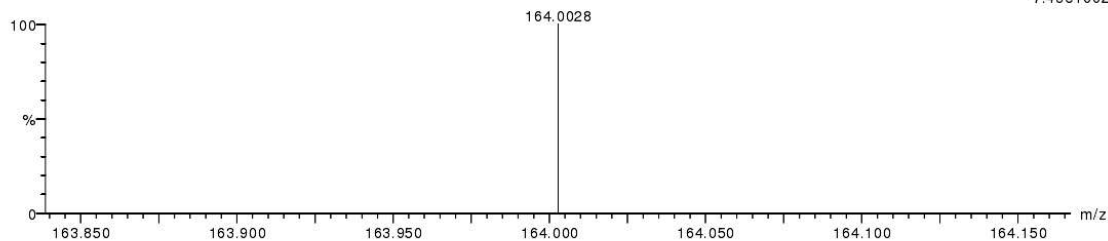
GCT Premier ZJU

TOF MS EI+

12-Apr-2018

yfl0412-3 609 (4.179)

7.43e+002



Minimum: -1.5
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
164.0028	164.0029	-0.1	-0.6	7.0	5546388.5	C9 H5 O Cl

Figure S24. High resolution mass spectrum of M8.

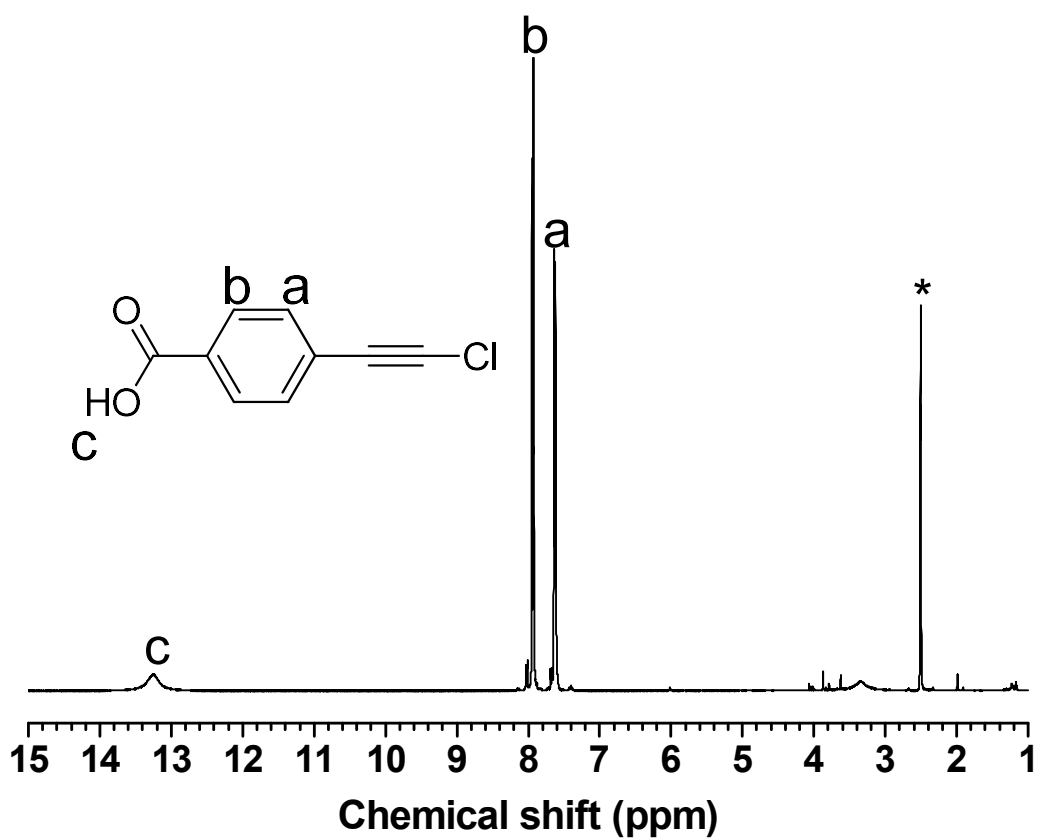


Figure S25. ¹H NMR spectrum of M9 in DMSO-*d*₆.

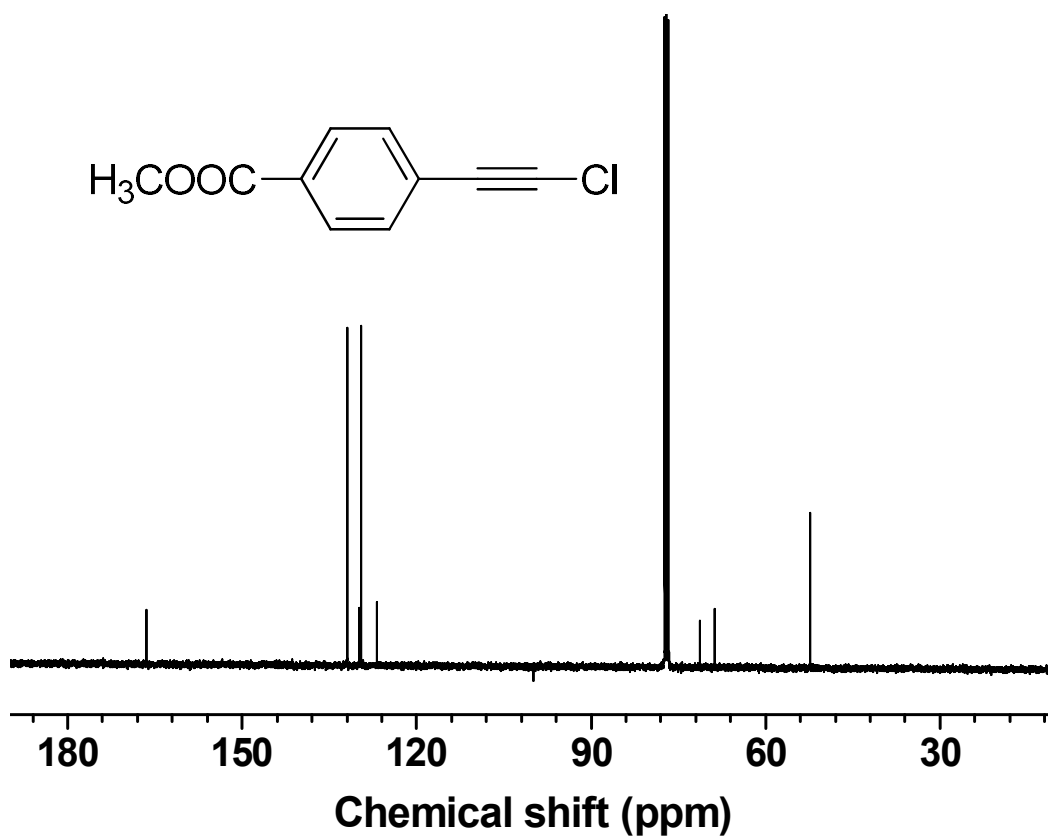


Figure S26. ¹³C NMR spectrum of M9 in DMSO-*d*₆.

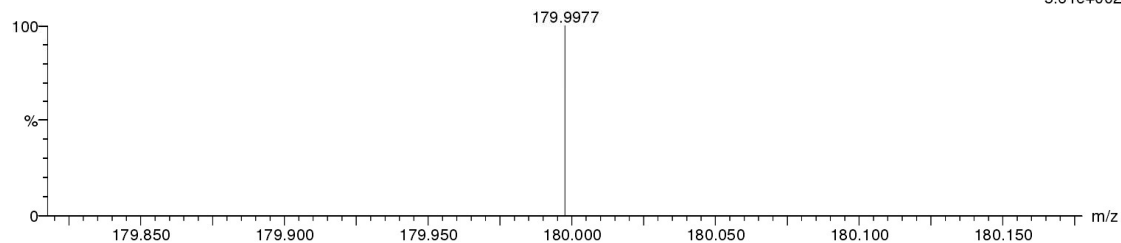
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-200 O: 0-6 Cl: 1-1
GCT Premier ZJU
TOF MS EI+

02-Jul-2018

yflcooh 443 (3.577)

5.61e+002



Minimum:				-1.5		
Maximum:	1.0	10.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
179.9977	179.9978	-0.1	-0.6	7.0	5546298.0	C9 H5 O2 Cl

Figure S27. High resolution mass spectrum of M9.

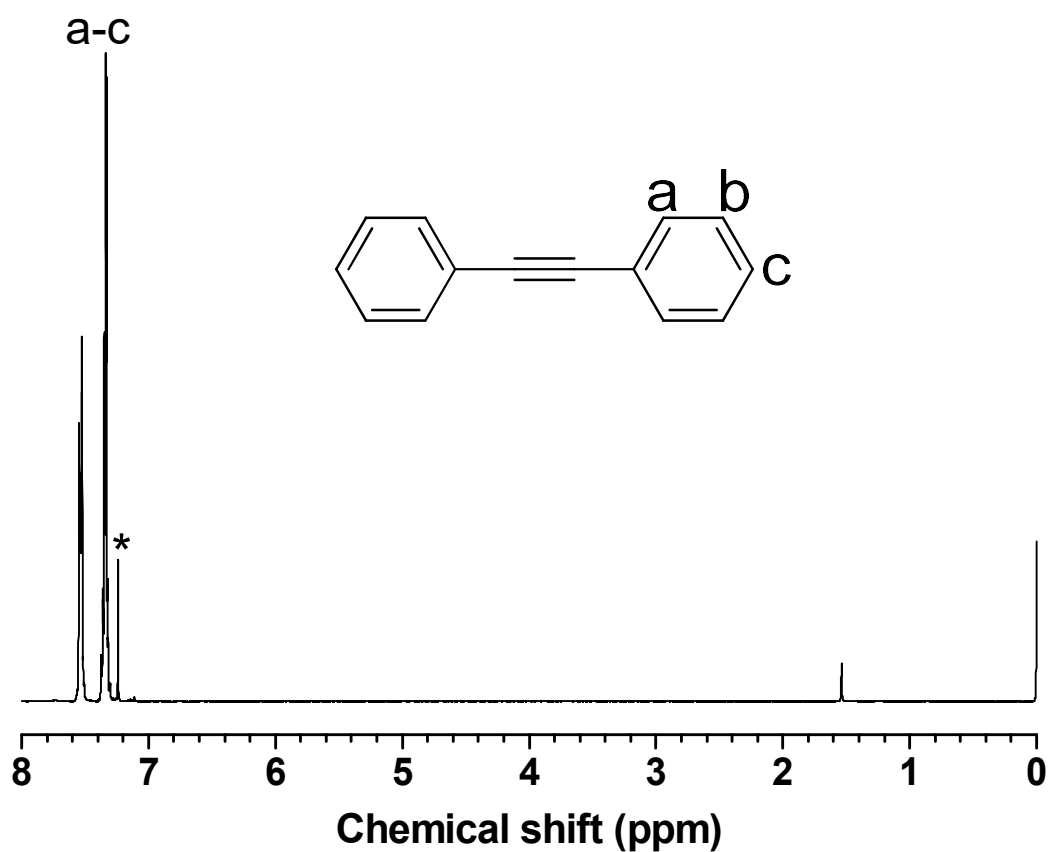


Figure S28. ¹H NMR spectrum of M10 in CDCl₃.

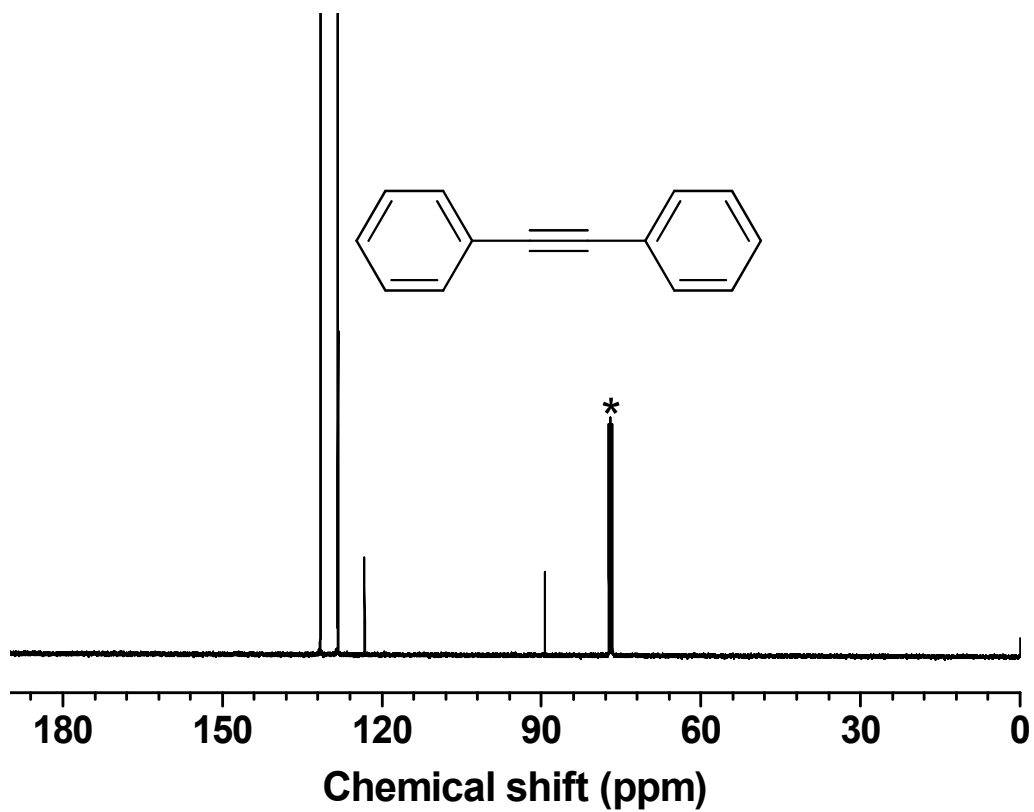


Figure S29. ^{13}C NMR spectrum of M10 in CDCl_3 .

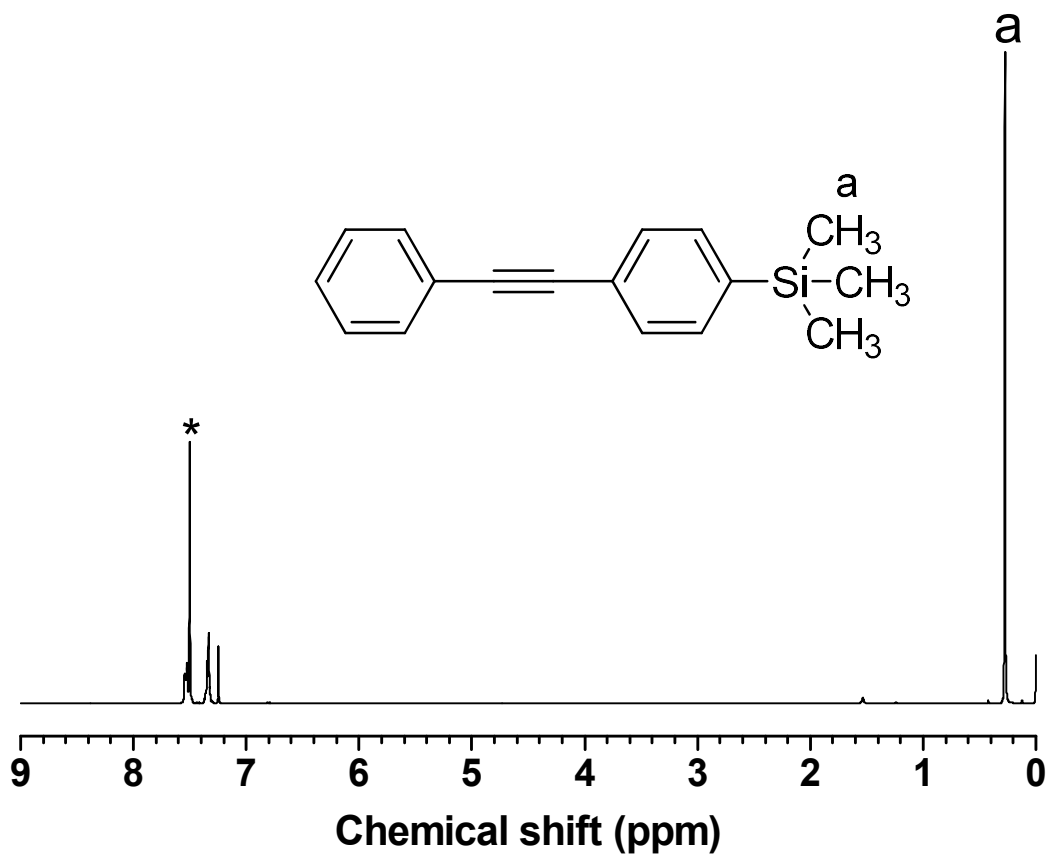


Figure S30. ^1H NMR spectrum of M11 in CDCl_3 .

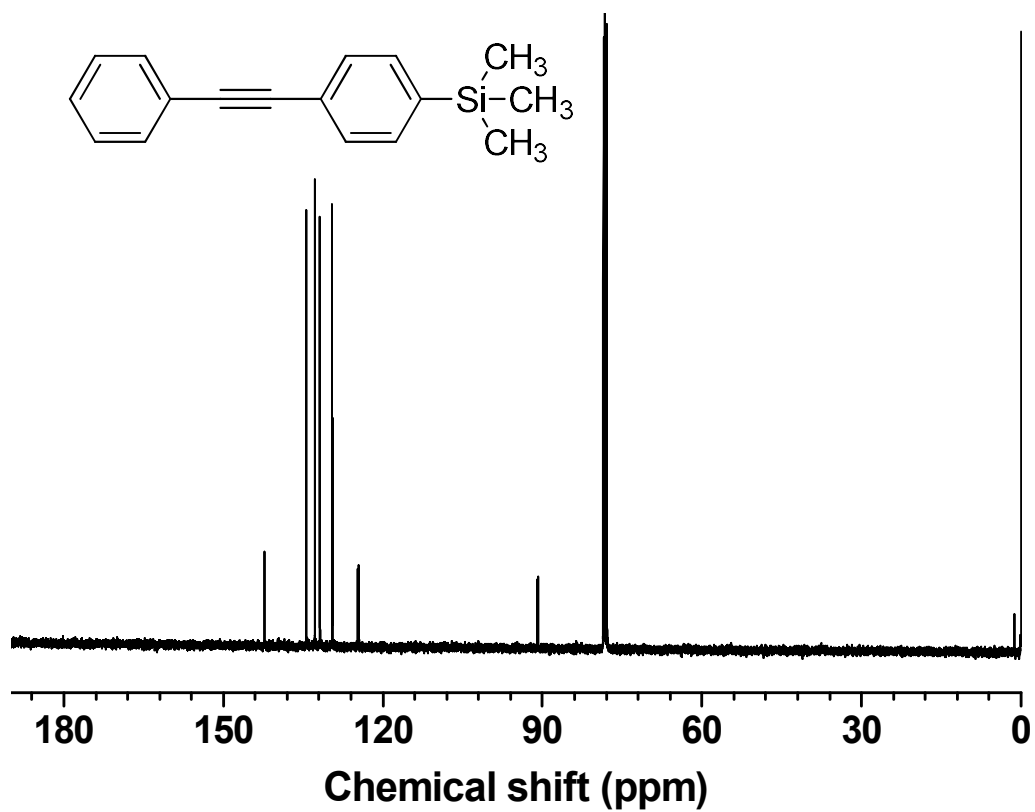


Figure S31. ^{13}C NMR spectrum of M11 in CDCl_3 .

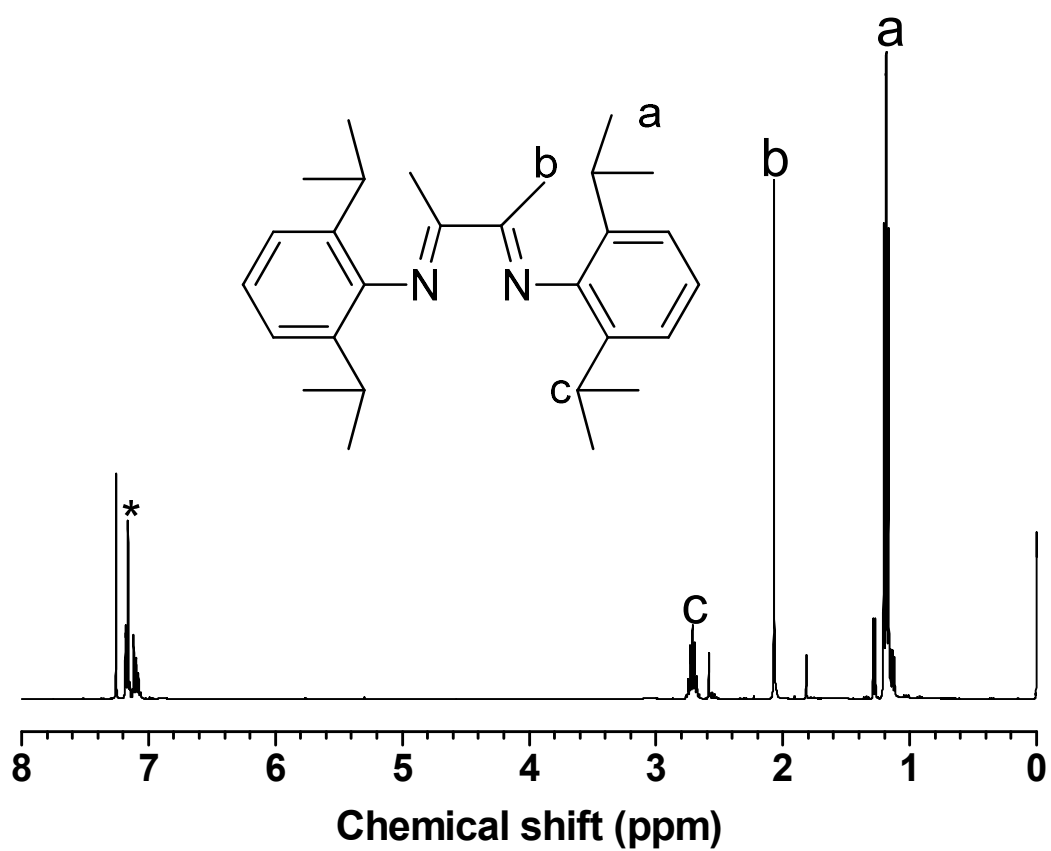


Figure S32. ^1H NMR spectrum of α -diimine ligand in CDCl_3 .

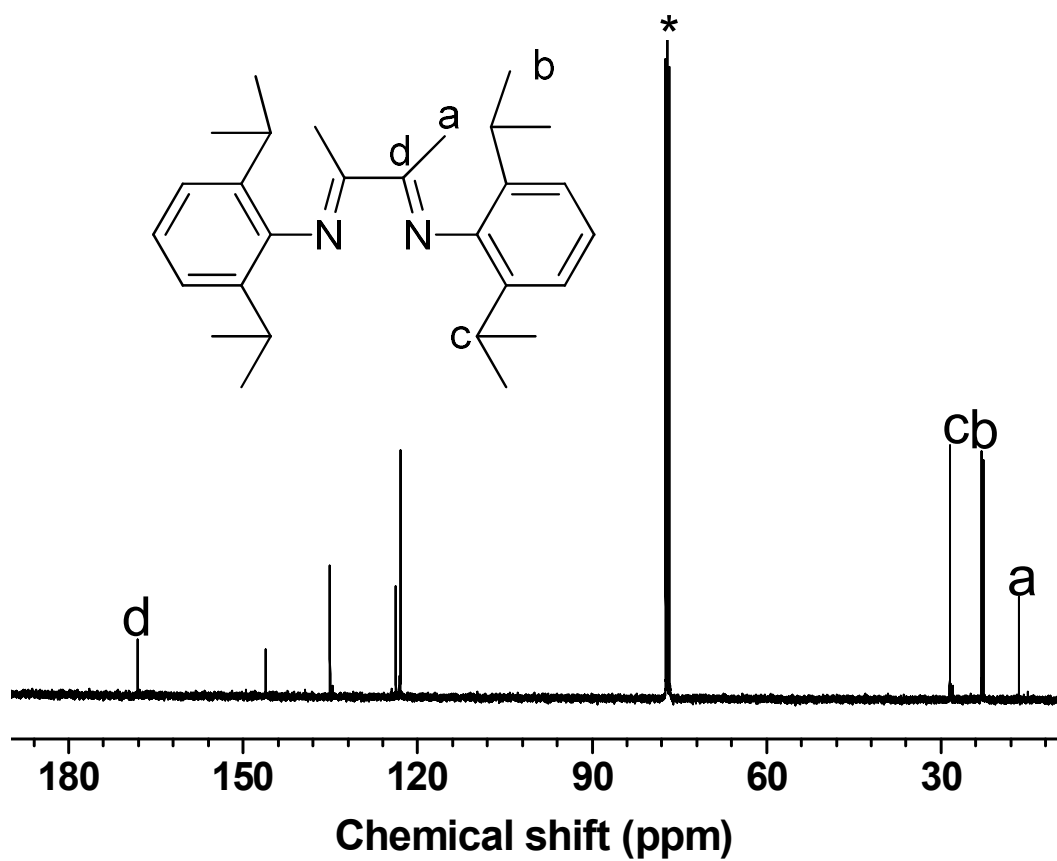


Figure S33. ^{13}C NMR spectrum of α -diimine ligand in CDCl_3 .

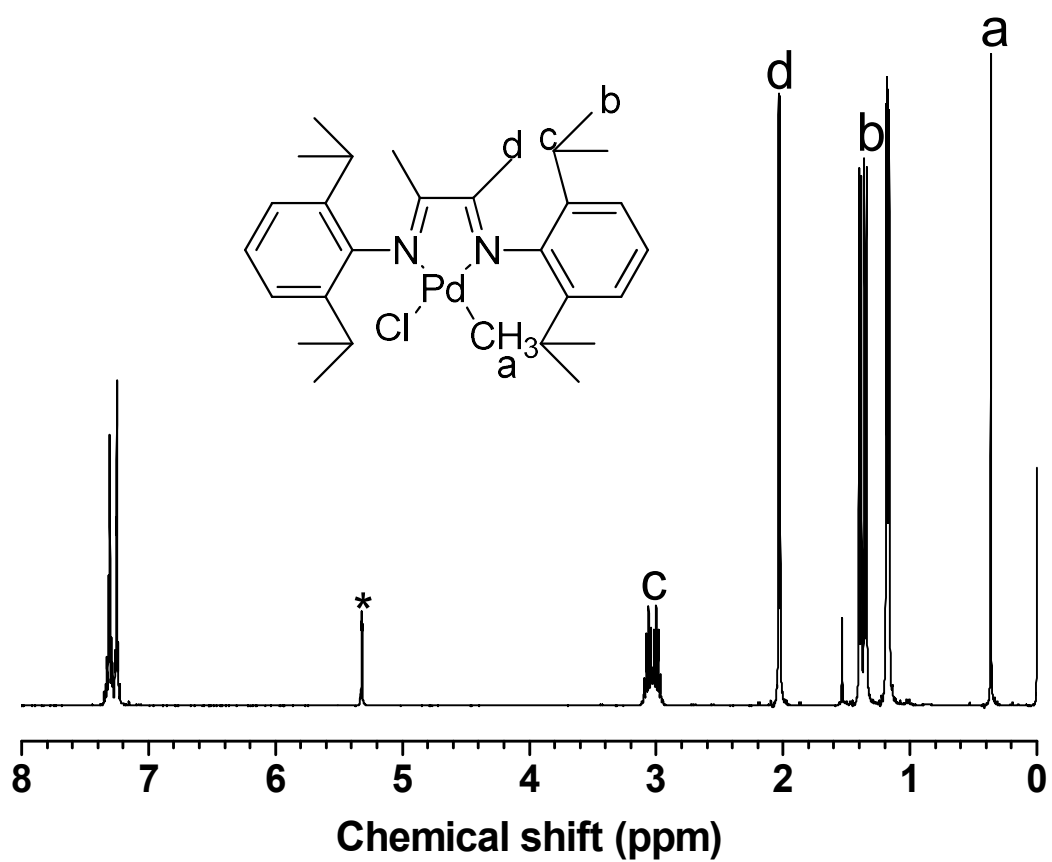


Figure S34. ^1H NMR spectrum of $(\alpha\text{-diimine})\text{PdMeCl}$ complex in CD_2Cl_2 .

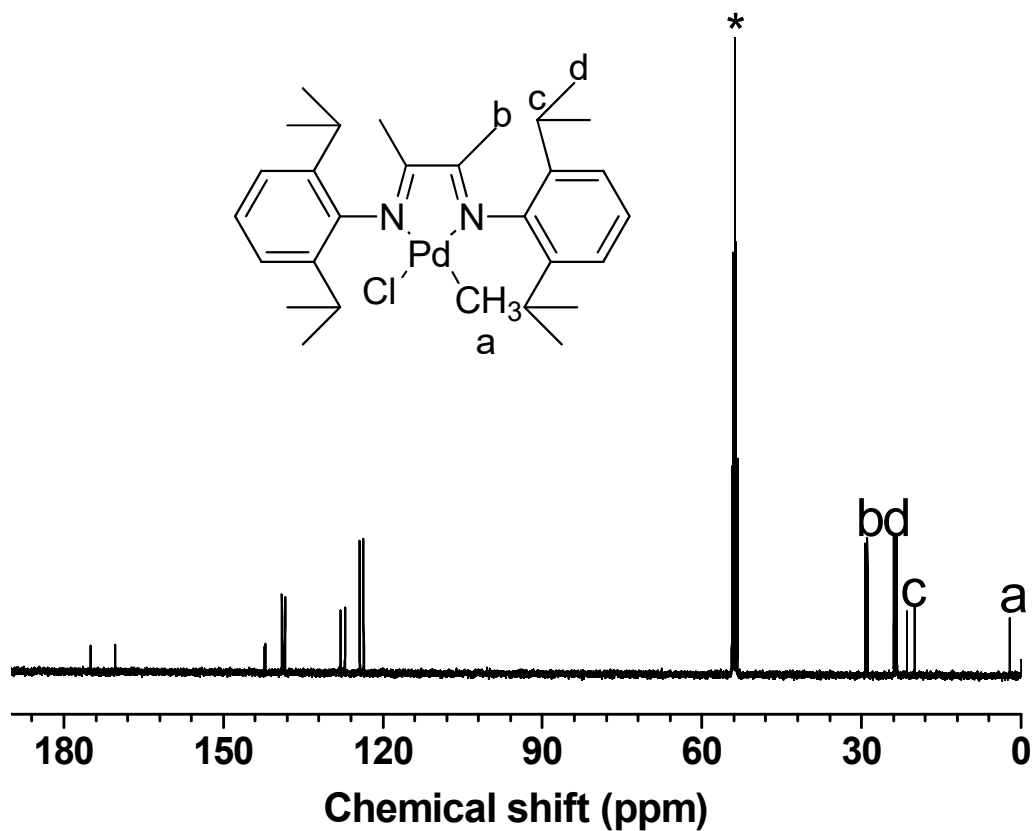


Figure S35. ^{13}C NMR spectrum of (α -diimine)PdMeCl complex in CD_2Cl_2 .

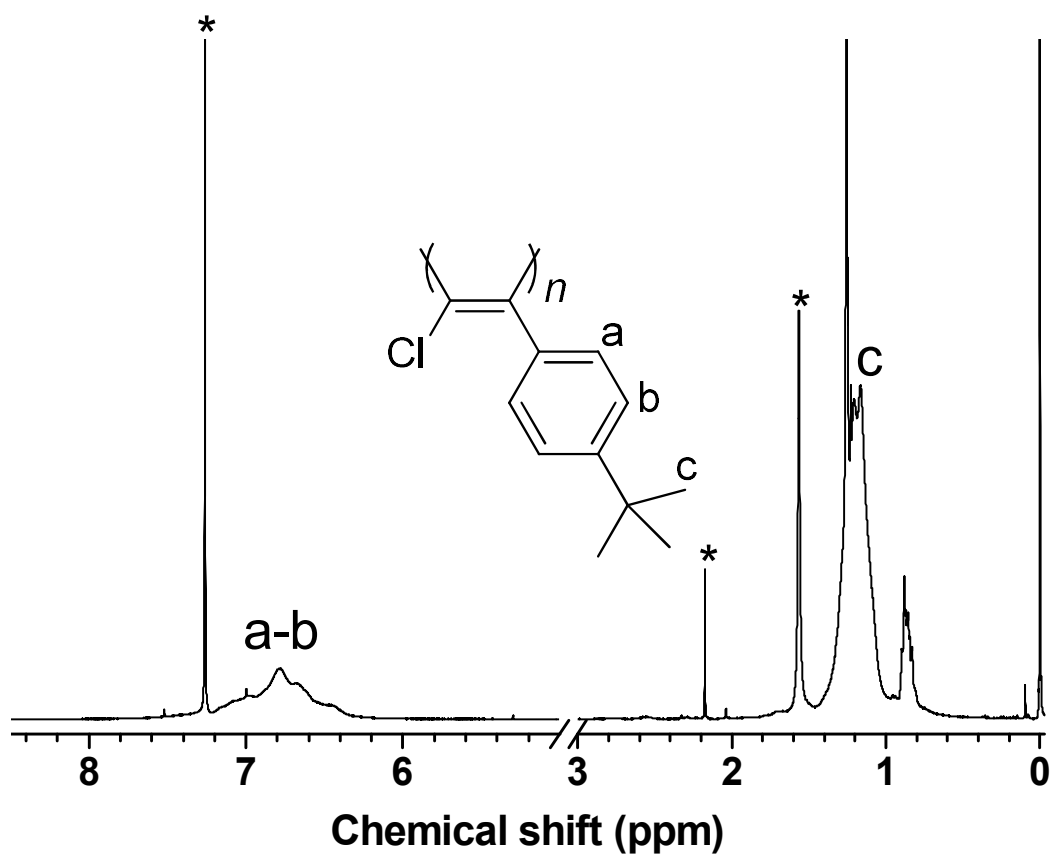


Figure S36. ^1H NMR spectrum of P1(Ag) in CDCl_3 .

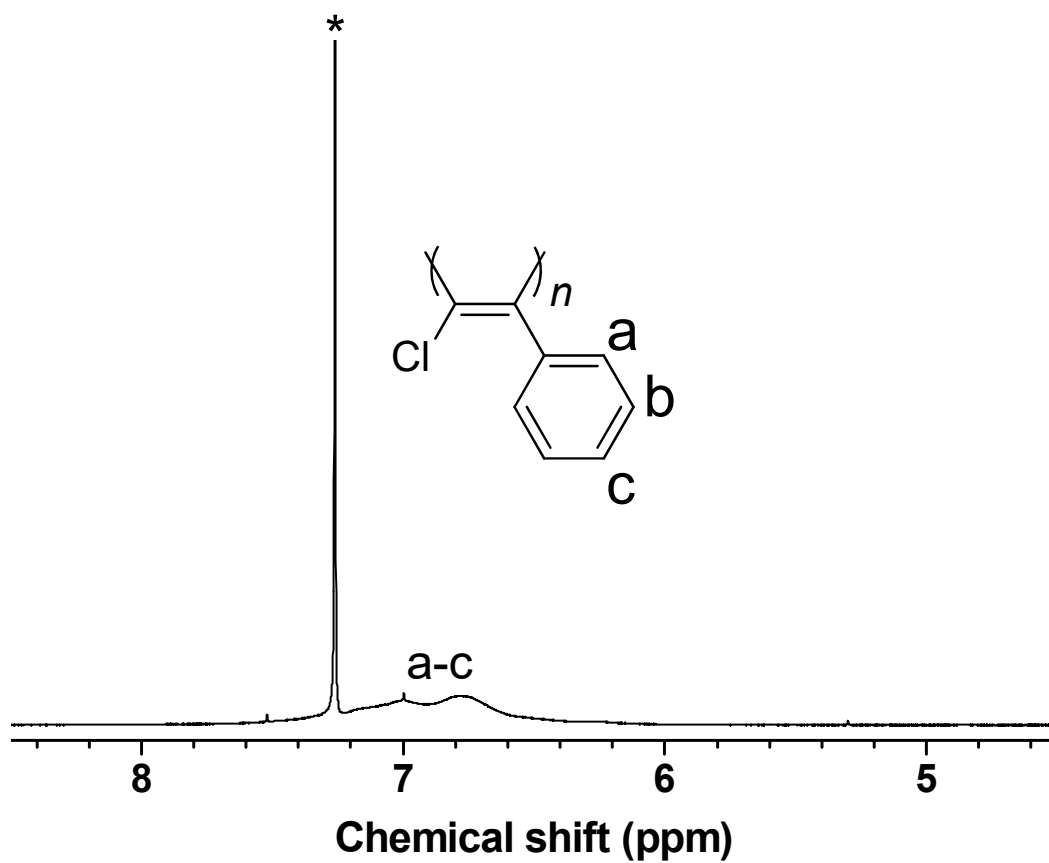


Figure S37. ^1H NMR spectrum of P2(Ag) in CDCl_3 .

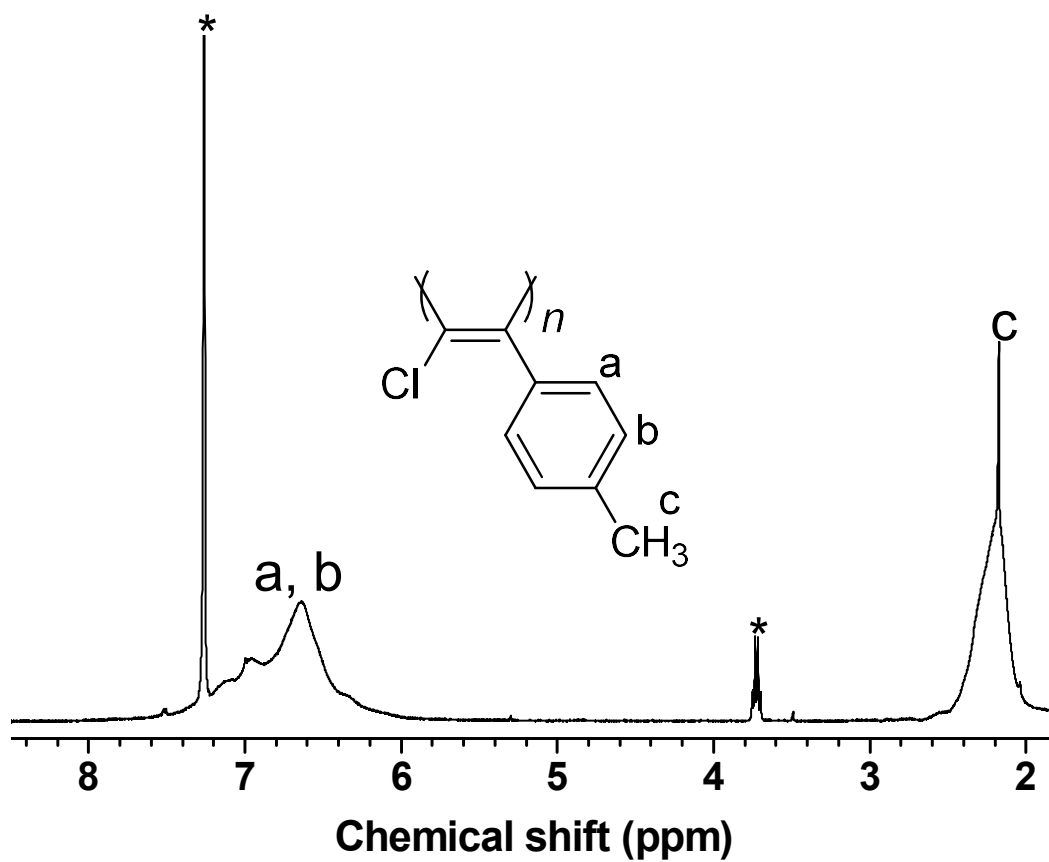


Figure S38. ^1H NMR spectrum of P3(Ag) in CDCl_3 .

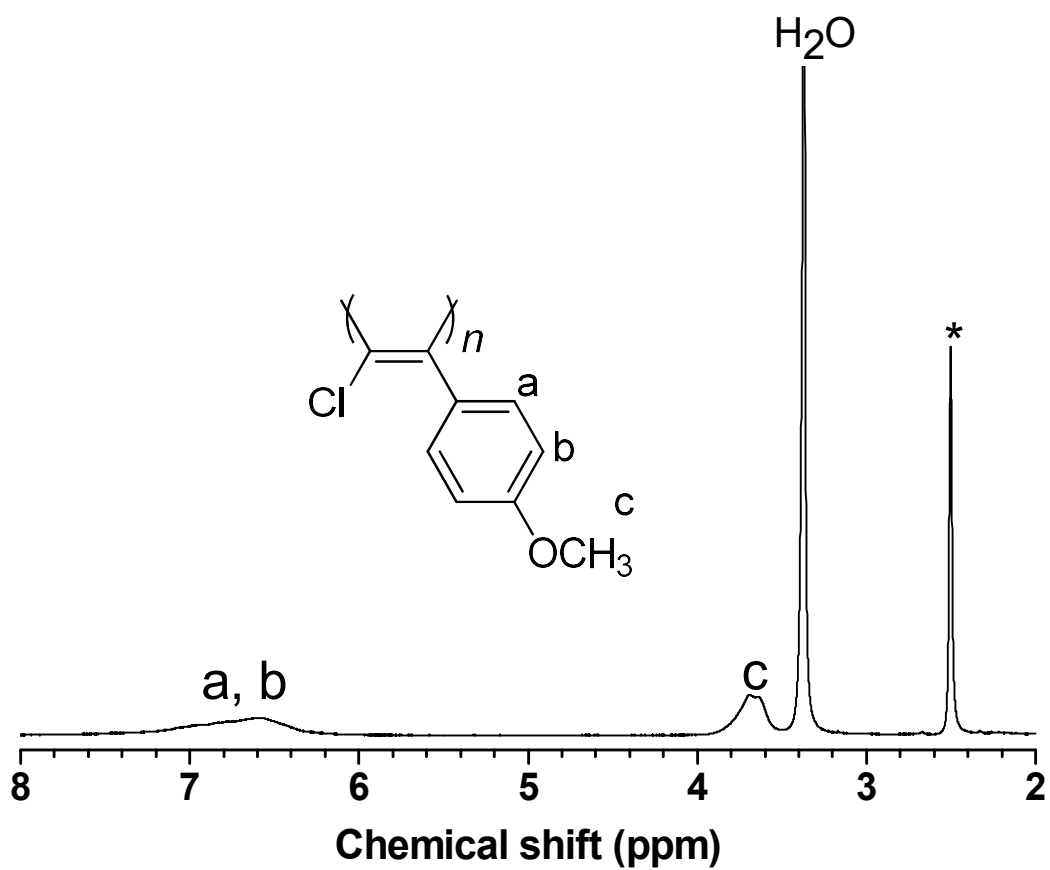


Figure S39. ^1H NMR spectrum of P4(Ag) in $\text{DMSO-}d_6$.

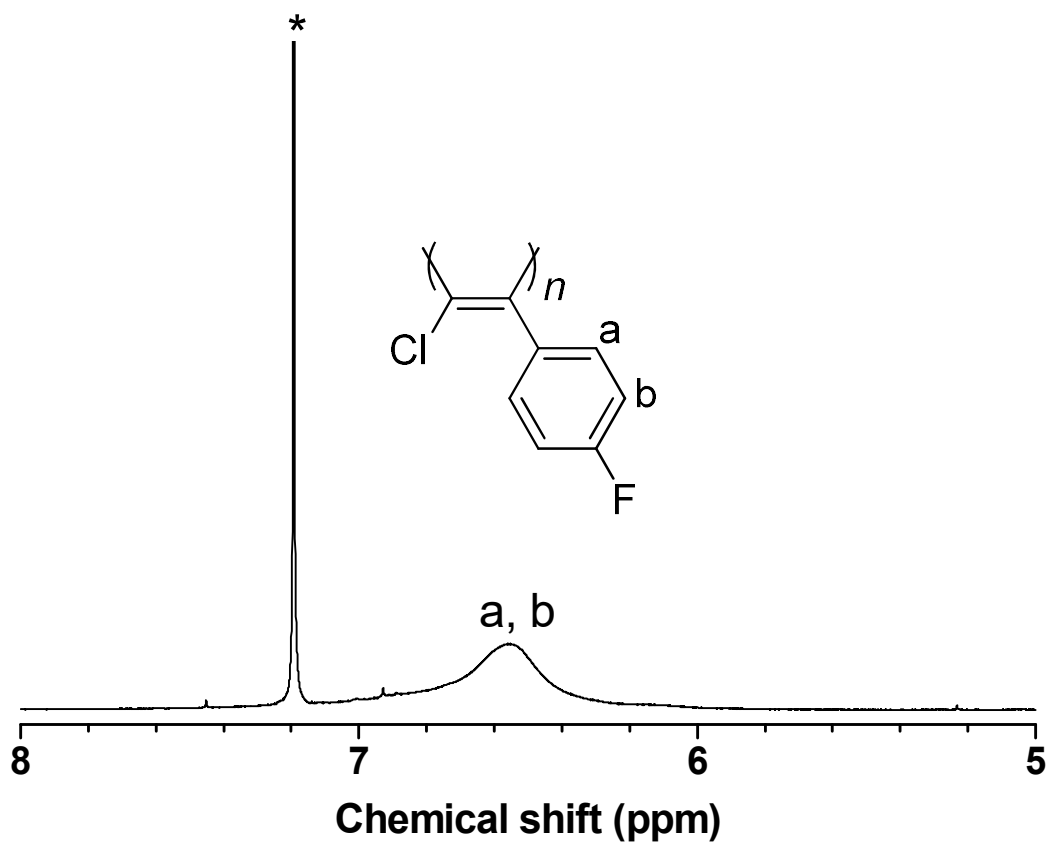


Figure S40. ^1H NMR spectrum of P5(Ag) in CDCl_3 .

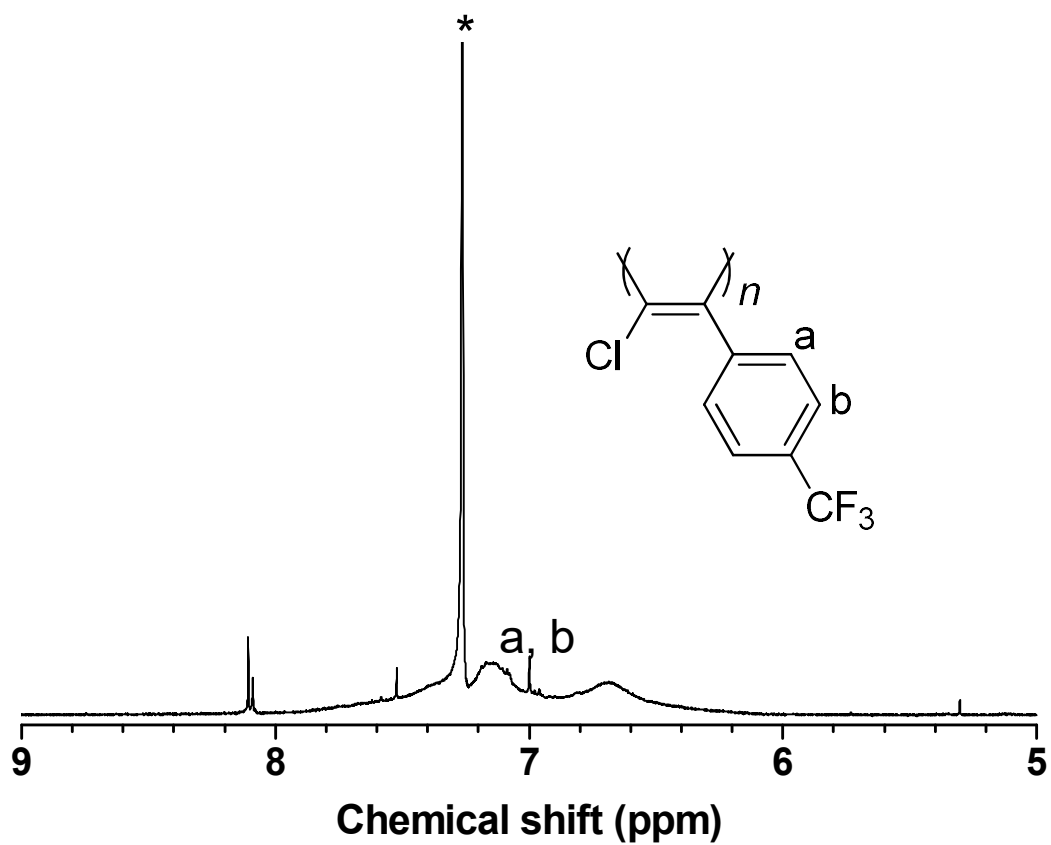


Figure S41. ^1H NMR spectrum of P6(Ag) in CDCl_3 .

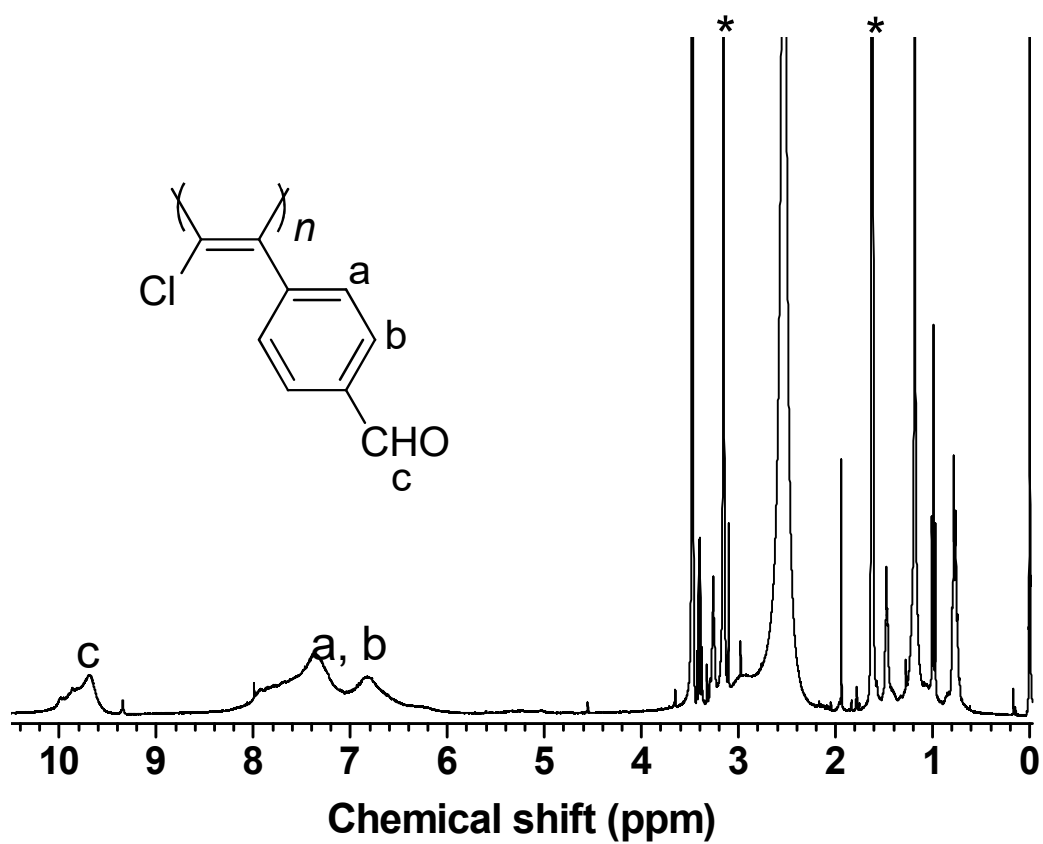


Figure S42. ^1H NMR spectrum of P8(Ag) in $(\text{THF-}d_3)$.

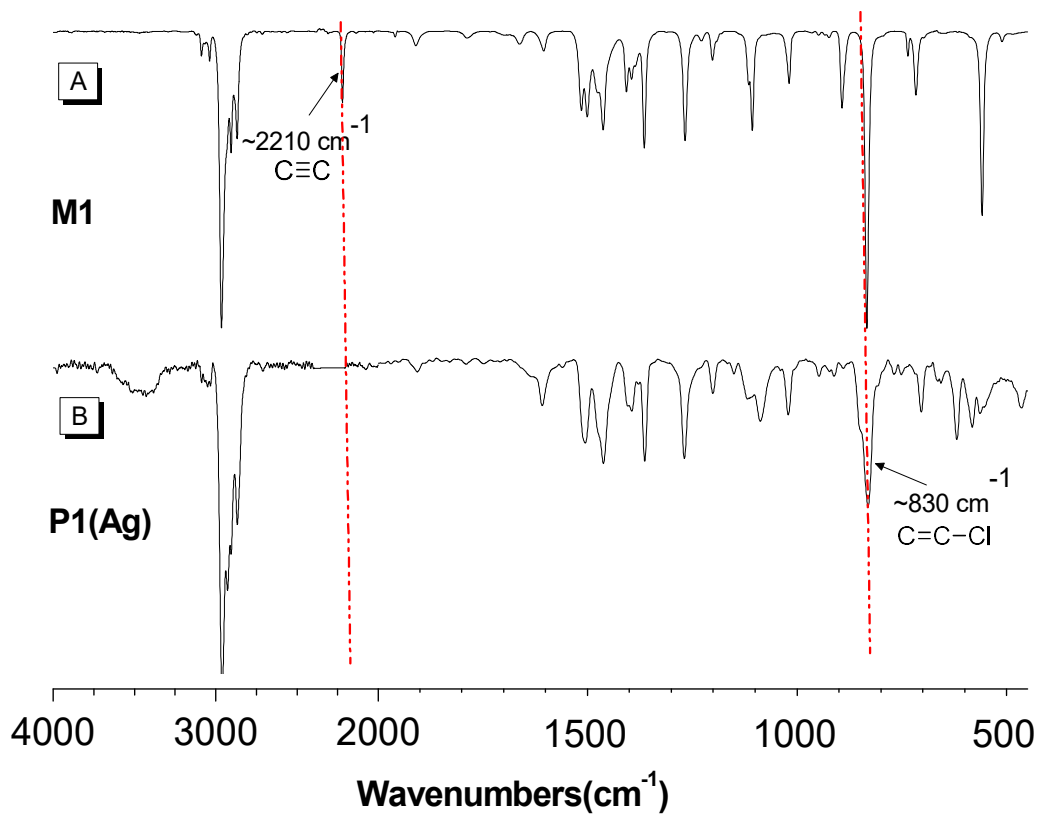


Figure S43. FTIR spectra of (A) M1 and (B) P1(Ag).

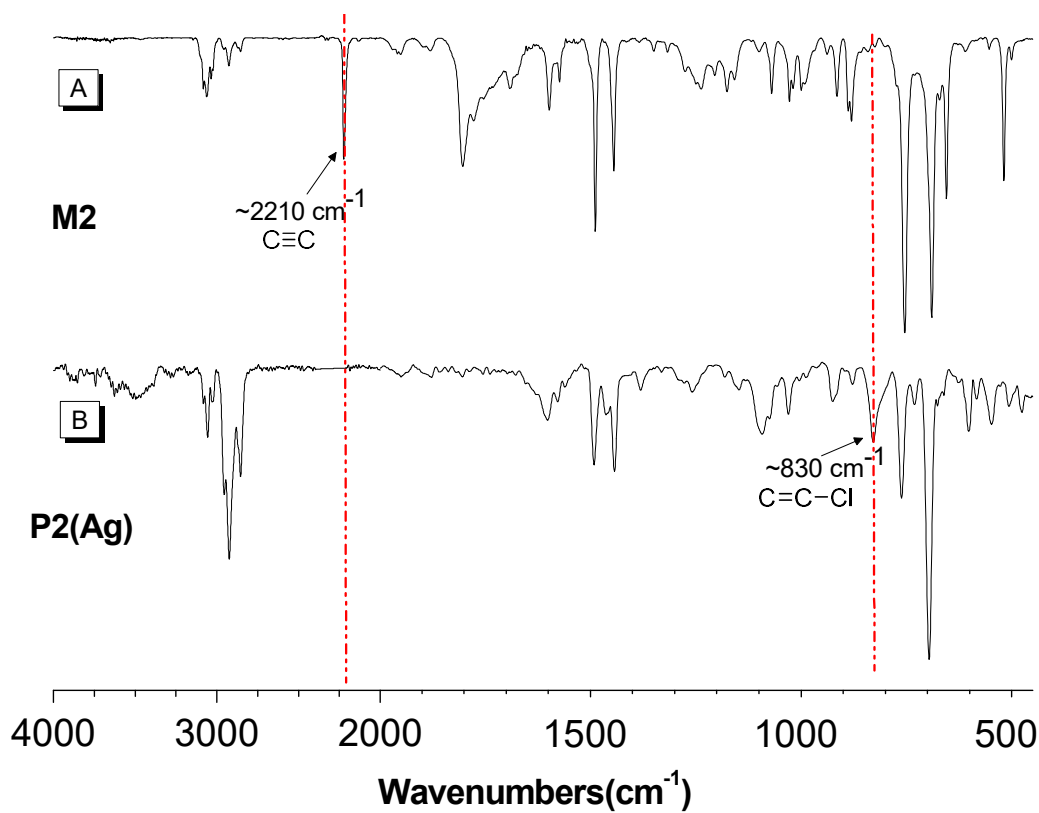


Figure S44. FTIR spectra of (A) M2 and (B) P2(Ag).

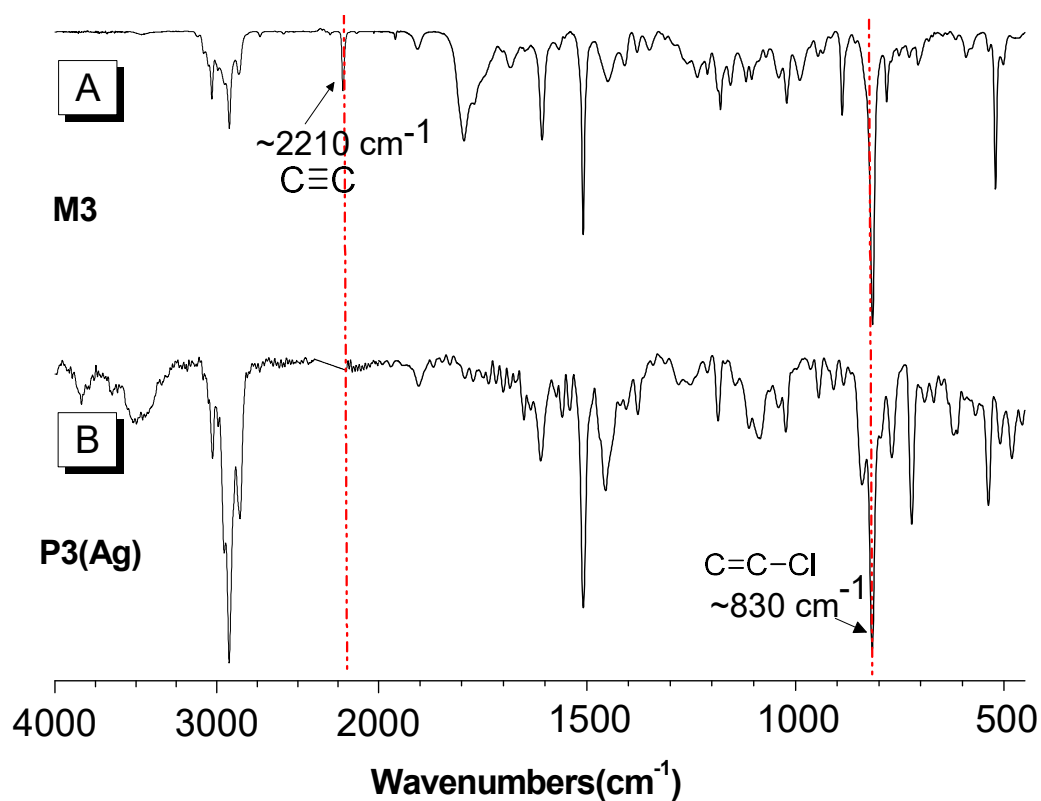


Figure S45. FTIR spectra of (A) M3 and (B) P3(Ag).

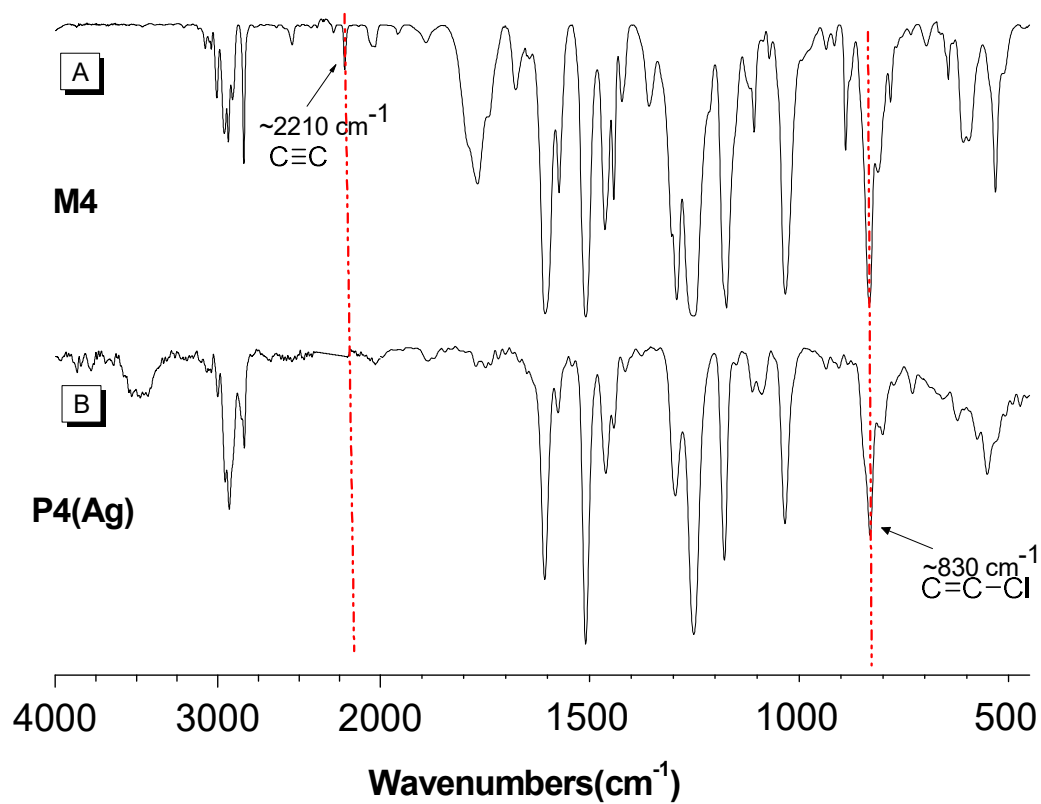


Figure S46. FTIR spectra of (A) M4 and (B) P4(Ag).

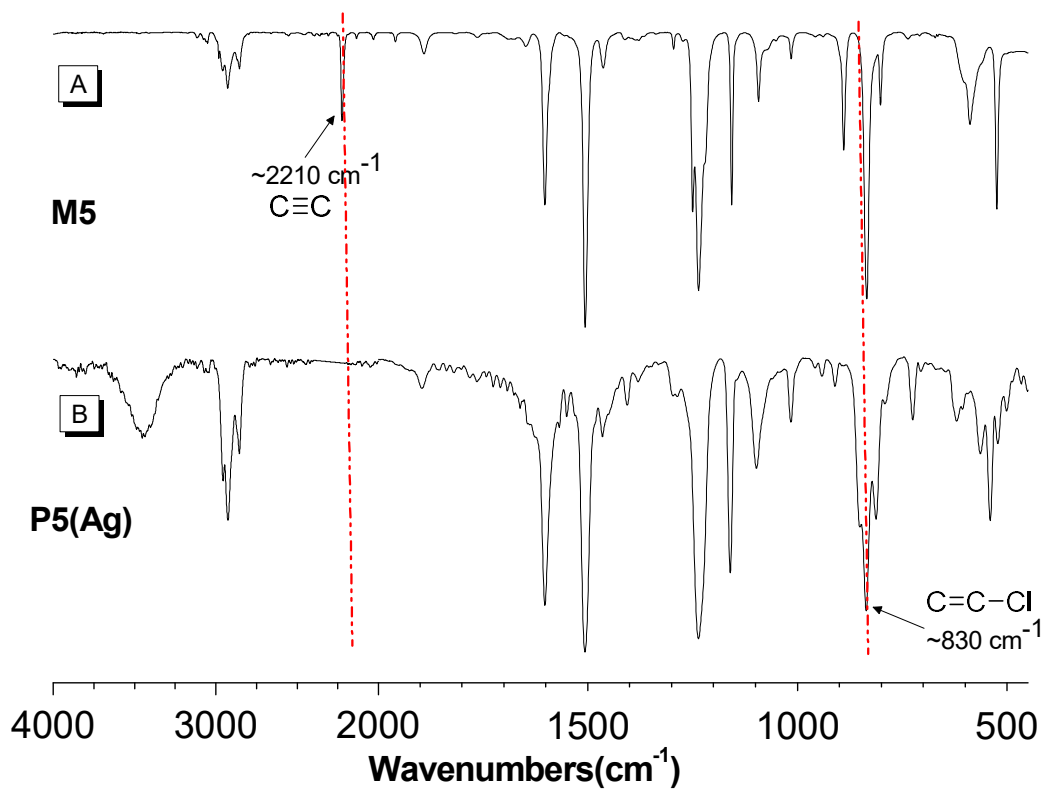


Figure S47. FTIR spectra of (A) M5 and (B) P5(Ag).

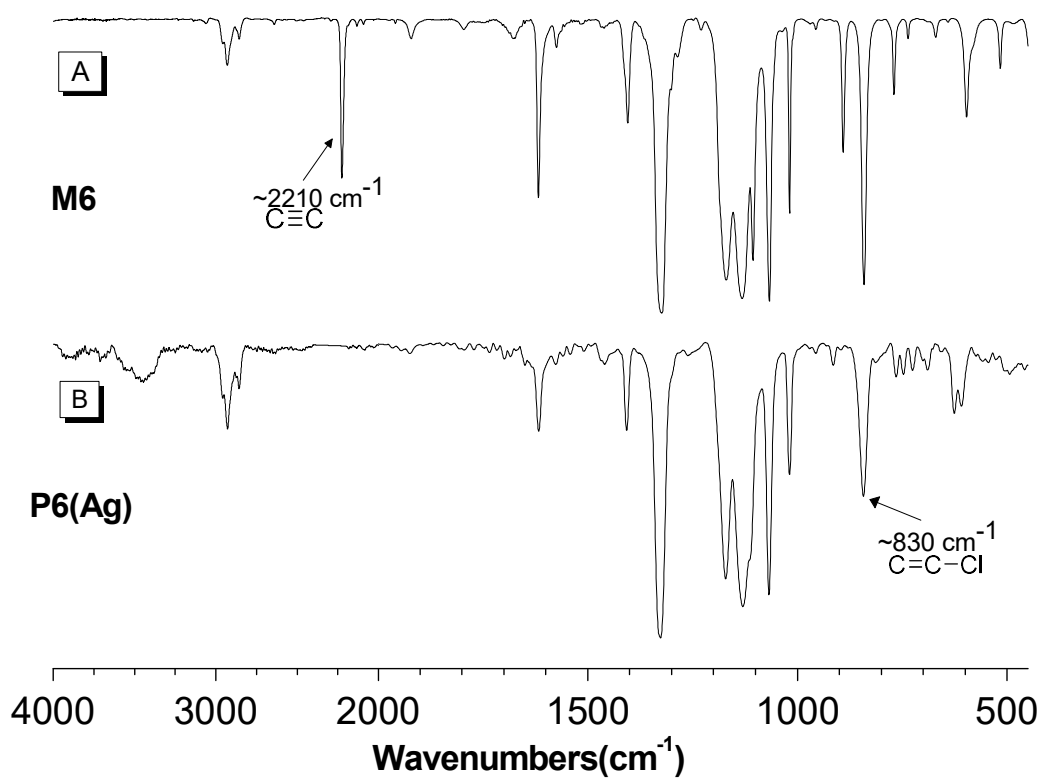


Figure S48. FTIR spectra of (A) M6 and (B) P6(Ag).

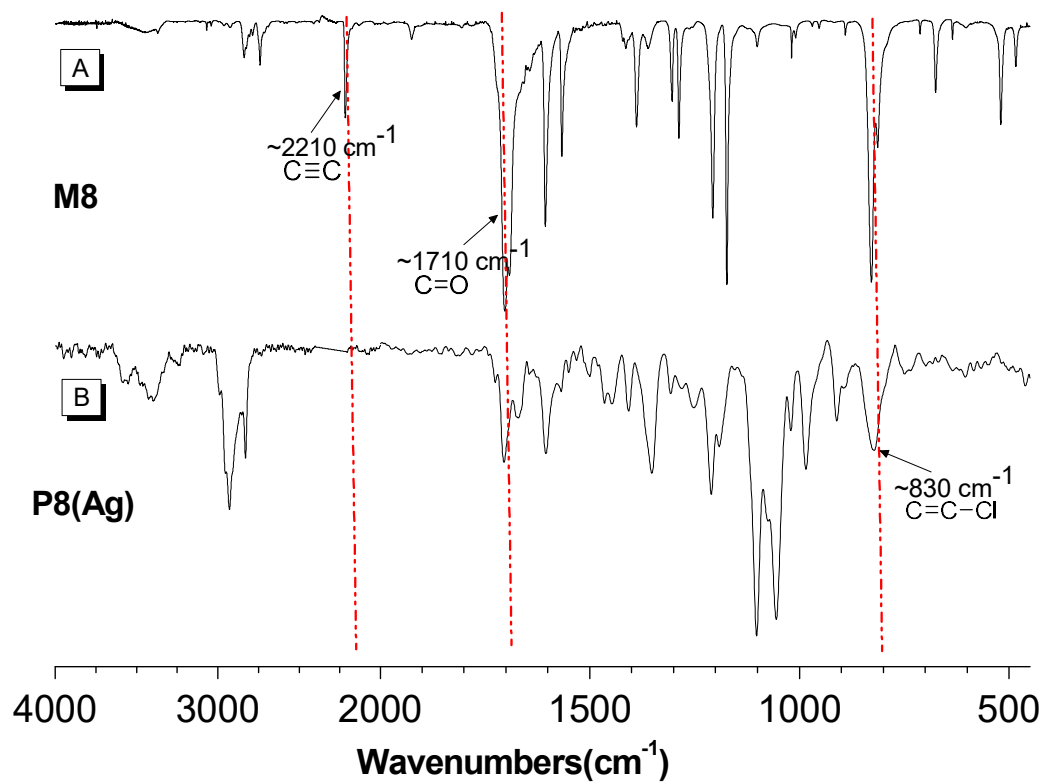


Figure S49. FTIR spectra of (A) M8 and (B) P8(Ag).