

Supplementary material for

Novel magnolol-sulforaphane hybrids as potent antitumor agents: Synthesis and biological characterization

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NMR and HRMS Spectra

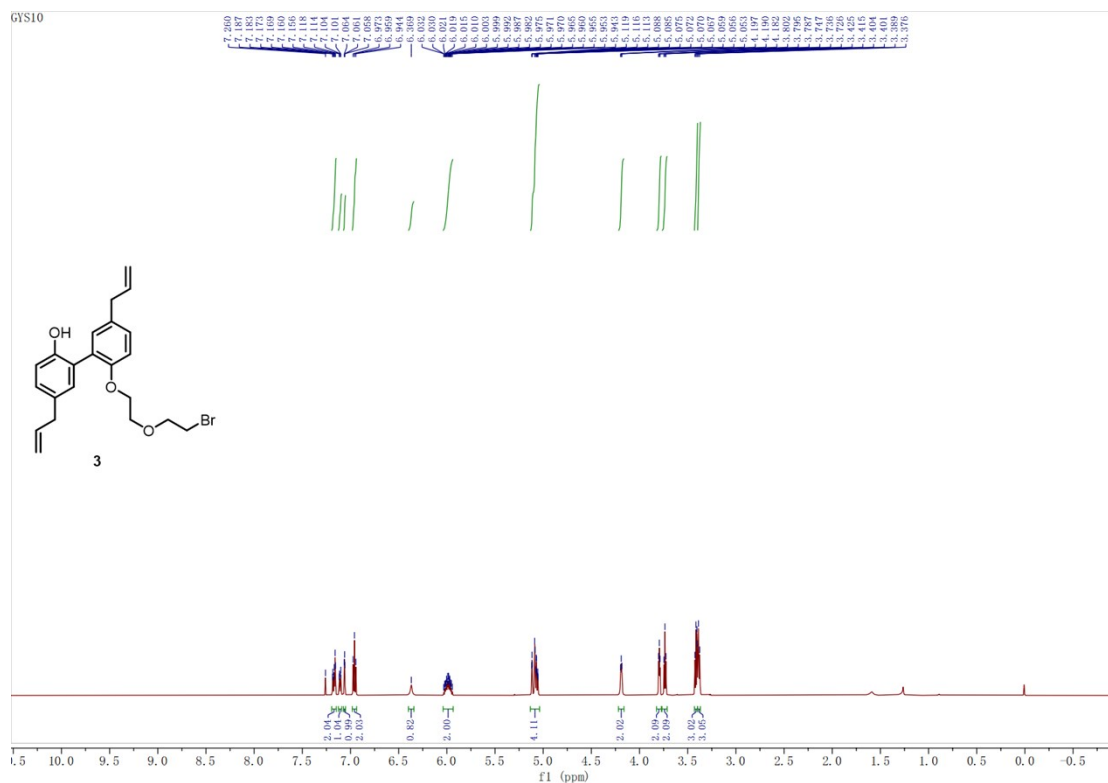


Figure S1. ¹H NMR of **3** (CDCl₃, 600 MHz)

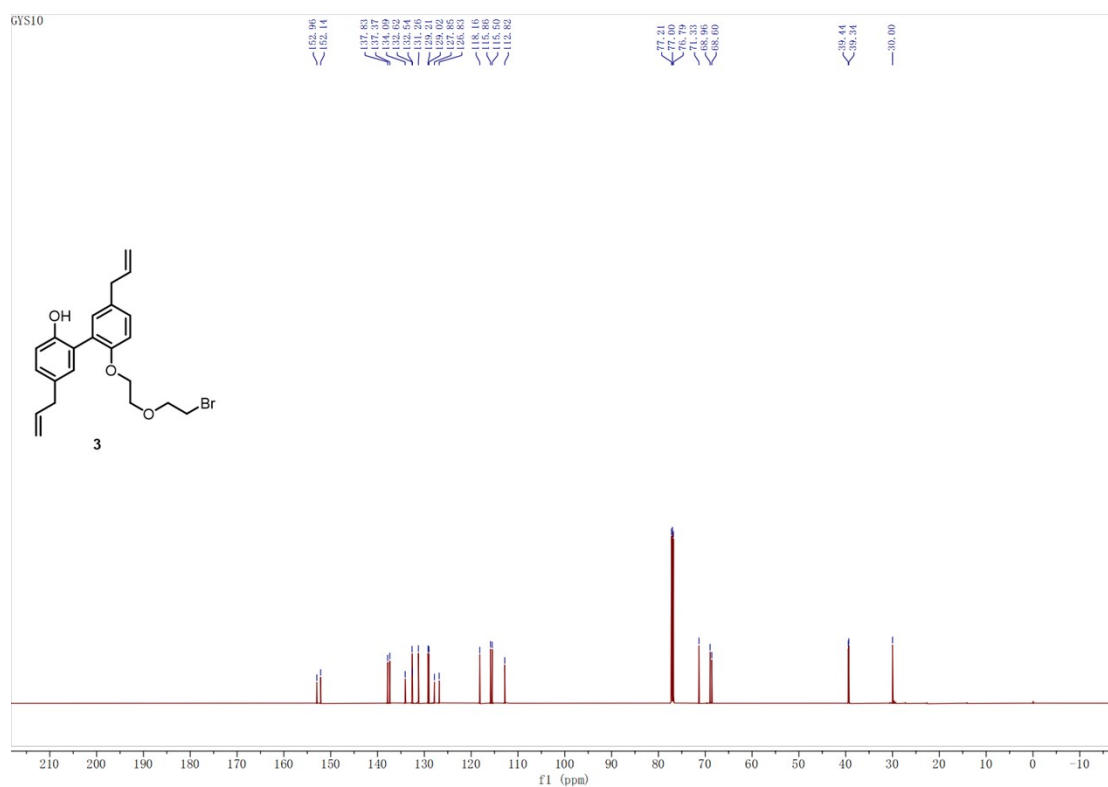


Figure S2. ¹³C NMR of **3** (CDCl₃, 150 MHz)

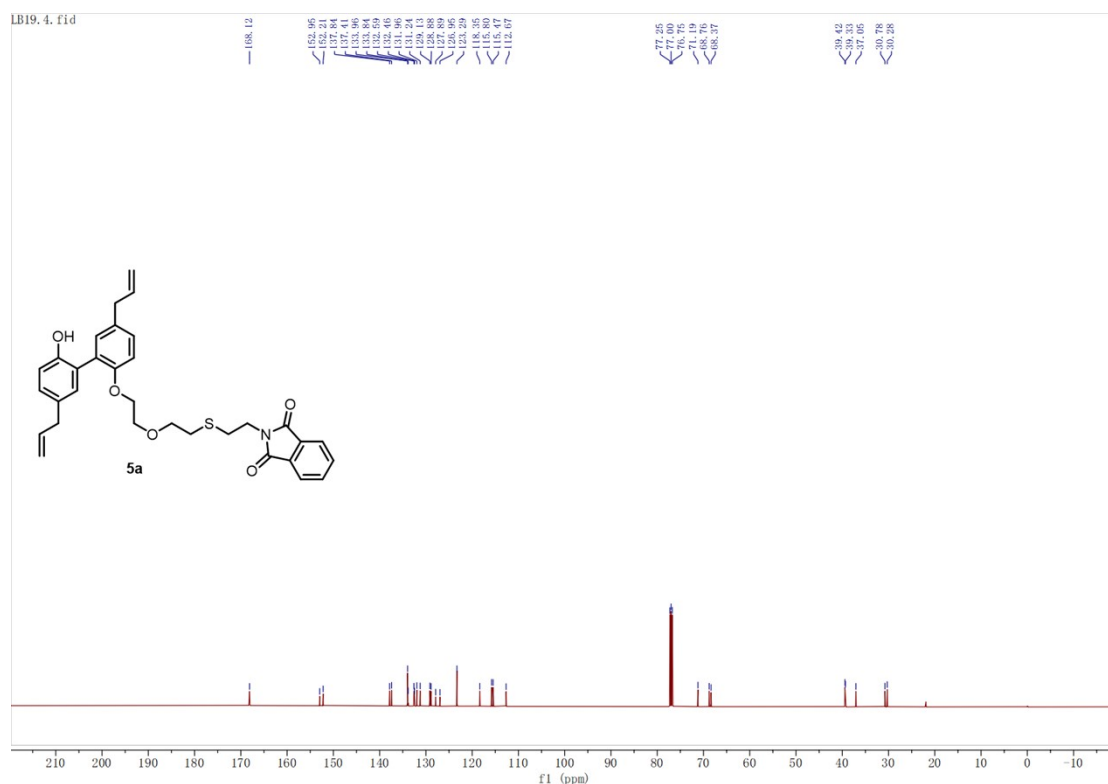


Figure S5. ^{13}C NMR of **5a** (CDCl_3 , 125 MHz)

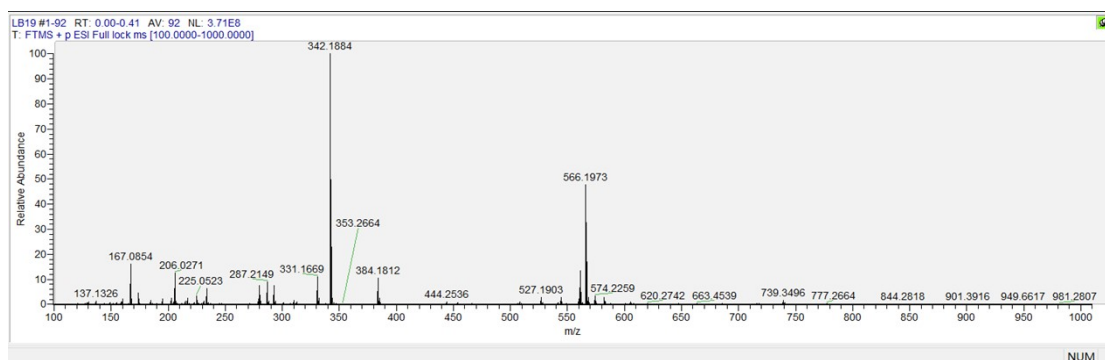


Figure S6. HRMS Spectra of **5a**

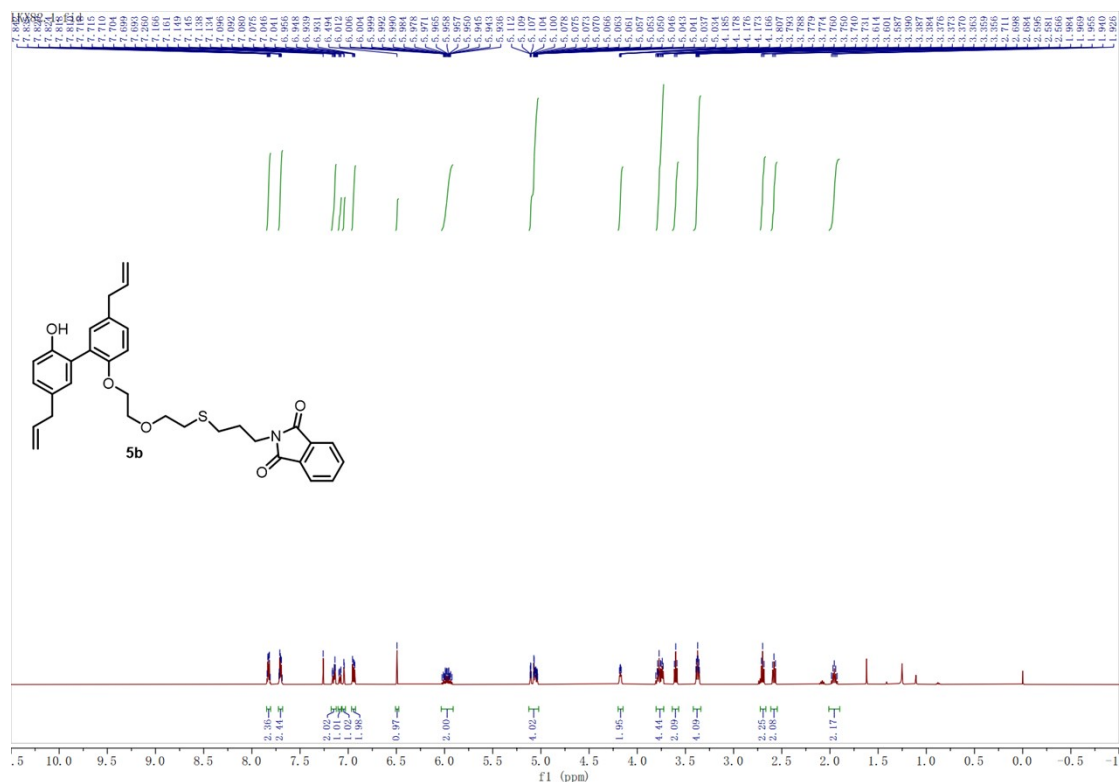


Figure S7. ¹H NMR of **5b** (CDCl₃, 500 MHz)

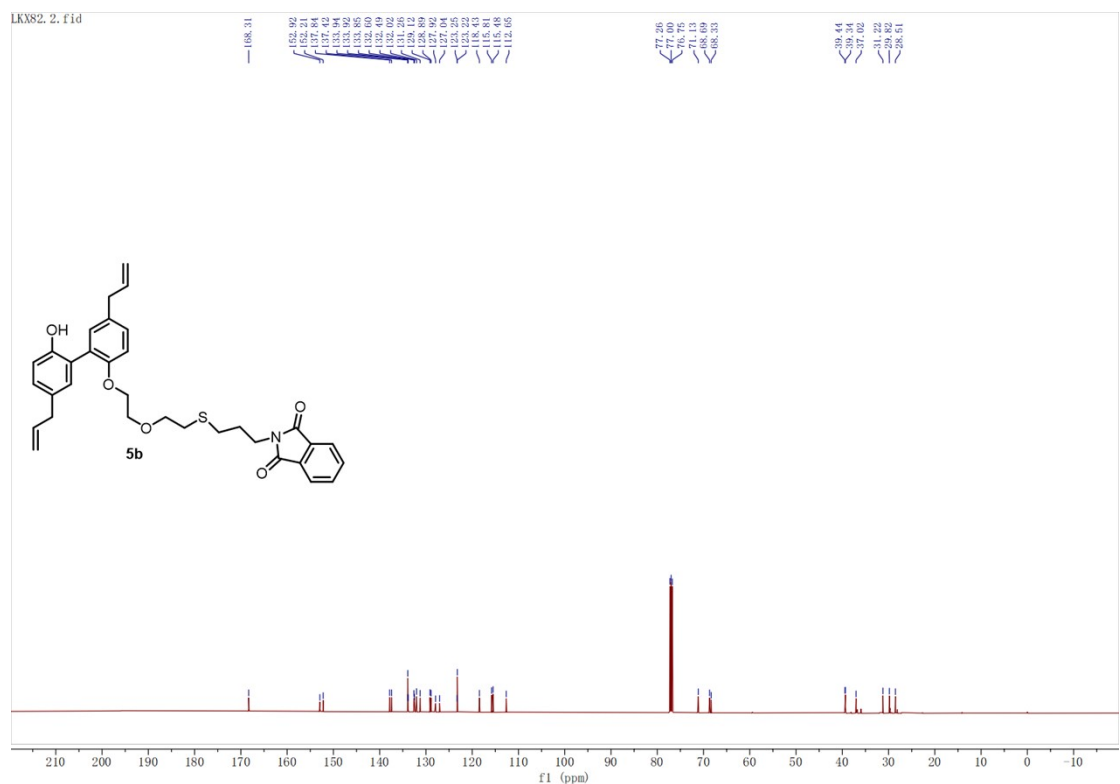


Figure S8. ¹³C NMR of **5b** (CDCl₃, 125 MHz)

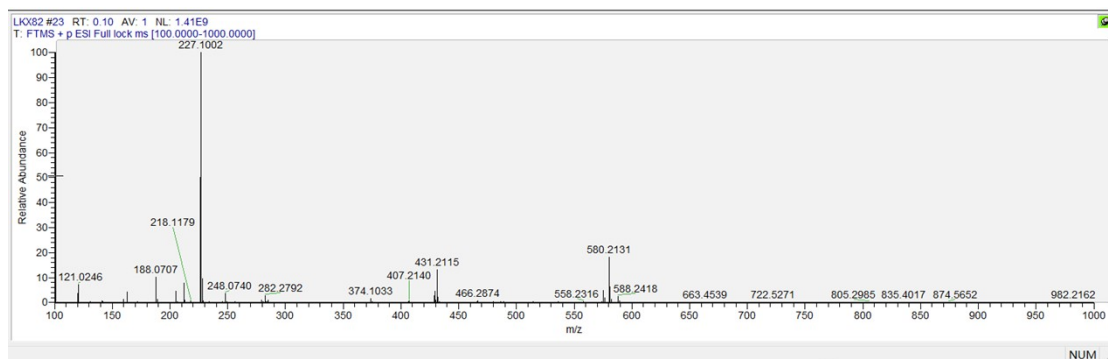


Figure S9. HRMS Spectra of **5b**

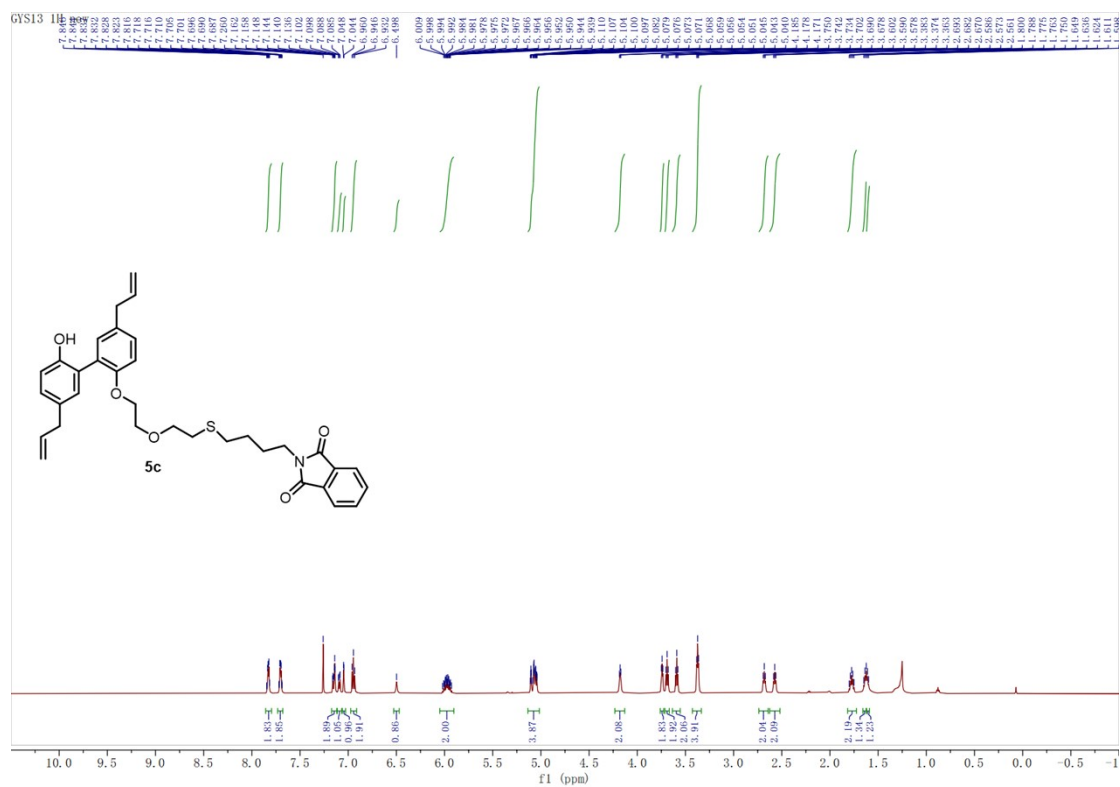


Figure S10. ^1H NMR of **5c** (CDCl_3 , 600 MHz)

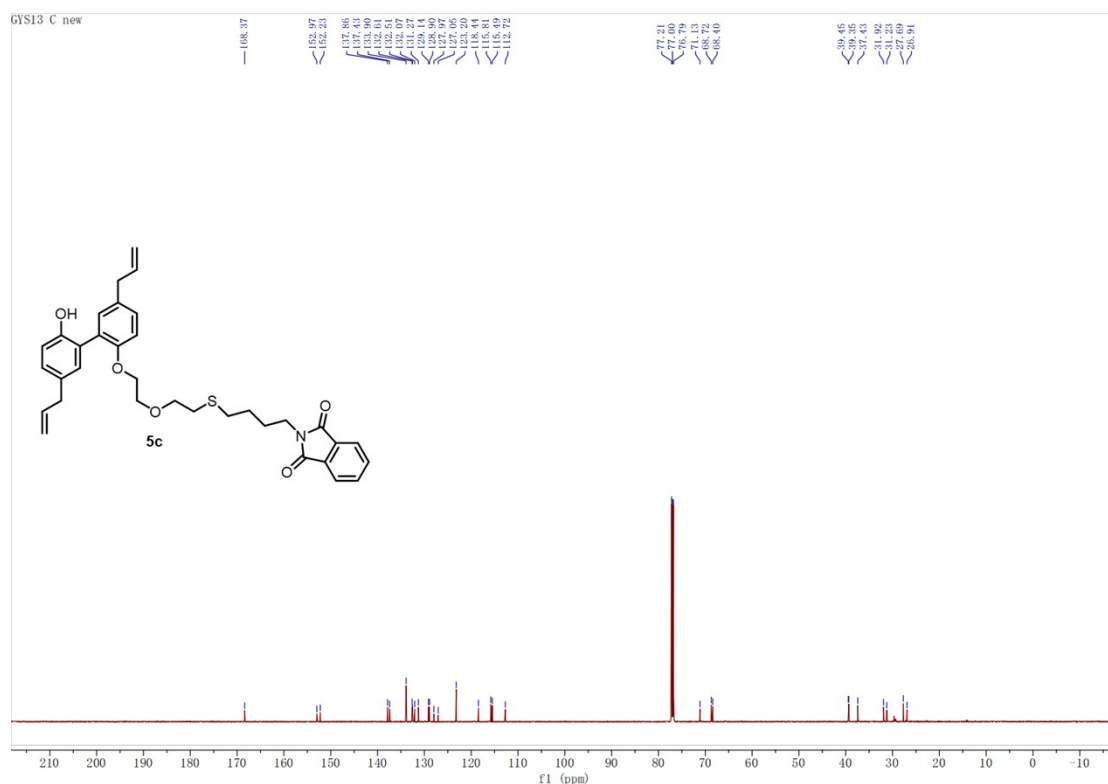


Figure S11. ^{13}C NMR of **5c** (CDCl_3 , 150 MHz)

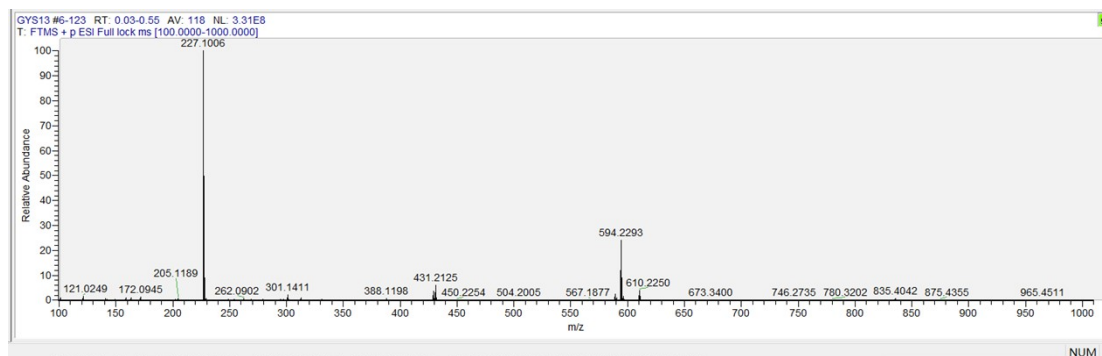
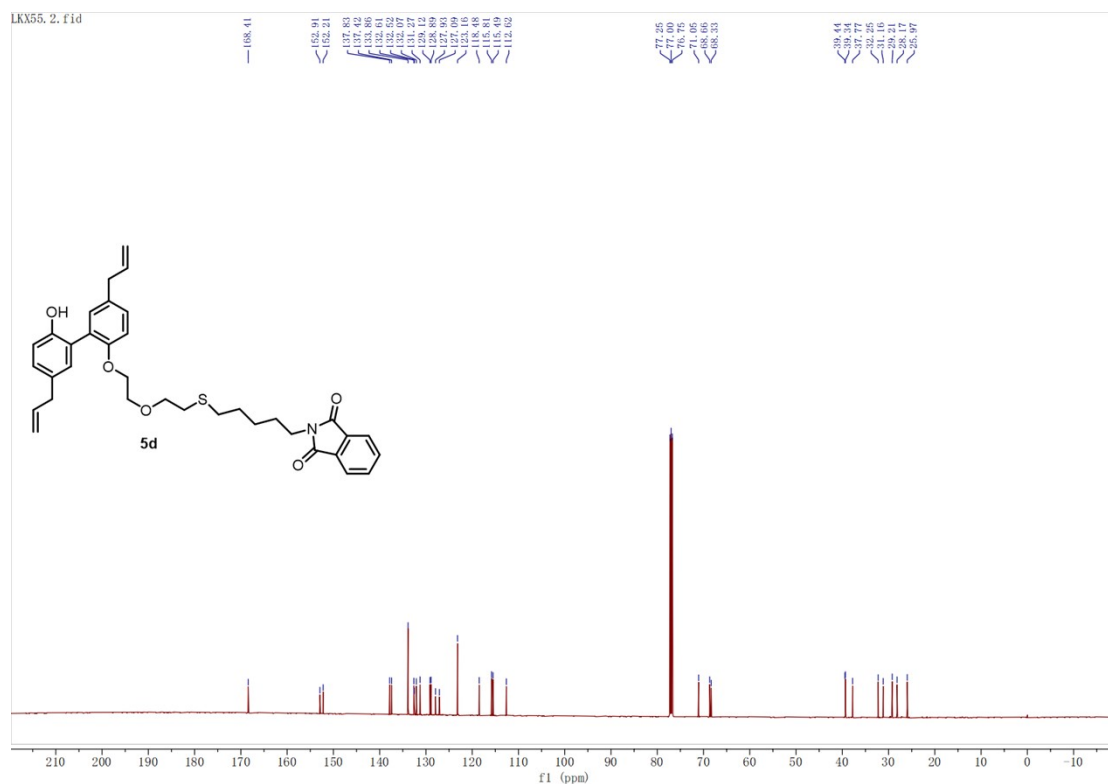
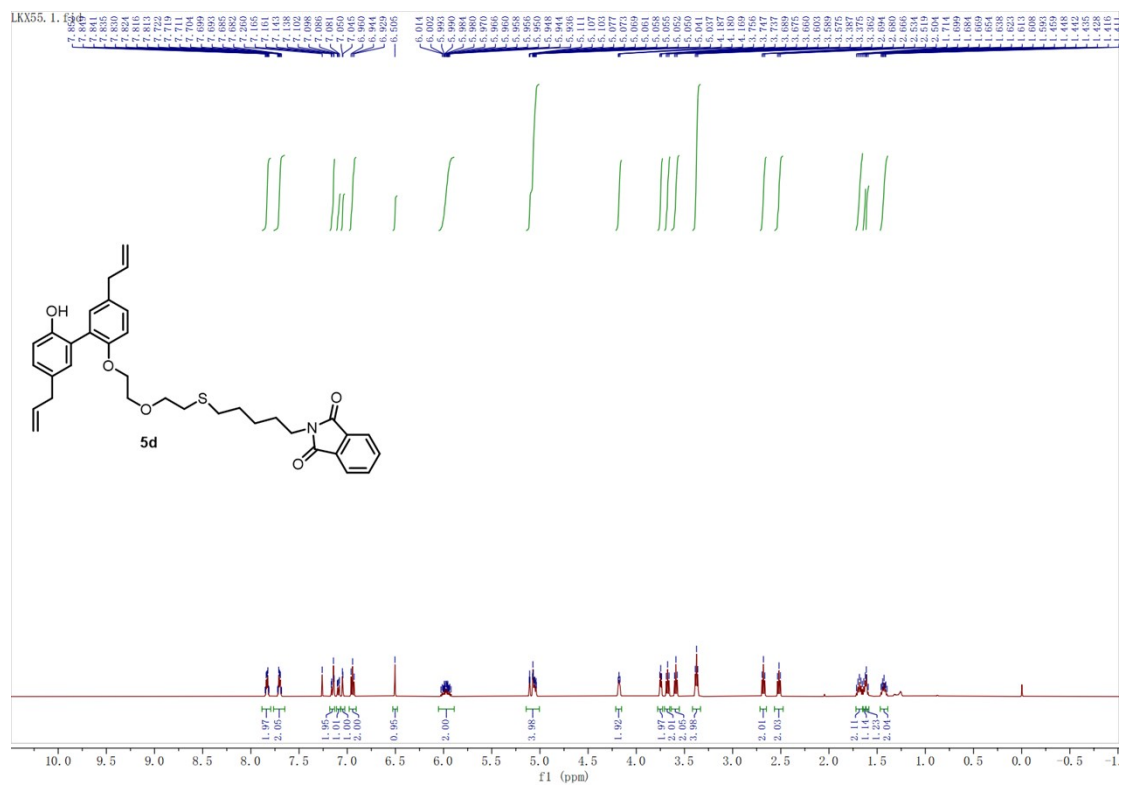


Figure S12. HRMS Spectra of **5c**



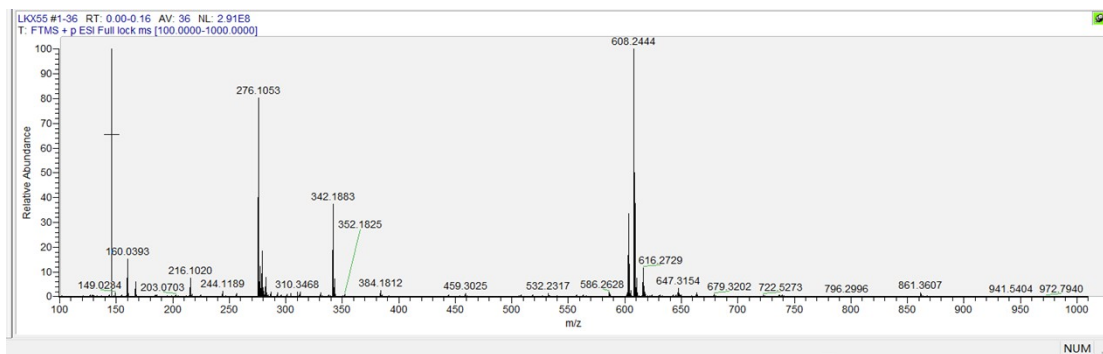


Figure S15. HRMS Spectra of **5d**

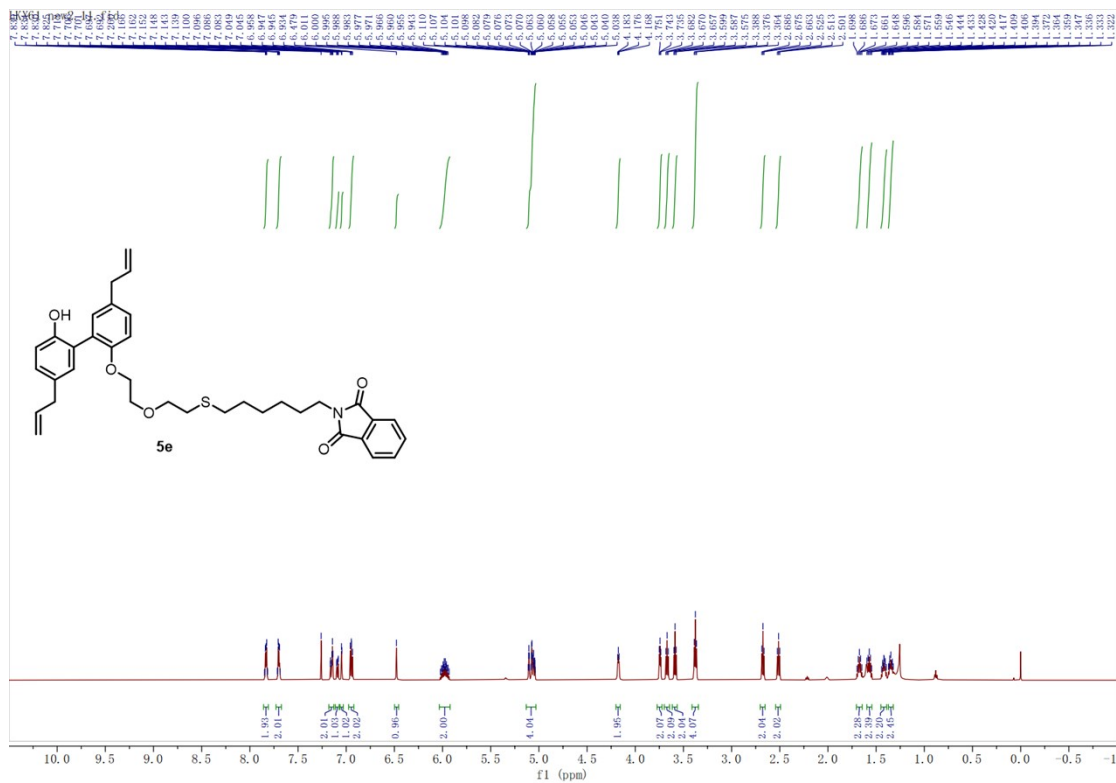


Figure S16. ^1H NMR of **5e** (CDCl_3 , 600 MHz)

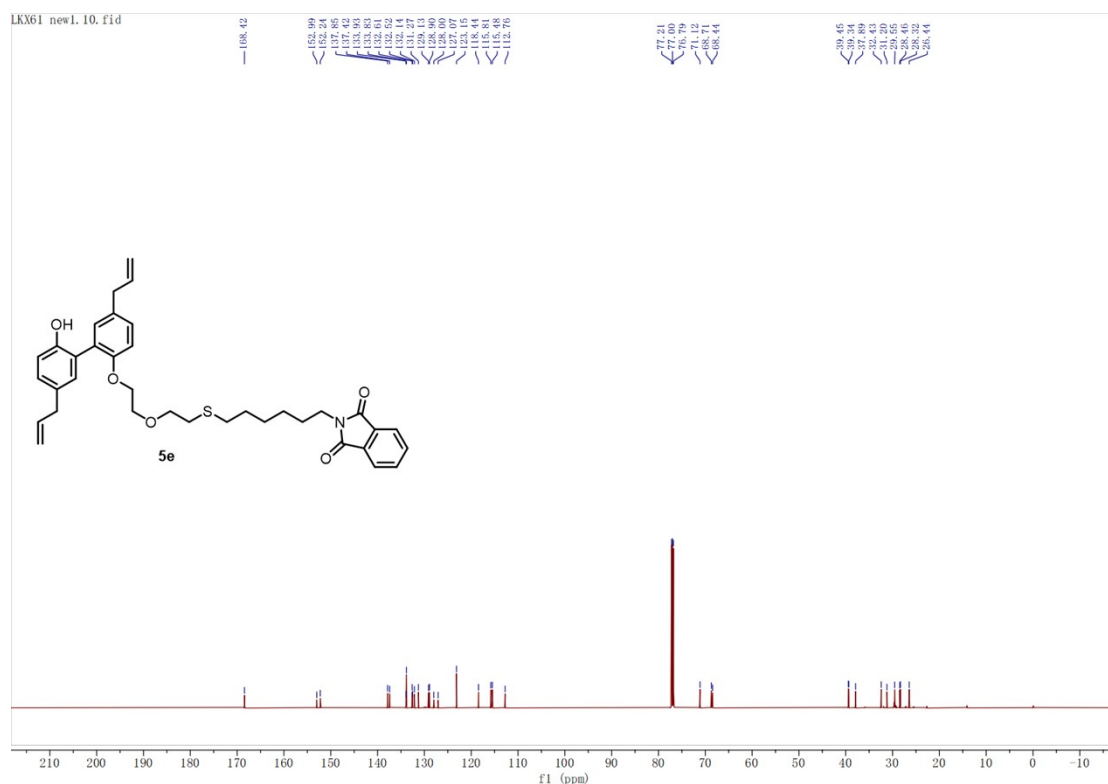


Figure S17. ^{13}C NMR of **5e** (CDCl_3 , 150 MHz)

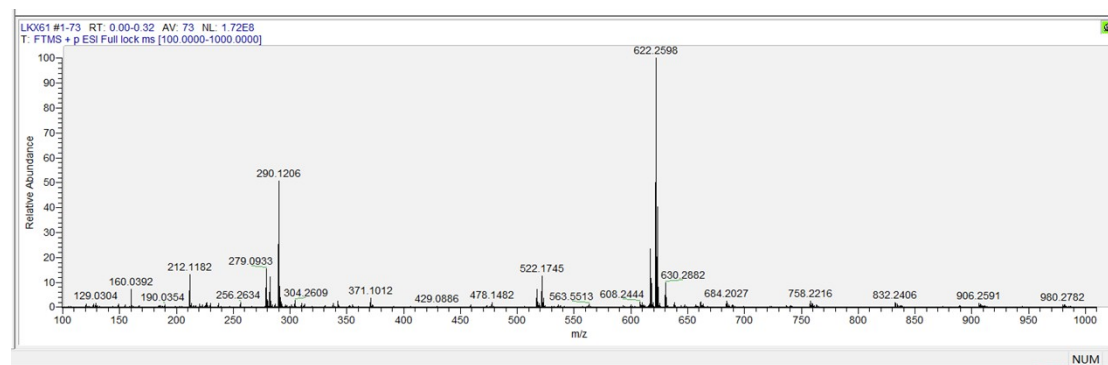


Figure S18. HRMS Spectra of **5e**

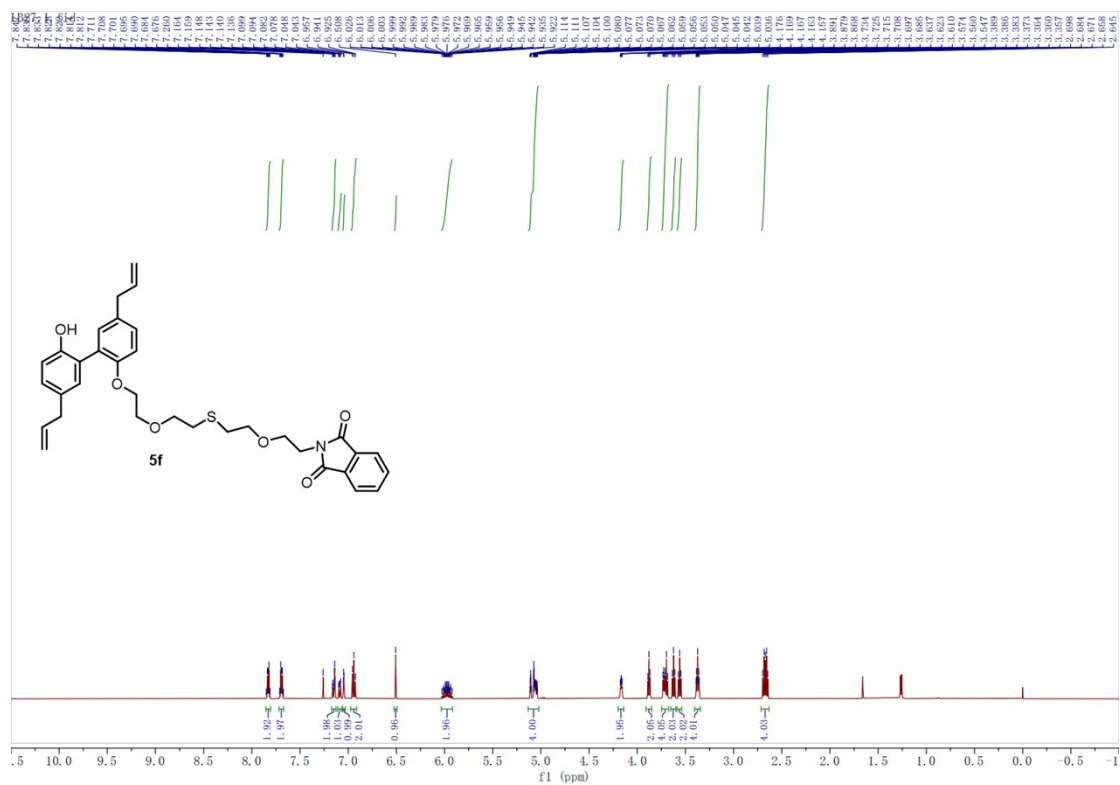


Figure S19. ¹H NMR of **5f** (CDCl₃, 500 MHz)

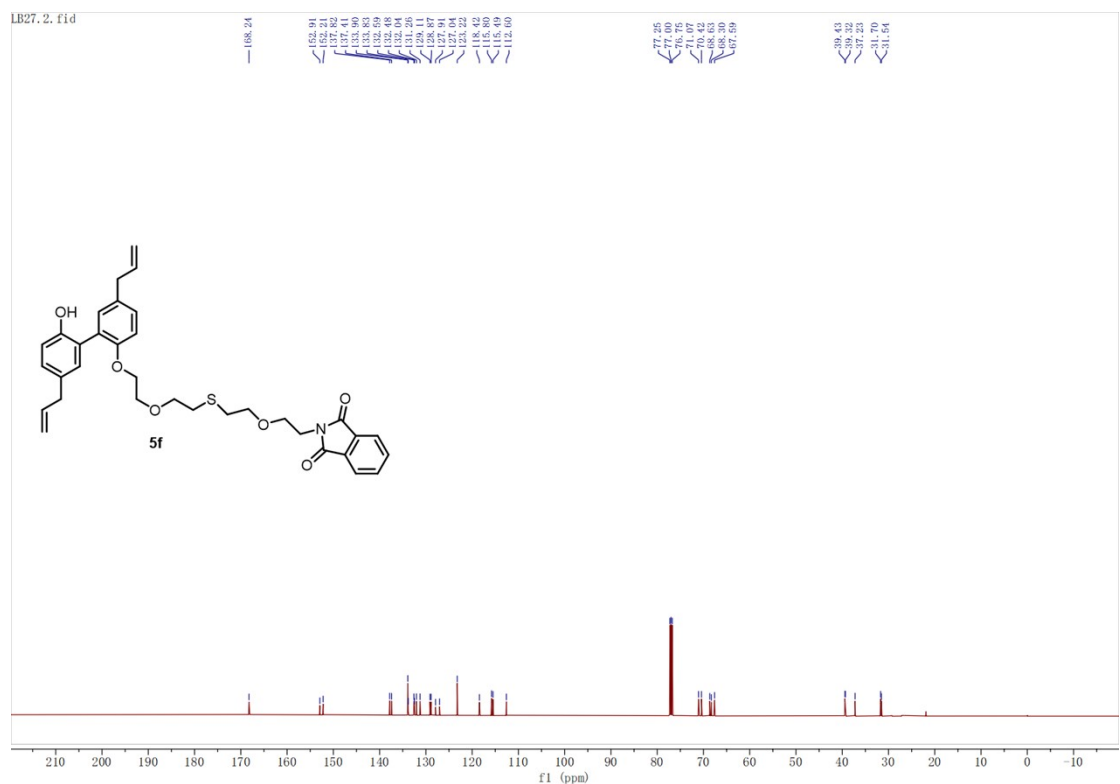


Figure S20. ¹³C NMR of **5f** (CDCl₃, 125 MHz)

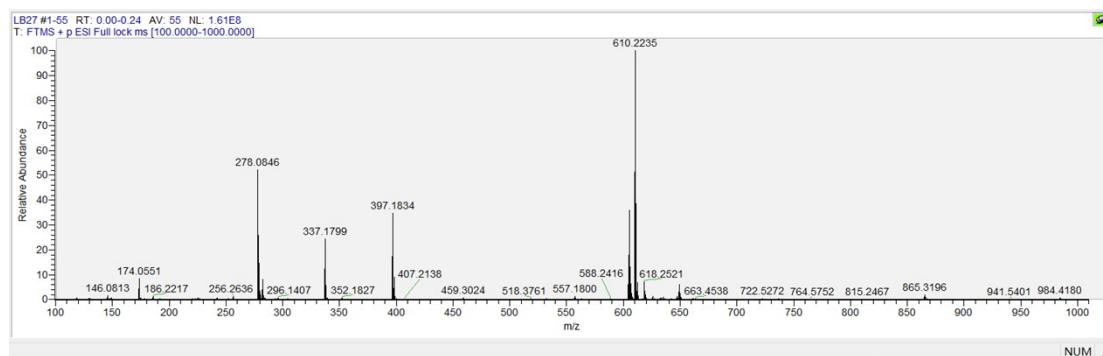


Figure S21. HRMS Spectra of **5f**

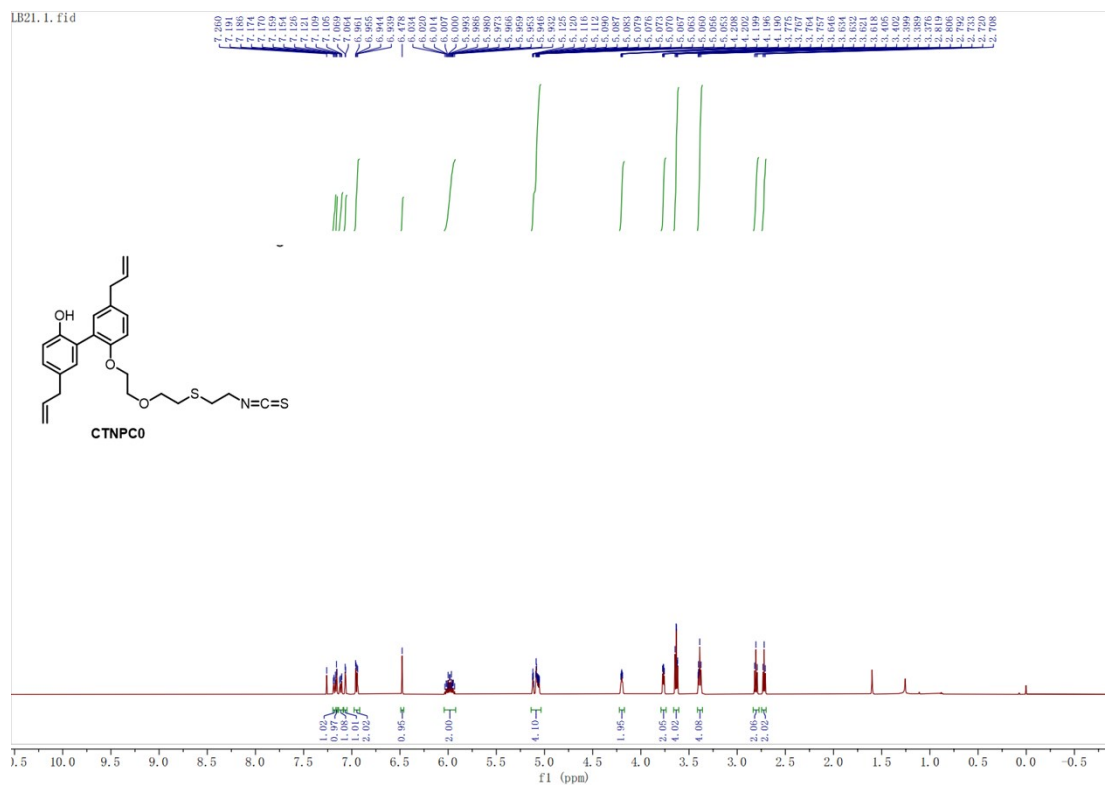


Figure S22. ^1H NMR of CTNPC0 (CDCl_3 , 500 MHz)

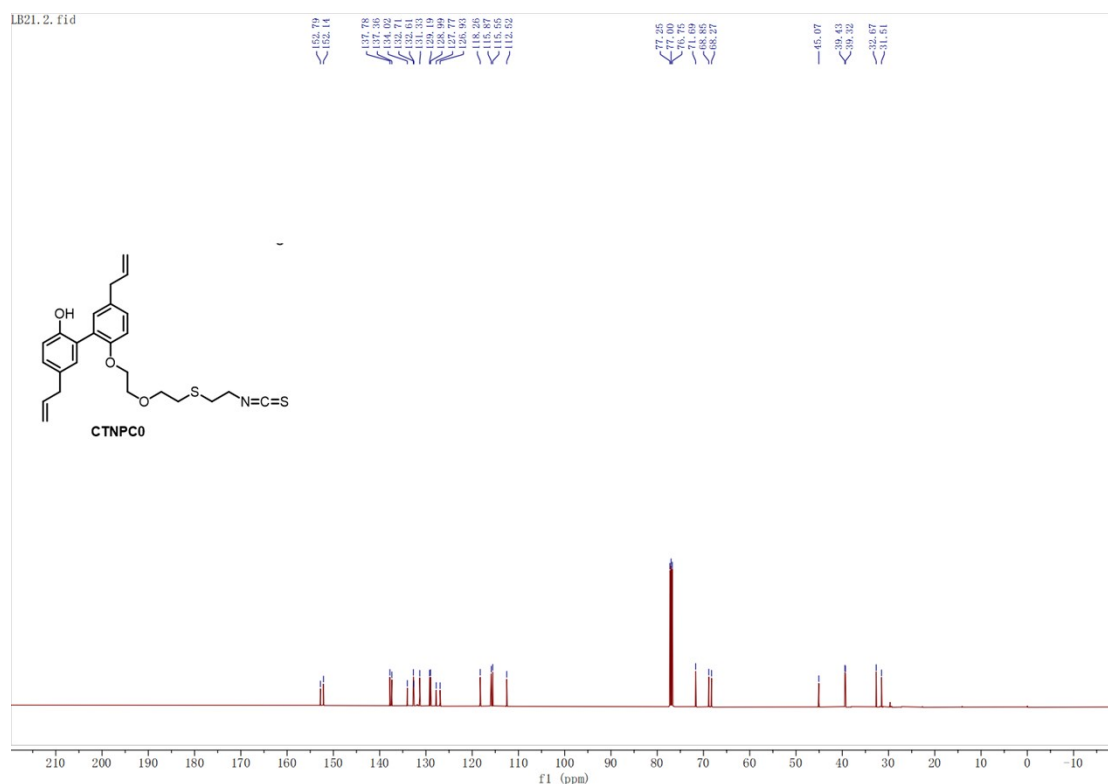


Figure S23. ^{13}C NMR of CTNPC0 (CDCl_3 , 125 MHz)

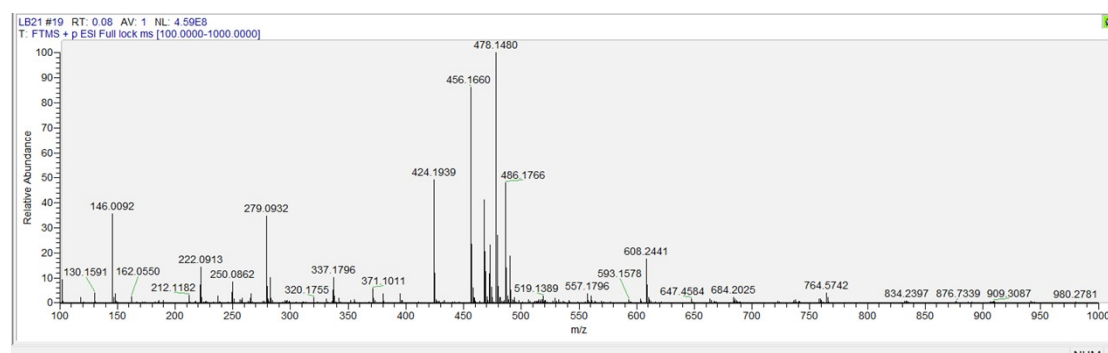


Figure S24. HRMS Spectra of CTNPC0

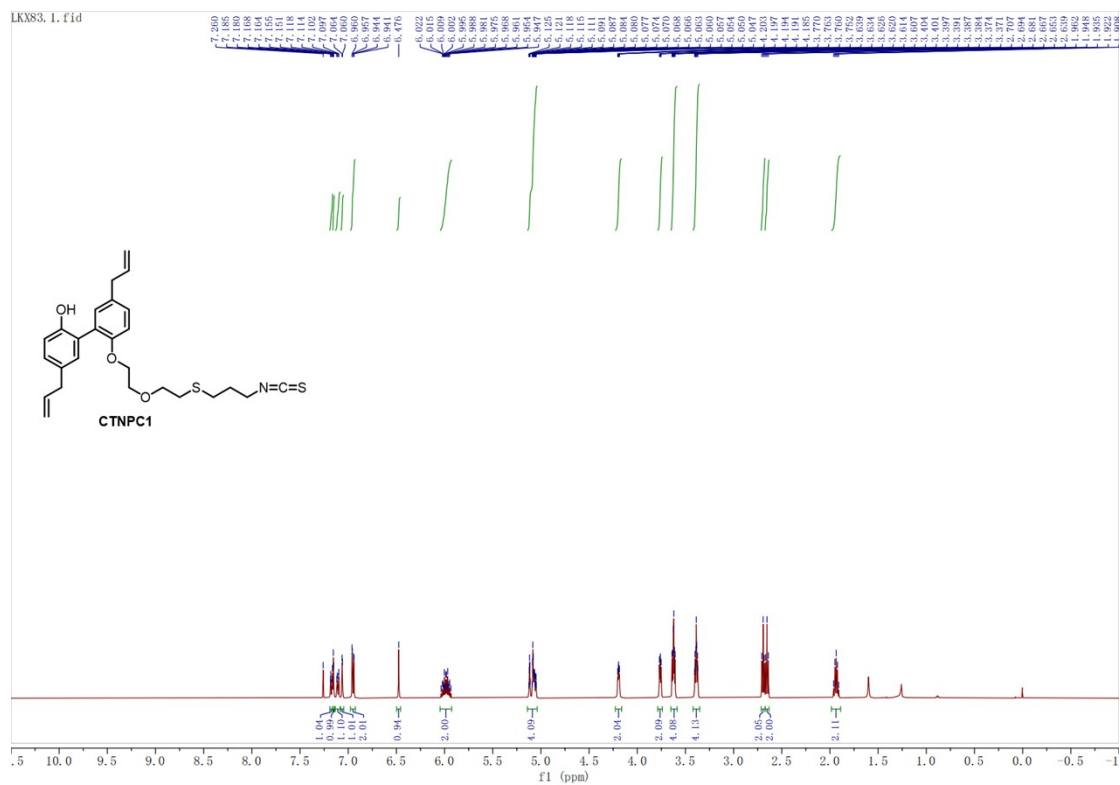


Figure S25. ^1H NMR of CTNPC1 (CDCl_3 , 500 MHz)

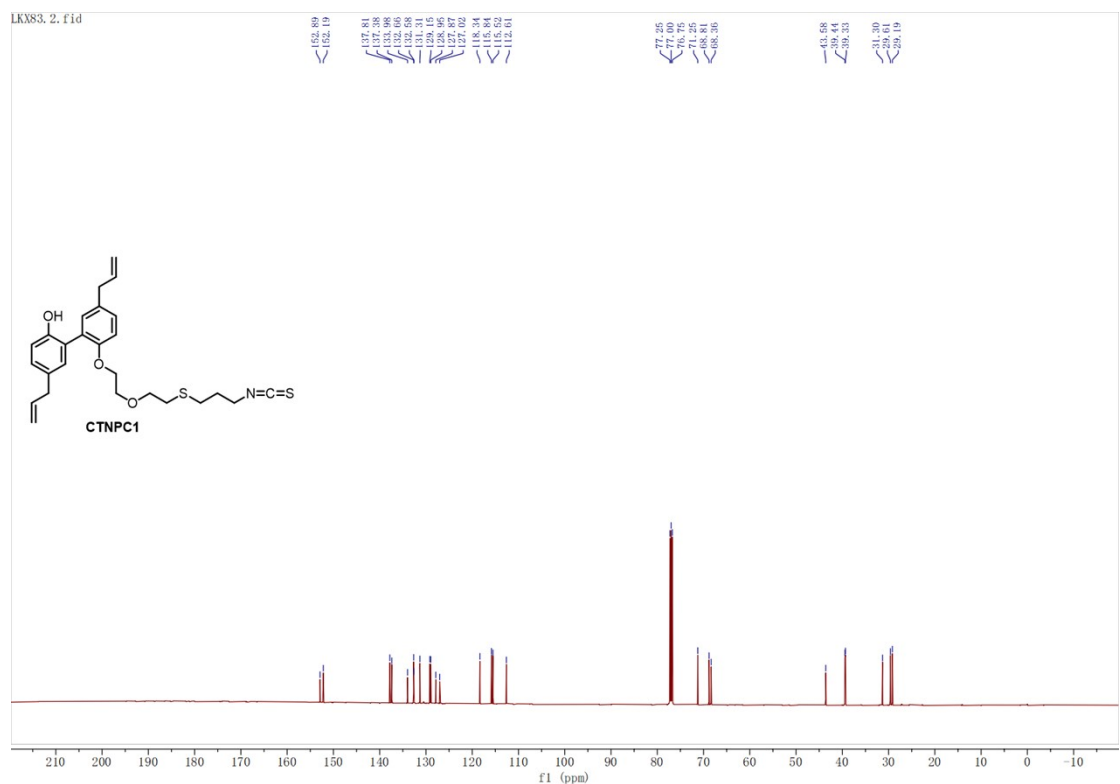


Figure S26. ^{13}C NMR of CTNPC1 (CDCl_3 , 125 MHz)

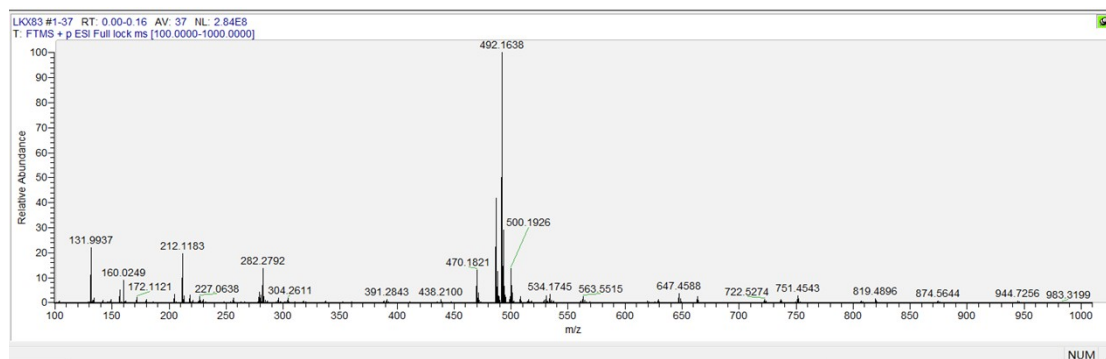


Figure S27. HRMS Spectra of CTNPC1

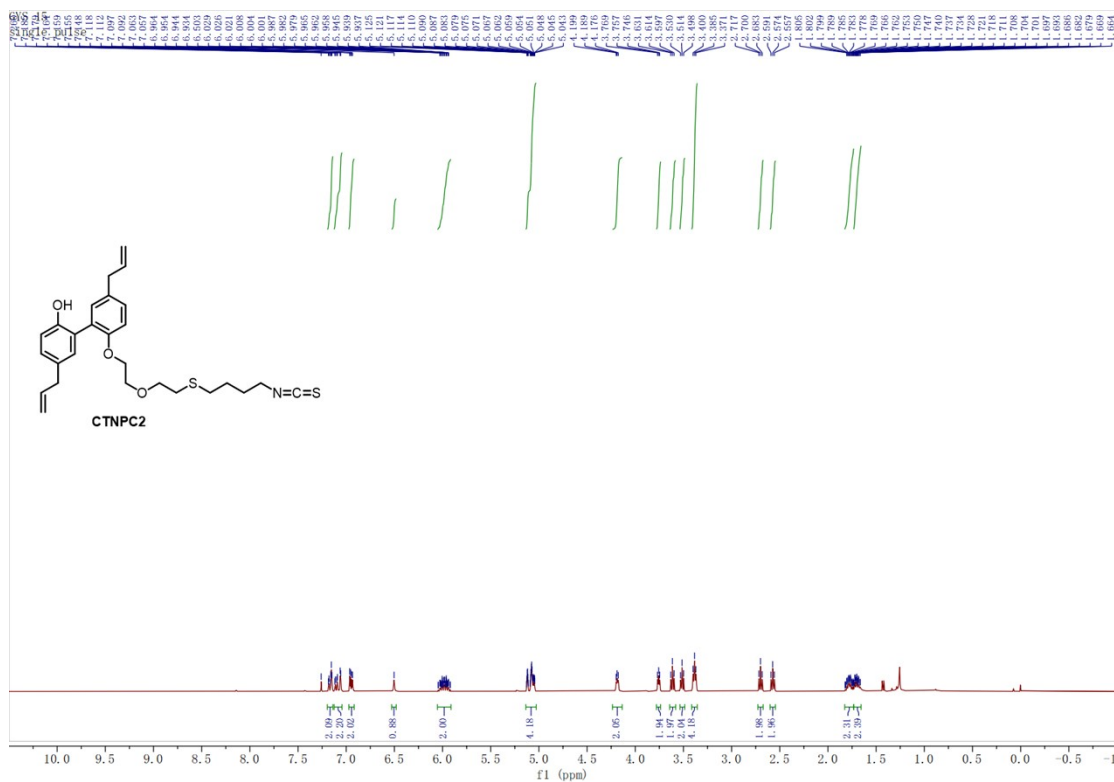


Figure S28. ^1H NMR of CTNPC2 (CDCl_3 , 400 MHz)

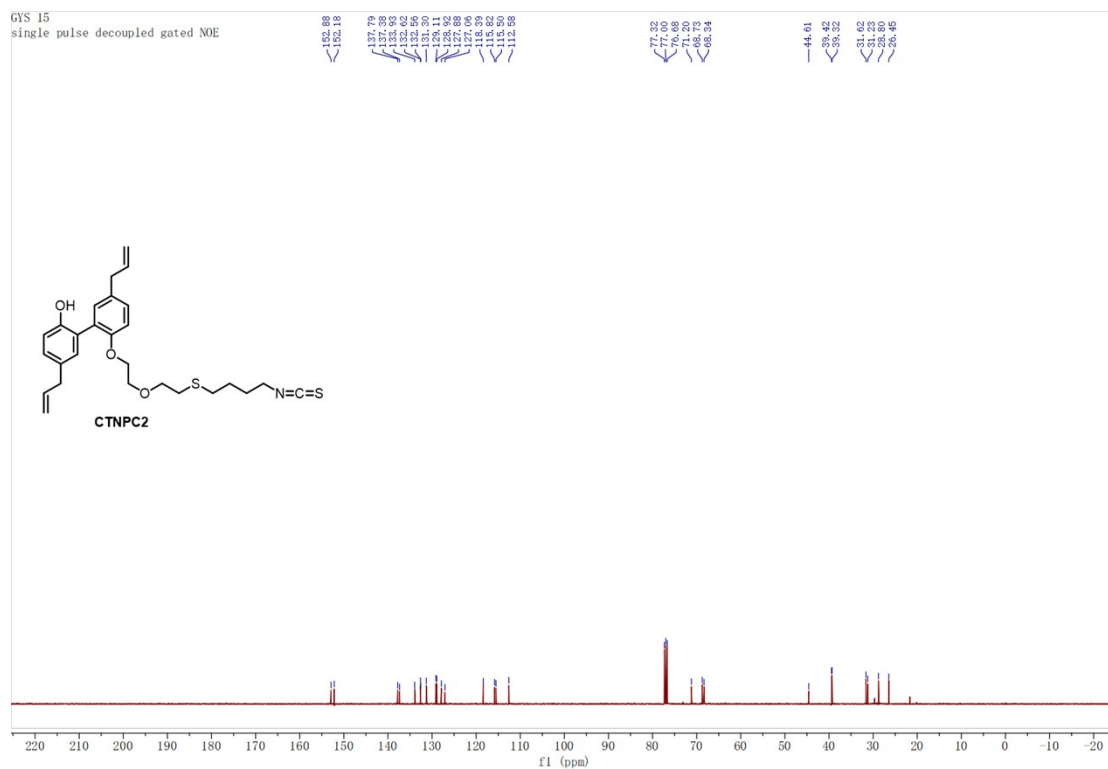


Figure S29. ^{13}C NMR of CTNPC2 (CDCl_3 , 100 MHz)

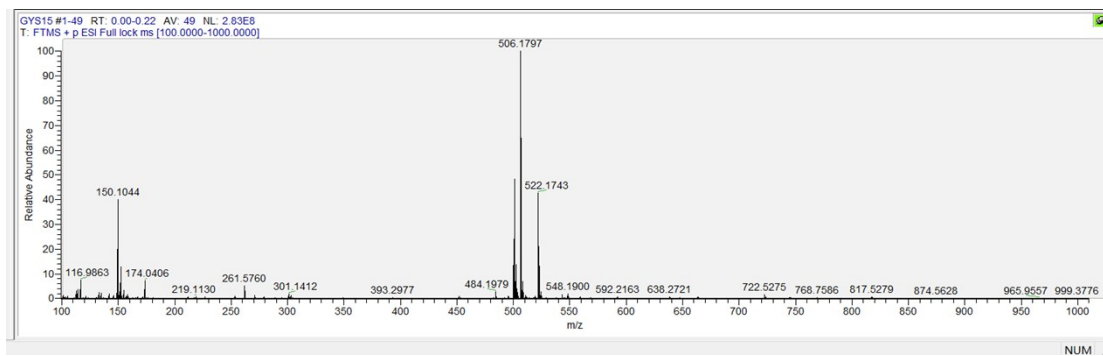


Figure S30. HRMS Spectra of CTNPC2

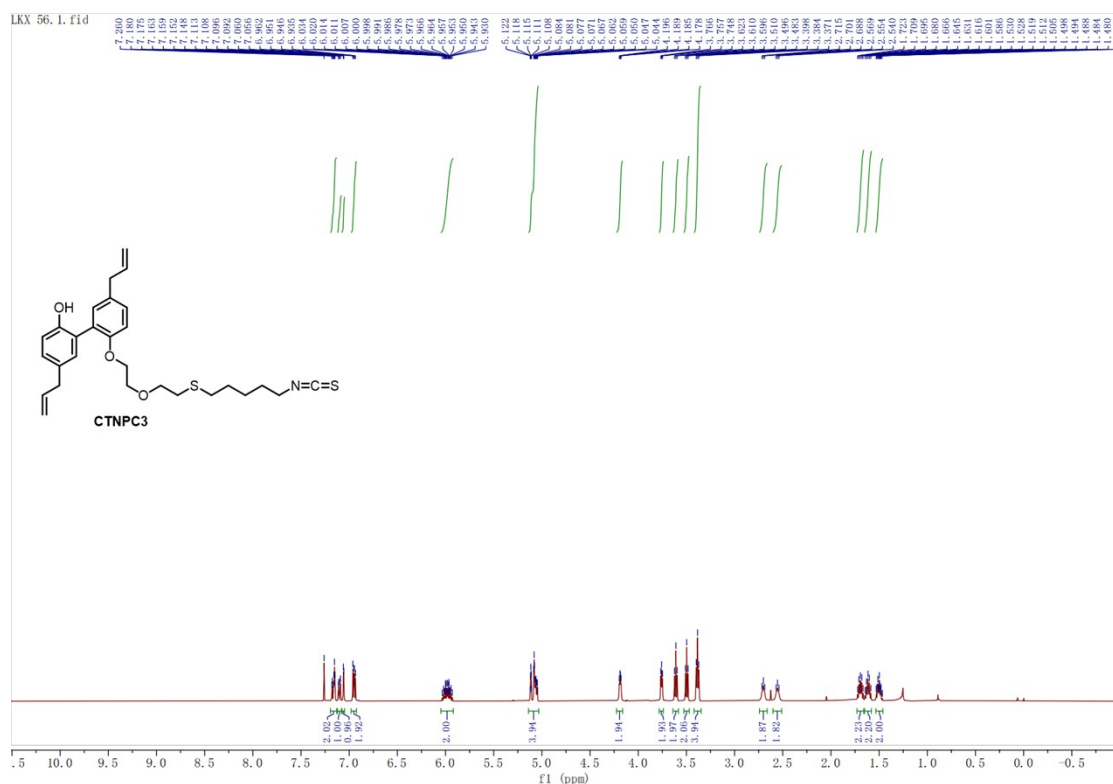


Figure S31. ^1H NMR of CTNPC3 (CDCl_3 , 500 MHz)

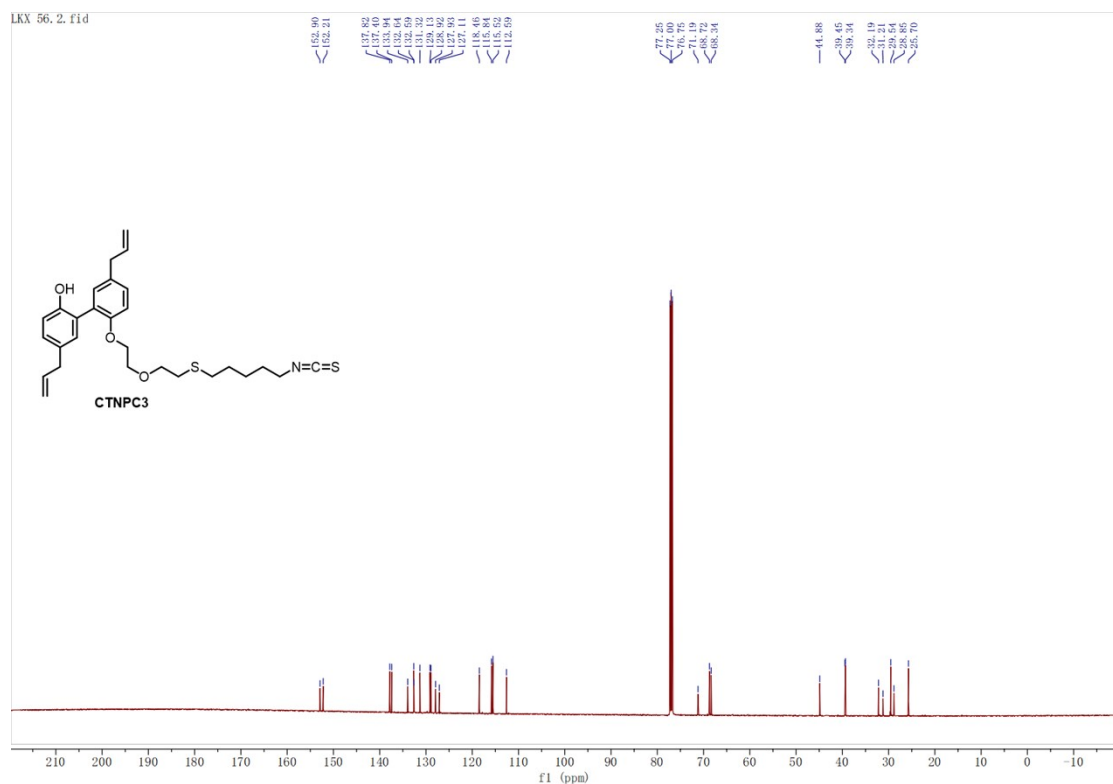


Figure S32. ^{13}C NMR of CTNPC3 (CDCl_3 , 125 MHz)

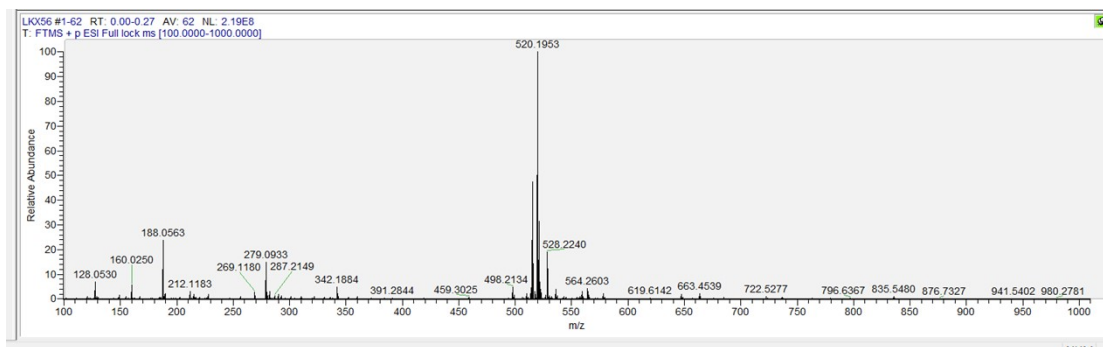


Figure S33. HRMS Spectra of CTNPC3

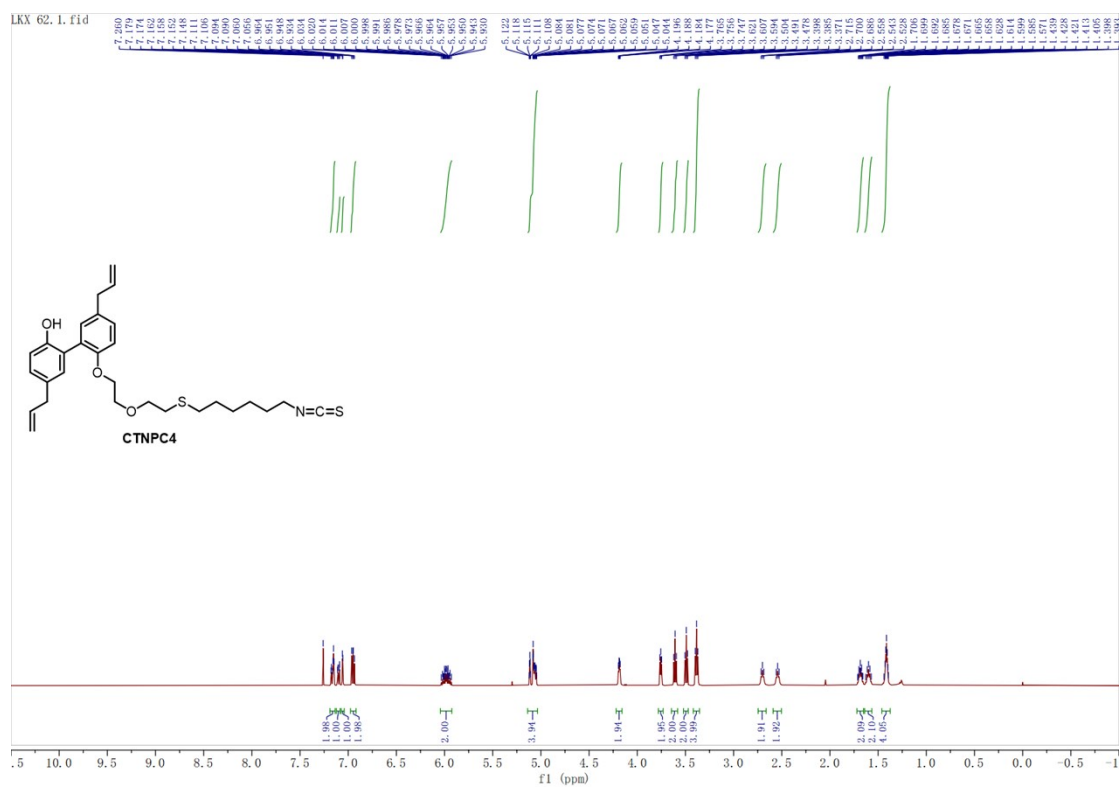


Figure S34. ¹H NMR of CTNPC4 (CDCl₃, 500 MHz)

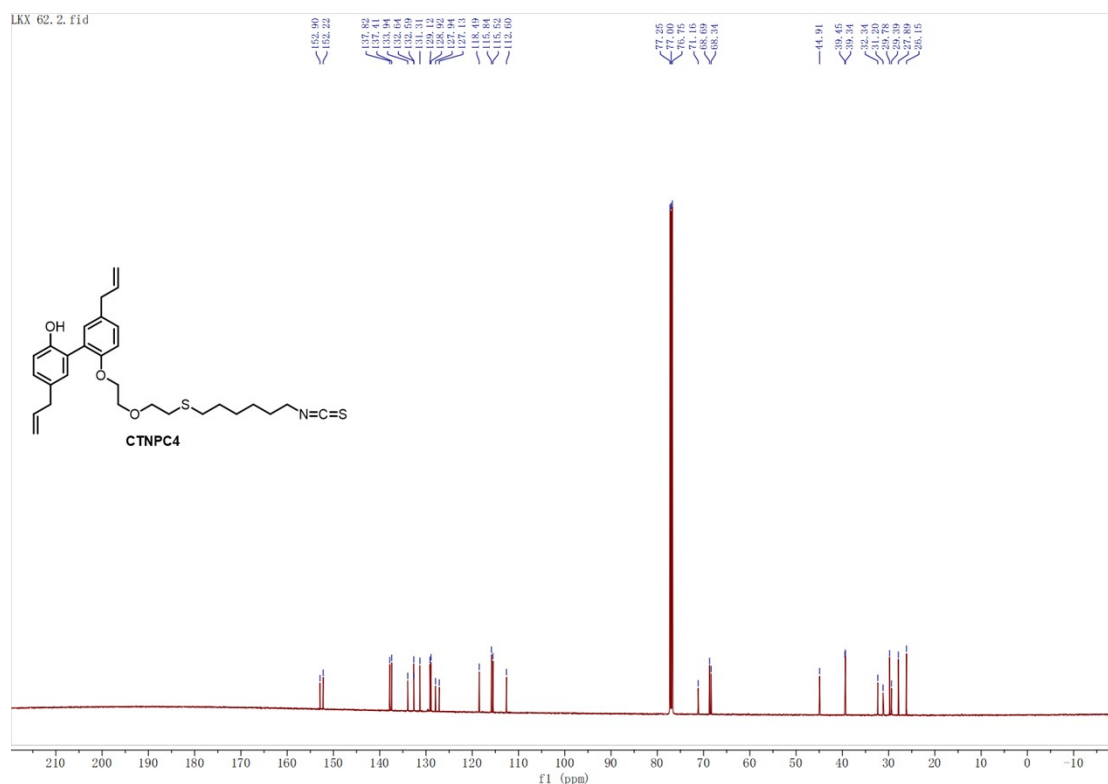


Figure S35. ^{13}C NMR of CTNPC4 (CDCl_3 , 125 MHz)

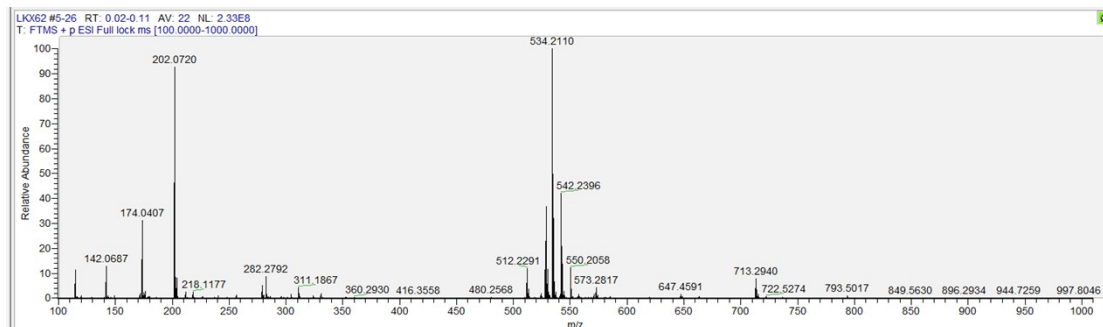


Figure S36. HRMS Spectra of CTNPC4

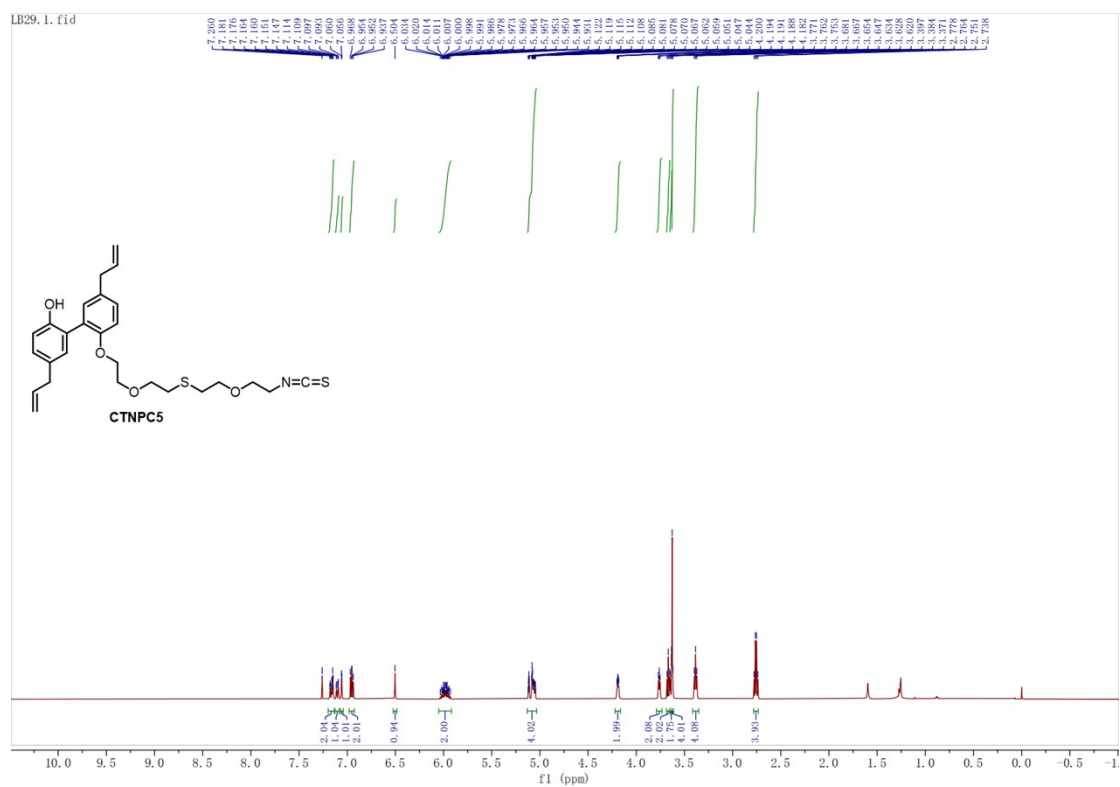


Figure S37. ^1H NMR of CTNPC5 (CDCl_3 , 500 MHz)

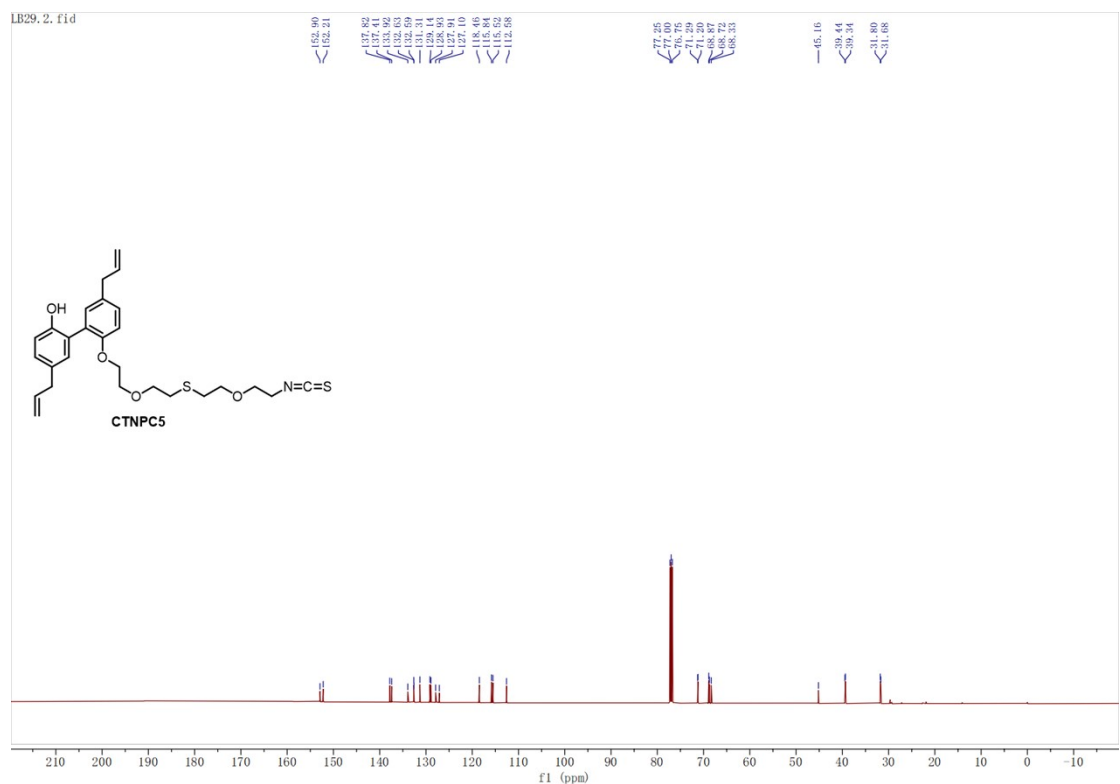


Figure S38. ^{13}C NMR of CTNPC5 (CDCl_3 , 125 MHz)

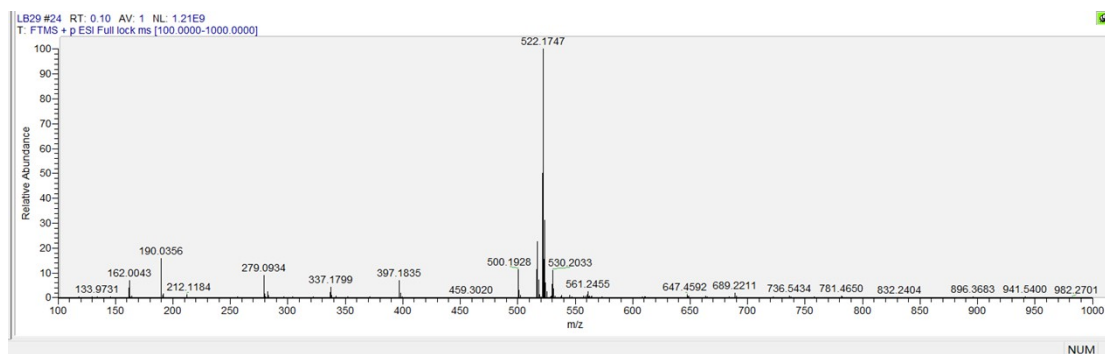


Figure S39. HRMS Spectra of CTNPC5

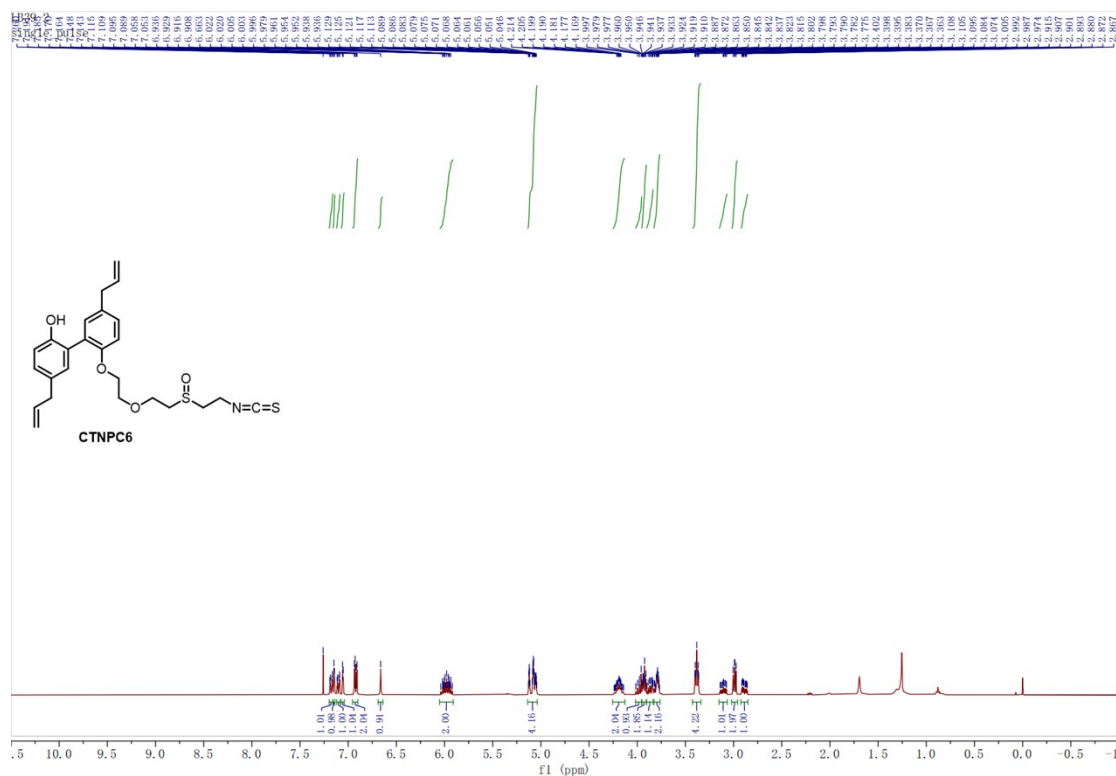


Figure S40. ¹H NMR of CTNPC6 (CDCl₃, 400 MHz)

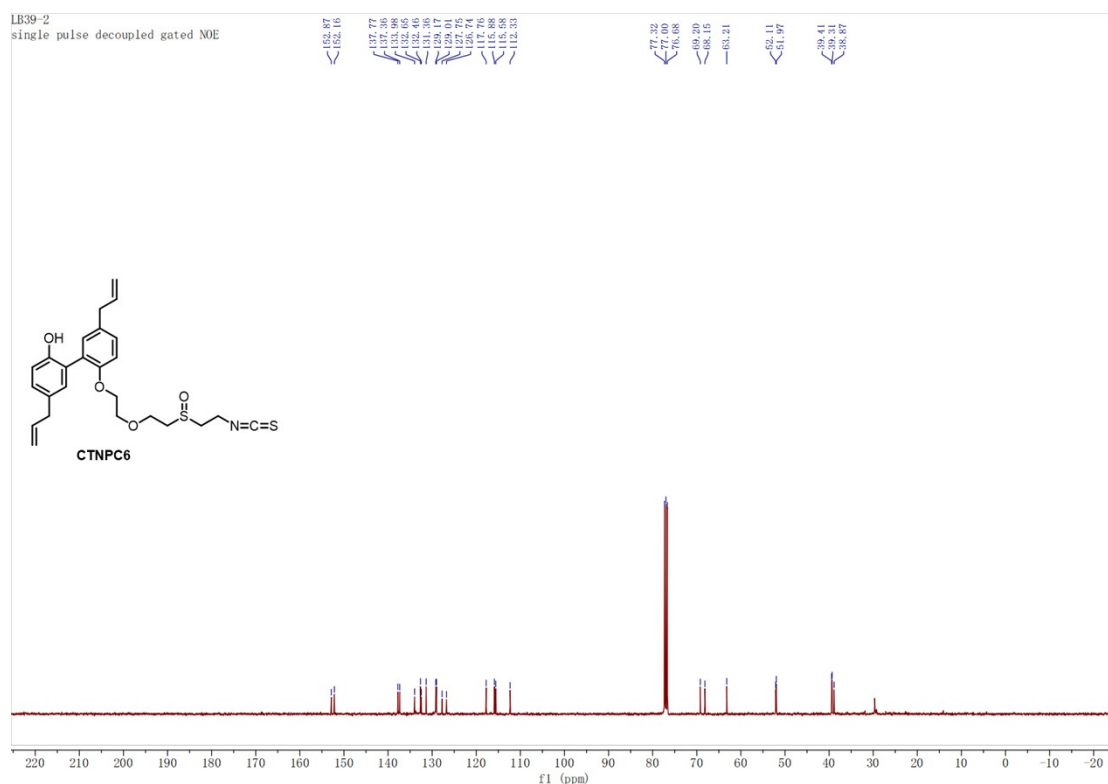


Figure S41. ^{13}C NMR of CTNPC6 (CDCl_3 , 100 MHz)

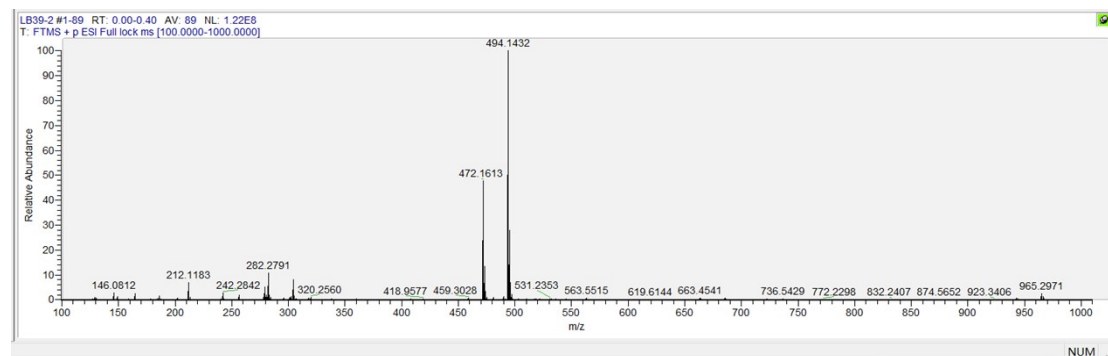


Figure S42. HRMS Spectra of CTNPC6

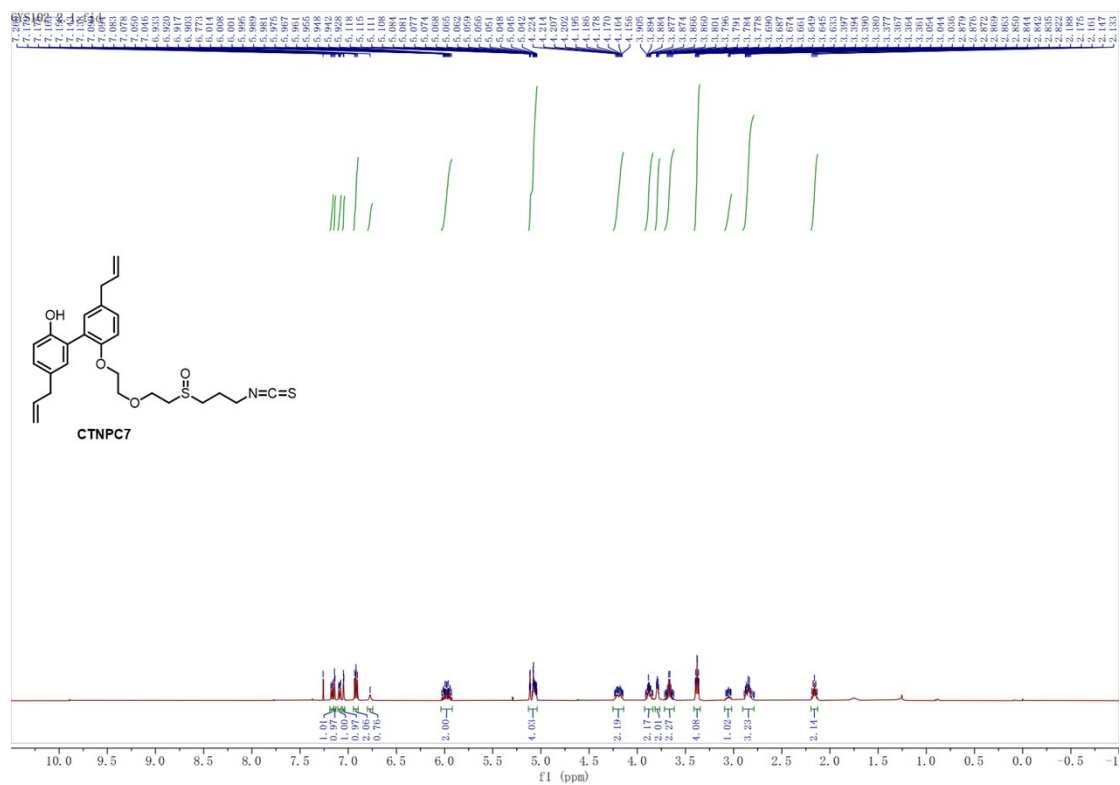


Figure S43. ¹H NMR of CTNPC7 (CDCl₃, 500 MHz)

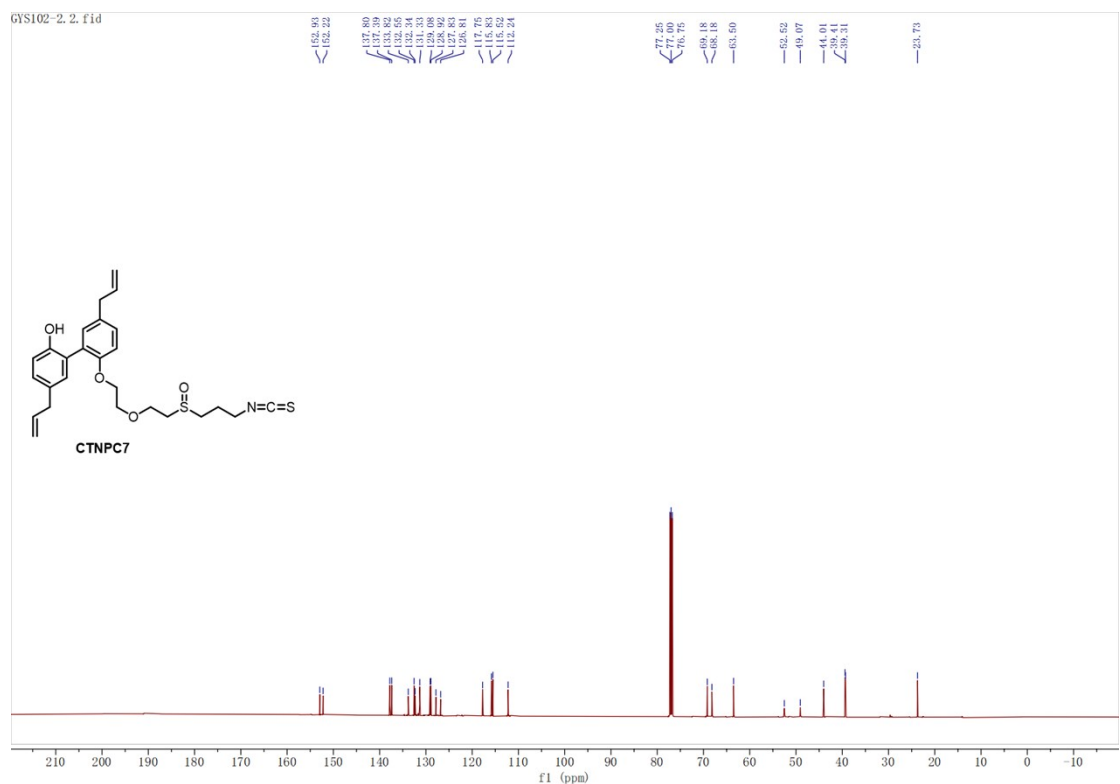


Figure S44. ¹³C NMR of CTNPC7 (CDCl₃, 125 MHz)

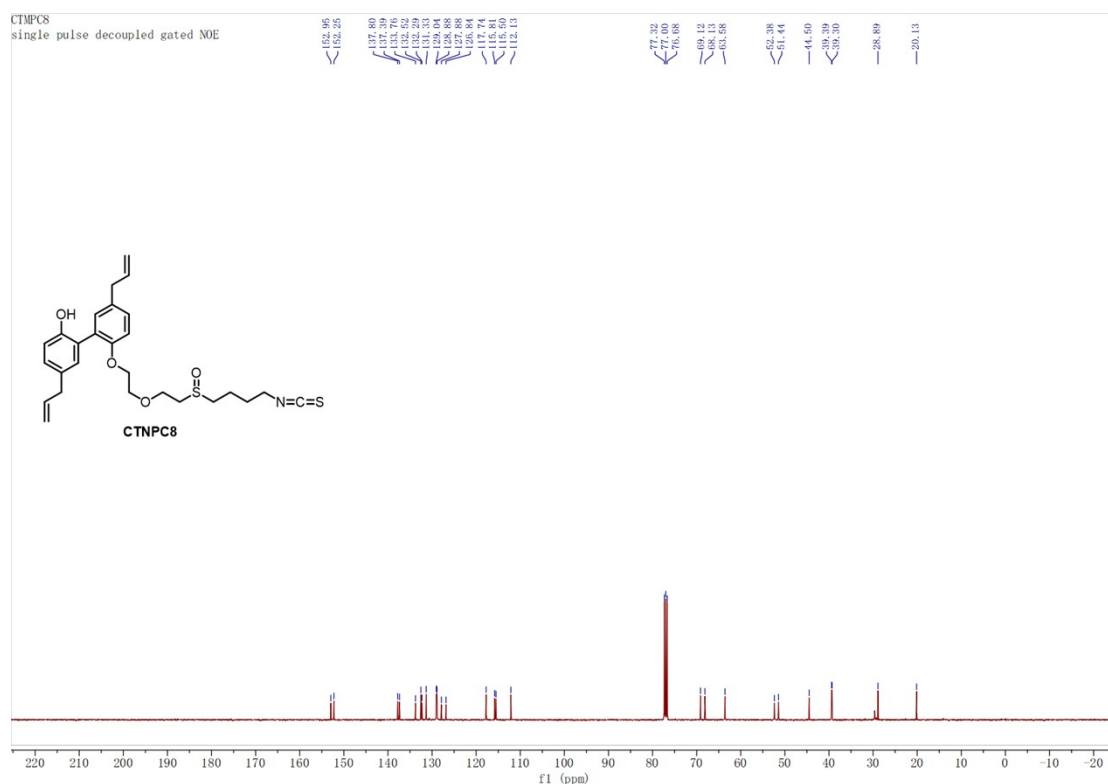


Figure S47. ^{13}C NMR of CTNPC8 (CDCl_3 , 100 MHz)

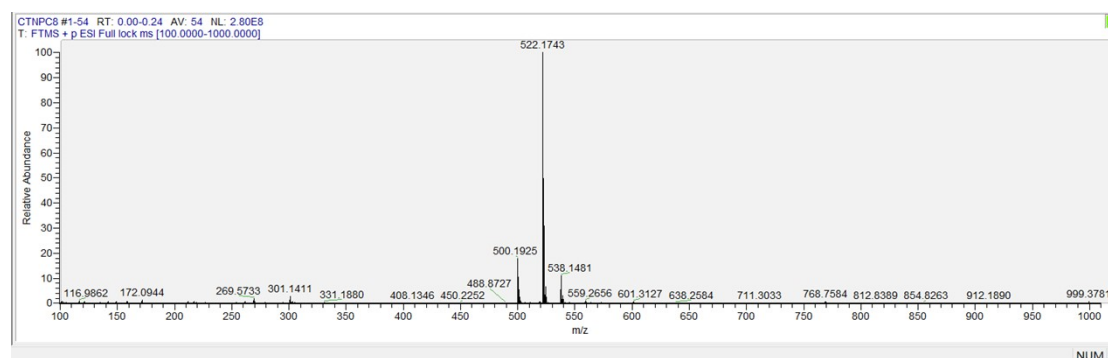


Figure S48. HRMS Spectra of CTNPC8

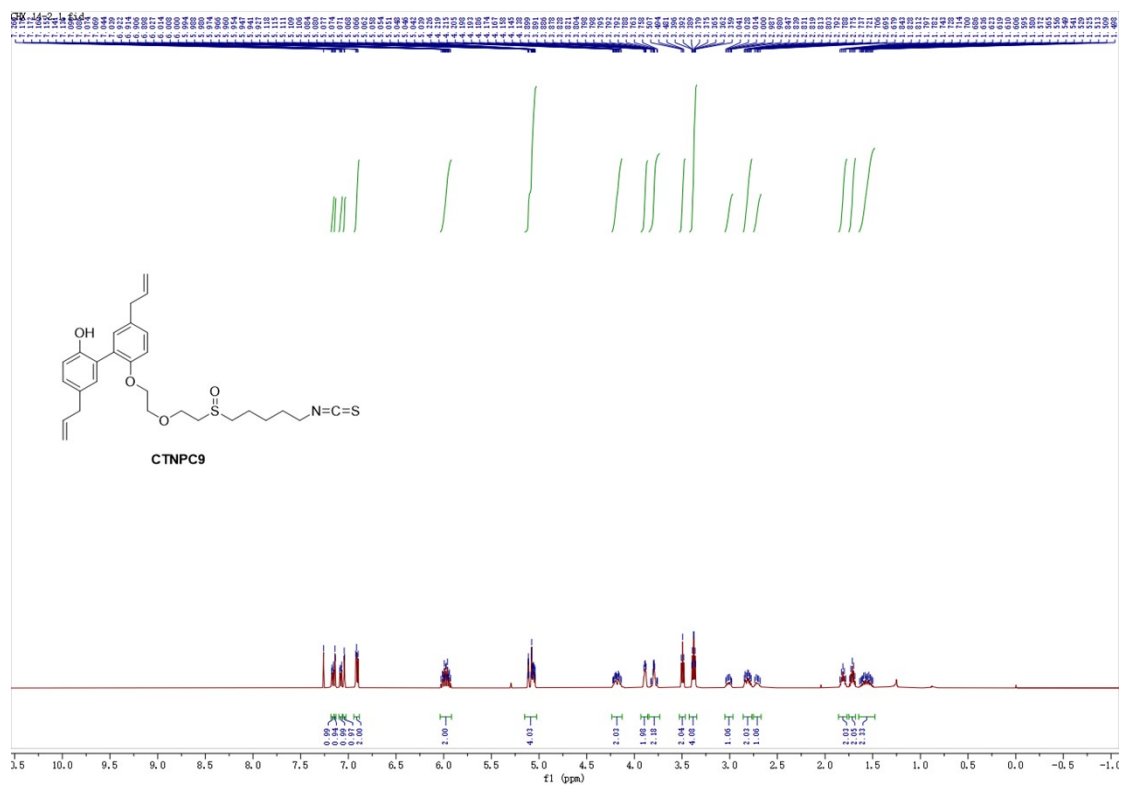


Figure S49. ¹H NMR of CTNPC9 (CDCl₃, 500 MHz)

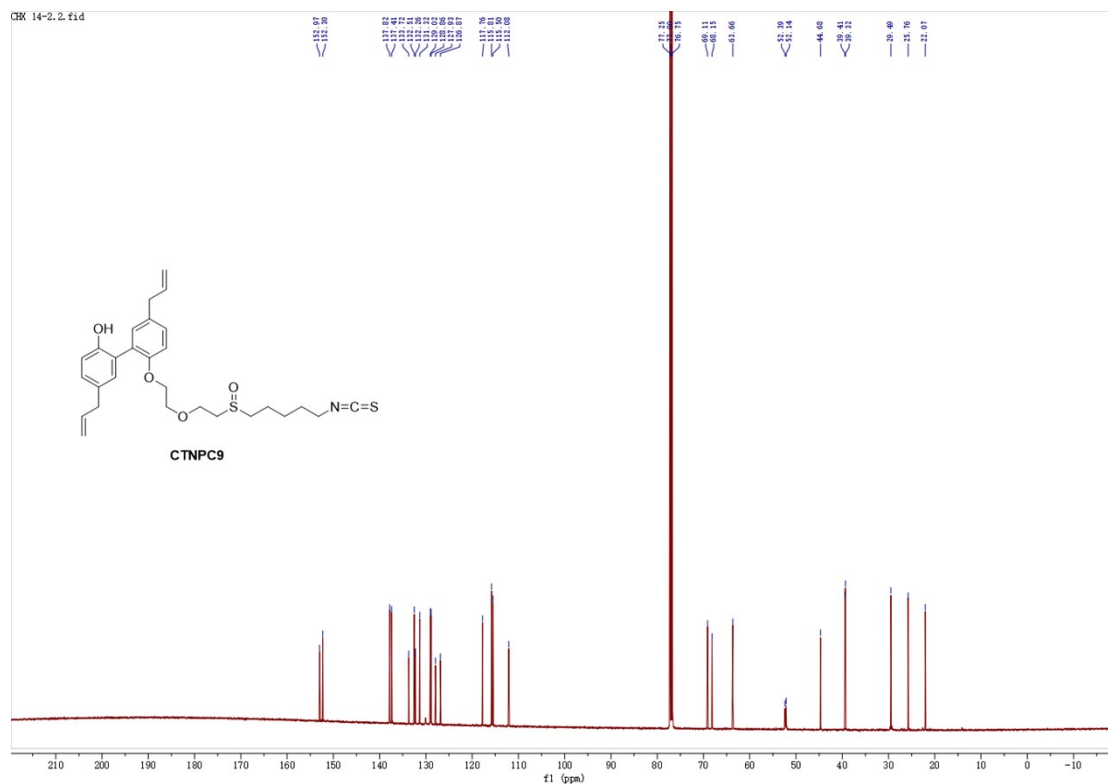


Figure S50. ¹³C NMR of CTNPC9 (CDCl₃, 125 MHz)

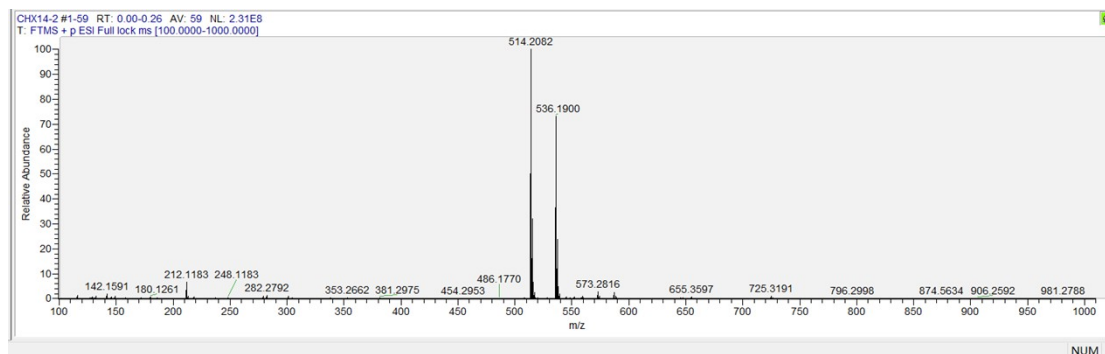


Figure S51. HRMS Spectra of CTNPC9

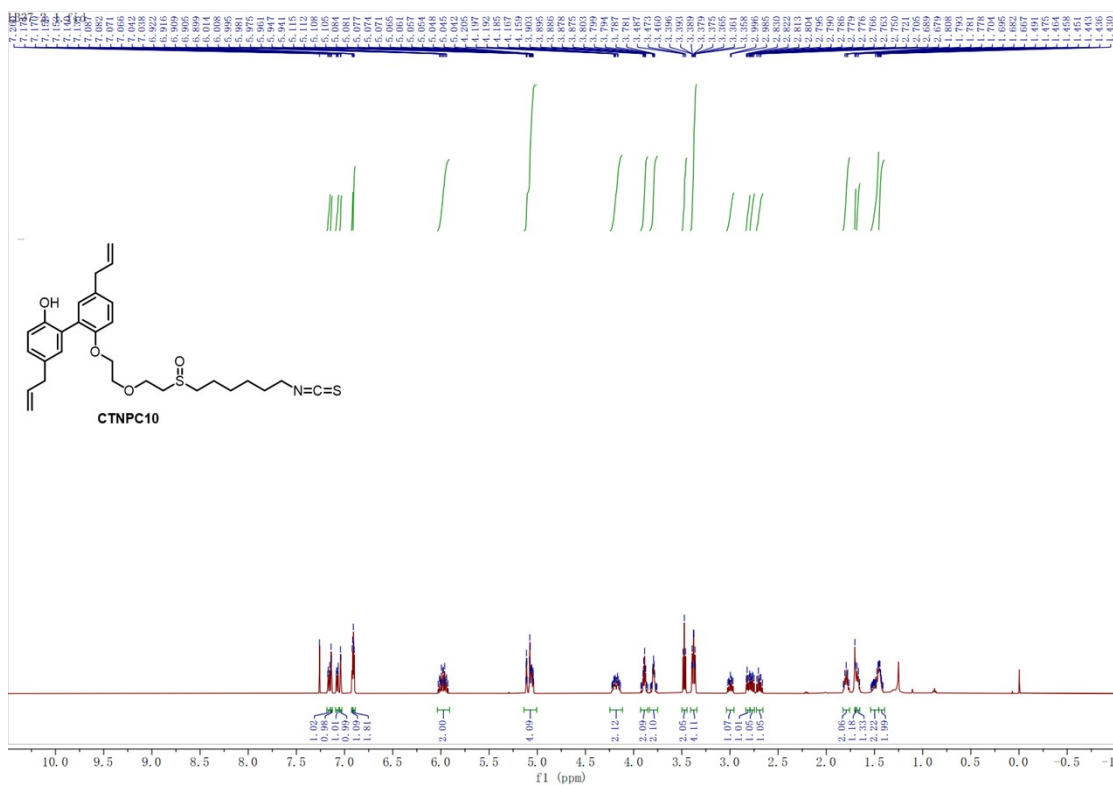


Figure S52. ^1H NMR of CTNPC10 (CDCl_3 , 500 MHz)

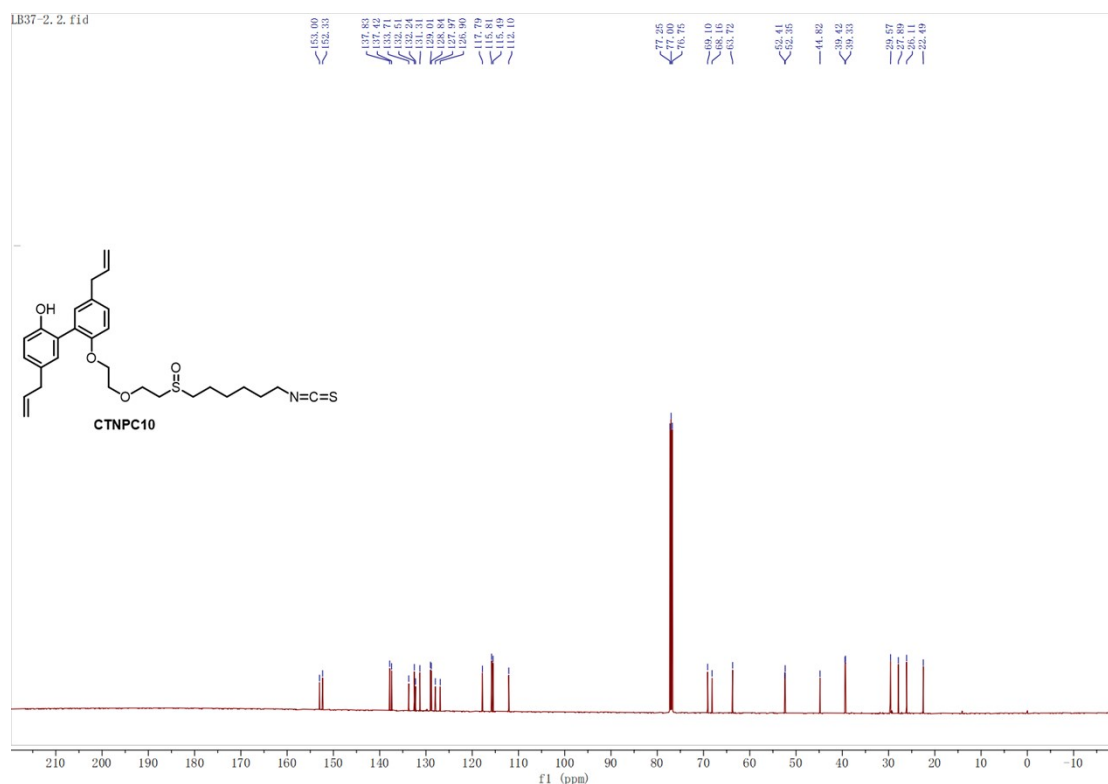


Figure S53. ^{13}C NMR of CTNPC10 (CDCl_3 , 125 MHz)

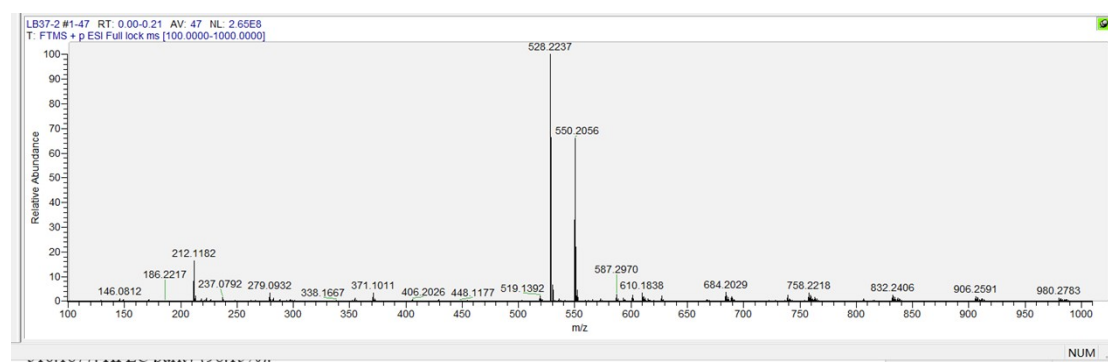


Figure S54. HRMS Spectra of CTNPC10

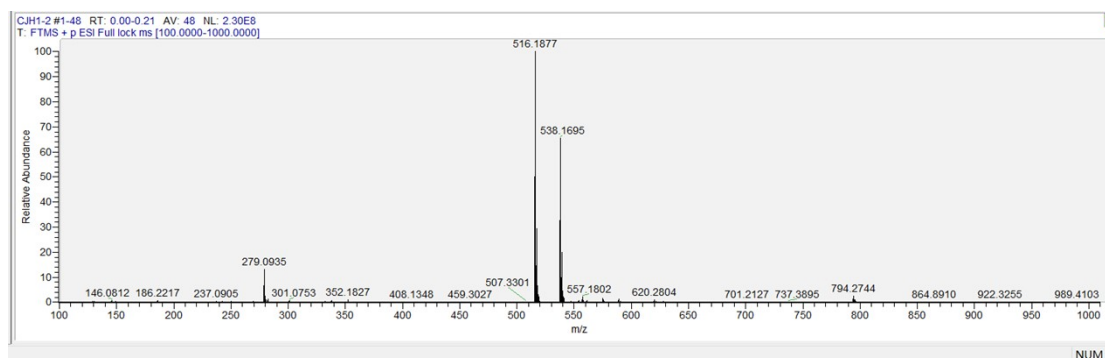


Figure S57. HRMS Spectra of CTNPC11

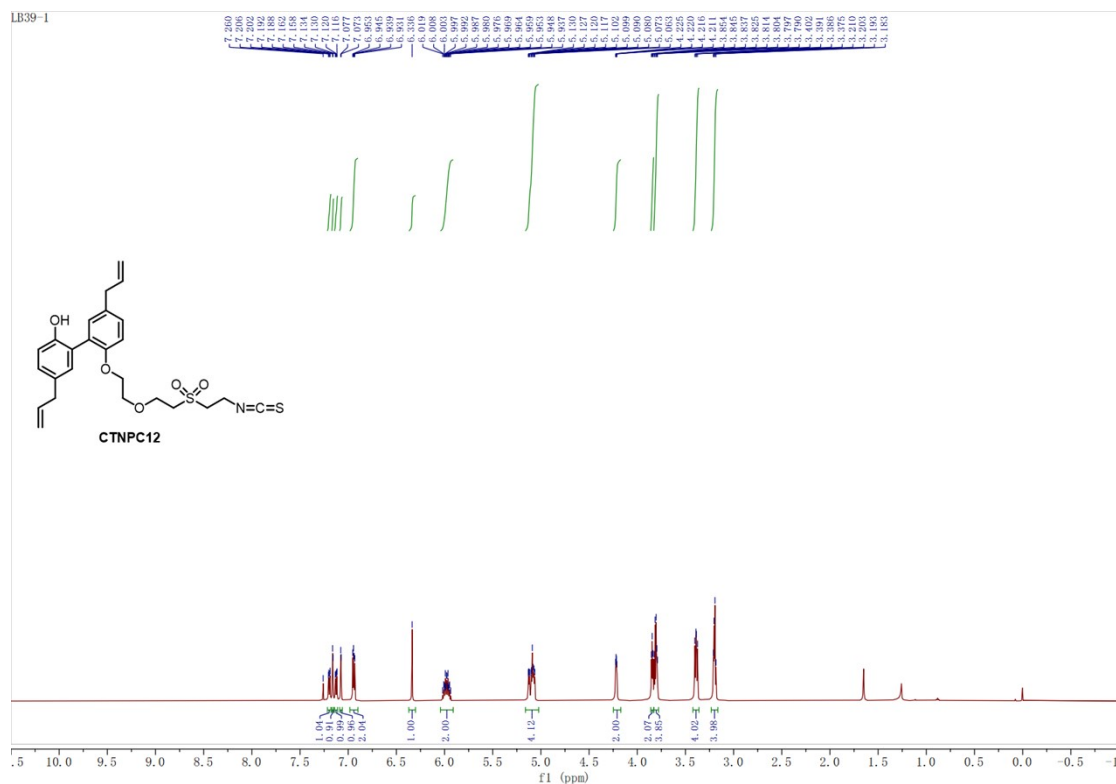
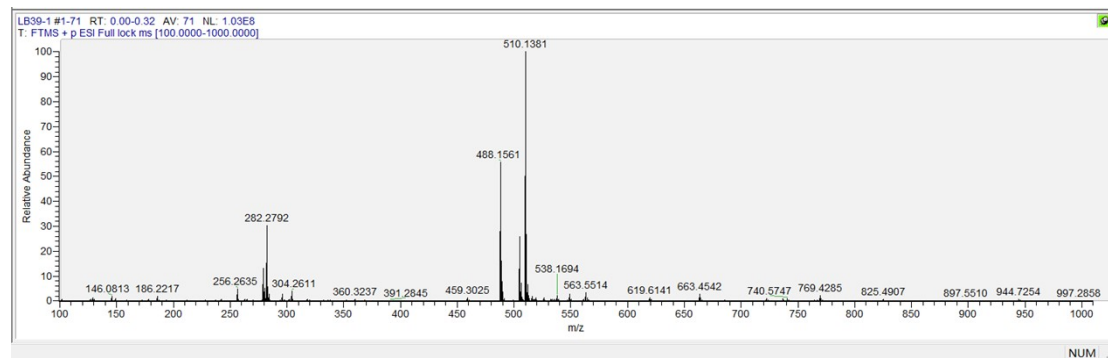
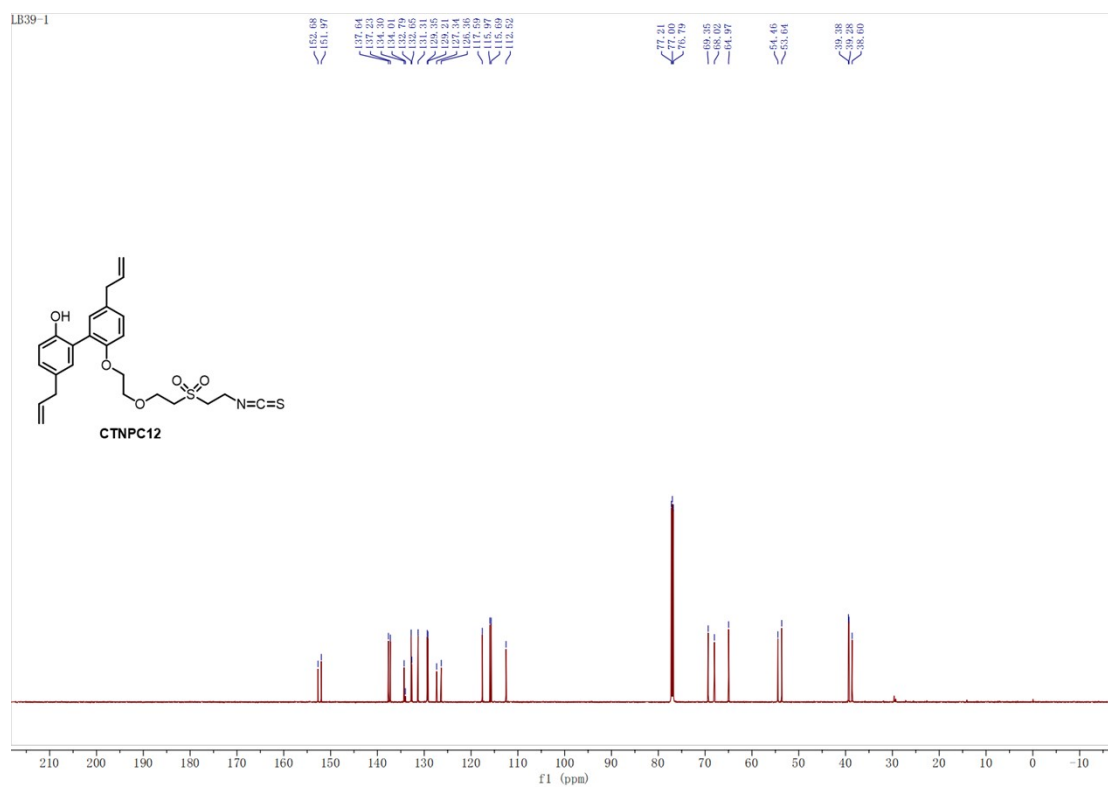


Figure S58. ¹H NMR of CTNPC12 (CDCl₃, 600 MHz)



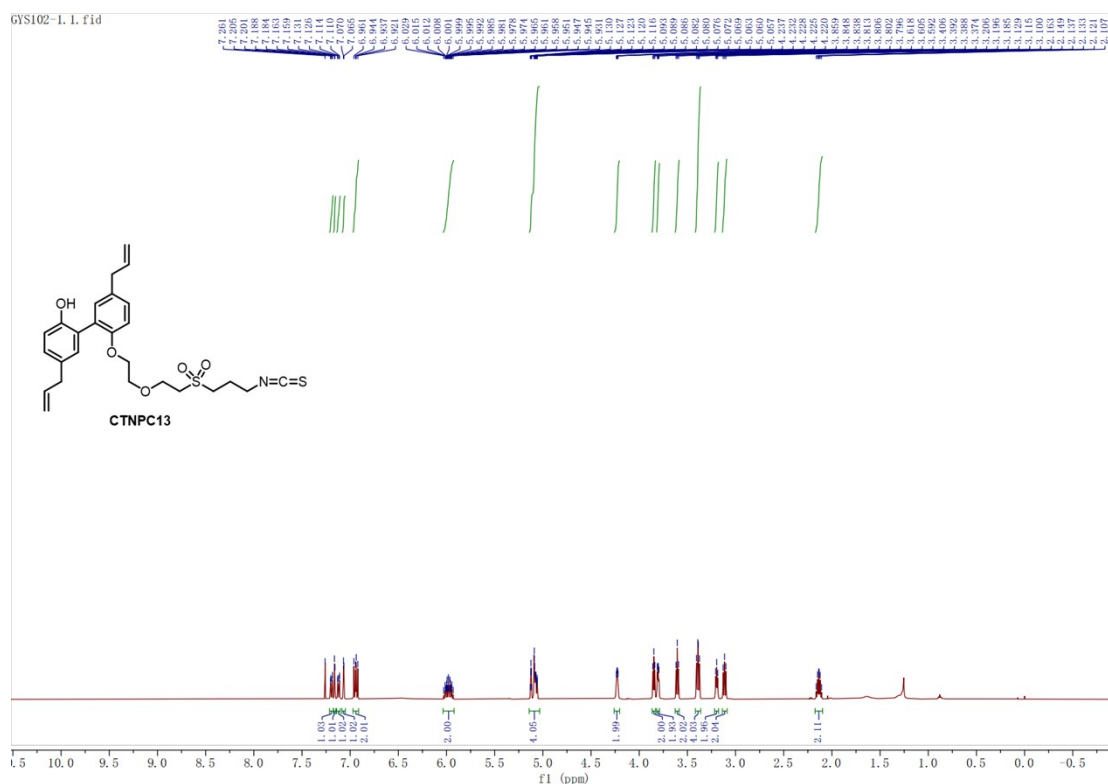


Figure S61. ^1H NMR of CTNPC13 (CDCl_3 , 500 MHz)

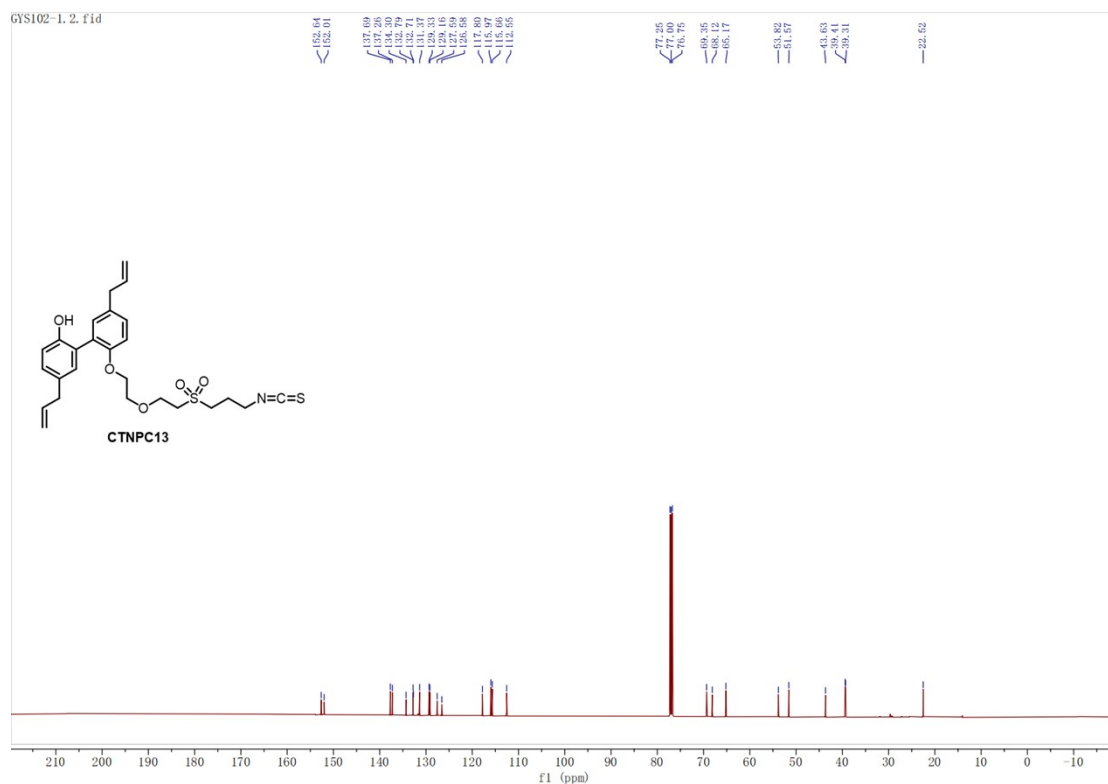


Figure S62. ^{13}C NMR of CTNPC13 (CDCl_3 , 125 MHz)

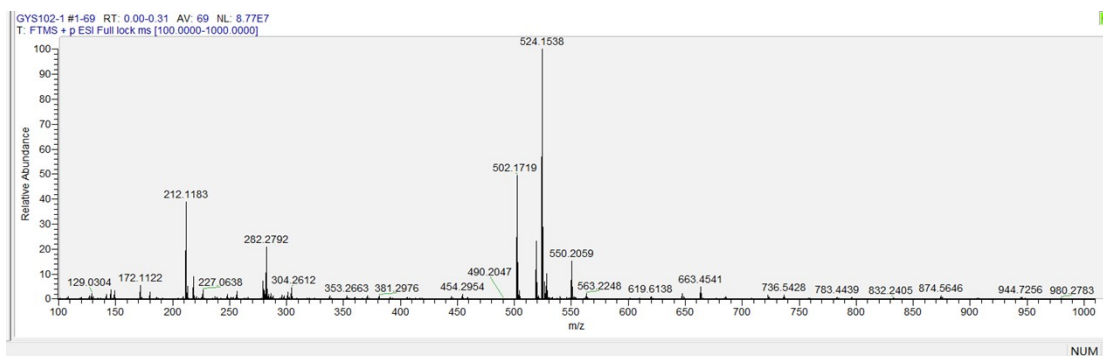


Figure S63. HRMS Spectra of CTNPC13

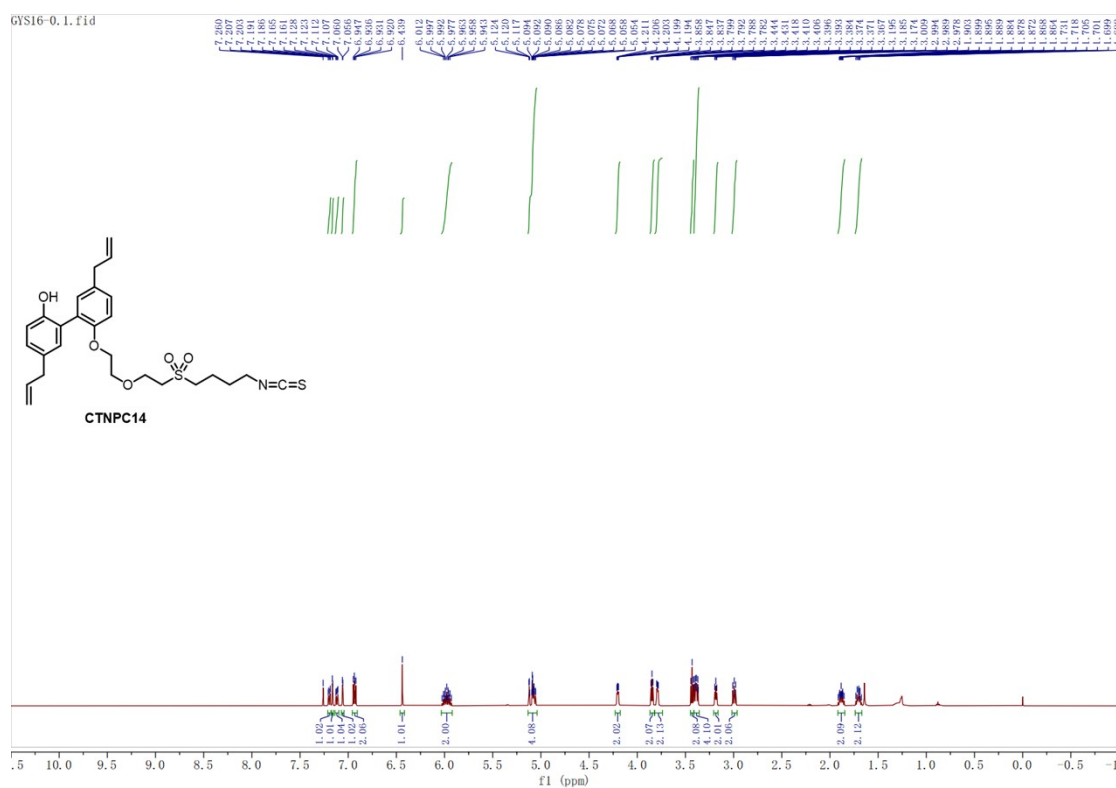


Figure S64. ^1H NMR of CTNPC14 (CDCl_3 , 500 MHz)

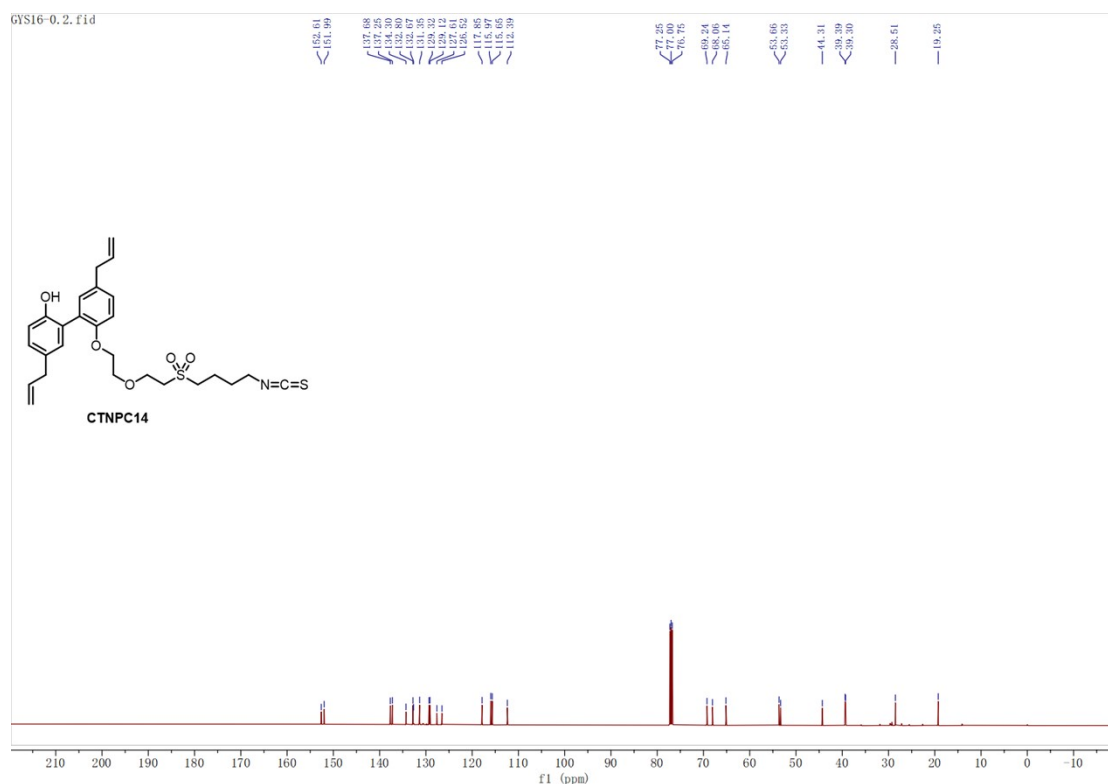


Figure S65. ^{13}C NMR of CTNPC14 (CDCl_3 , 125 MHz)

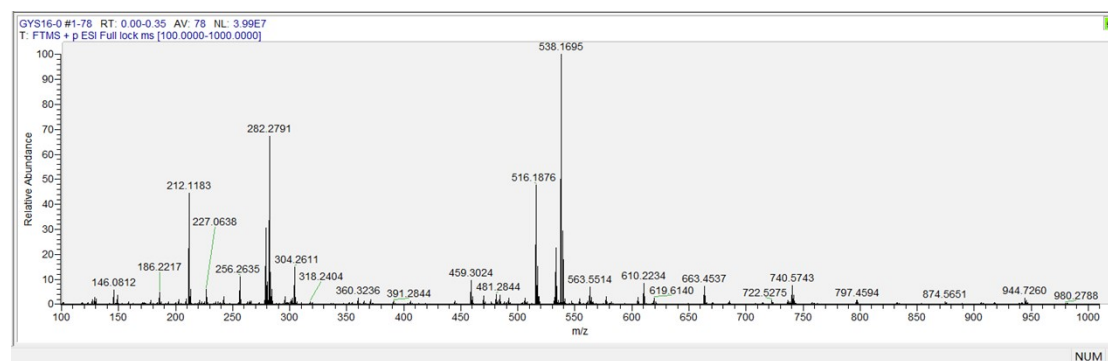


Figure S66. HRMS Spectra of CTNPC14

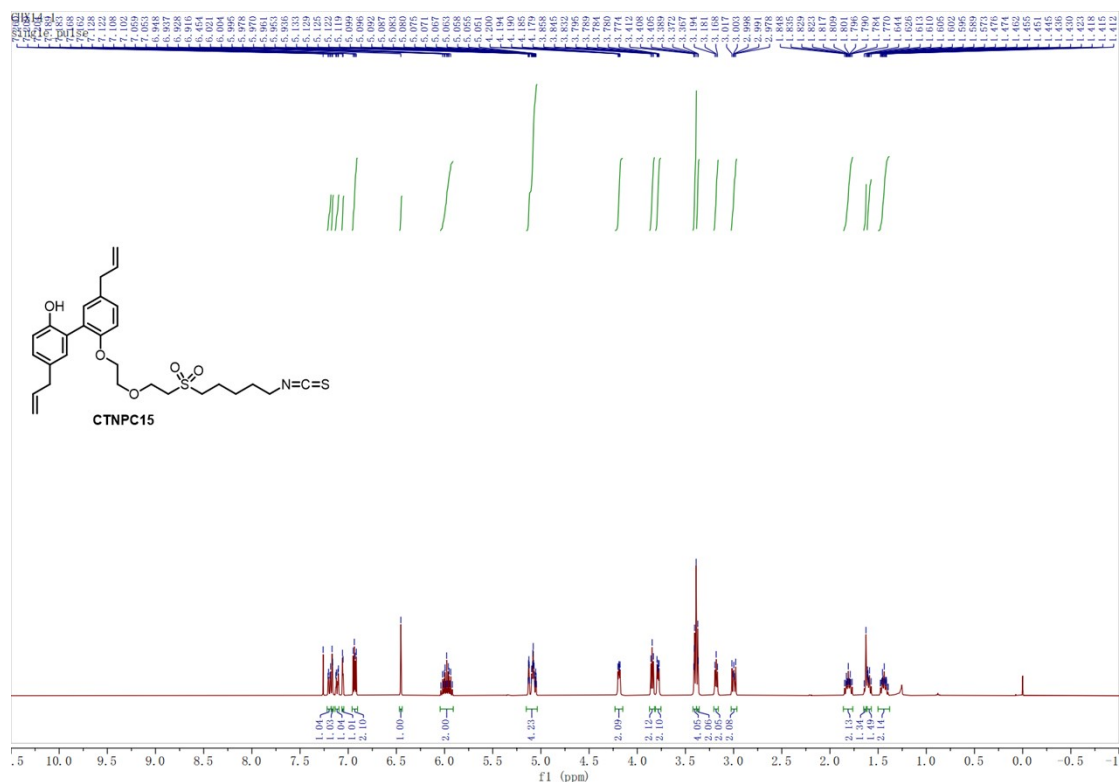


Figure S67. ¹H NMR of CTNPC15 (CDCl₃, 400 MHz)

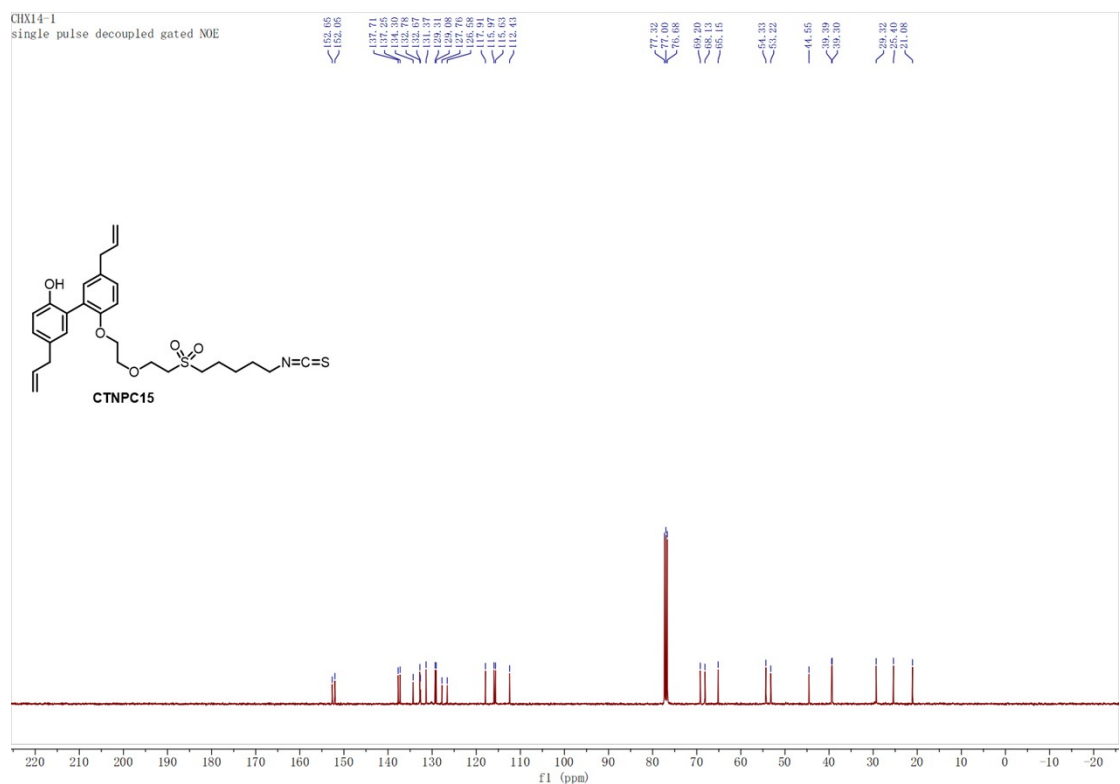


Figure S68. ¹³C NMR of CTNPC15 (CDCl₃, 100 MHz)

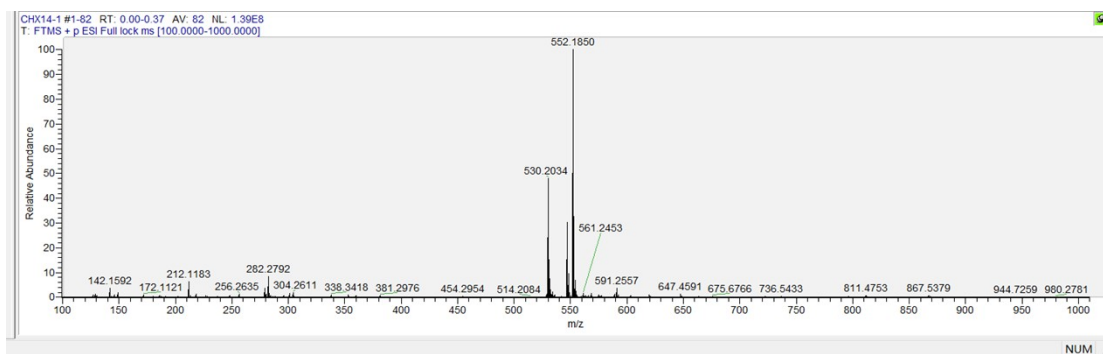


Figure S69. HRMS Spectra of CTNPC15

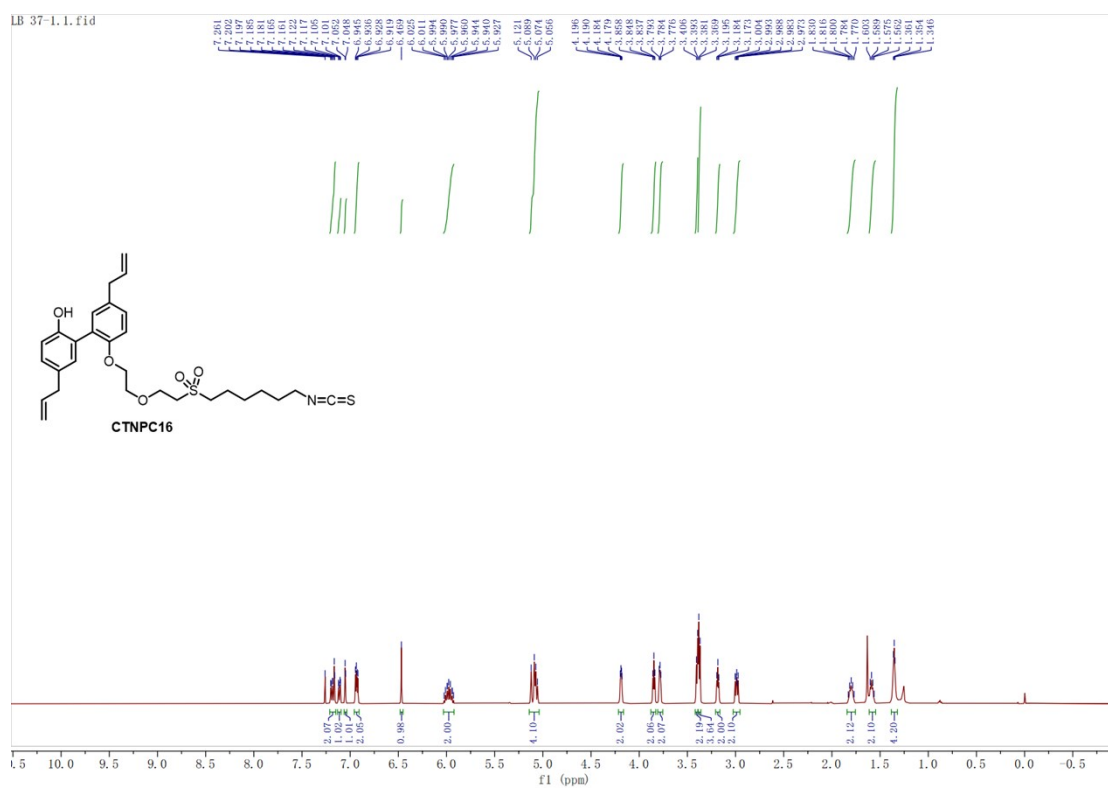


Figure S70. ^1H NMR of CTNPC16 (CDCl_3 , 500 MHz)

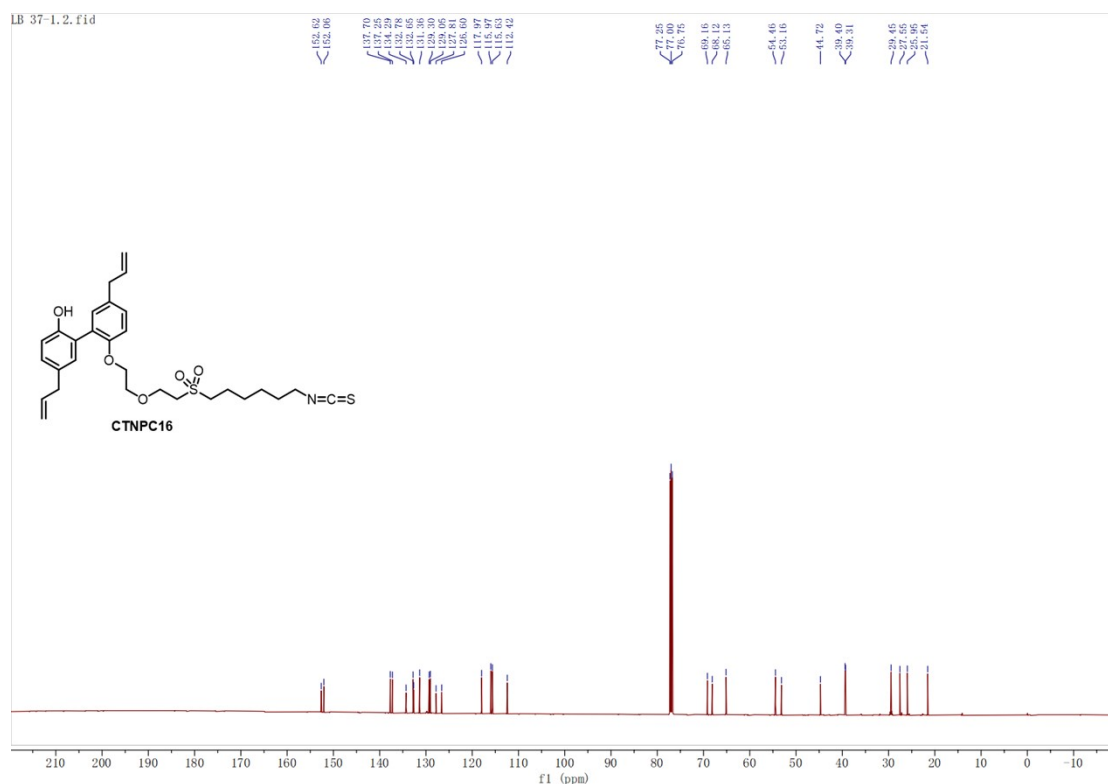


Figure S71. ^{13}C NMR of CTNPC16 (CDCl_3 , 125 MHz)

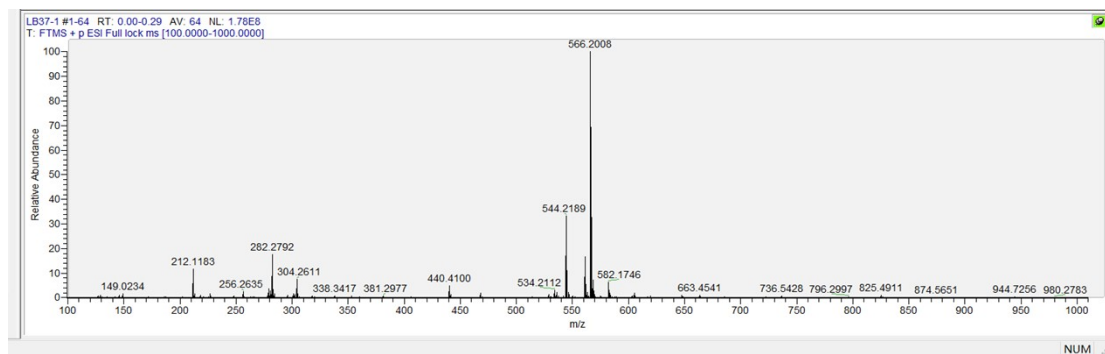


Figure S72. HRMS Spectra of CTNPC16

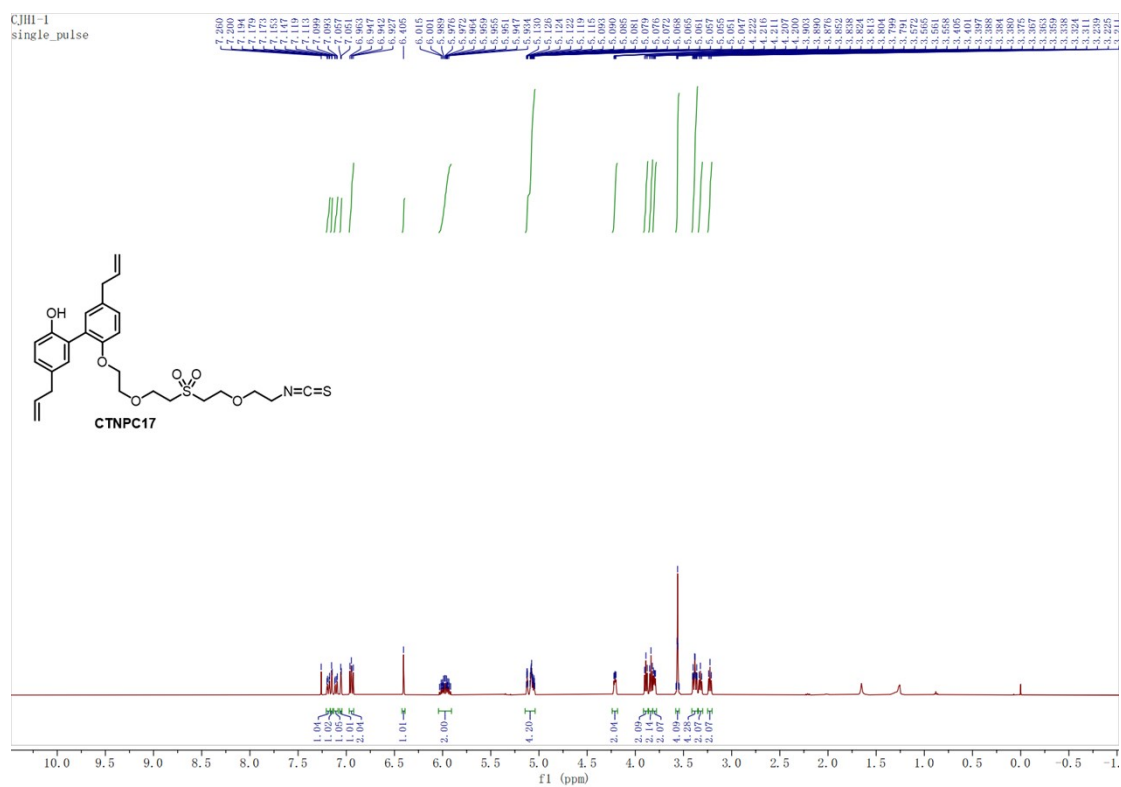


Figure S73. ^1H NMR of CTNPC17 (CDCl_3 , 400 MHz)

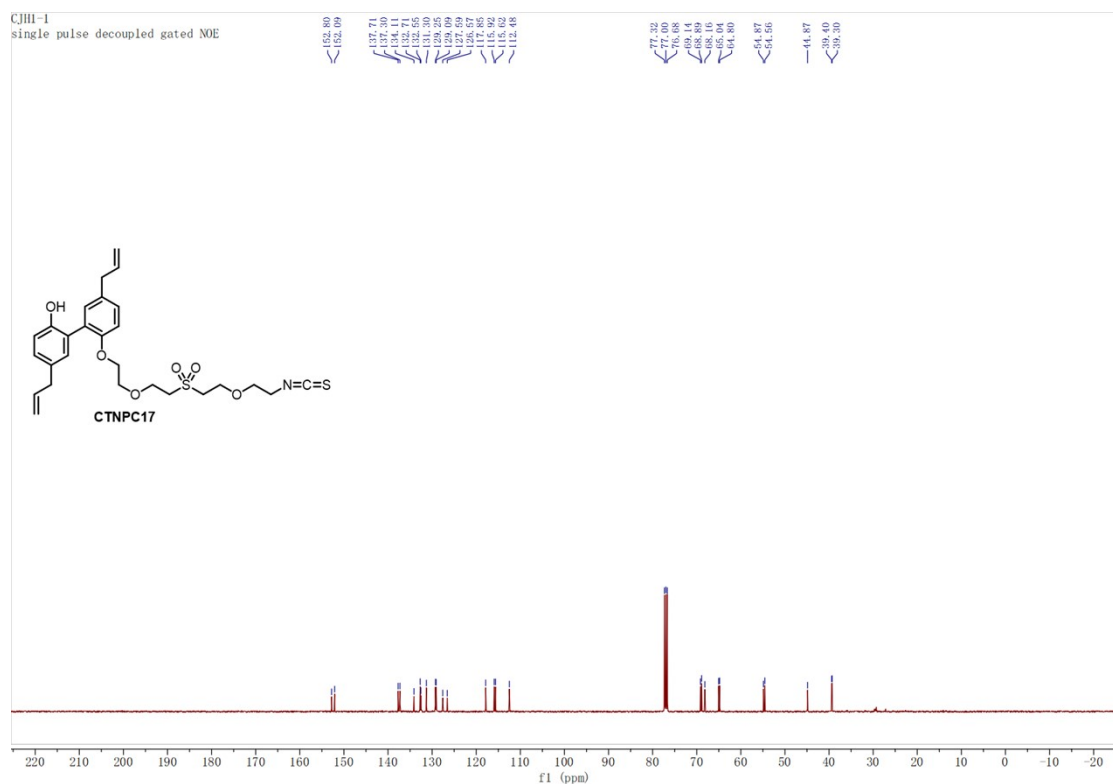


Figure S74. ^{13}C NMR of CTNPC17 (CDCl_3 , 100 MHz)

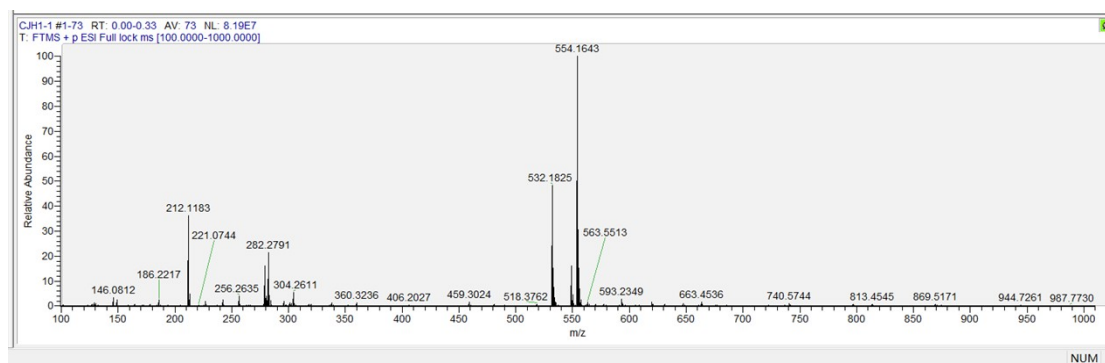
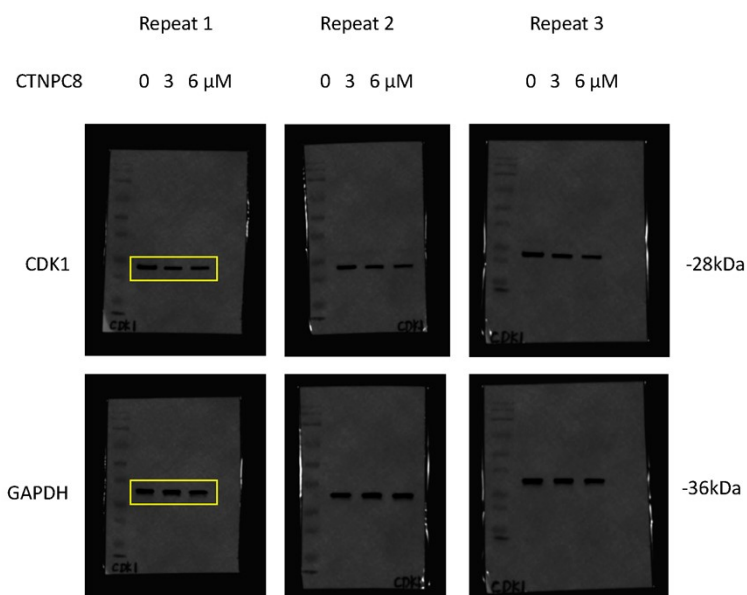
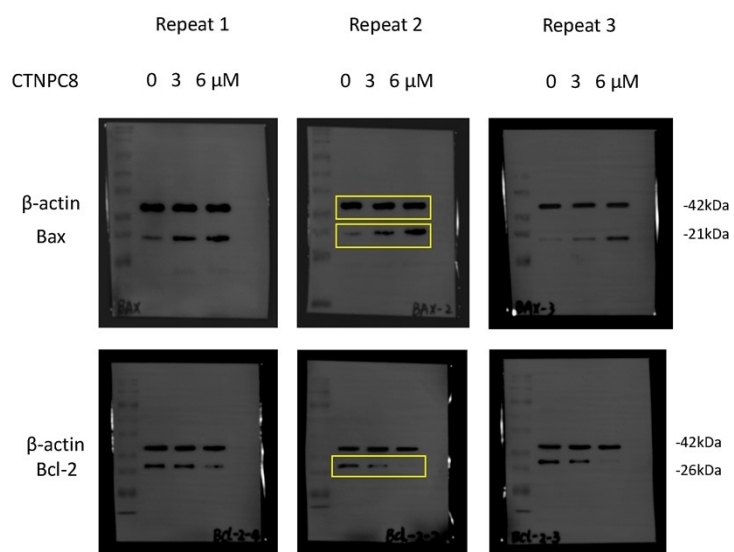


Figure S75. HRMS Spectra of CTNPC17

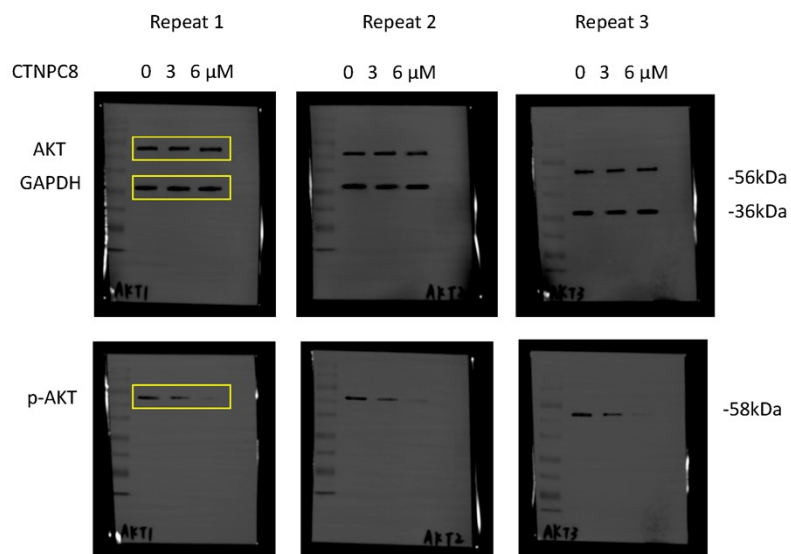
(A)



(B)



(C)



(D)

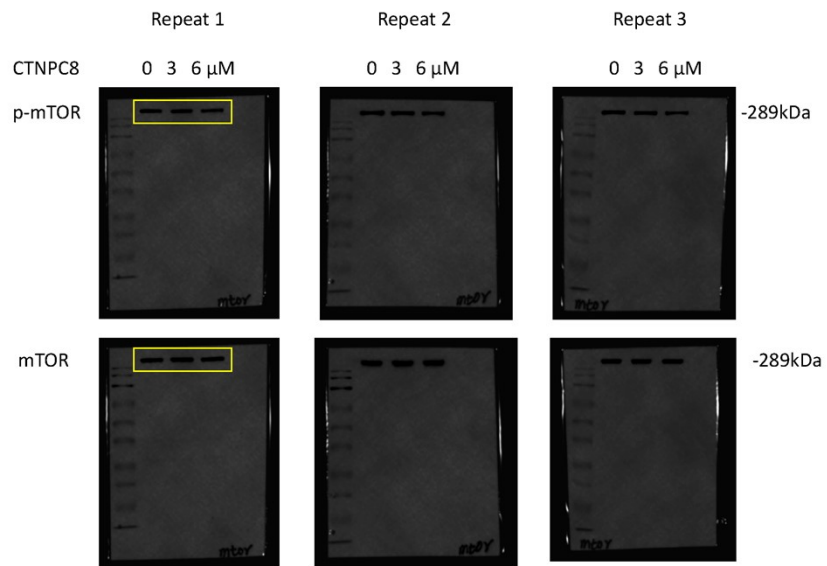


Figure S51. Original Western blot images for three repeats