

Supplementary Information

Simultaneous Regioselective Synthesis of Trifluoromethyl-Containing 1,7-Phenanthrolines and Quinolines from Cyclocondensation Reaction of *N,N'*-Bis(oxotrifluoroalkenyl)-1,3-Phenylenediamines

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NMR spectra of compounds

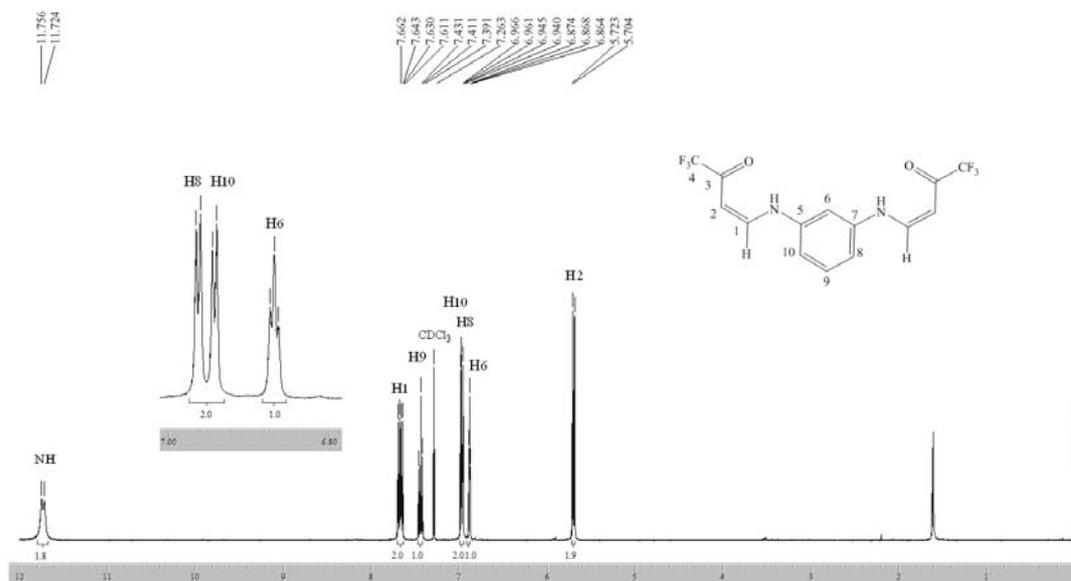


Figure S1. ¹H NMR (100 MHz, CDCl₃) spectrum of (Z,Z)-*N,N'*-bis(4,4,4-trifluoro-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2a**).

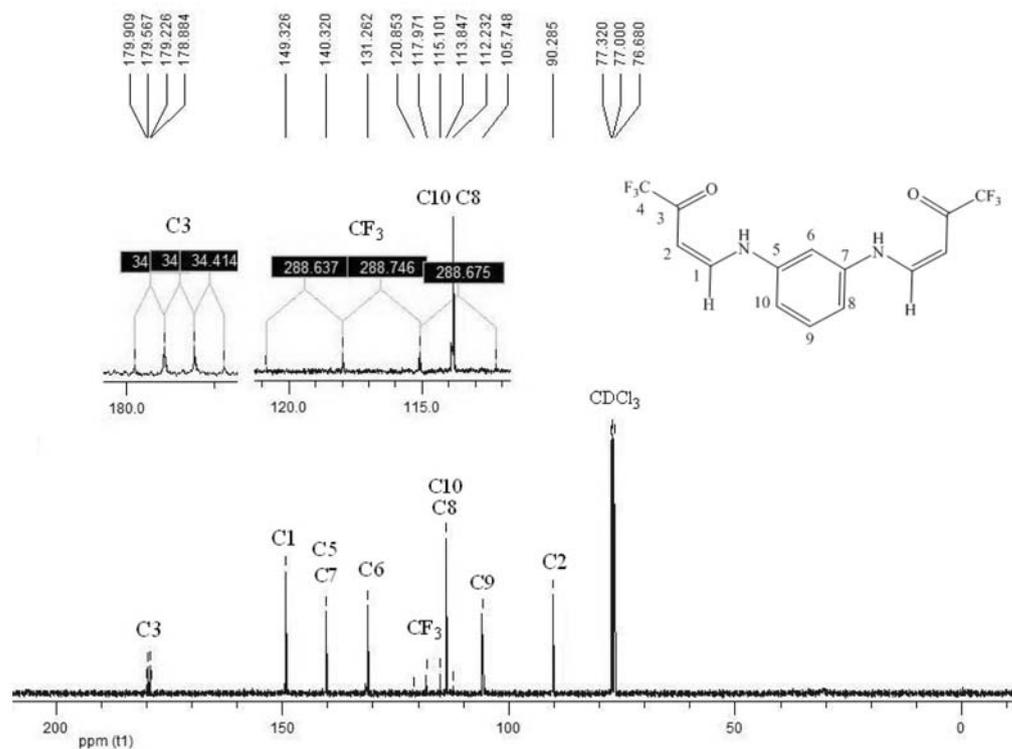


Figure S2. ^{13}C NMR (200 MHz, CDCl_3) spectrum of (Z,Z) - N,N' -bis(4,4,4-trifluoro-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2a**).



Figure S3. ^{19}F NMR (376 MHz, CDCl_3) spectrum of (Z,Z) - N,N' -bis(4,4,4-trifluoro-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2a**).

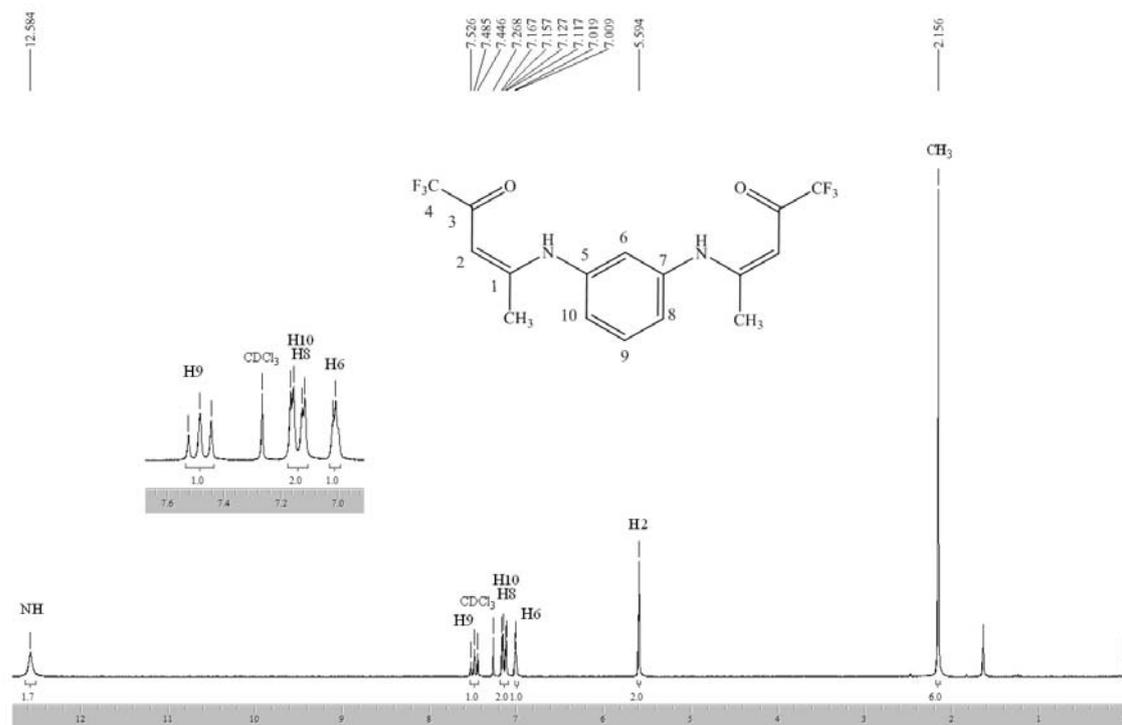


Figure S4. ^1H NMR (100 MHz, CDCl_3) spectrum of *(Z,Z)*-*N,N'*-bis(5,5,5-trifluoro-4-oxo-2-penten-2-yl)-1,3-phenylenediamine (**2b**).

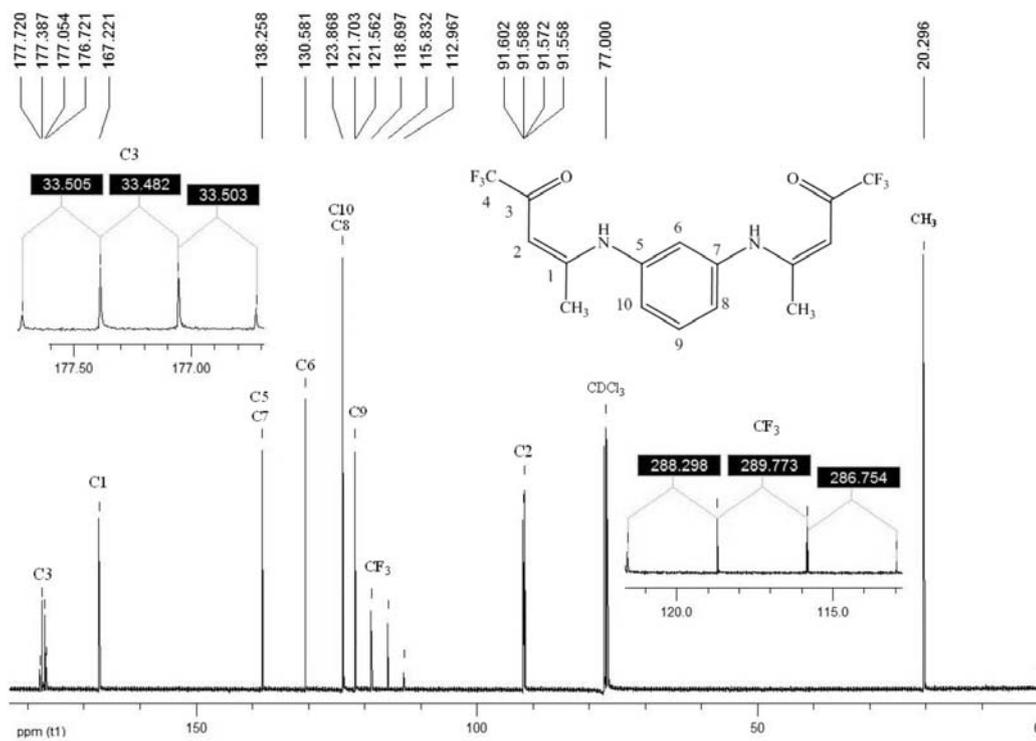


Figure S5. ^{13}C NMR (200 MHz, CDCl_3) spectrum of *(Z,Z)*-*N,N'*-bis(5,5,5-trifluoro-4-oxo-2-penten-2-yl)-1,3-phenylenediamine (**2b**).

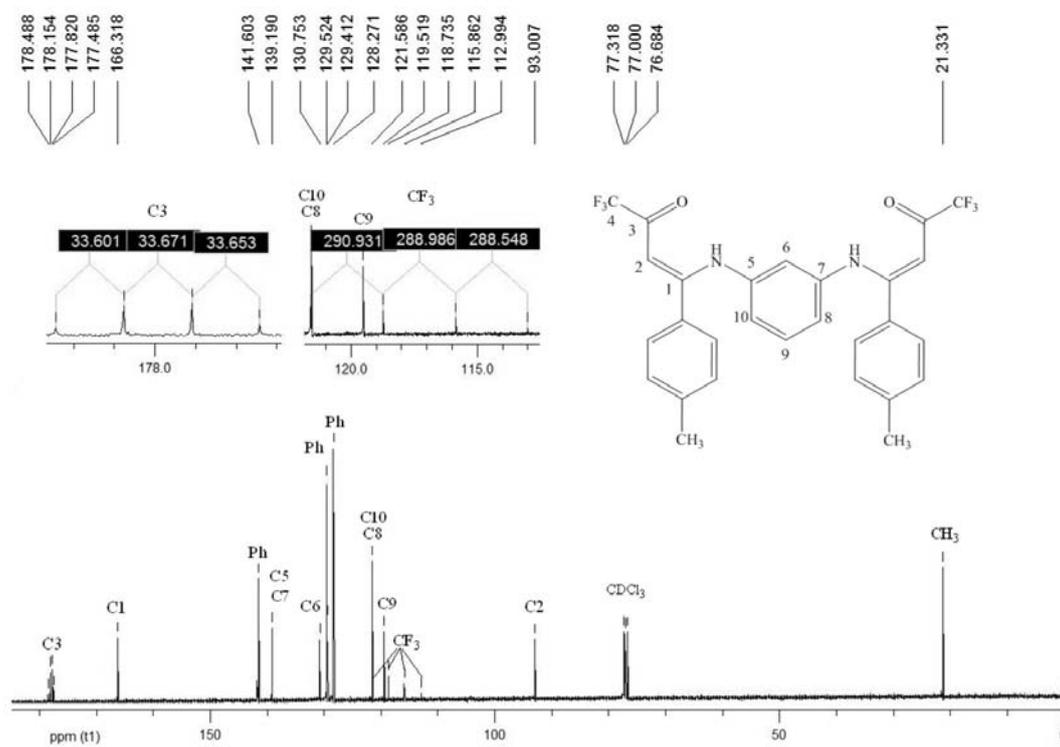
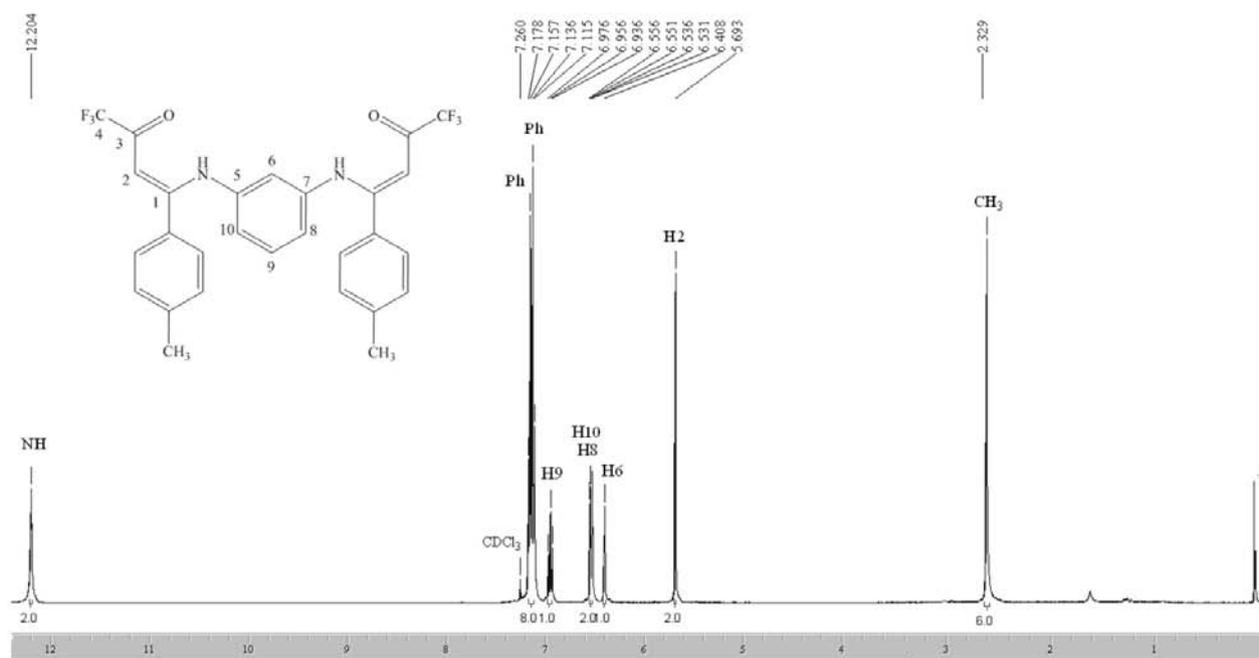


Figure S9. ^{13}C NMR (200 MHz, CDCl_3) spectrum of *(Z,Z)*-*N,N'*-bis(4,4,4-trifluoro-1-[4-methylphenyl]-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2d**).

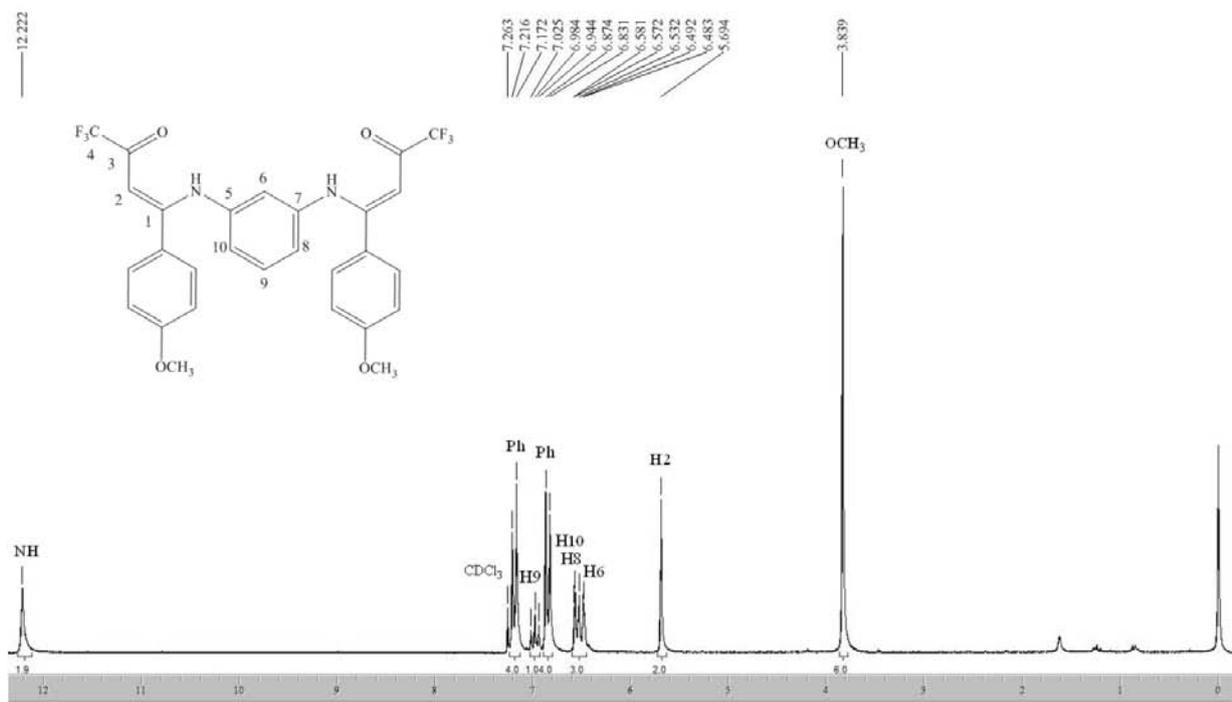


Figure S10. ^1H NMR (100 MHz, CDCl_3) spectrum of (*Z,Z*)-*N,N'*-bis(4,4,4-trifluoro-1-[4-methoxyphenyl]-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2e**).

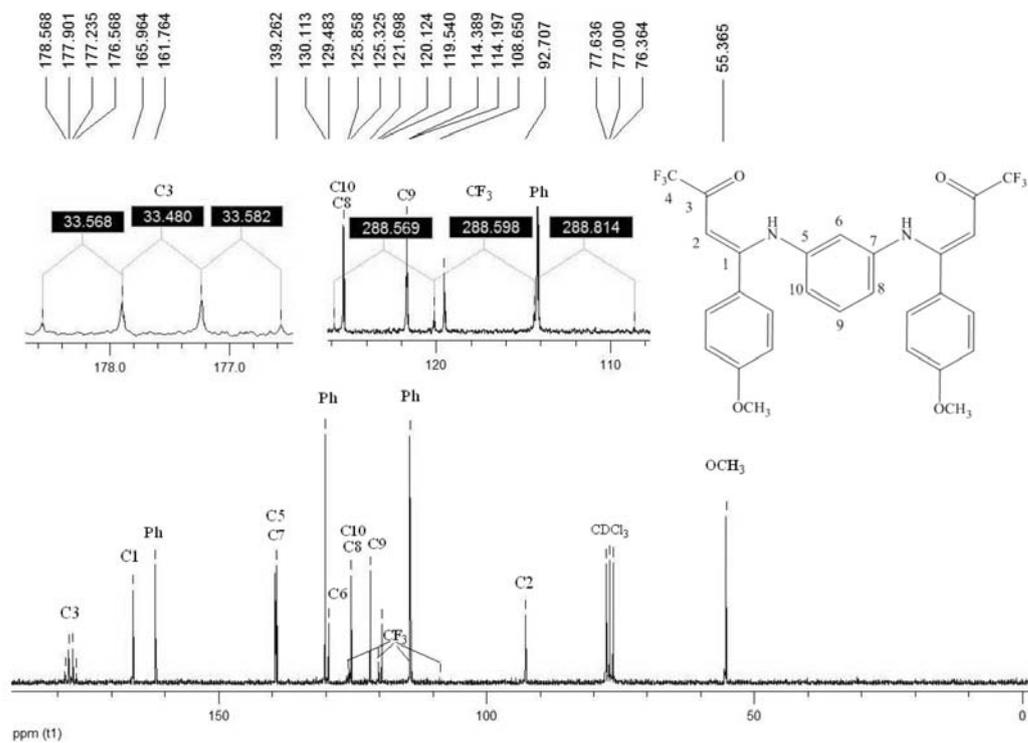


Figure S11. ^{13}C NMR (200 MHz, CDCl_3) spectrum of (*Z,Z*)-*N,N'*-bis(4,4,4-trifluoro-1-[4-methoxyphenyl]-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2e**).

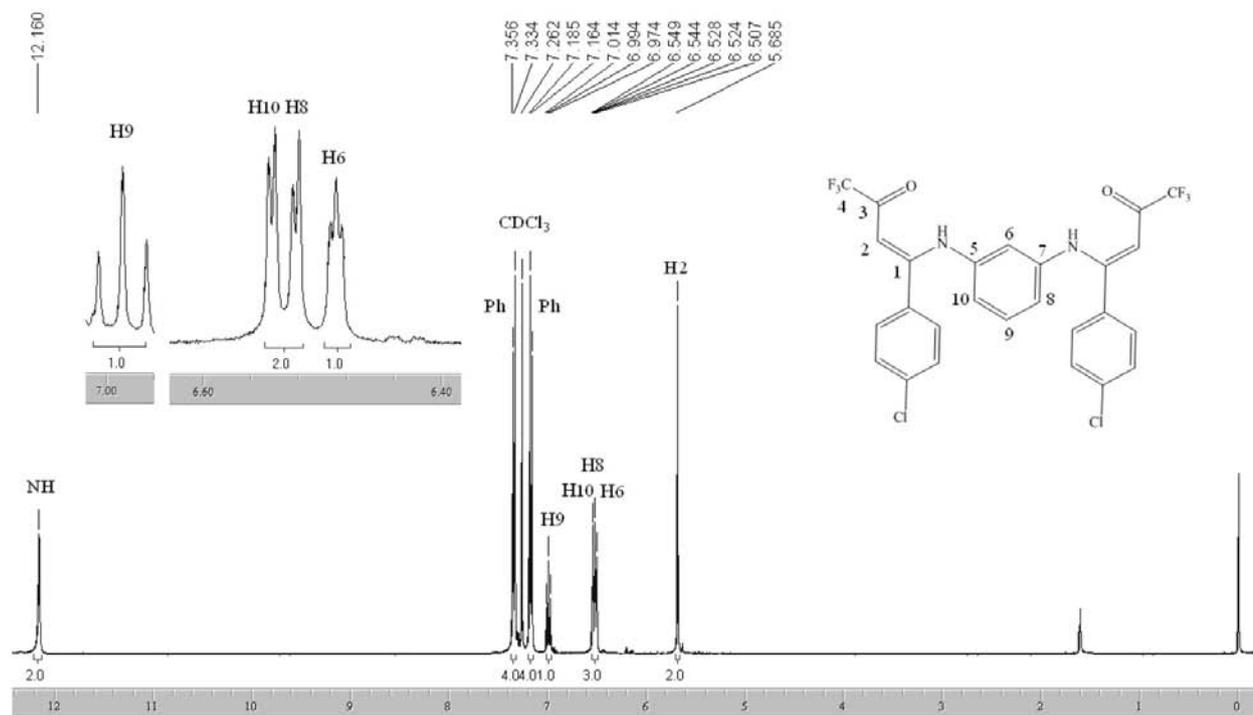


Figure S14. ^1H NMR (100 MHz, CDCl_3) spectrum of (Z,Z)-N,N'-[1-[4-chlorophenyl]-4,4,4-trifluoro-3-oxo-1-buten-1-yl]-1,3-phenylenediamine (**2g**).

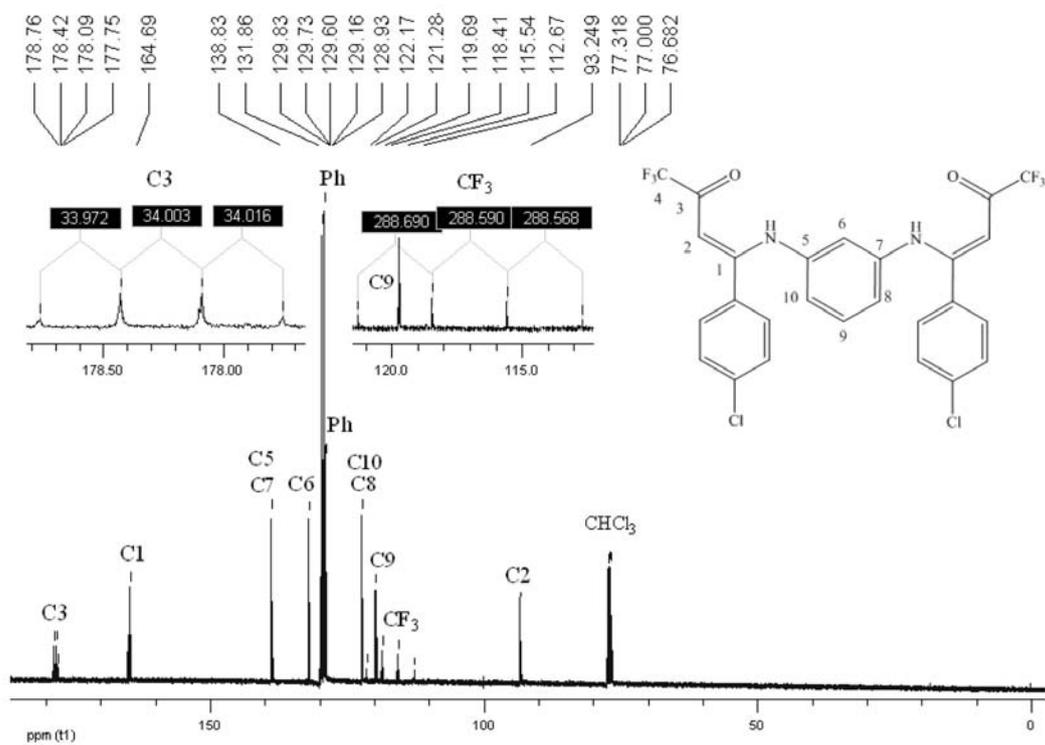


Figure S15. ^{13}C NMR (200 MHz, CDCl_3) spectrum of (Z,Z)-N,N'-[1-[4-chlorophenyl]-4,4,4-trifluoro-3-oxo-1-buten-1-yl]-1,3-phenylenediamine (**2g**).

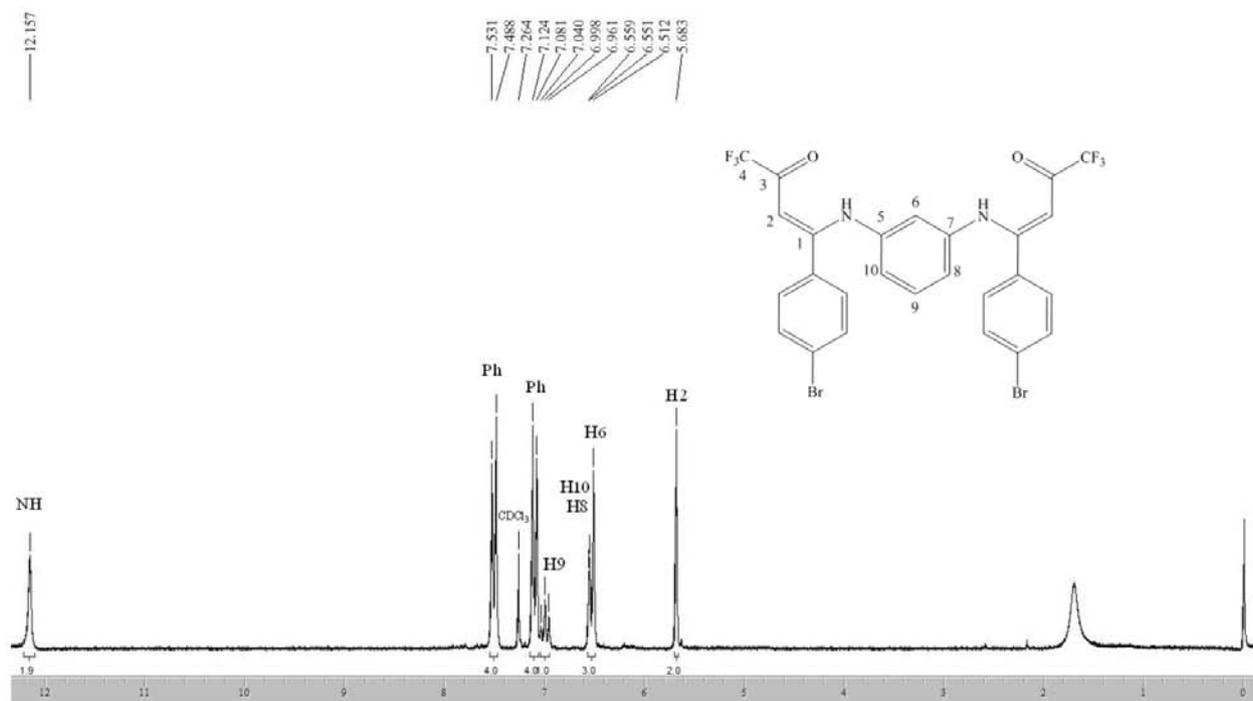


Figure S16. ^1H NMR (100 MHz, CDCl_3) spectrum of (Z,Z) - N,N' -bis(1-[4-bromophenyl]-4,4,4-trifluoro-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2h**).

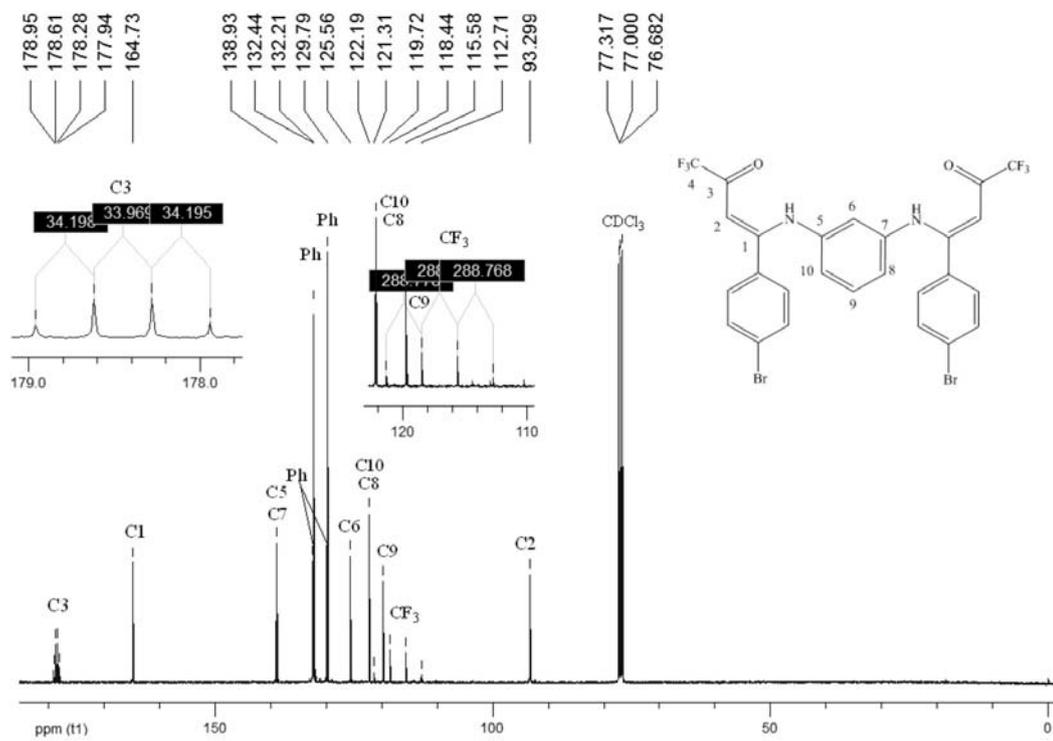


Figure S17. ^{13}C NMR (200 MHz, CDCl_3) spectrum of (Z,Z) - N,N' -bis(1-[4-bromophenyl]-4,4,4-trifluoro-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2h**).

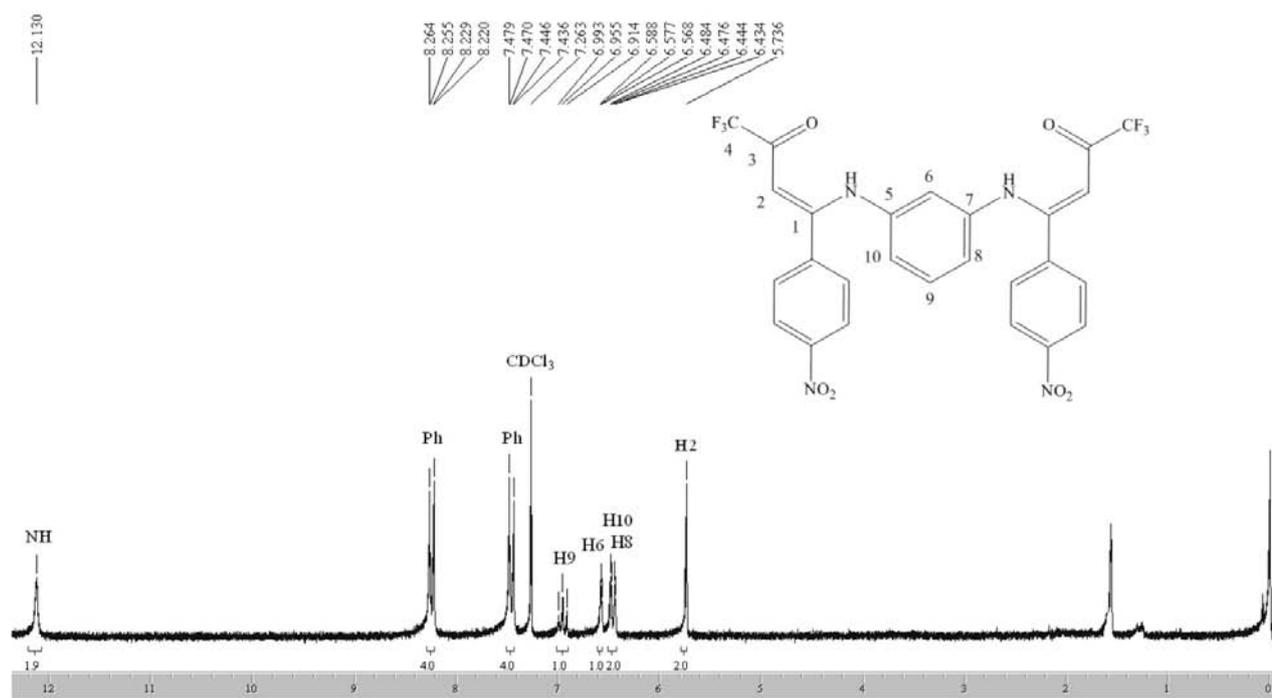


Figure S18. ^1H NMR (100 MHz, CDCl_3) spectrum of (Z,Z)-N,N'-bis(4,4,4-trifluoro-1-(4-nitrophenyl)-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2i**).

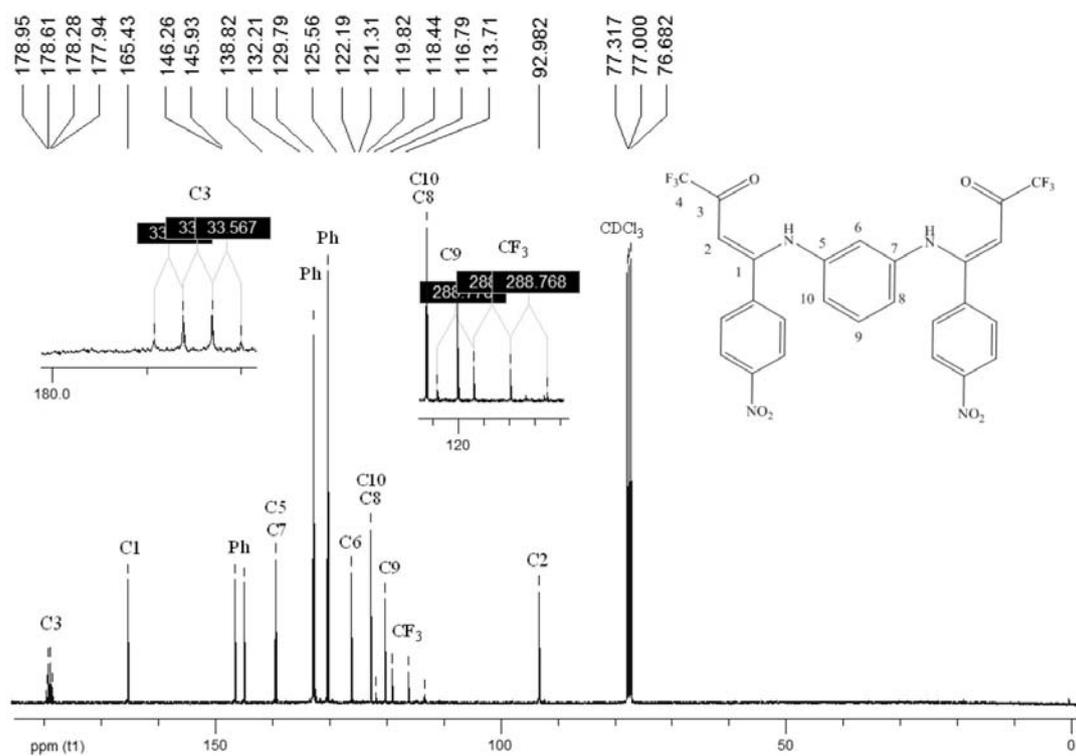


Figure S19. ^{13}C NMR (200 MHz, CDCl_3) spectrum of (Z,Z)-N,N'-bis(4,4,4-trifluoro-1-(4-nitrophenyl)-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2i**).

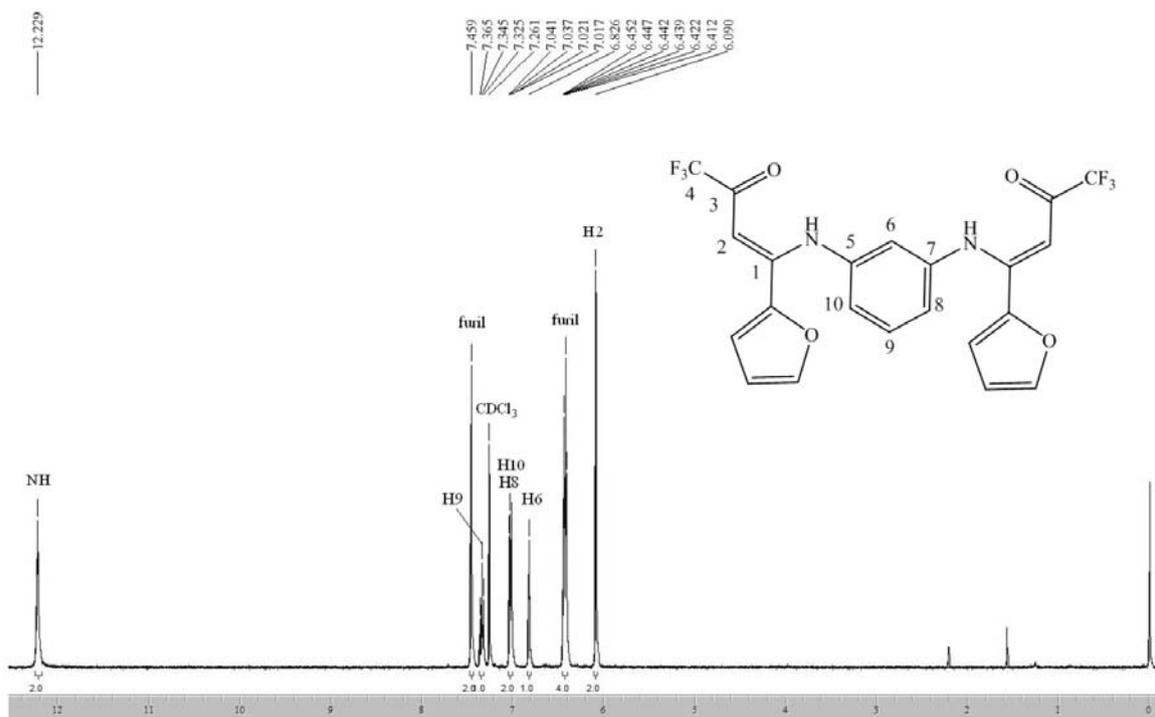


Figure S20. ^1H NMR (100 MHz, CDCl_3) spectrum of (*Z,Z*)-*N,N'*-bis(4,4,4-trifluoro-1-[2-furyl]-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2j**).

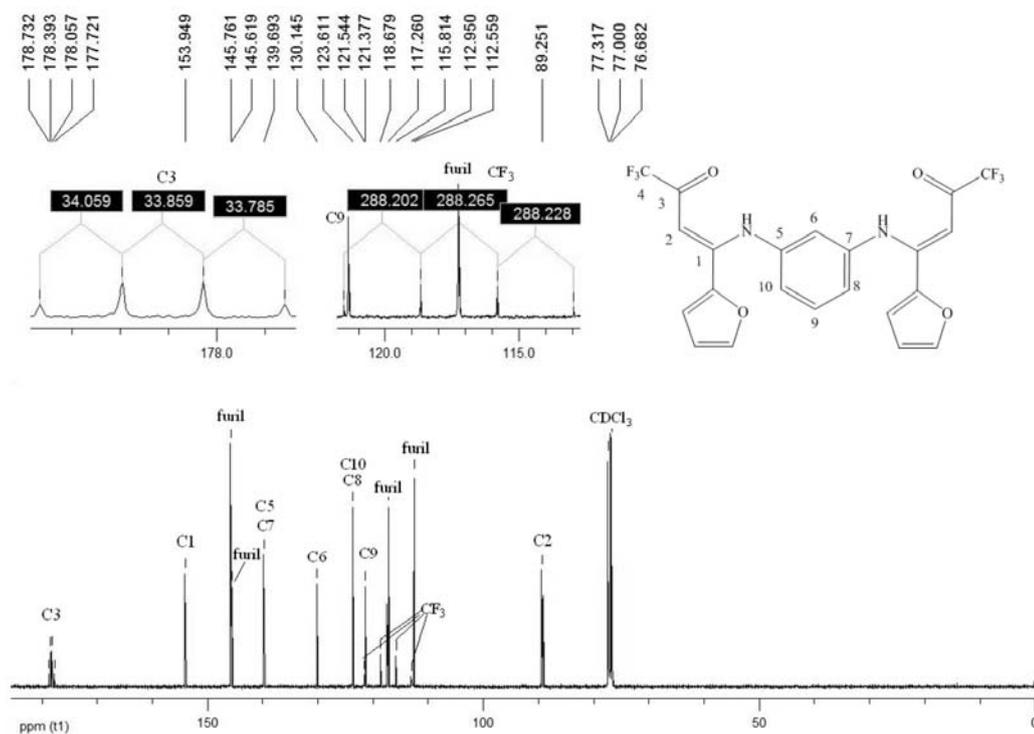


Figure S21. ^{13}C NMR (200 MHz, CDCl_3) spectrum of (*Z,Z*)-*N,N'*-bis(4,4,4-trifluoro-1-[2-furyl]-3-oxo-1-buten-1-yl)-1,3-phenylenediamine (**2j**).

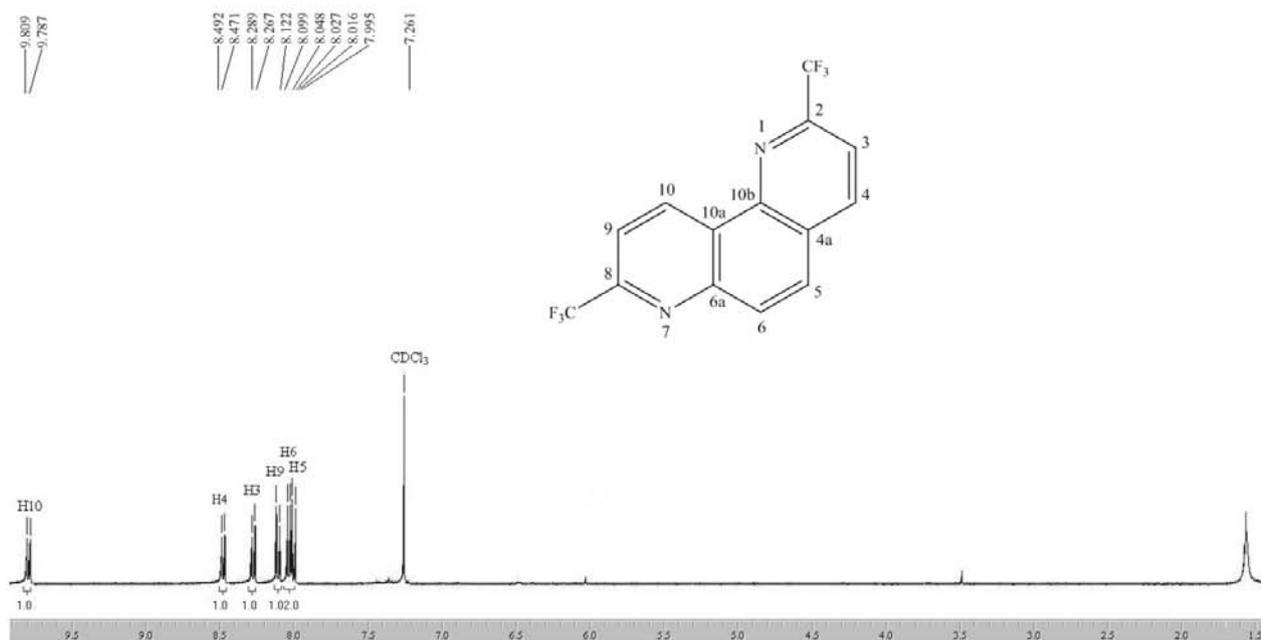


Figure S22. ¹H NMR (100 MHz, CDCl₃) spectrum of 2,8-bis(trifluoromethyl)-1,7-phenanthroline (**3a**).

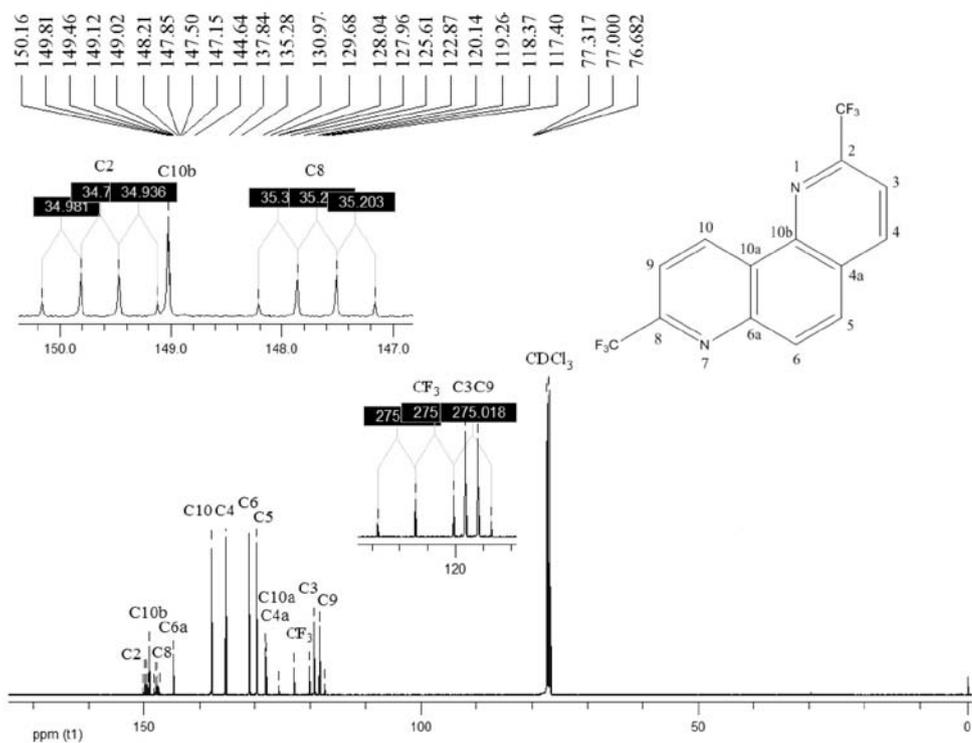


Figure S23. ¹³C NMR (200 MHz, CDCl₃) spectrum of 2,8-bis(trifluoromethyl)-1,7-phenanthroline (**3a**).

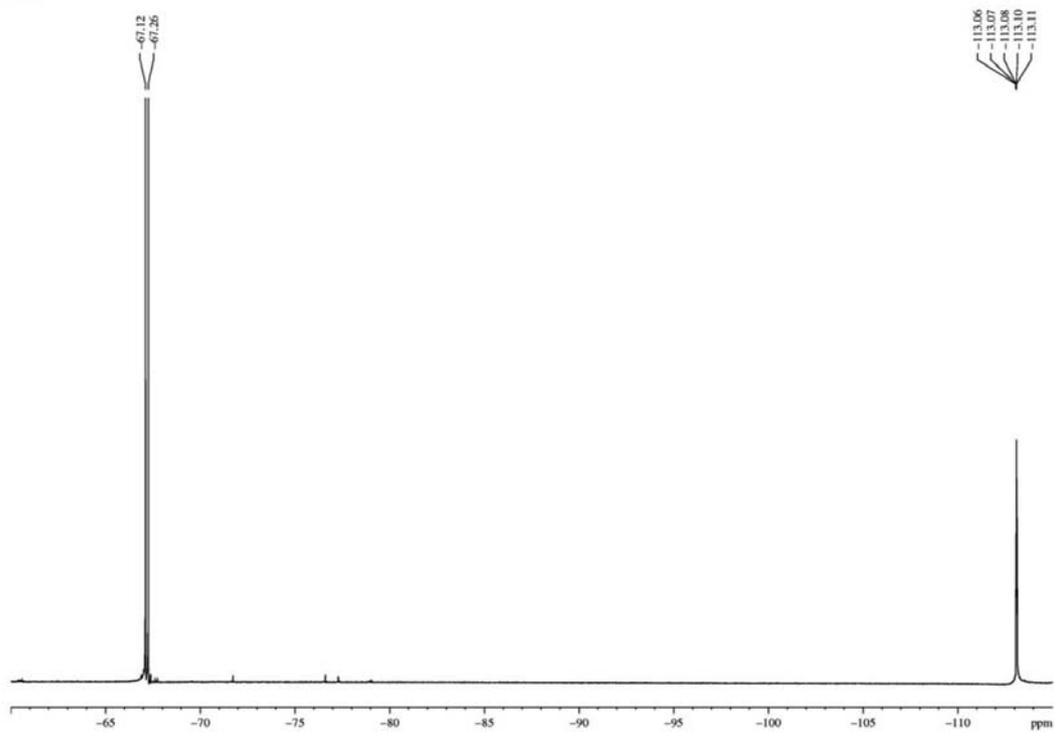


Figure S24. ^{19}F NMR (376 MHz, CDCl_3) spectrum of 2,8-bis(trifluoromethyl)-1,7-phenanthroline (**3a**).

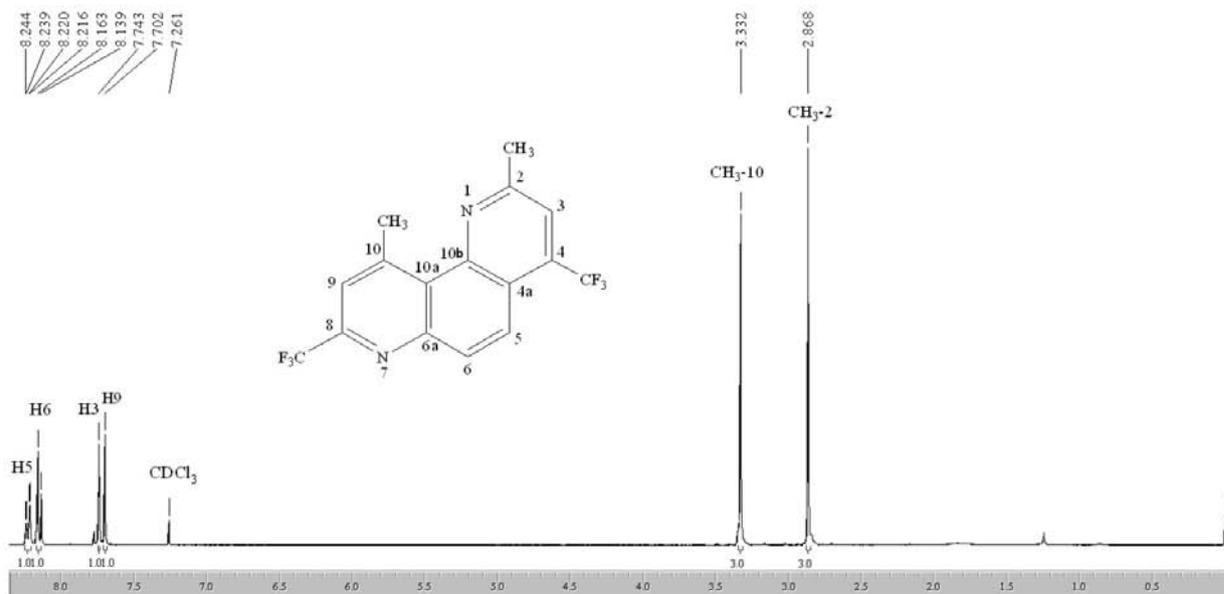


Figure S25. ^1H NMR (100 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(methyl)-1,7-phenanthroline (**3b**).

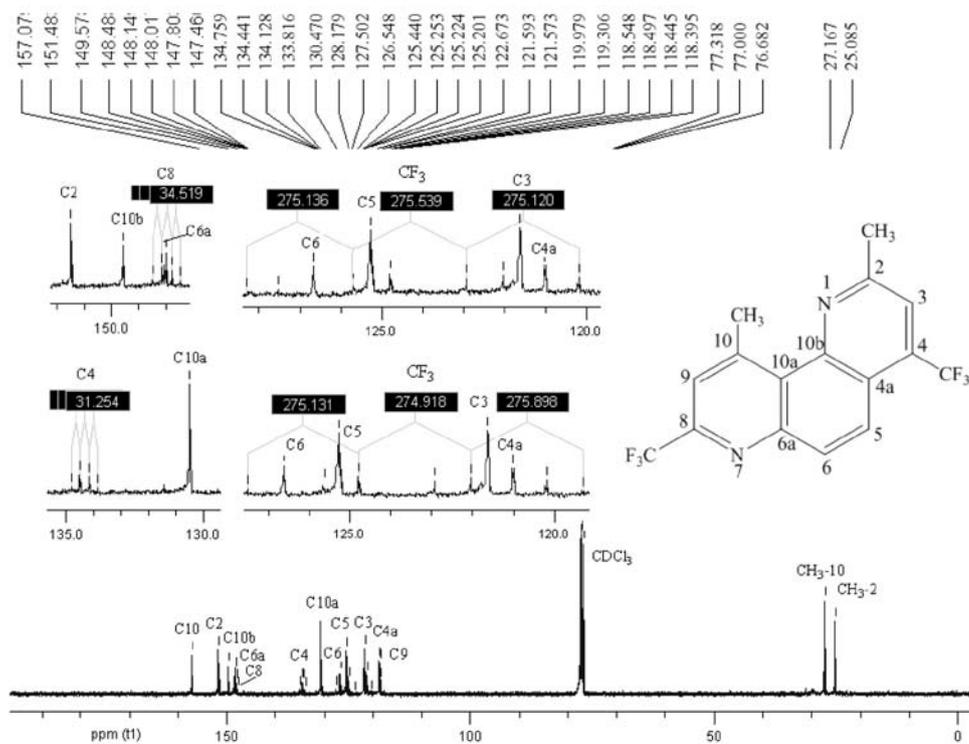


Figure S26. ^{13}C NMR (200 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(methyl)-1,7-phenanthroline (**3b**).

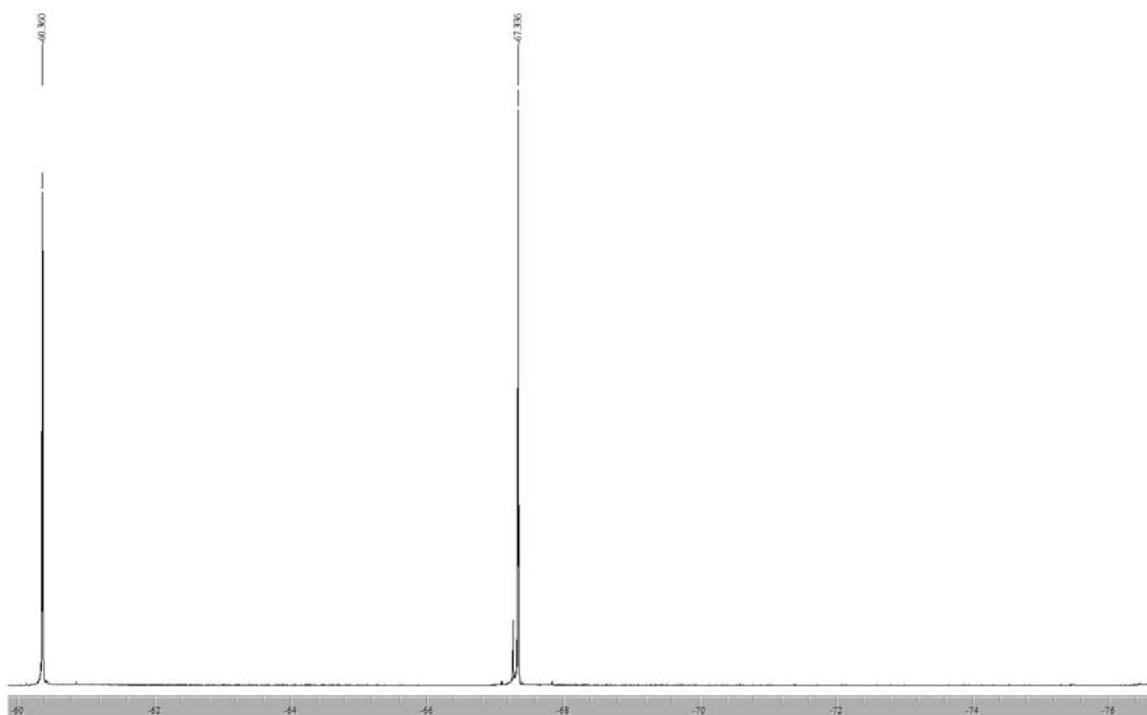


Figure S27. ^{19}F NMR (376 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(methyl)-1,7-phenanthroline (**3b**).

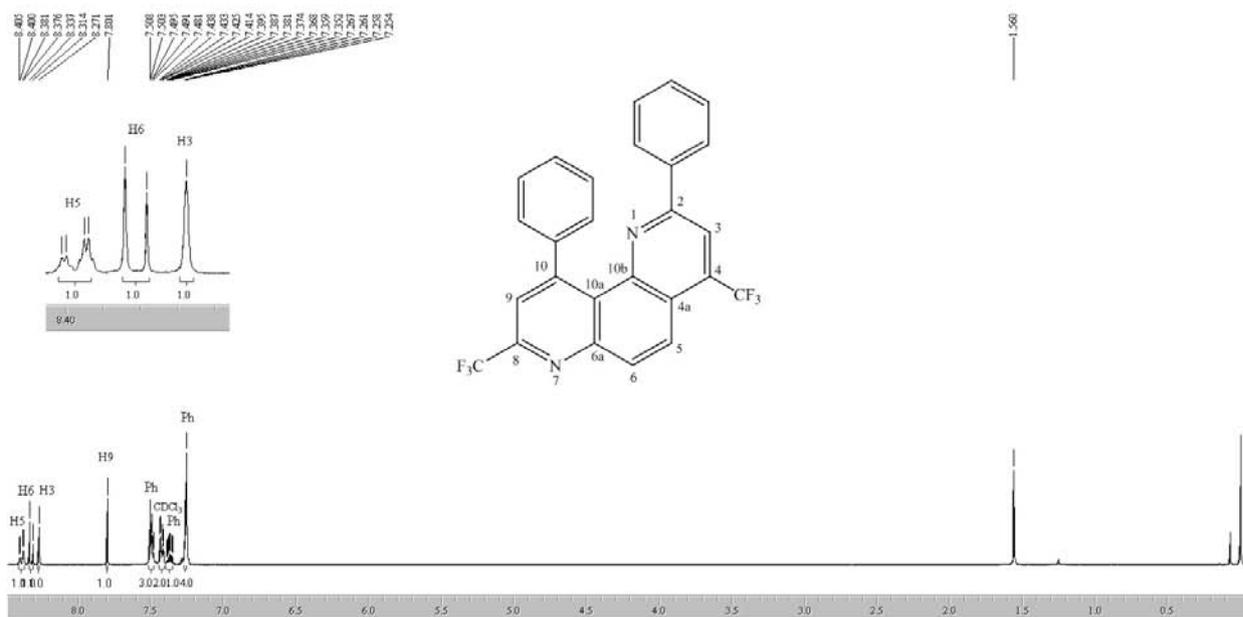


Figure S28. ^1H NMR (100 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(phenyl)-1,7-phenanthroline (**3c**).

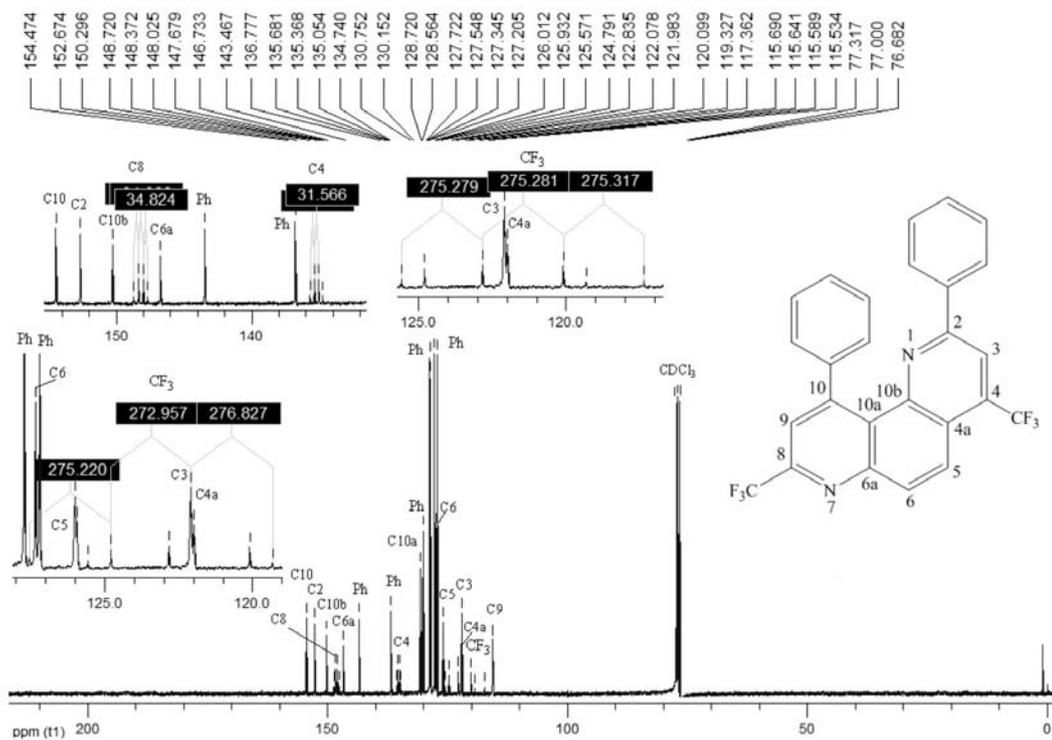


Figure S29. ^{13}C NMR (200 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(phenyl)-1,7-phenanthroline (**3c**).

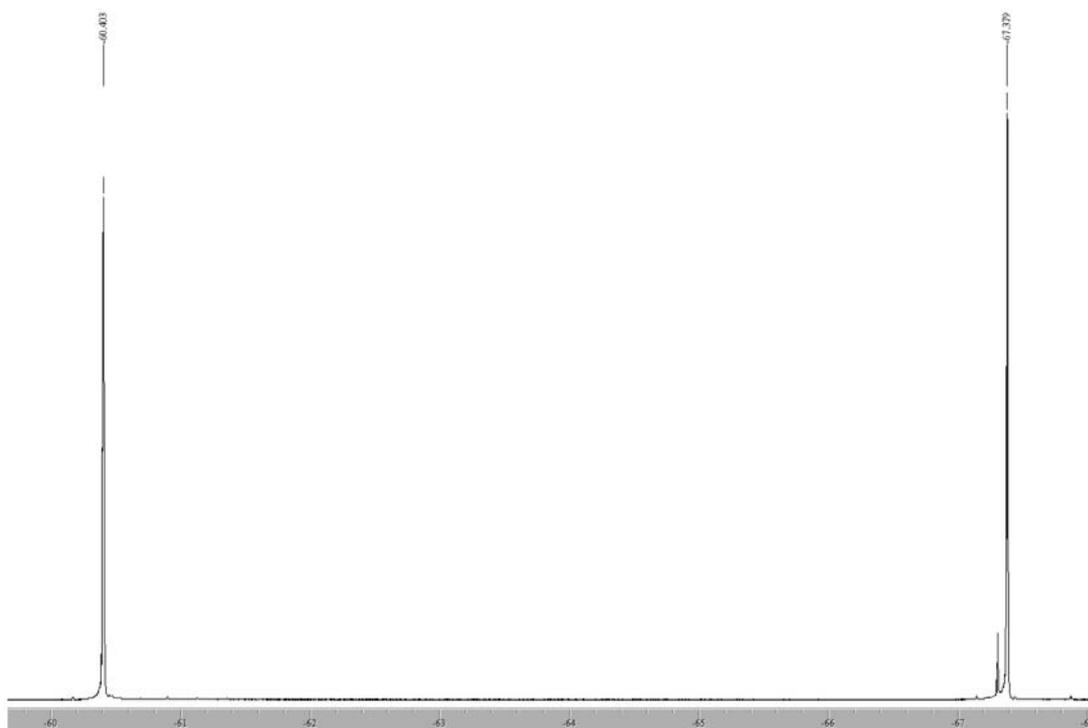


Figure S30. ^{19}F NMR (376 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(phenyl)-1,7-phenanthroline (**3c**).

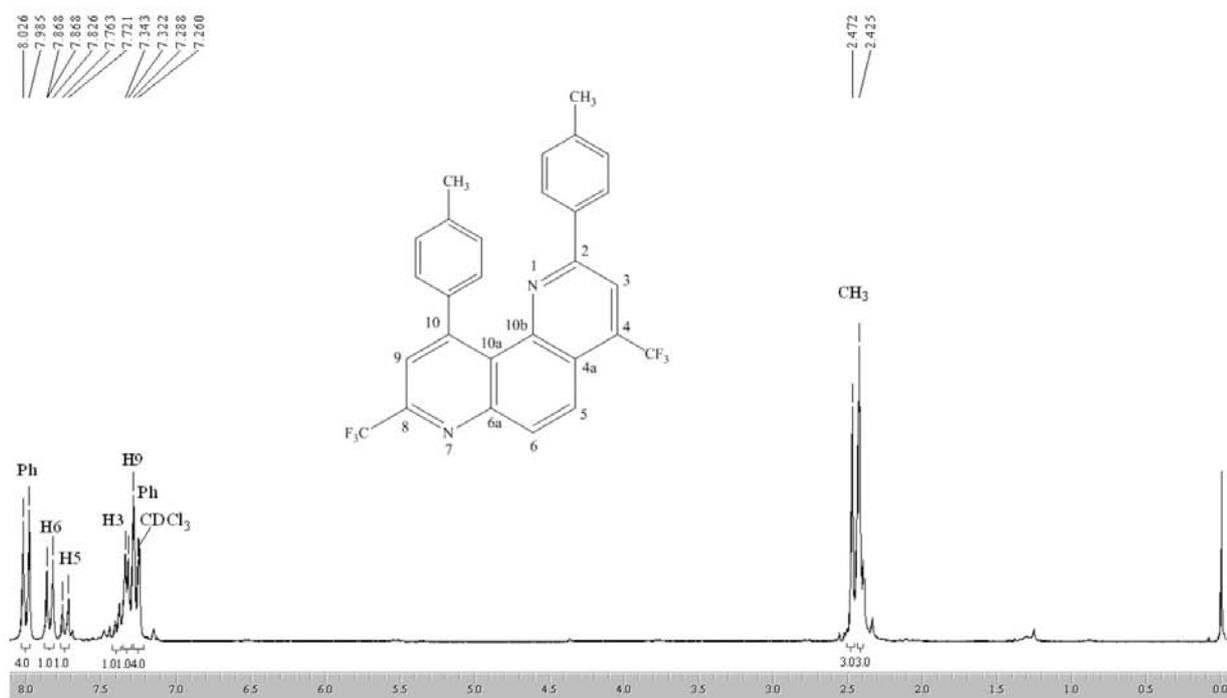


Figure S31. ^1H NMR (100 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-methylphenyl)-1,7-phenanthroline (**3d**).

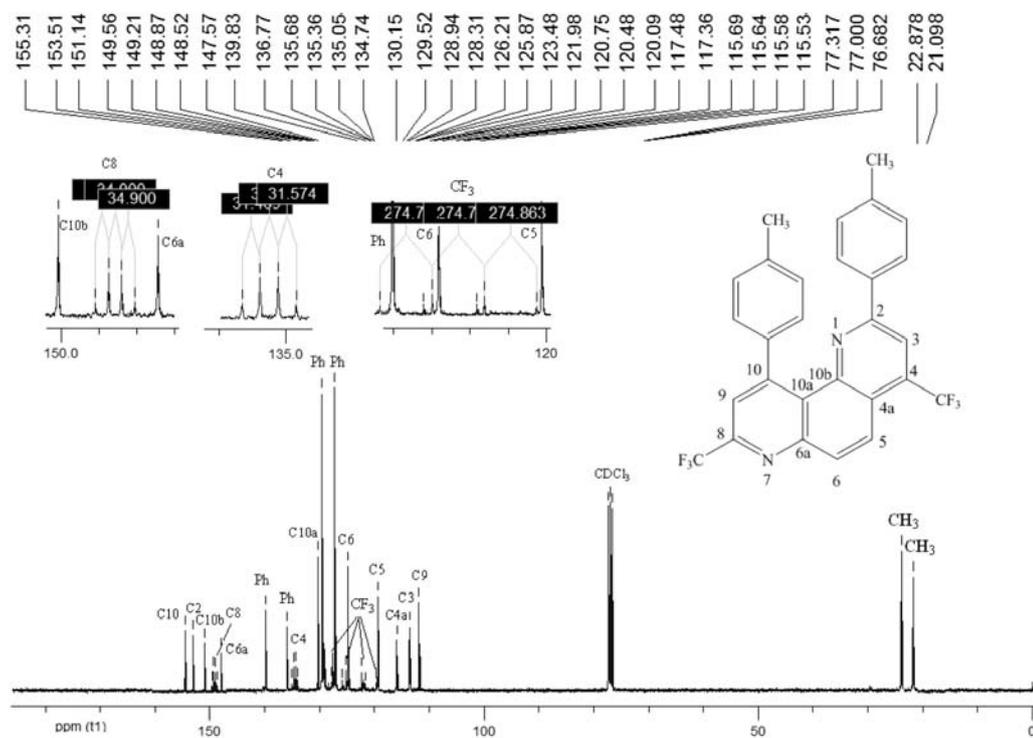


Figure S32. ^{13}C NMR (200 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-methylphenyl)-1,7-phenanthroline (**3d**).

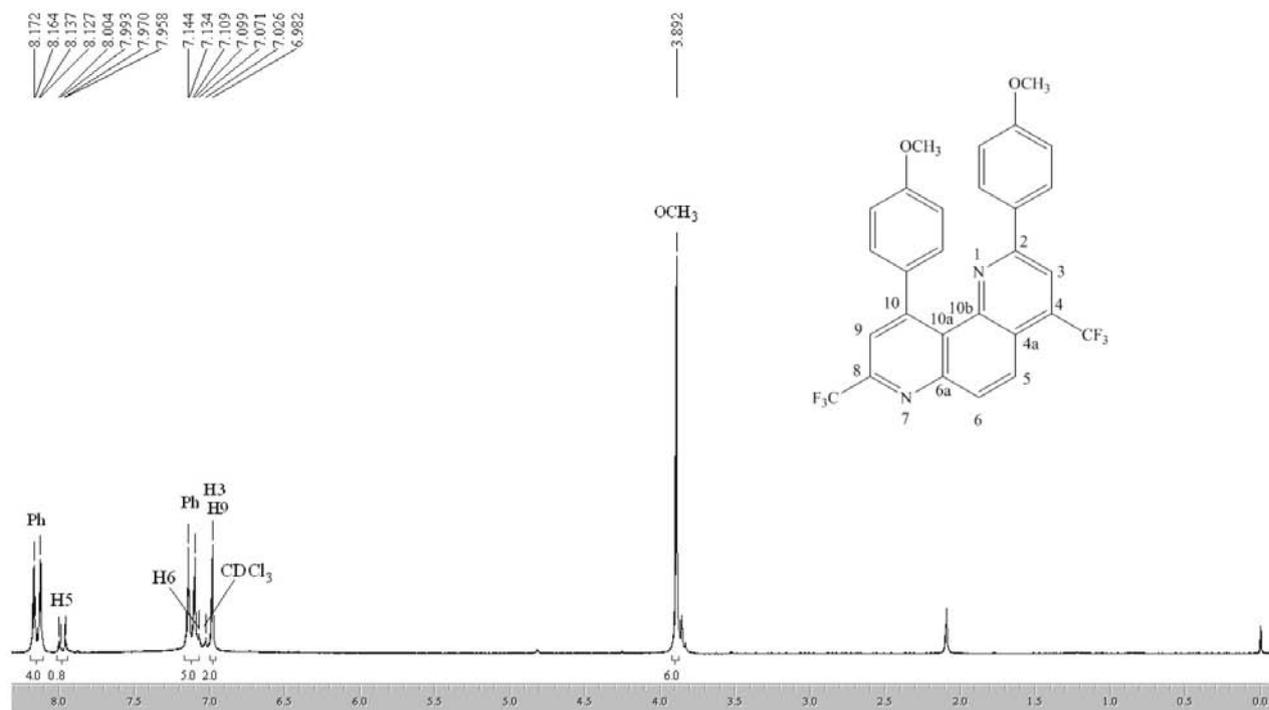


Figure S33. ^1H NMR (100 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-methoxyphenyl)-1,7-phenanthroline (**3e**).

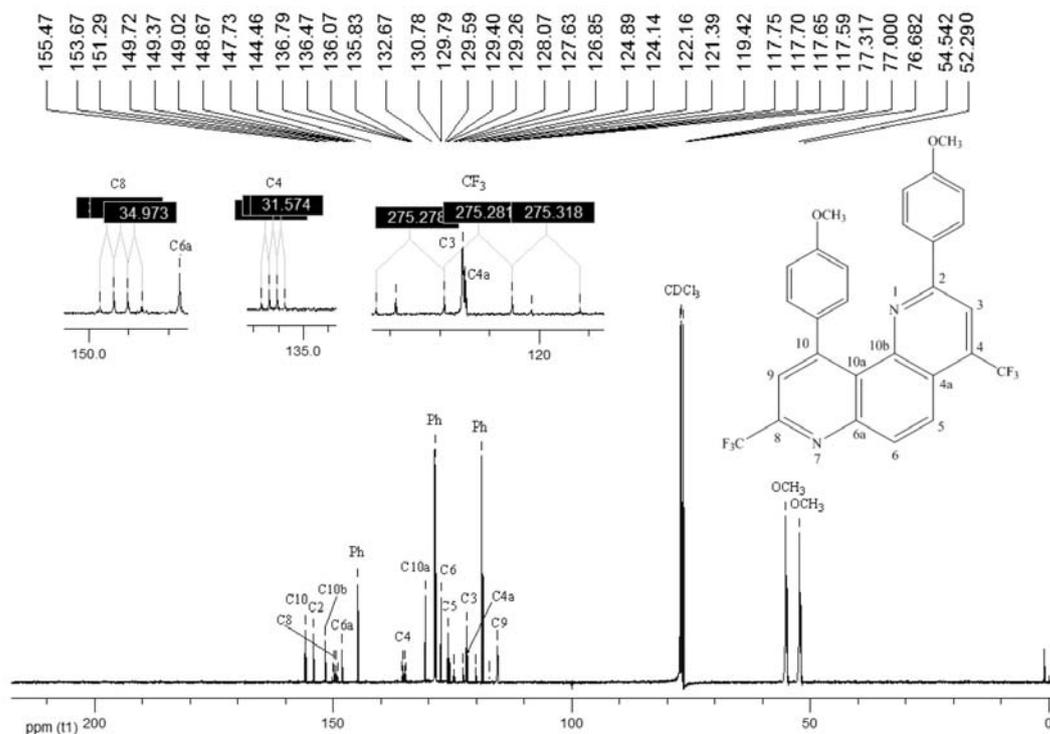


Figure S34. ¹³C NMR (200 MHz, CDCl₃) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-methoxyphenyl)-1,7-phenanthroline (**3e**).

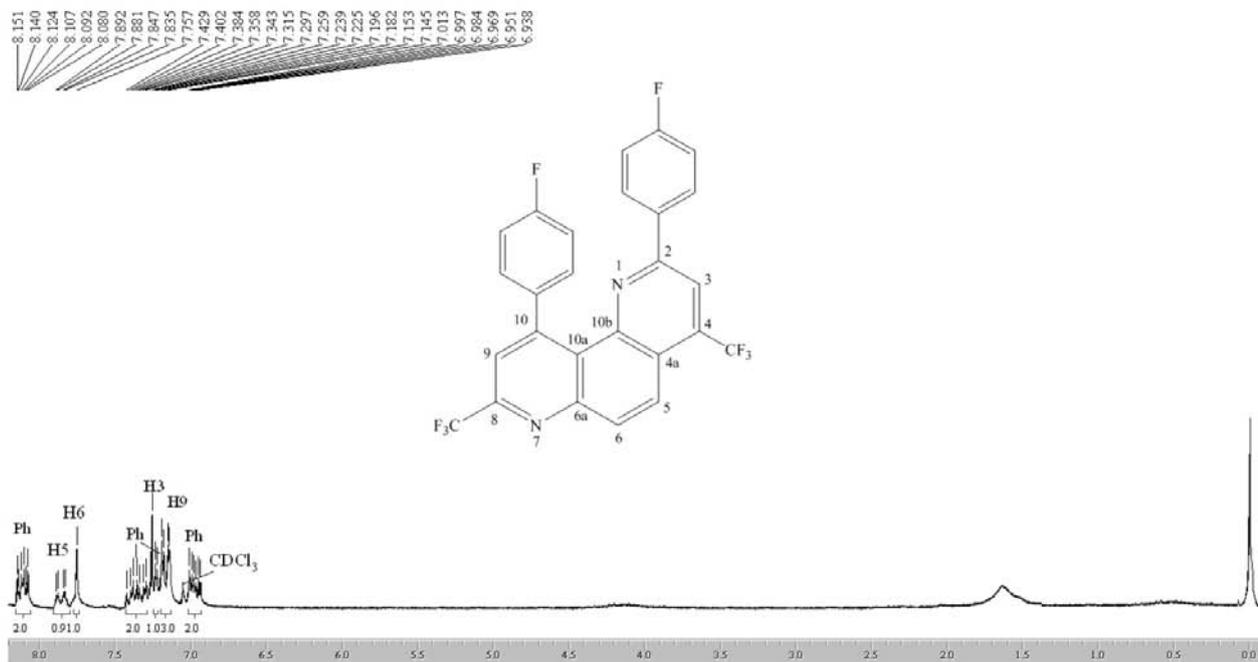


Figure S35. ¹H NMR (100 MHz, CDCl₃) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-fluorophenyl)-1,7-phenanthroline (**3f**).

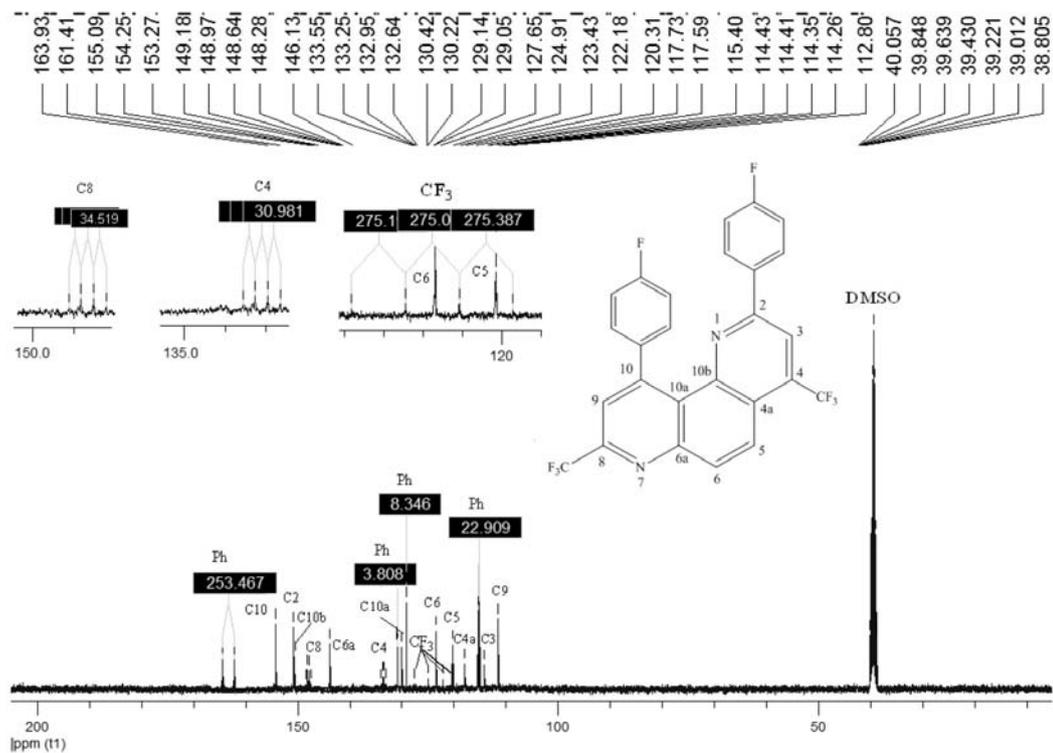


Figure S36. ^{13}C NMR (200 MHz, CDCl_3) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-fluorophenyl)-1,7-phenanthroline (**3f**).

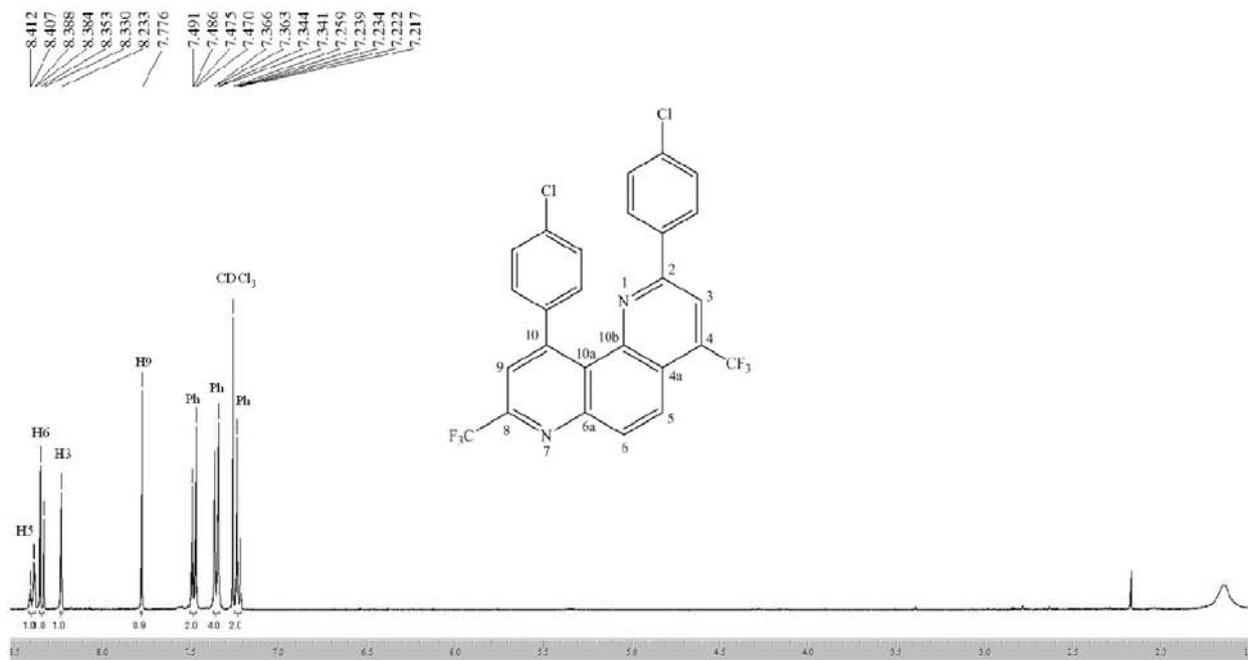


Figure S37. ^1H NMR (100 MHz, CDCl_3) spectrum of 2,10-di(4-chlorophenyl)-4,8-bis(trifluoromethyl)-1,7-phenanthroline (**3g**).

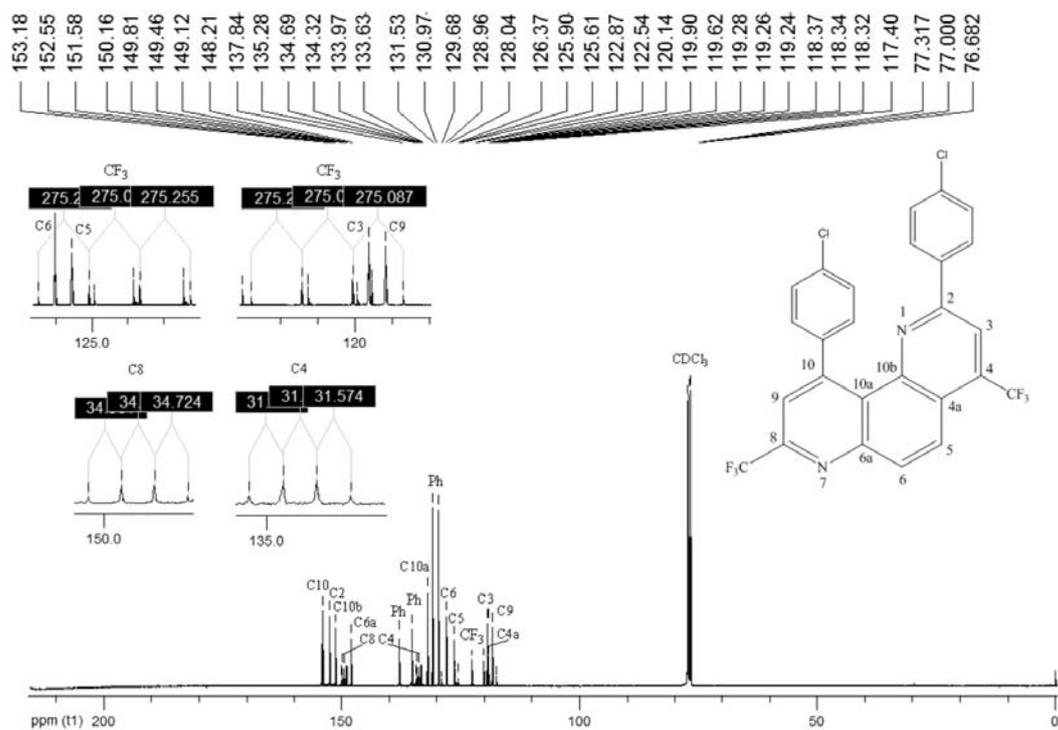


Figure S38. ^{13}C NMR (200 MHz, CDCl_3) spectrum of 2,10-di(4-chlorophenyl)-4,8-bis(trifluoromethyl)-1,7-phenanthroline (**3g**).

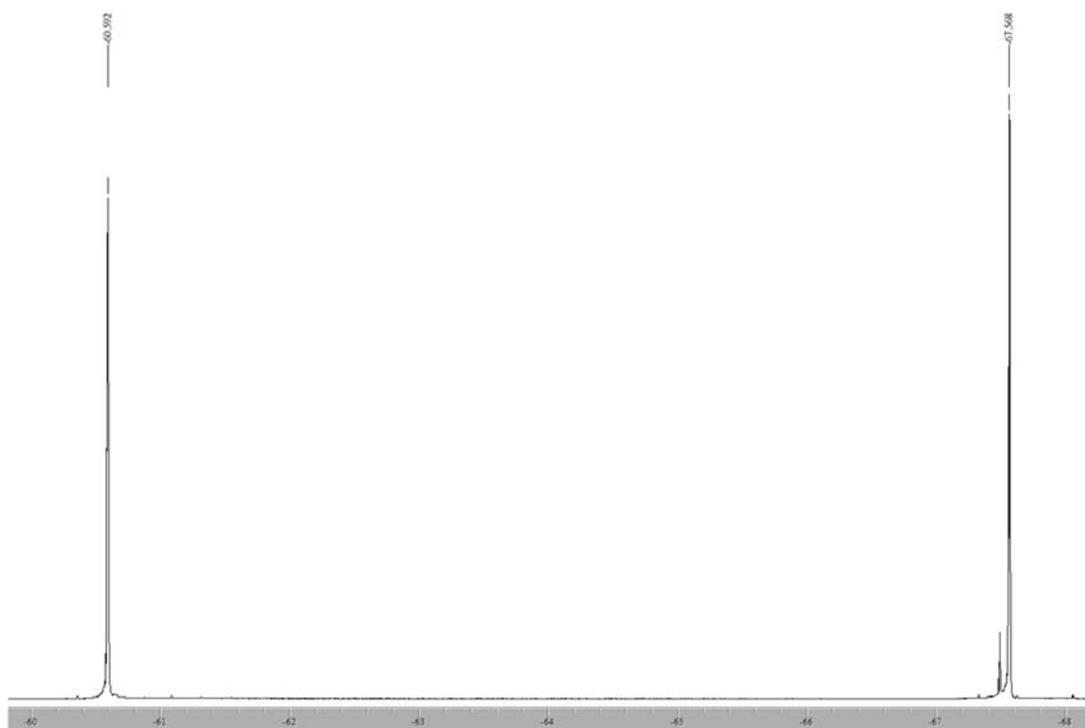


Figure S39. ^{19}F NMR (376 MHz, CDCl_3) spectrum of 2,10-di(4-chlorophenyl)-4,8-bis(trifluoromethyl)-1,7-phenanthroline (**3g**).

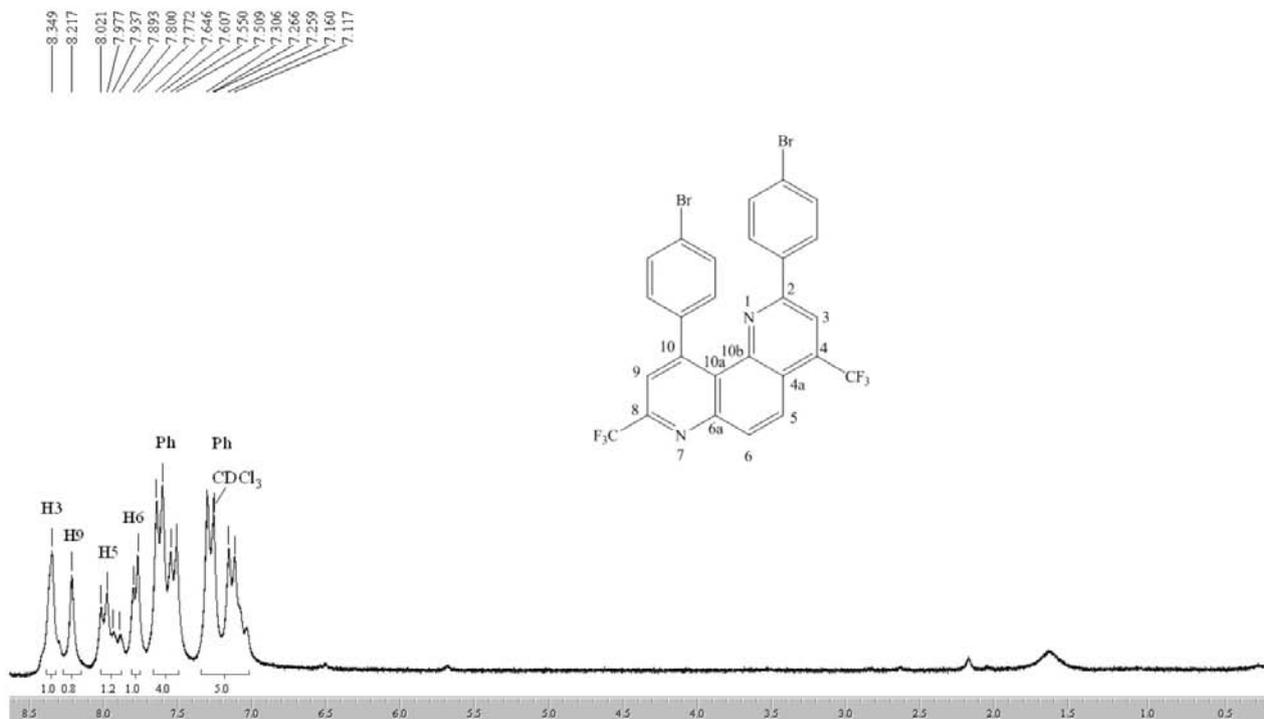


Figure S40. ¹H NMR (100 MHz, CDCl₃) spectrum of 2,10-di(4-bromophenyl)-4,8-bis(trifluoromethyl)-1,7-phenanthroline (**3h**).

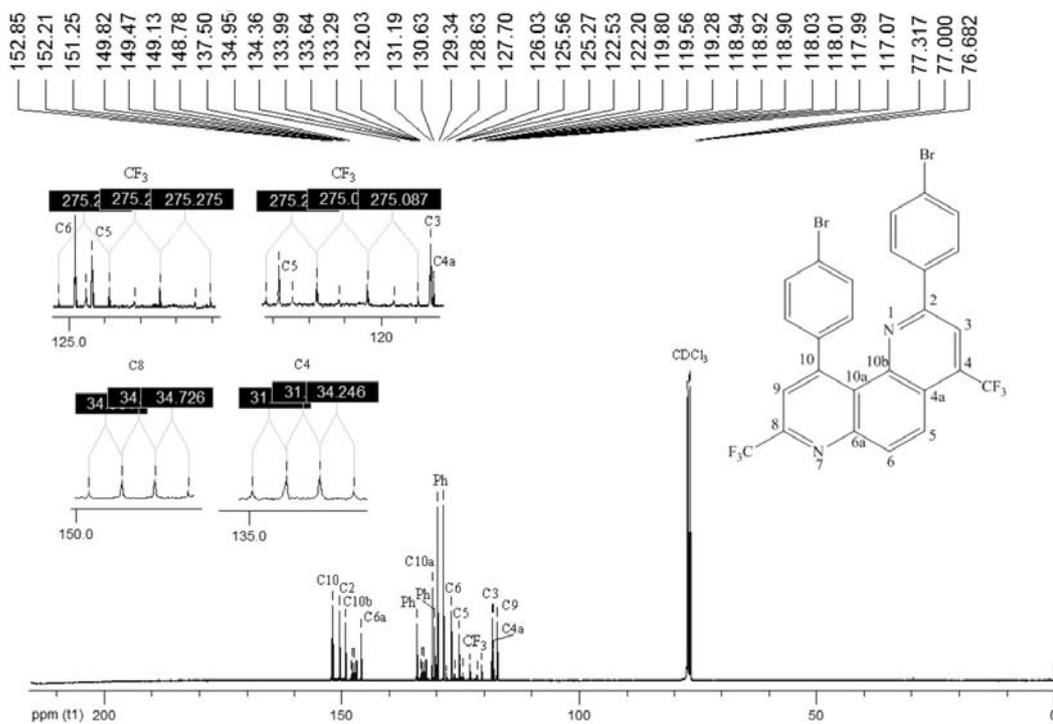


Figure S41. ¹³C NMR (200 MHz, CDCl₃) spectrum of 2,10-di(4-bromophenyl)-4,8-bis(trifluoromethyl)-1,7-phenanthroline (**3h**).

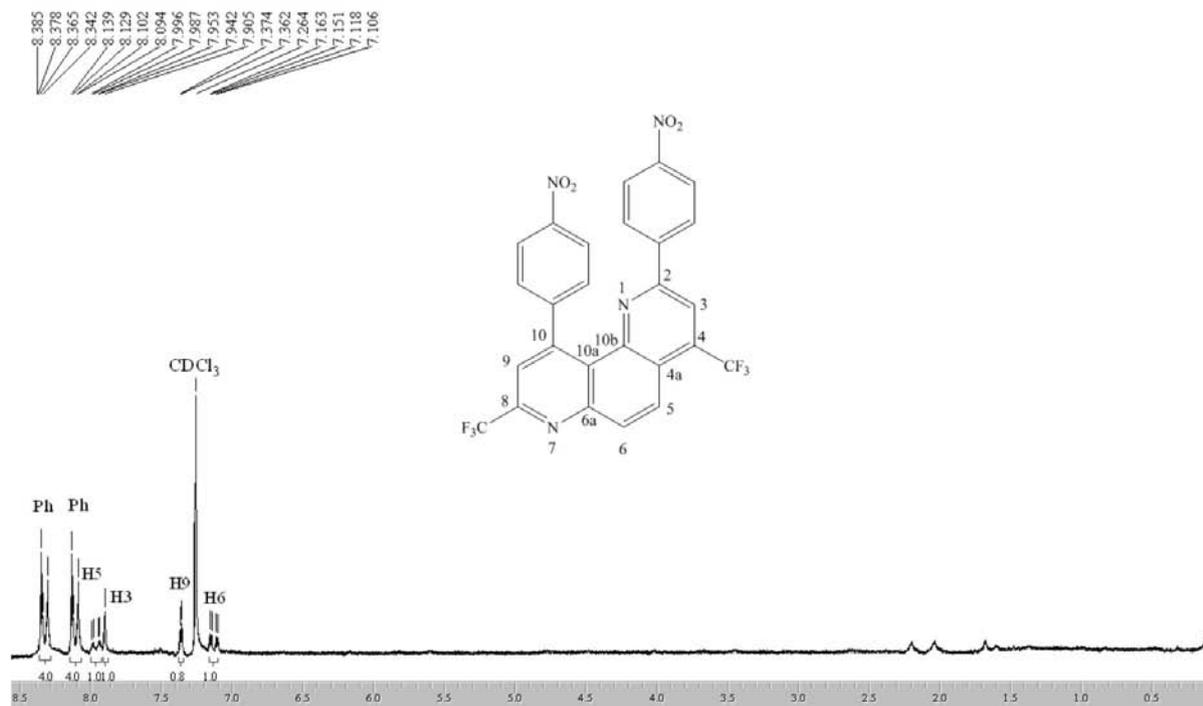


Figure S42. ¹H NMR (100 MHz, CDCl₃) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-nitrophenyl)-1,7-phenanthroline (3i).

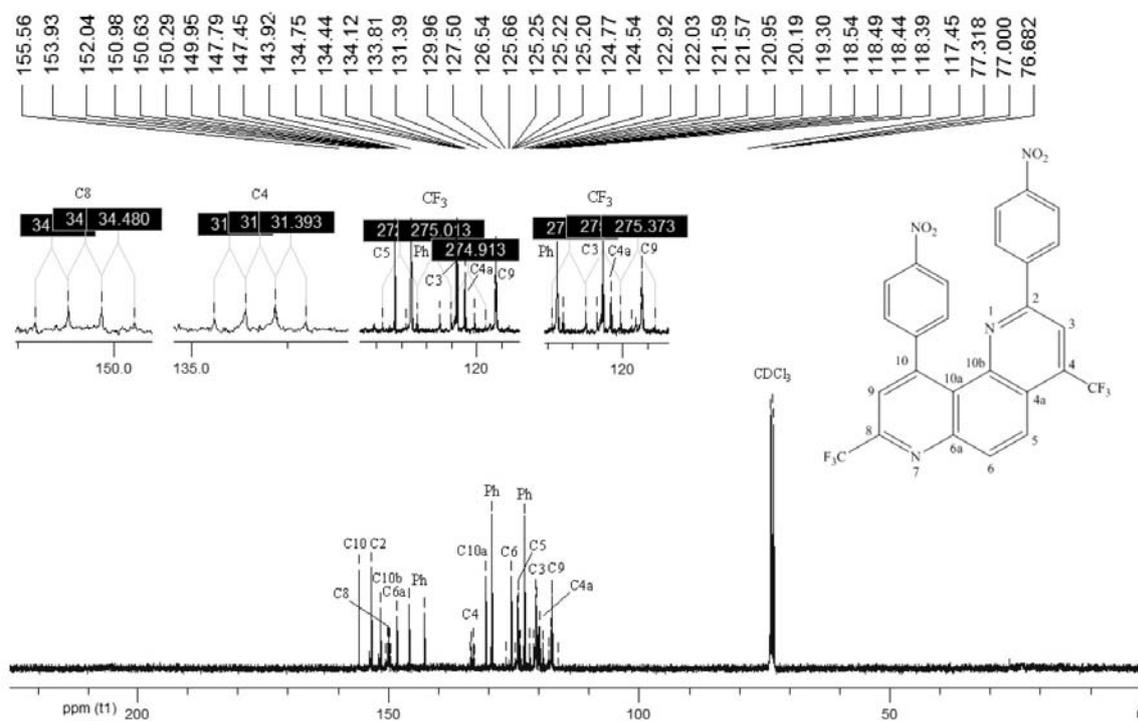


Figure S43. ¹³C NMR (200 MHz, CDCl₃) spectrum of 4,8-bis(trifluoromethyl)-2,10-di(4-nitrophenyl)-1,7-phenanthroline (3i).

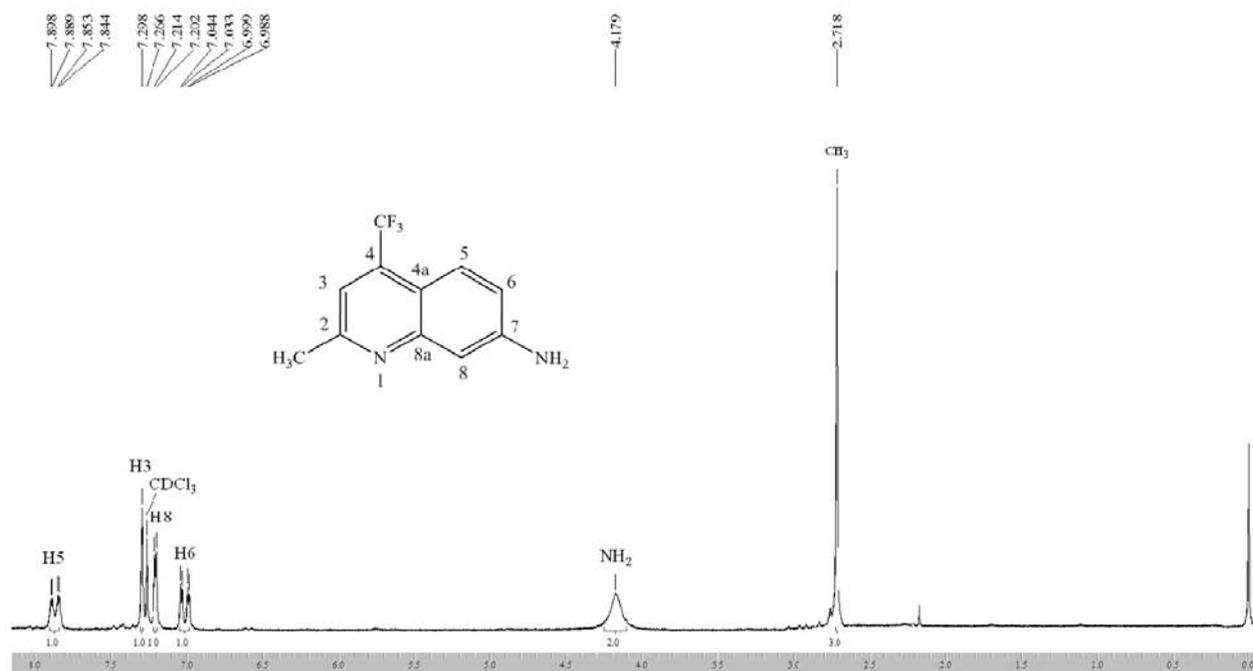


Figure S44. ¹H NMR (100 MHz, CDCl₃) spectrum of 4-trifluoromethyl-2-methyl-7-aminoquinoline (**4b**).

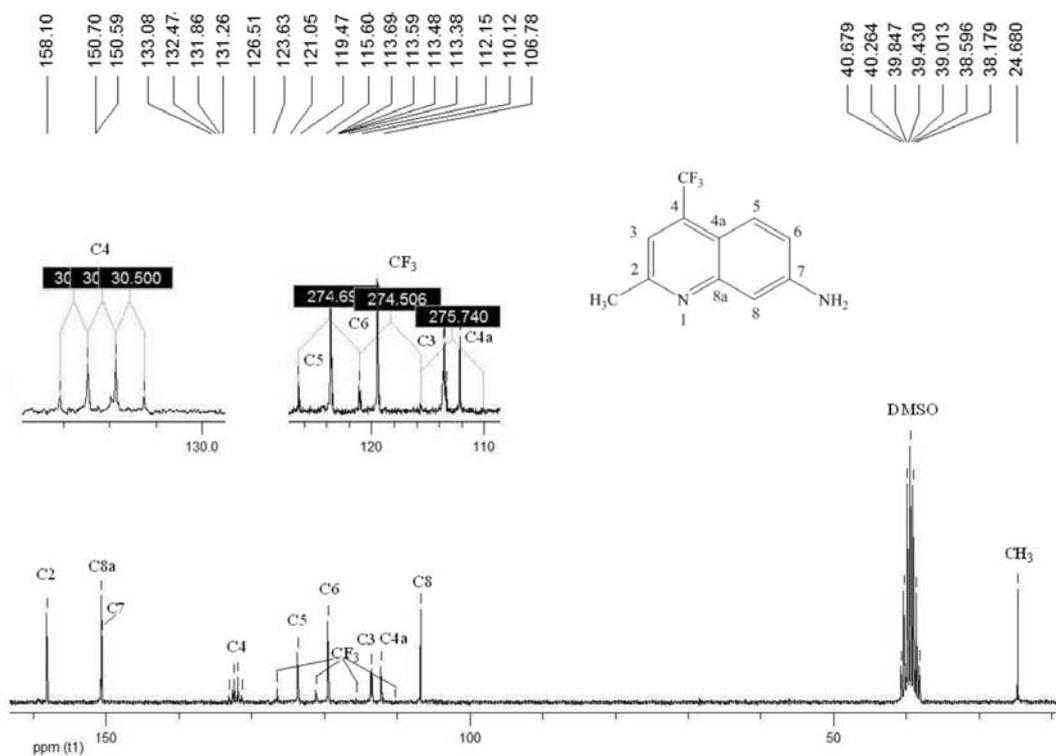


Figure S45. ¹³C NMR (200 MHz, DMSO-*d*₆) spectrum of 4-trifluoromethyl-2-methyl-7-aminoquinoline (**4b**).

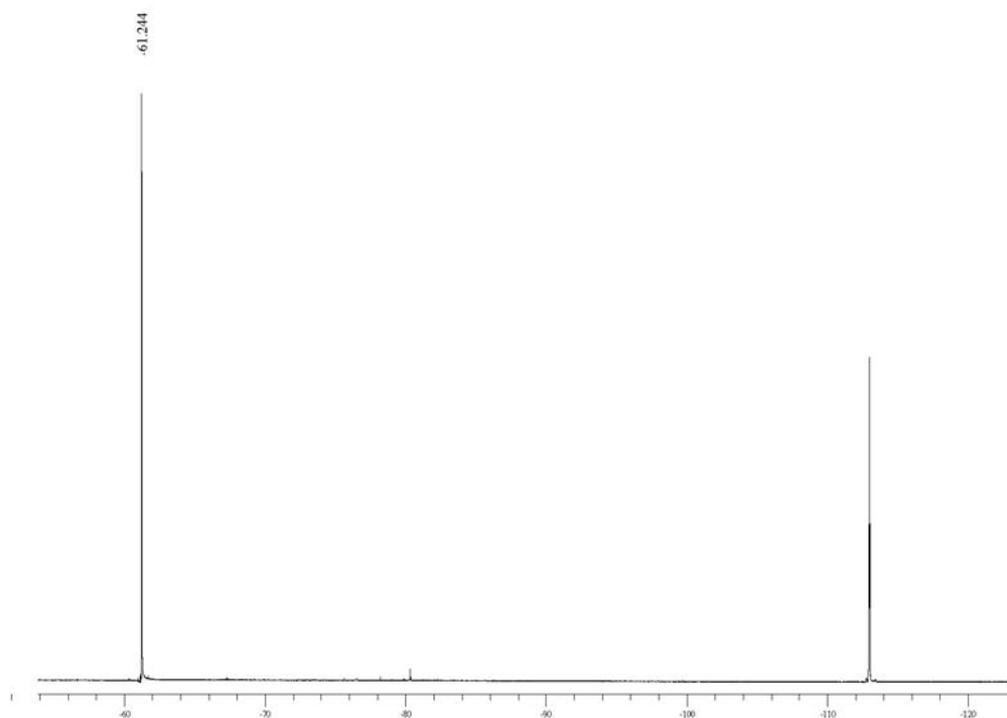


Figure S46. ^{19}F NMR (376 MHz, CDCl_3) spectrum of 4-trifluoromethyl-2-methyl-7-aminoquinoline (**4b**).

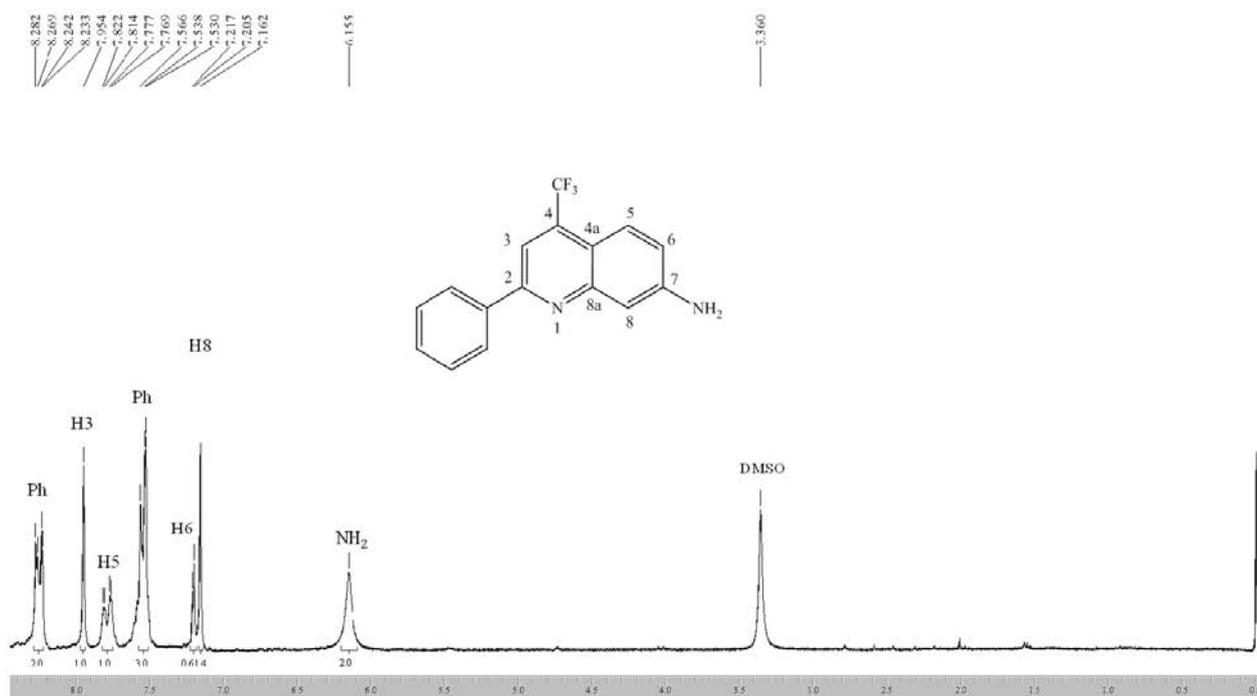


Figure S47. ^1H NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of 4-trifluoromethyl-2-phenyl-7-aminoquinoline (**4c**).

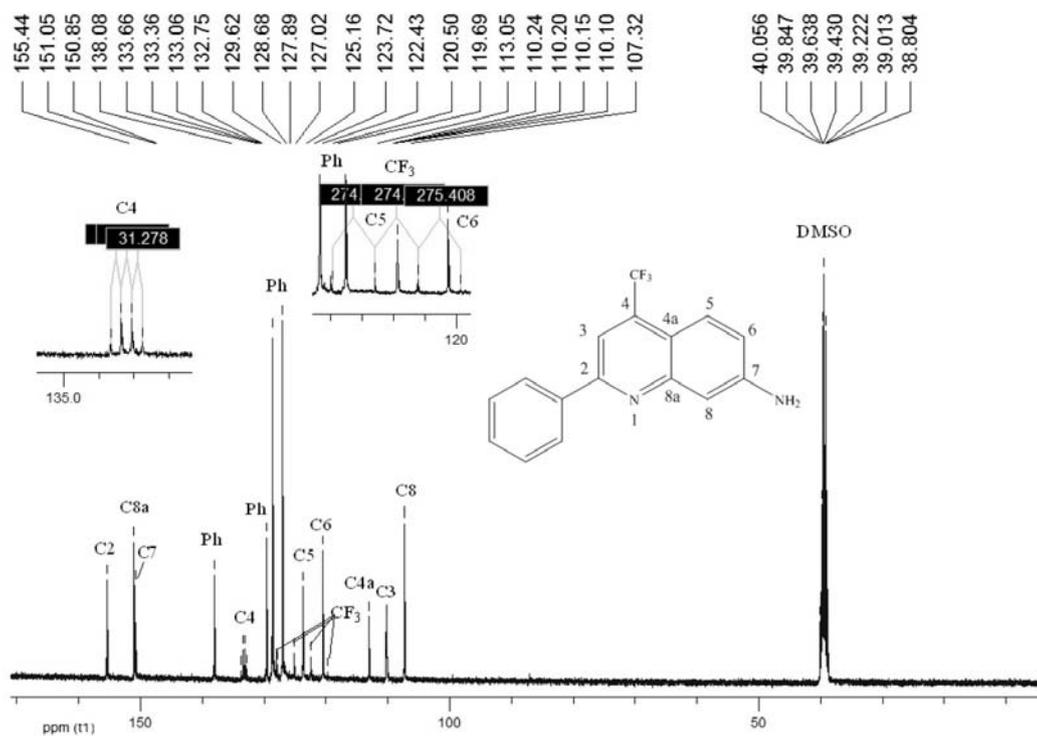


Figure S48. ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of 4-trifluoromethyl-2-phenyl-7-aminoquinoline (**4c**).



Figure S49. ^{19}F NMR (376 MHz, CDCl_3) spectrum of 4-trifluoromethyl-2-phenyl-7-aminoquinoline (**4c**).

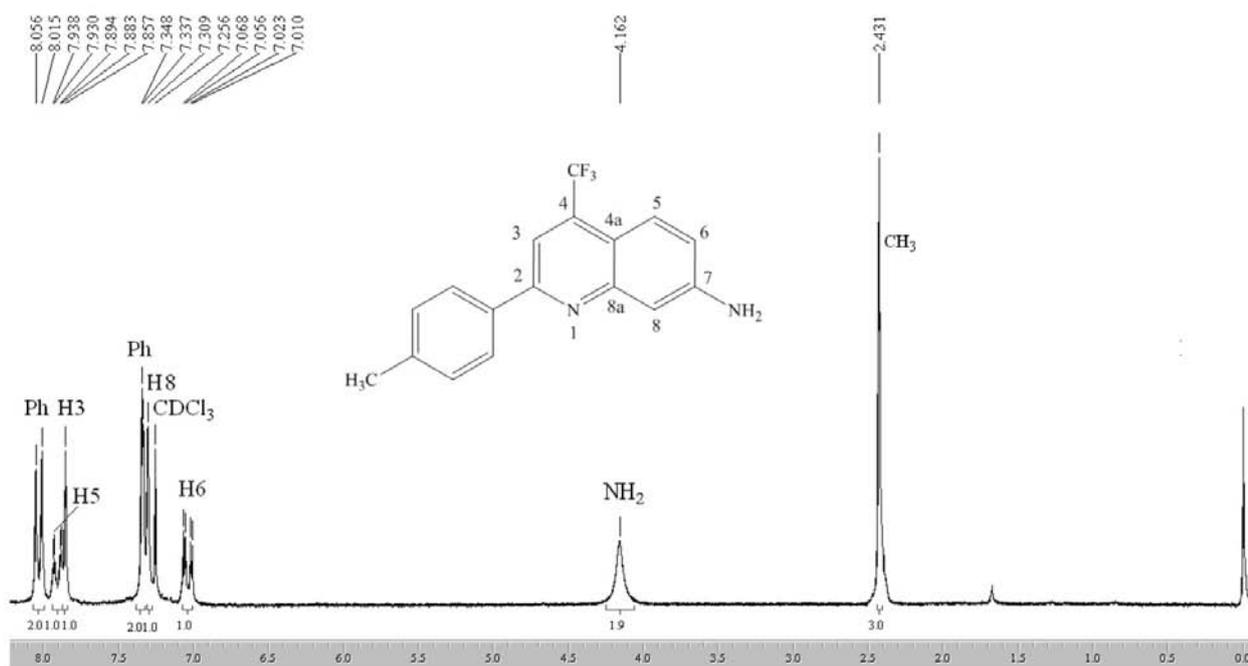


Figure S50. ^1H NMR (100 MHz, CDCl_3) spectrum of 4-trifluoromethyl-2-(4-methylphenyl)-7-aminoquinoline (**4d**).

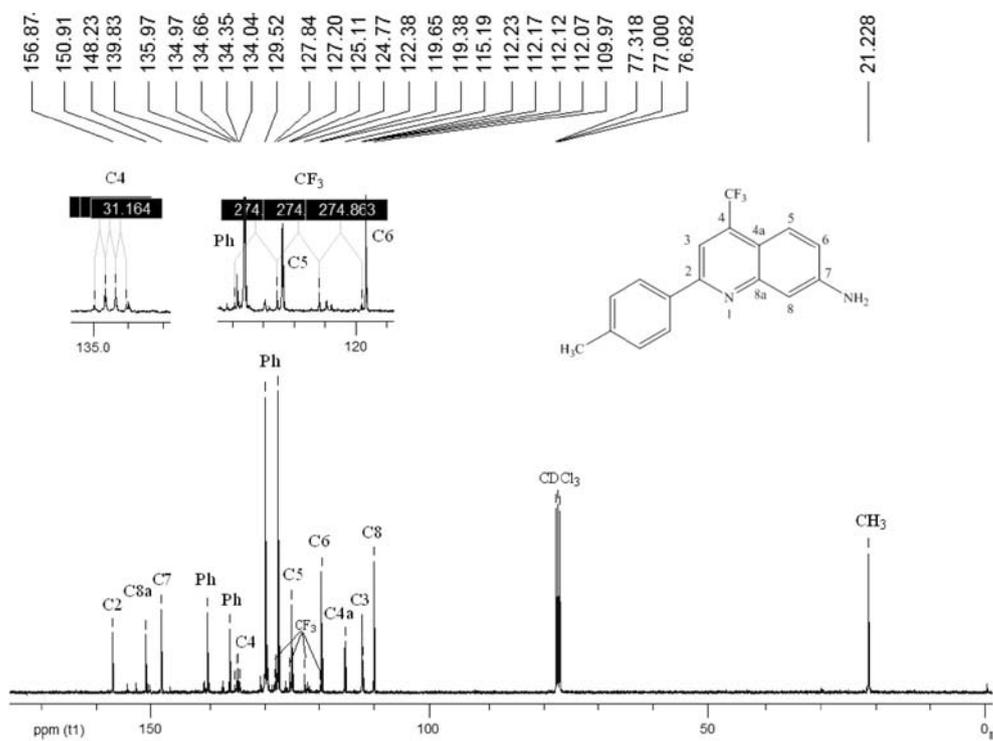


Figure S51. ^{13}C NMR (200 MHz, CDCl_3) spectrum of 4-trifluoromethyl-2-(4-methylphenyl)-7-aminoquinoline (**4d**).

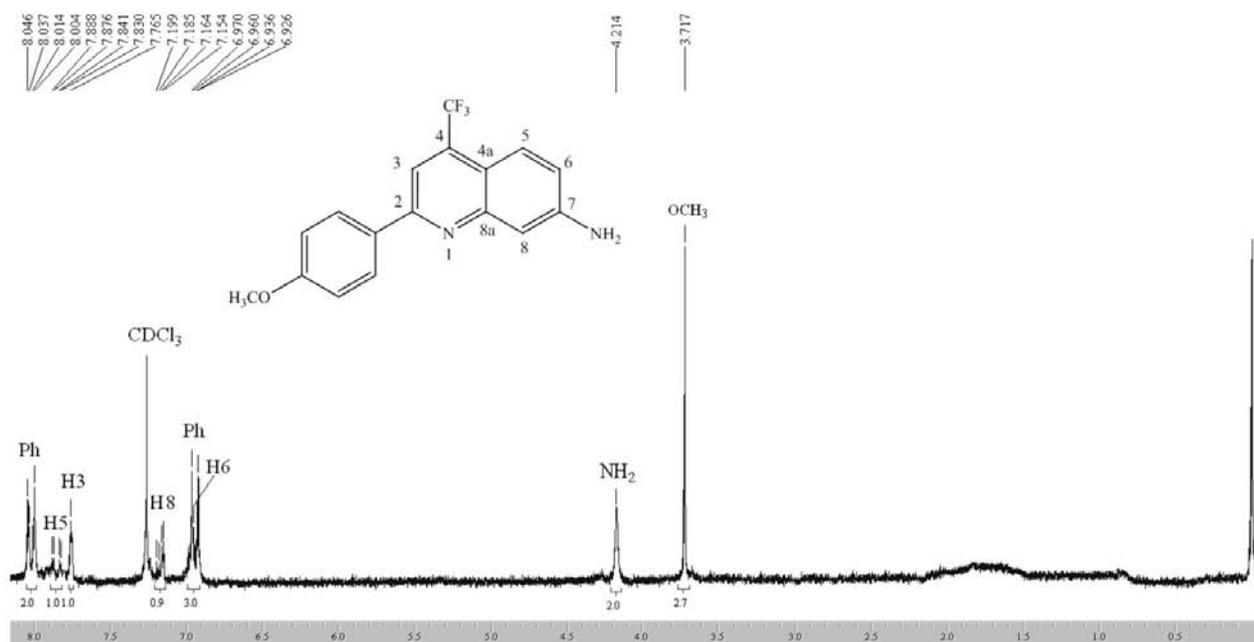


Figure S52. ¹H NMR (100 MHz, CDCl₃) spectrum of 4-trifluoromethyl-2-(4-methoxyphenyl)-7-aminoquinoline (**4e**).

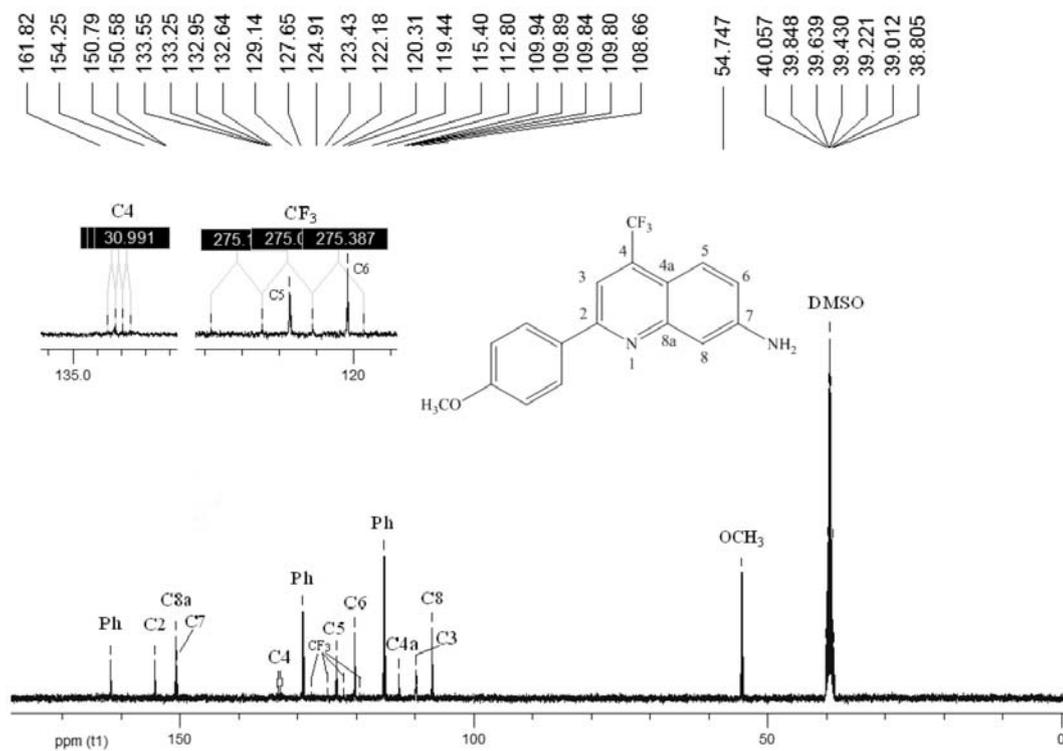


Figure S53. ¹³C NMR (200 MHz, DMSO-*d*₆) spectrum of 4-trifluoromethyl-2-(4-methoxyphenyl)-7-aminoquinoline (**4e**).

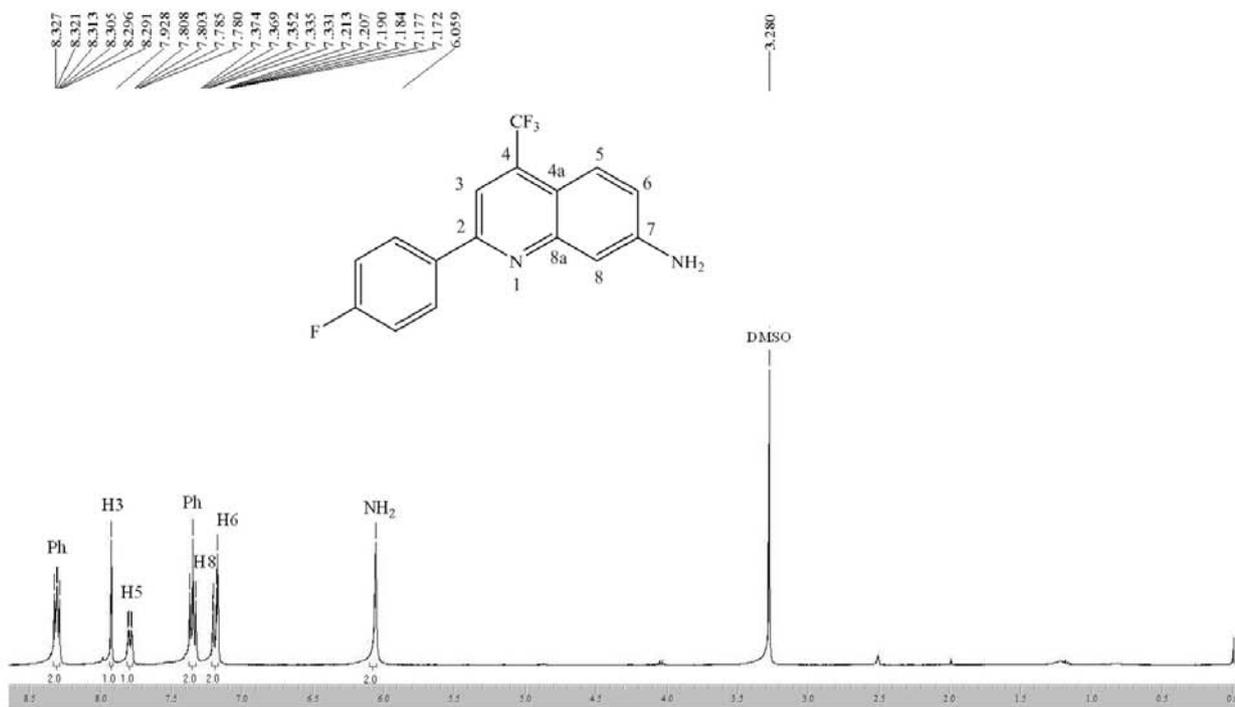


Figure S54. ¹H NMR (100 MHz, DMSO-*d*₆) spectrum of 4-trifluoromethyl-2-(4-fluorophenyl)-7-aminoquinoline (4f).

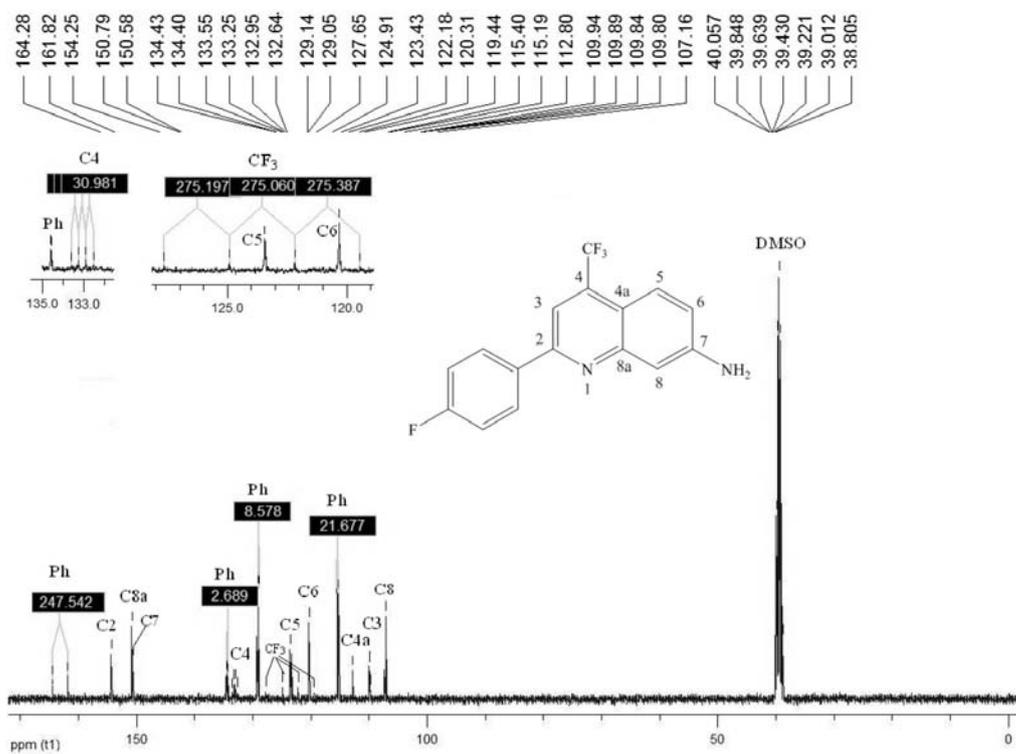


Figure S55. ¹³C NMR (200 MHz, DMSO-*d*₆) spectrum of 4-trifluoromethyl-2-(4-fluorophenyl)-7-aminoquinoline (4f).

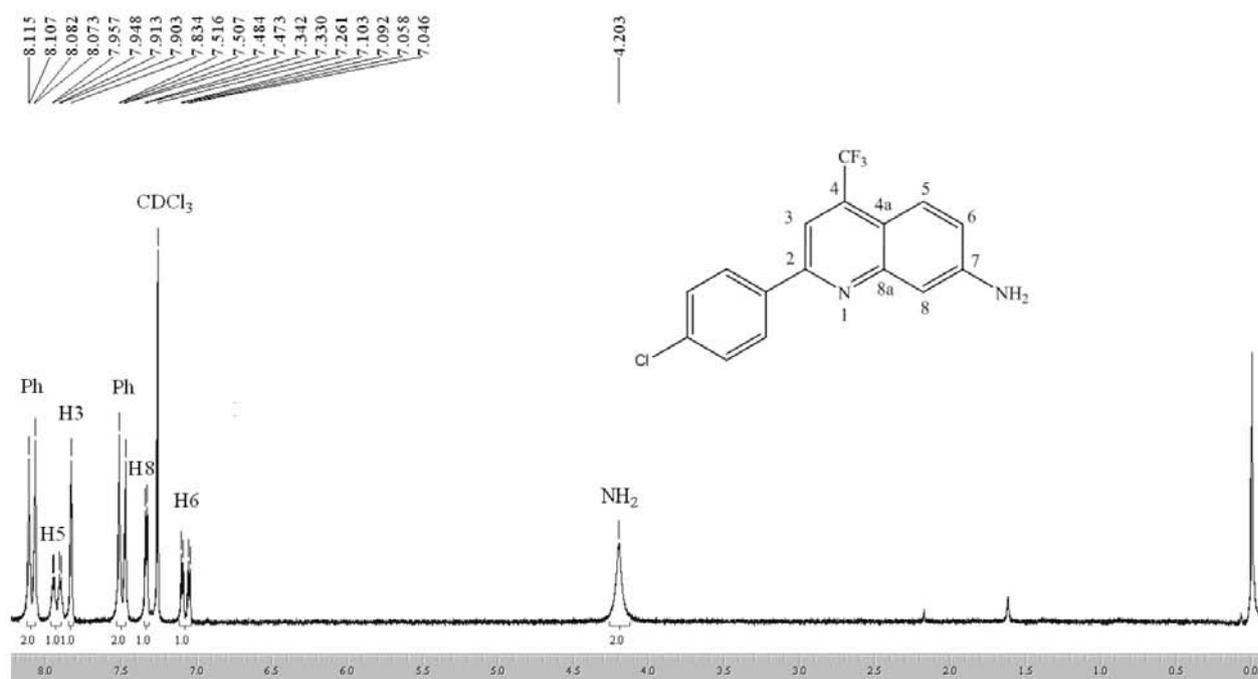


Figure S56. ¹H NMR (100 MHz, CDCl₃) spectrum of 2-(4-chlorophenyl)-4-trifluoromethyl-7-aminoquinoline (**4g**).

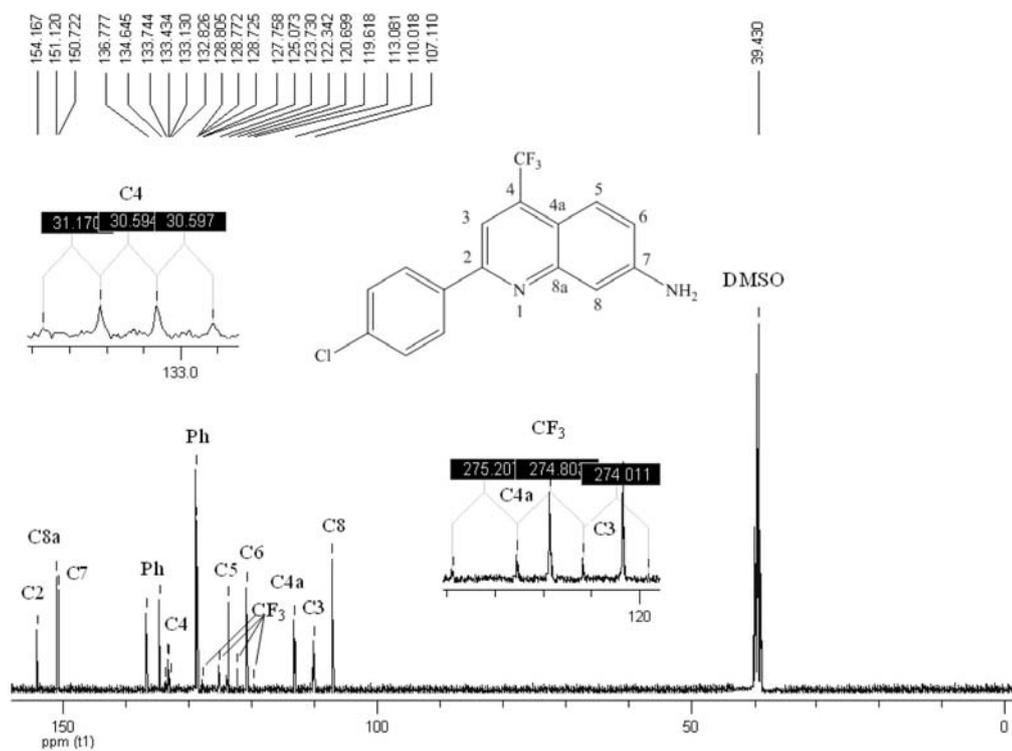


Figure S57. ¹³C NMR (200 MHz, DMSO-*d*₆) spectrum of 2-(4-chlorophenyl)-4-trifluoromethyl-7-aminoquinoline (**4g**).

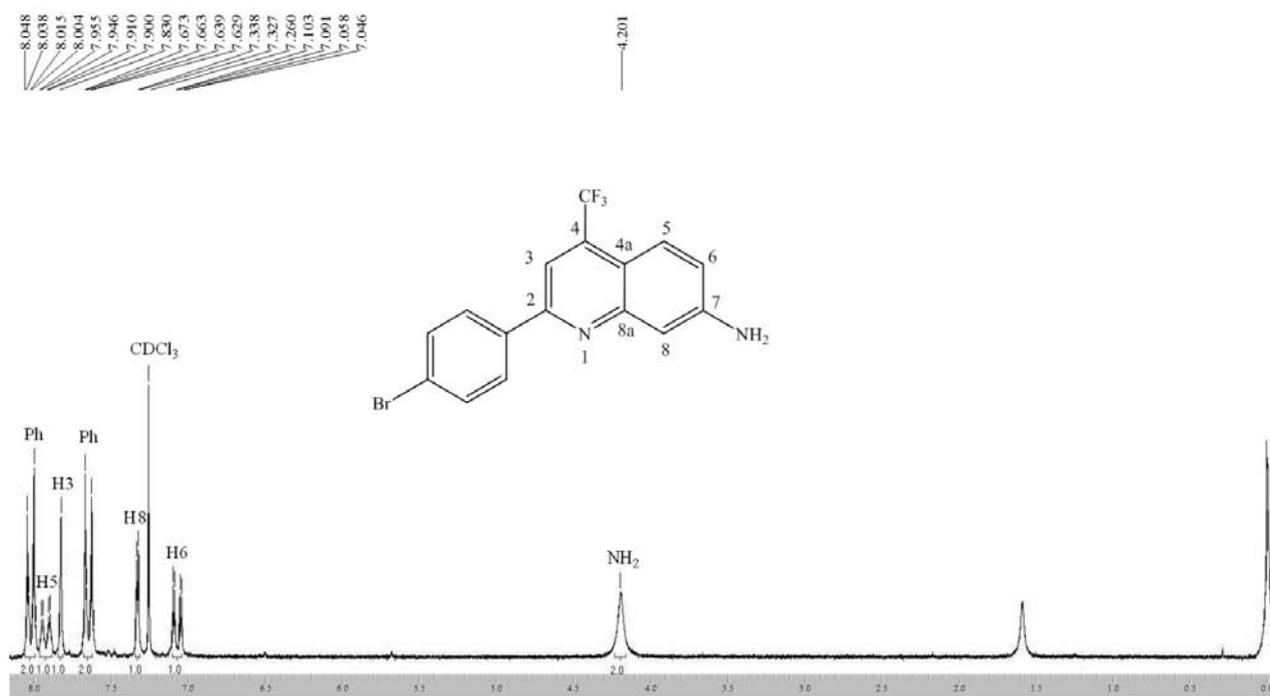


Figure S58. ¹H NMR (100 MHz, CDCl₃) spectrum of 2-(4-bromophenyl)-4-trifluoromethyl-7-aminoquinoline (**4h**).

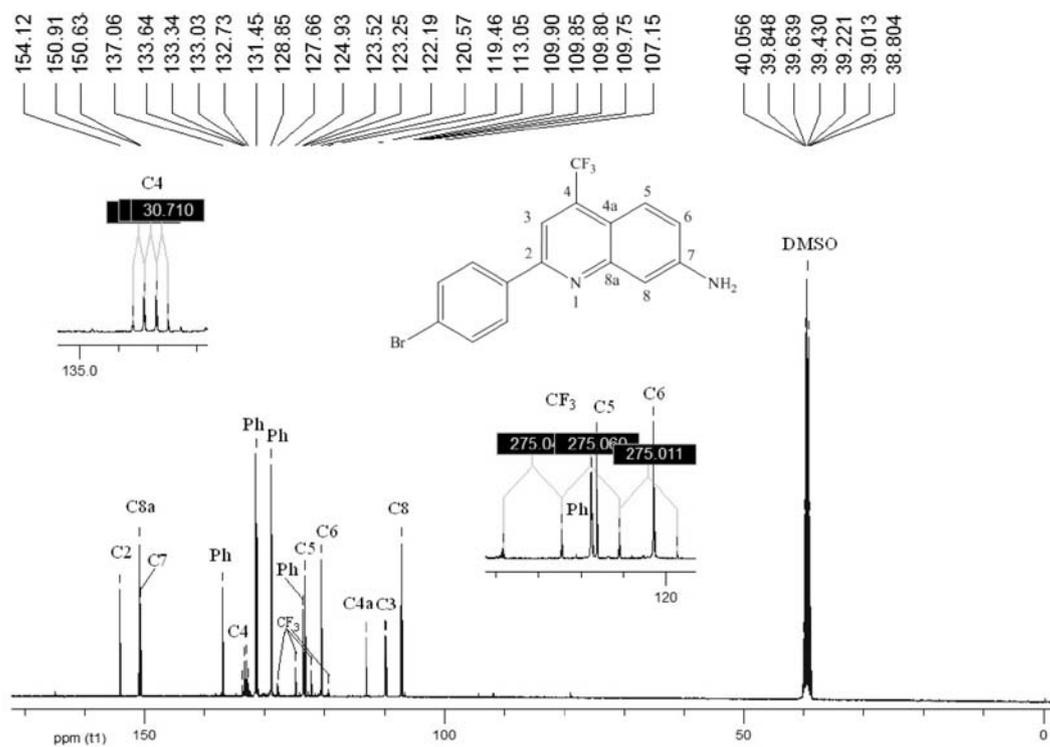


Figure S59. ¹³C NMR (200 MHz, DMSO-*d*₆) spectrum of 2-(4-bromophenyl)-4-trifluoromethyl-7-aminoquinoline (**4h**).

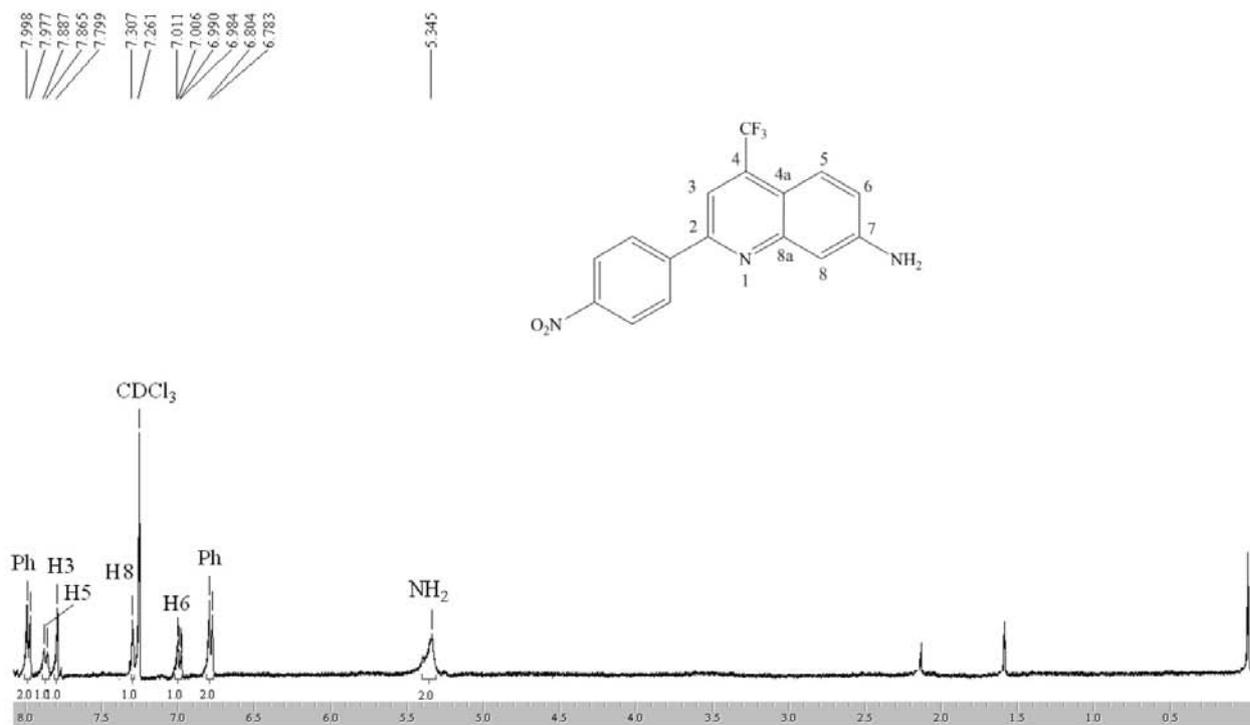


Figure S60. ¹H NMR (100 MHz, CDCl₃) spectrum of 4-trifluoromethyl-2-(4-nitrophenyl)-7-aminoquinoline (**4i**).

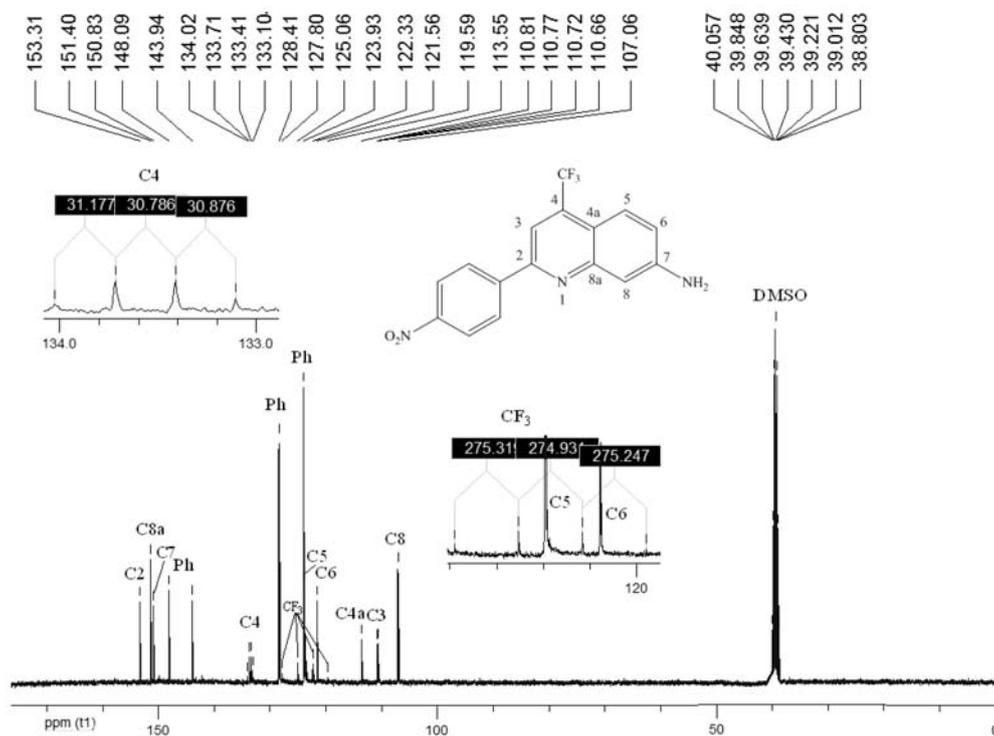


Figure S61. ¹³C NMR (200 MHz, DMSO-*d*₆) spectrum of 4-trifluoromethyl-2-(4-nitrophenyl)-7-aminoquinoline (**4i**).