

Supporting information *for*

Synthesis of novel 5-amino-1,2,3-triazole-2,1,3-benzothiadiazoles and their derivatives via dipolar azide-nitrile cycloaddition and buchwald–hartwig reaction

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Table of contents

NMR spectra	S2
Electrochemistry	S66

NMR spectra

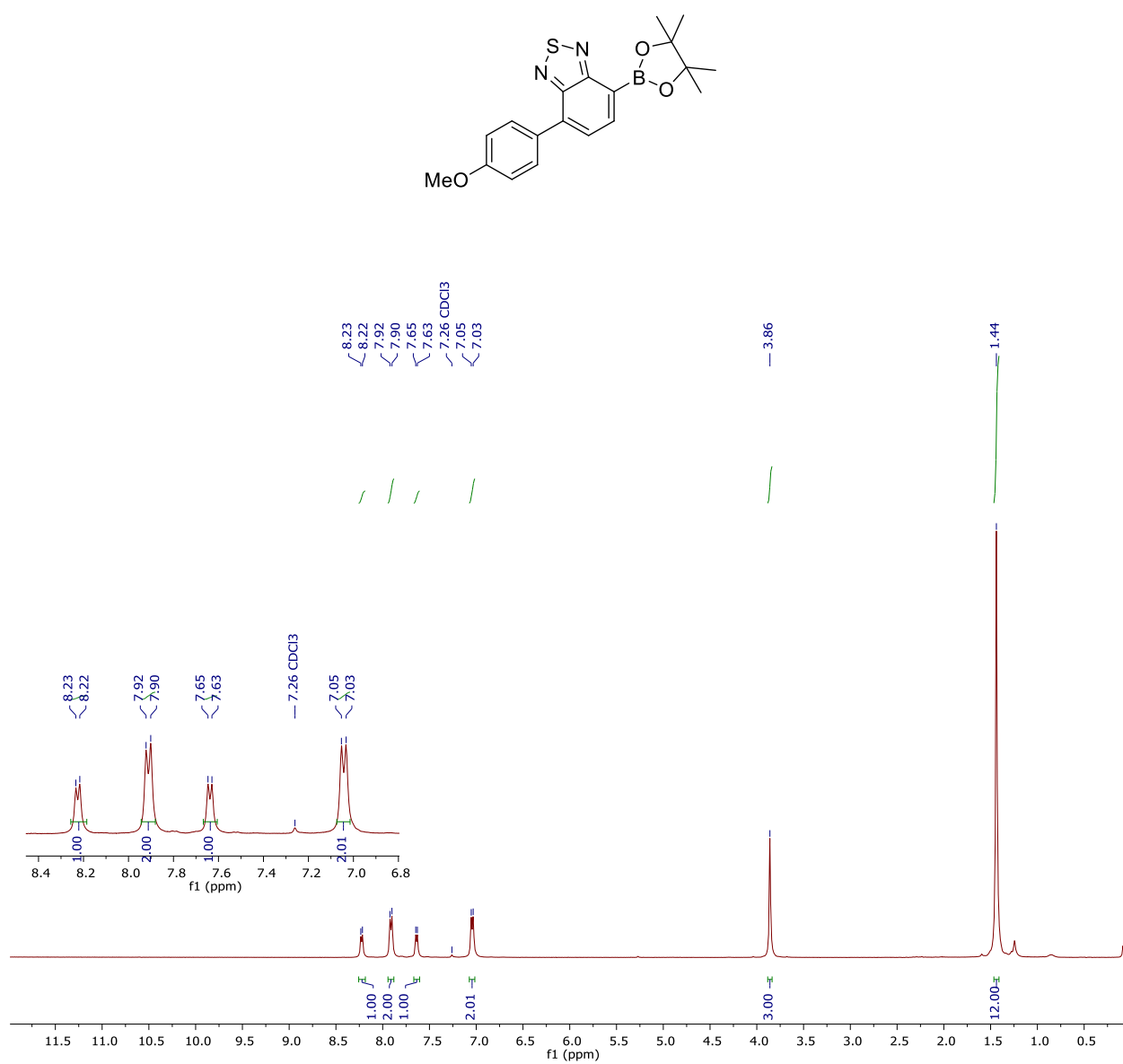


Figure S1. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **2**

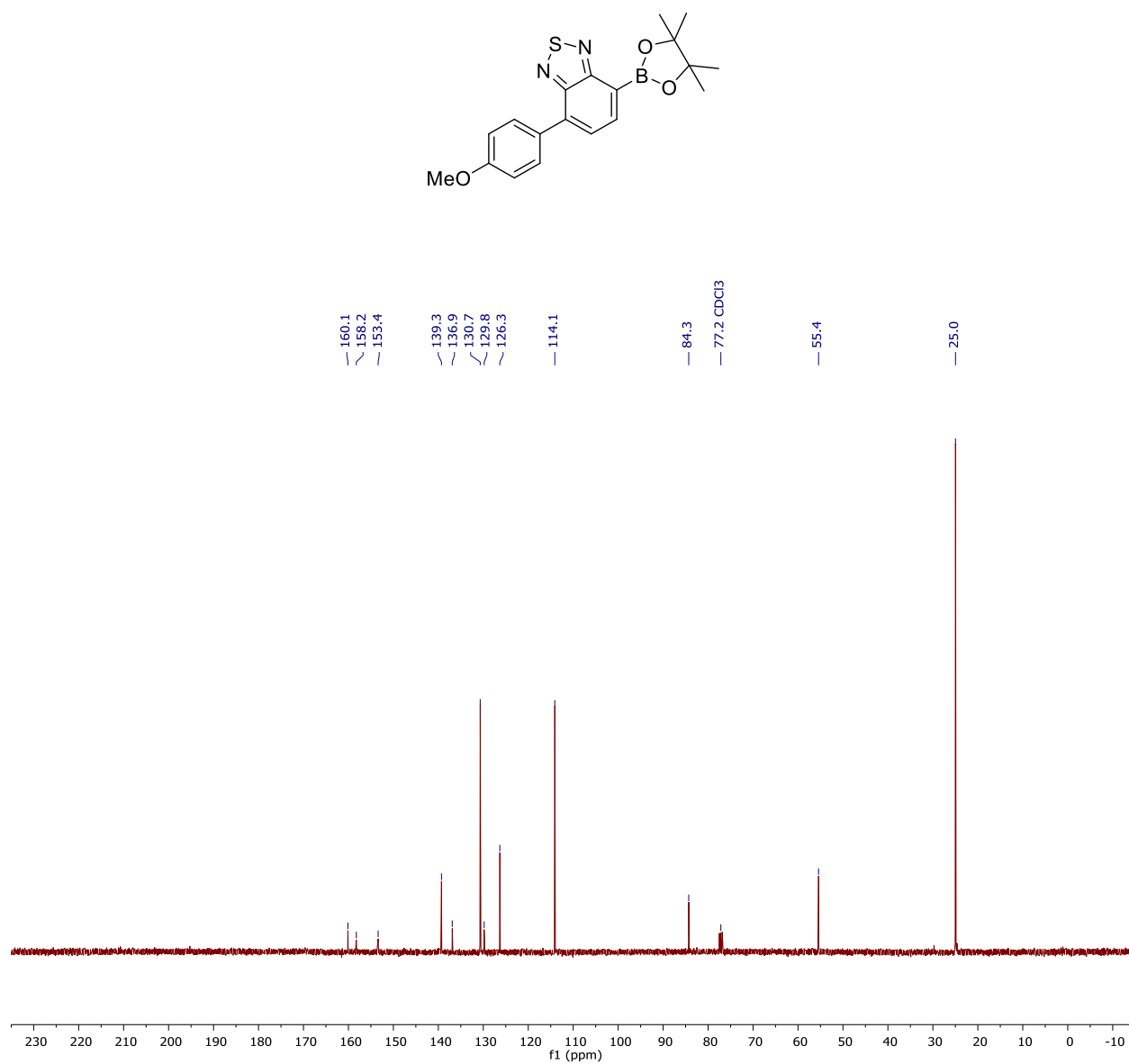


Figure S2. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **2**

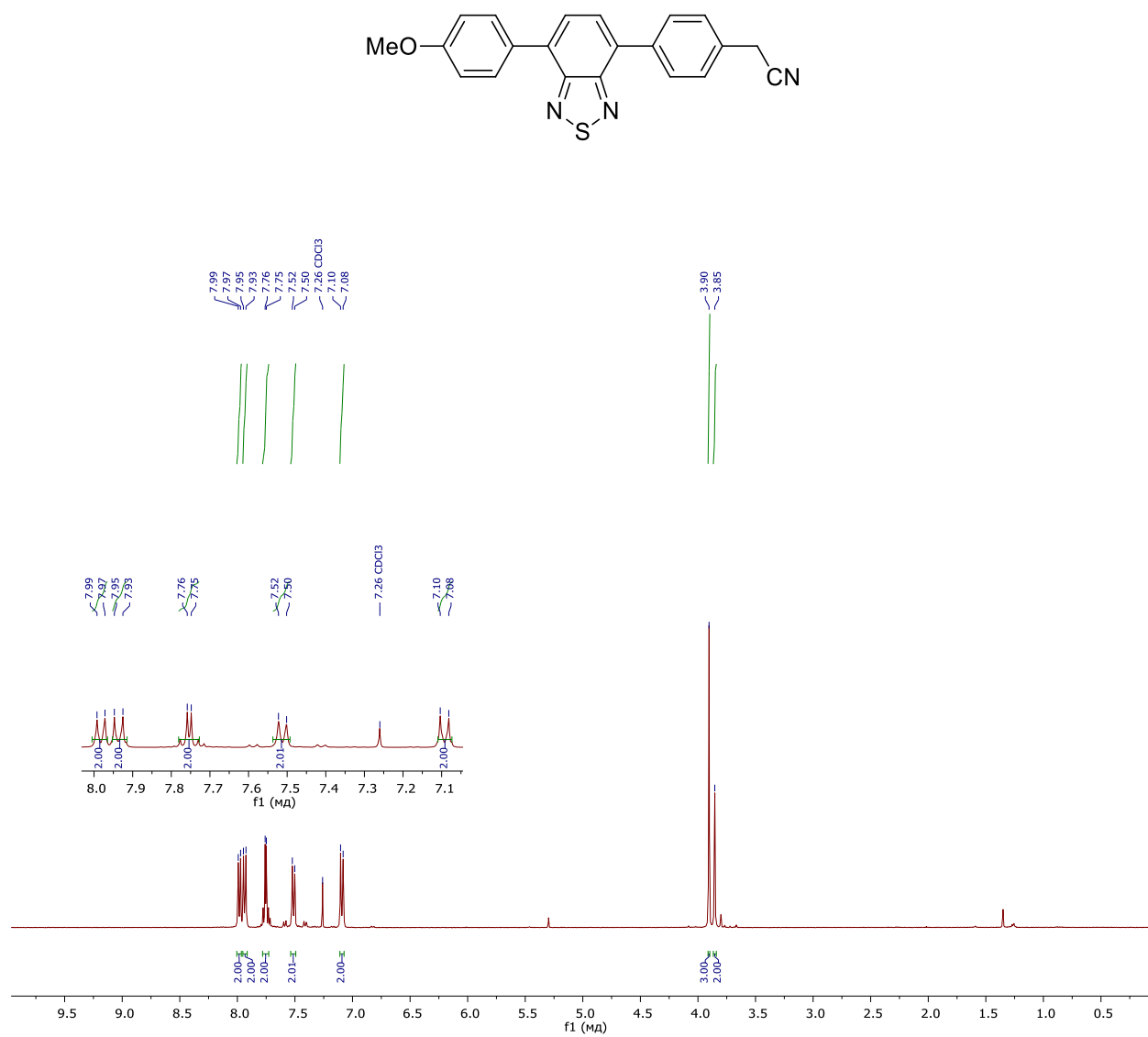


Figure S3. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **3a**

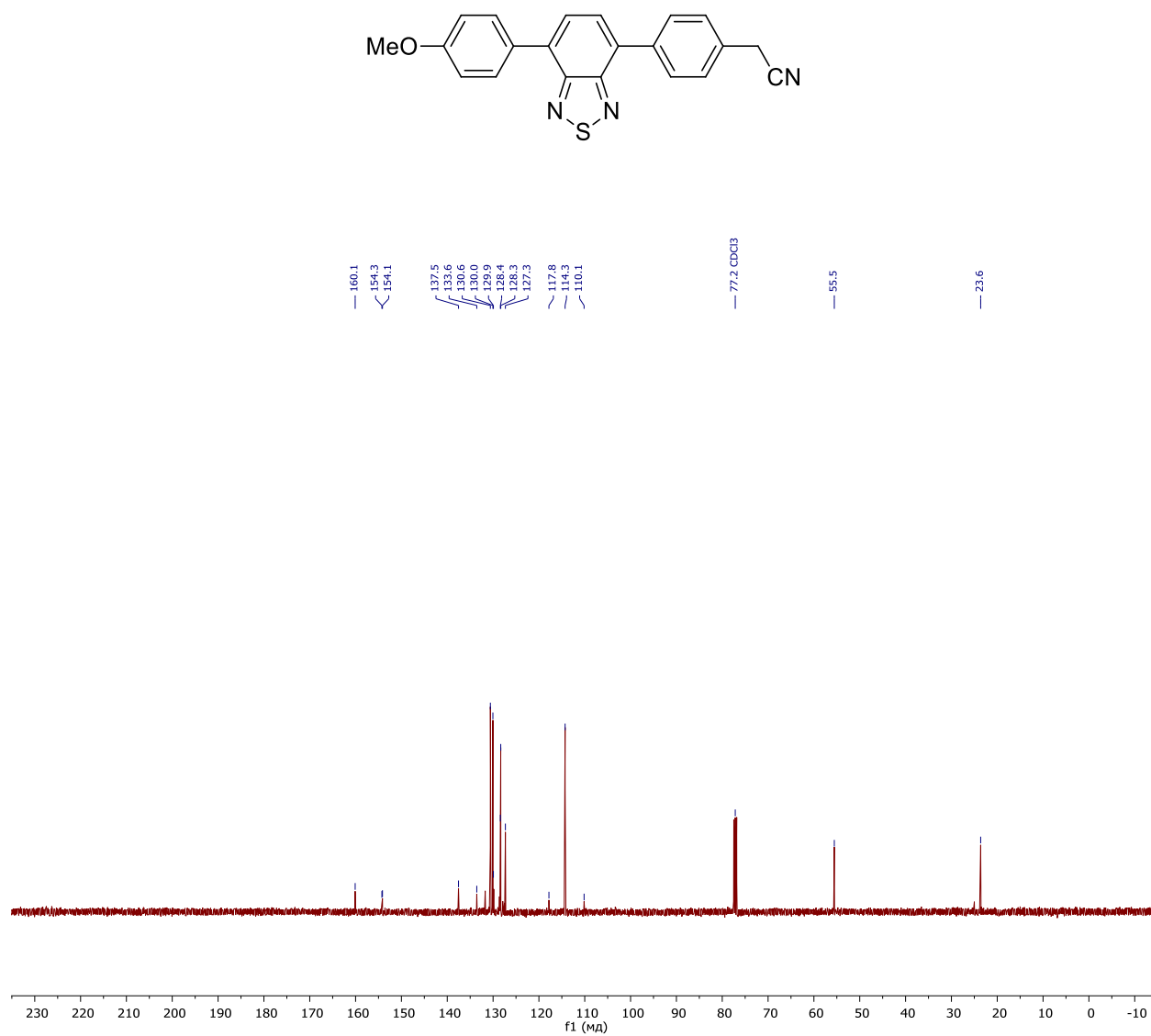


Figure S4. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **3a**

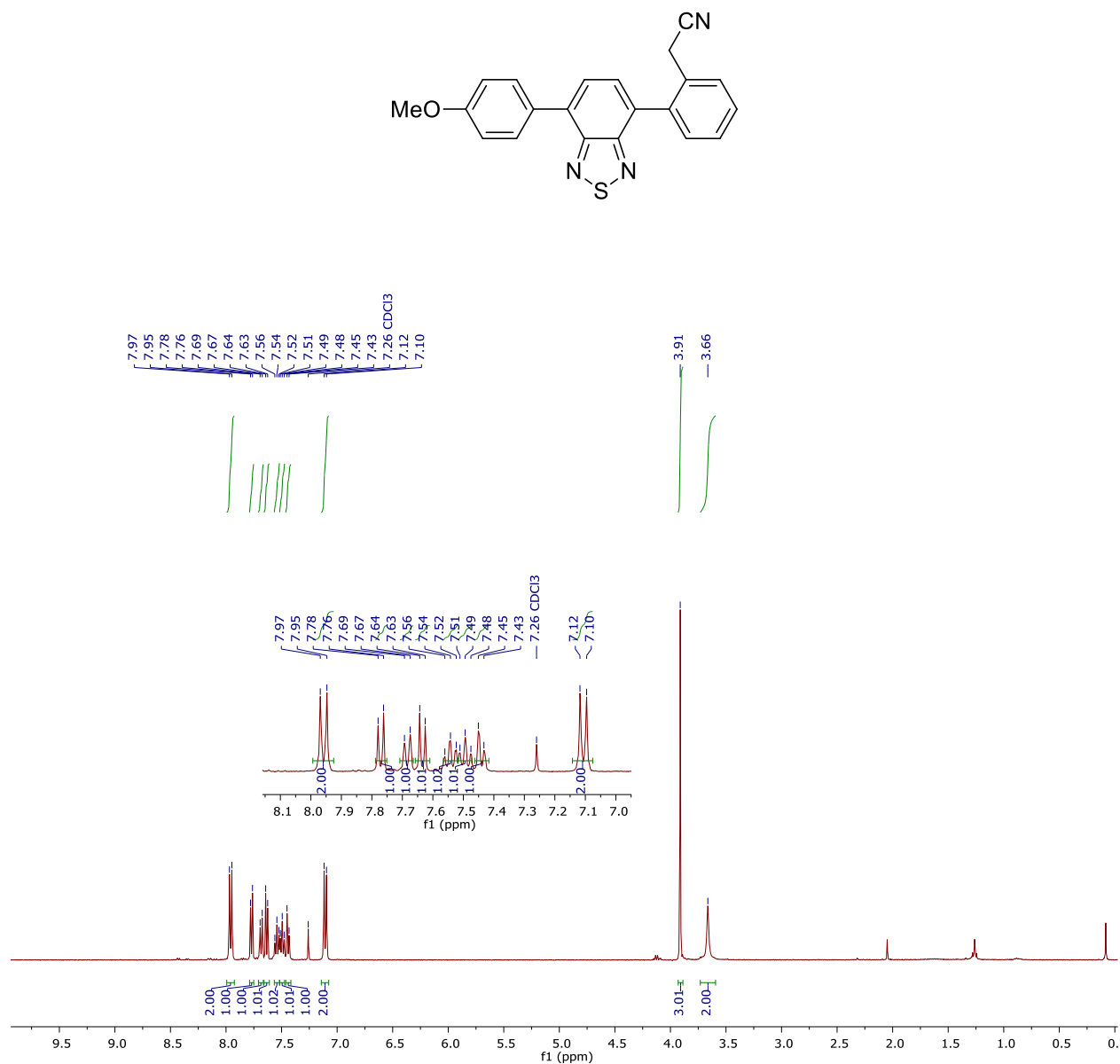


Figure S5. ^1H NMR (400 MHz, chloroform-d) spectrum of compound **3b**

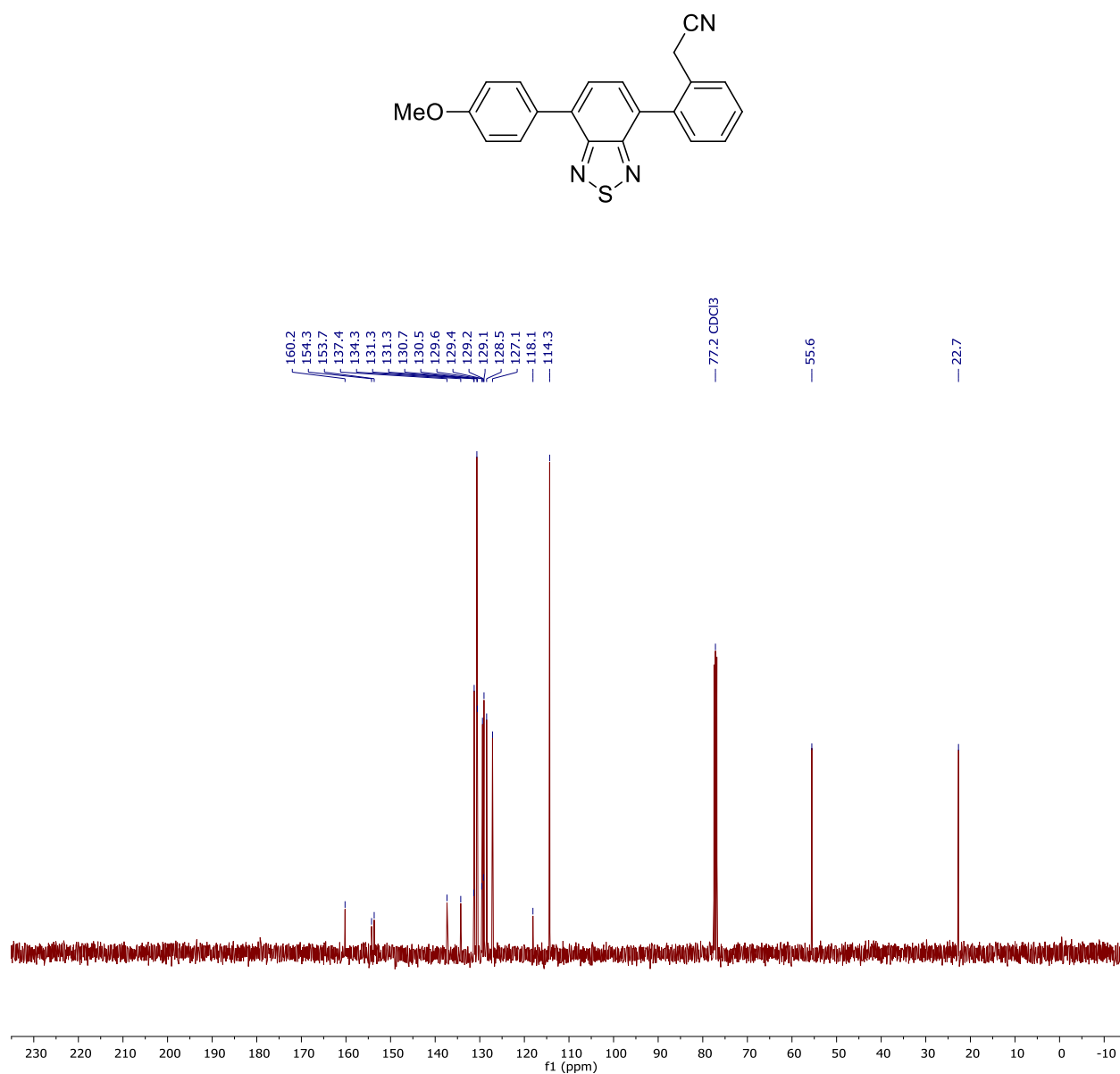


Figure S6. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **3b**

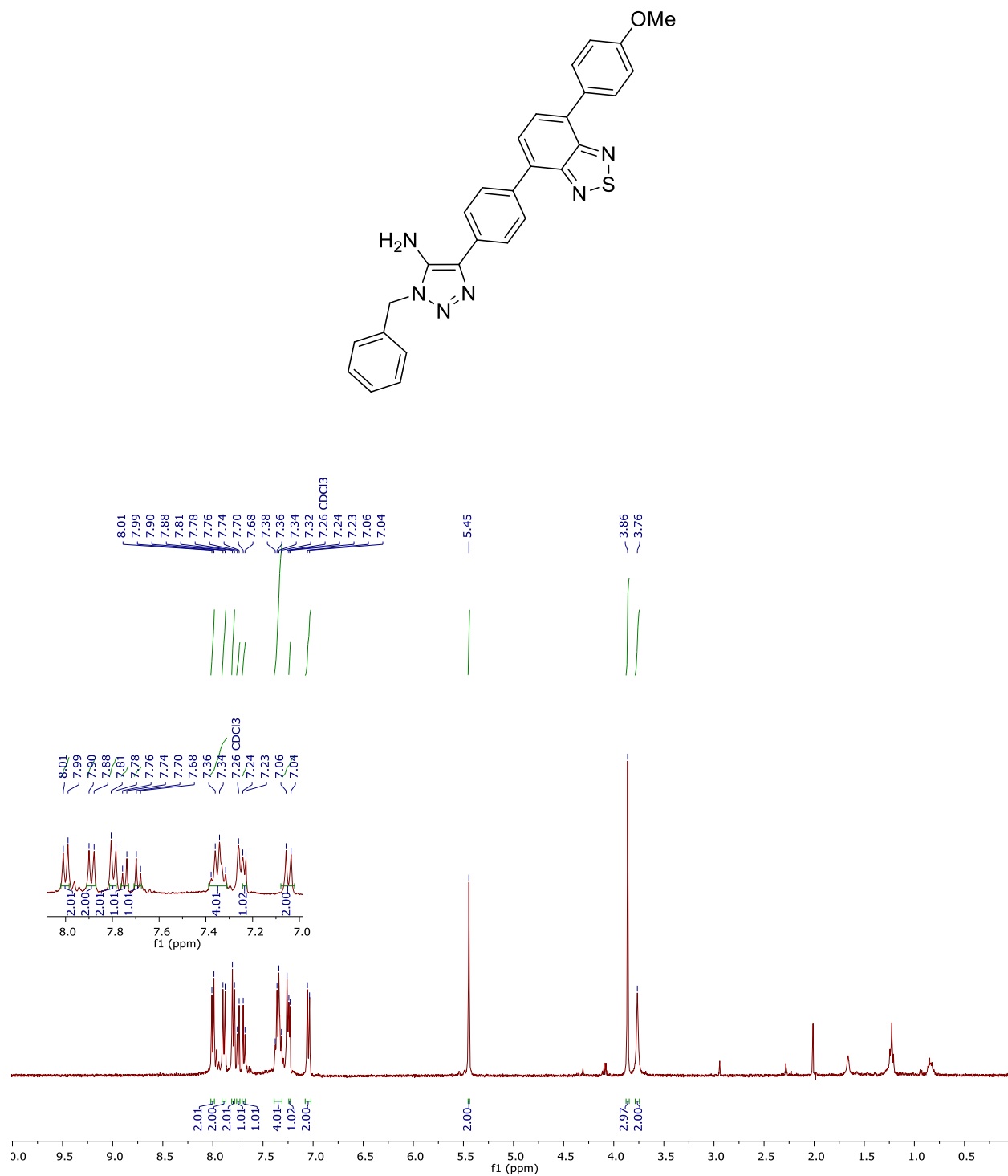


Figure S7. ^1H NMR (400 MHz, chloroform-d) spectrum of compound **4a**

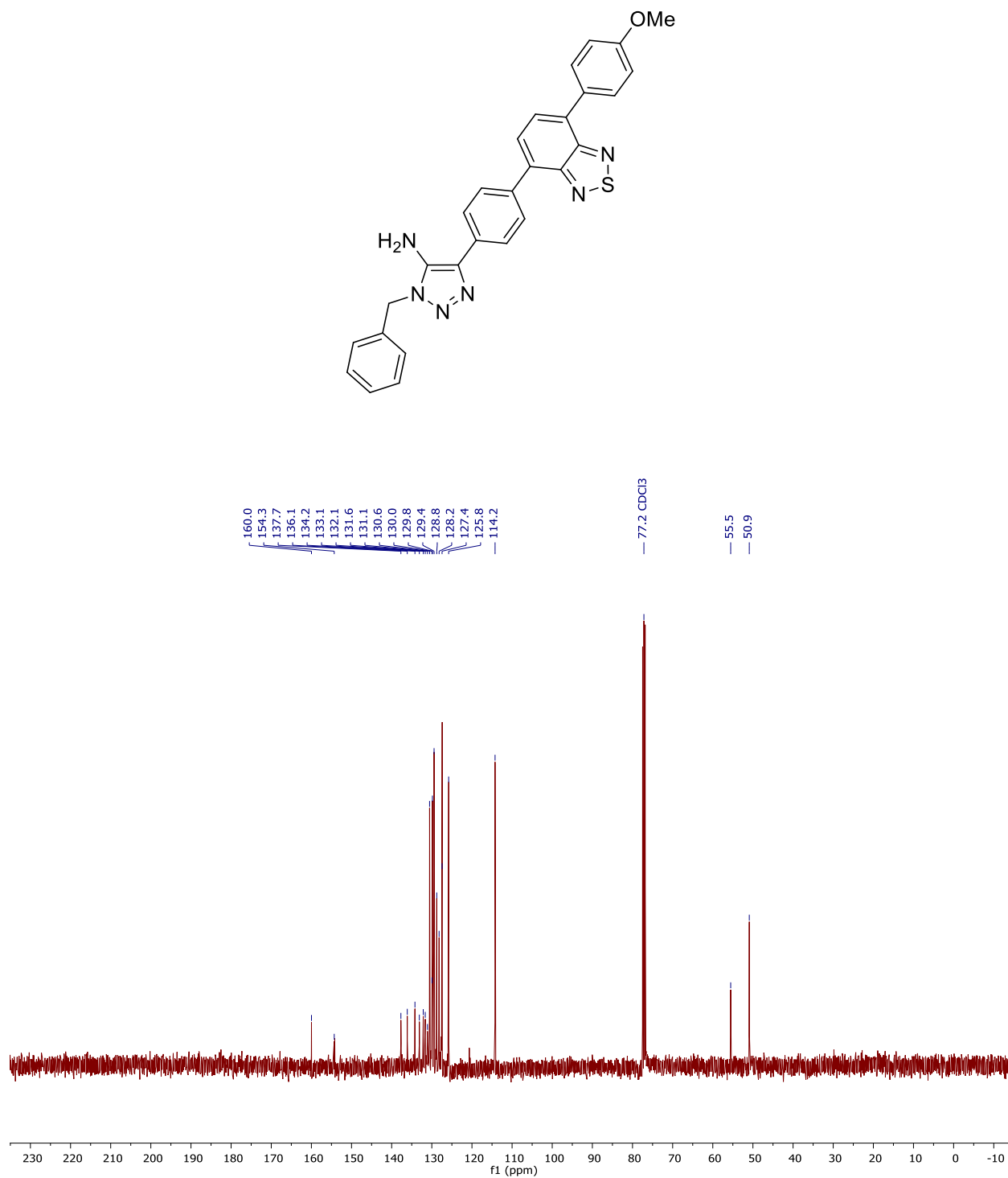


Figure S8. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **4a**

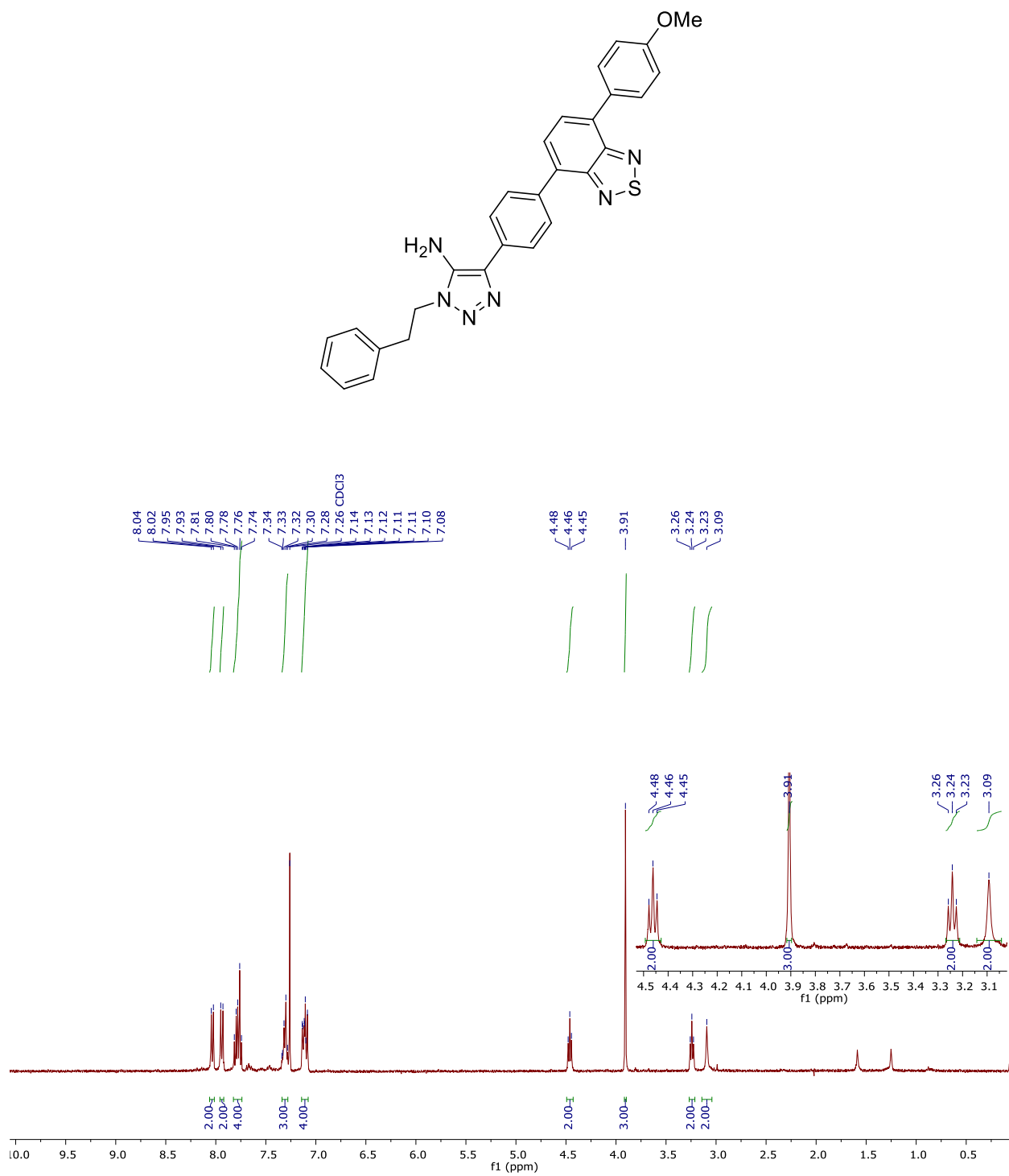


Figure S9. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4b**

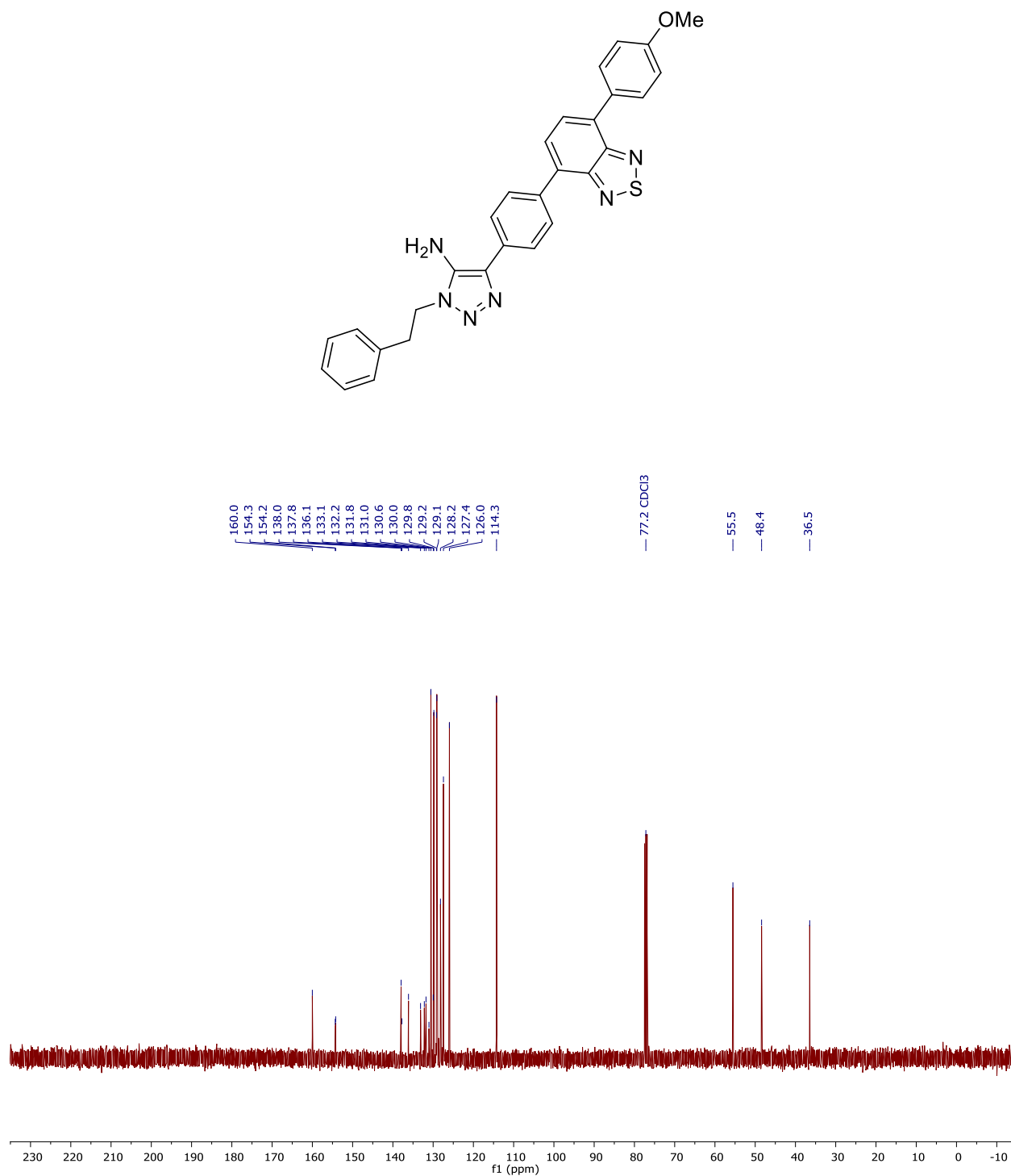


Figure S10. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **4b**

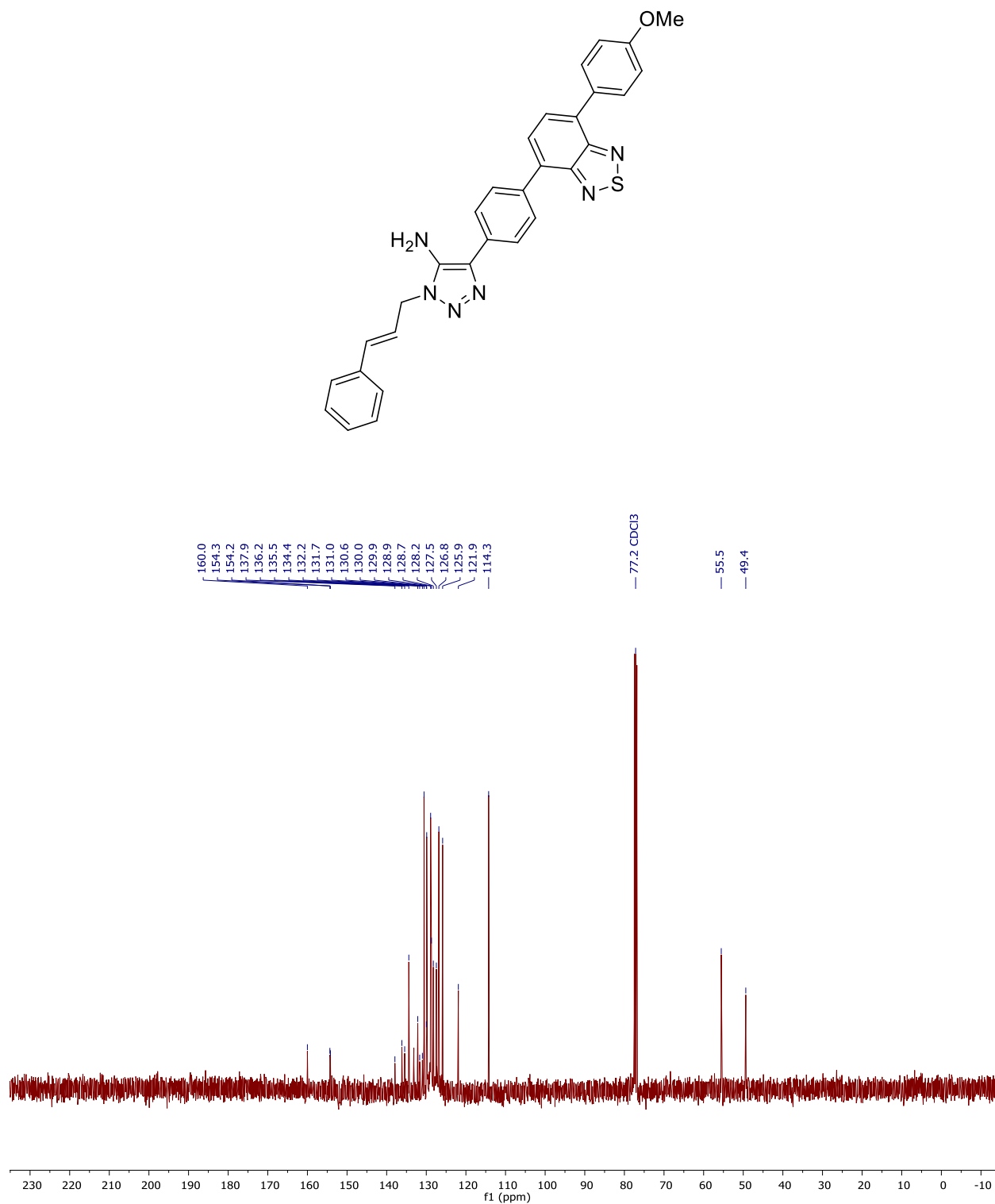


Figure S12. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **4c**

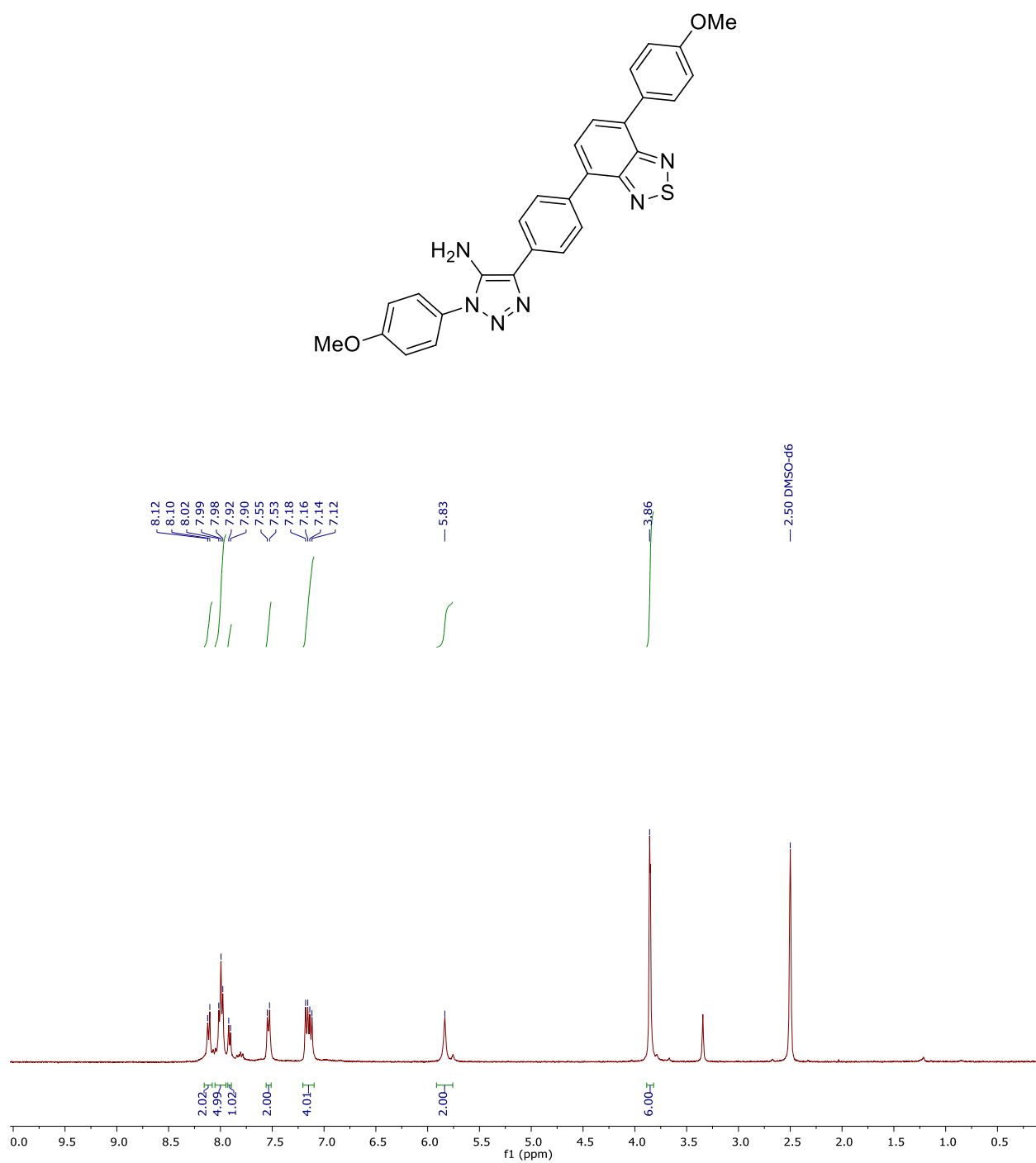


Figure S13. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **4d**

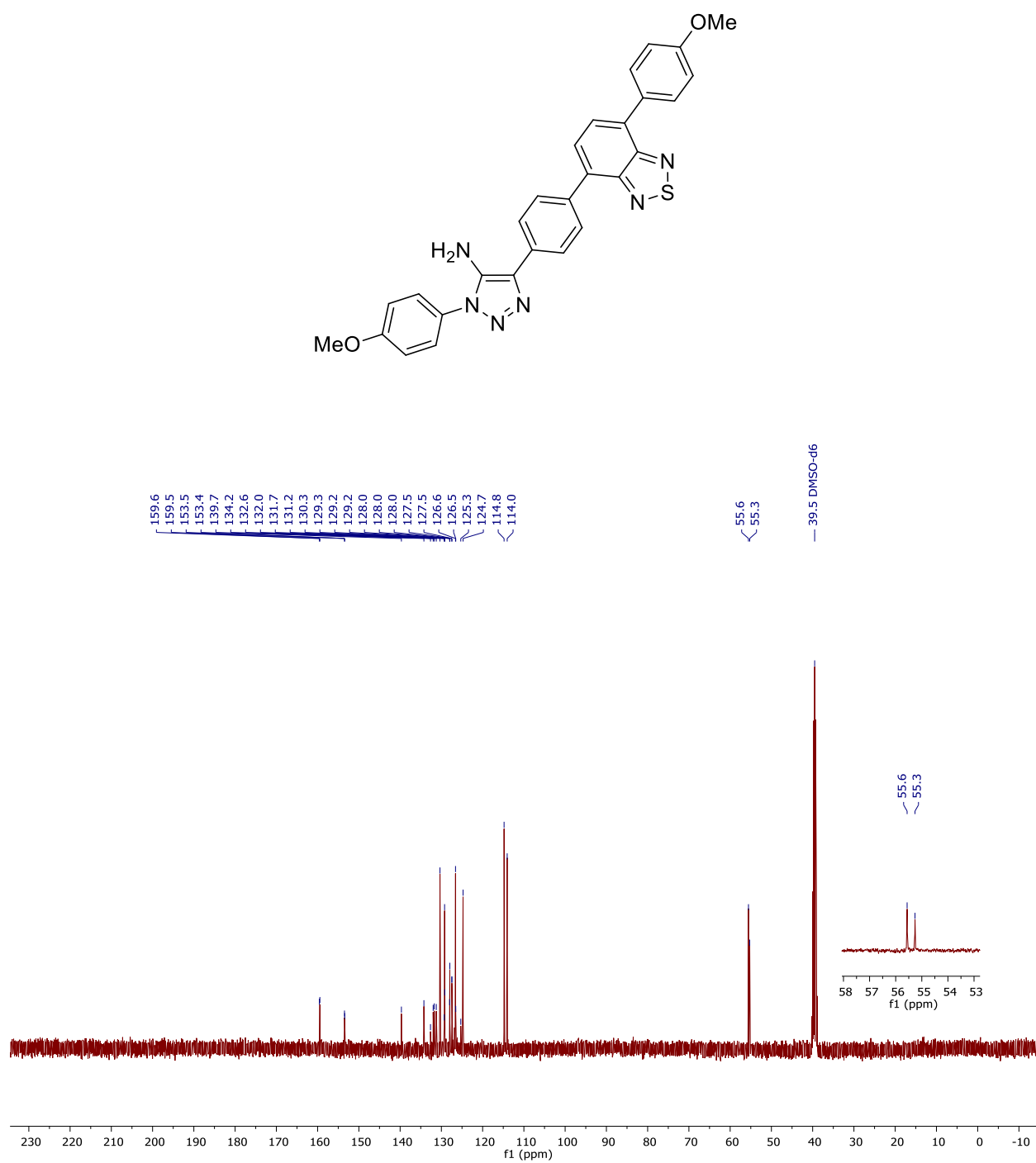


Figure S14. ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) spectrum of compound **4d**

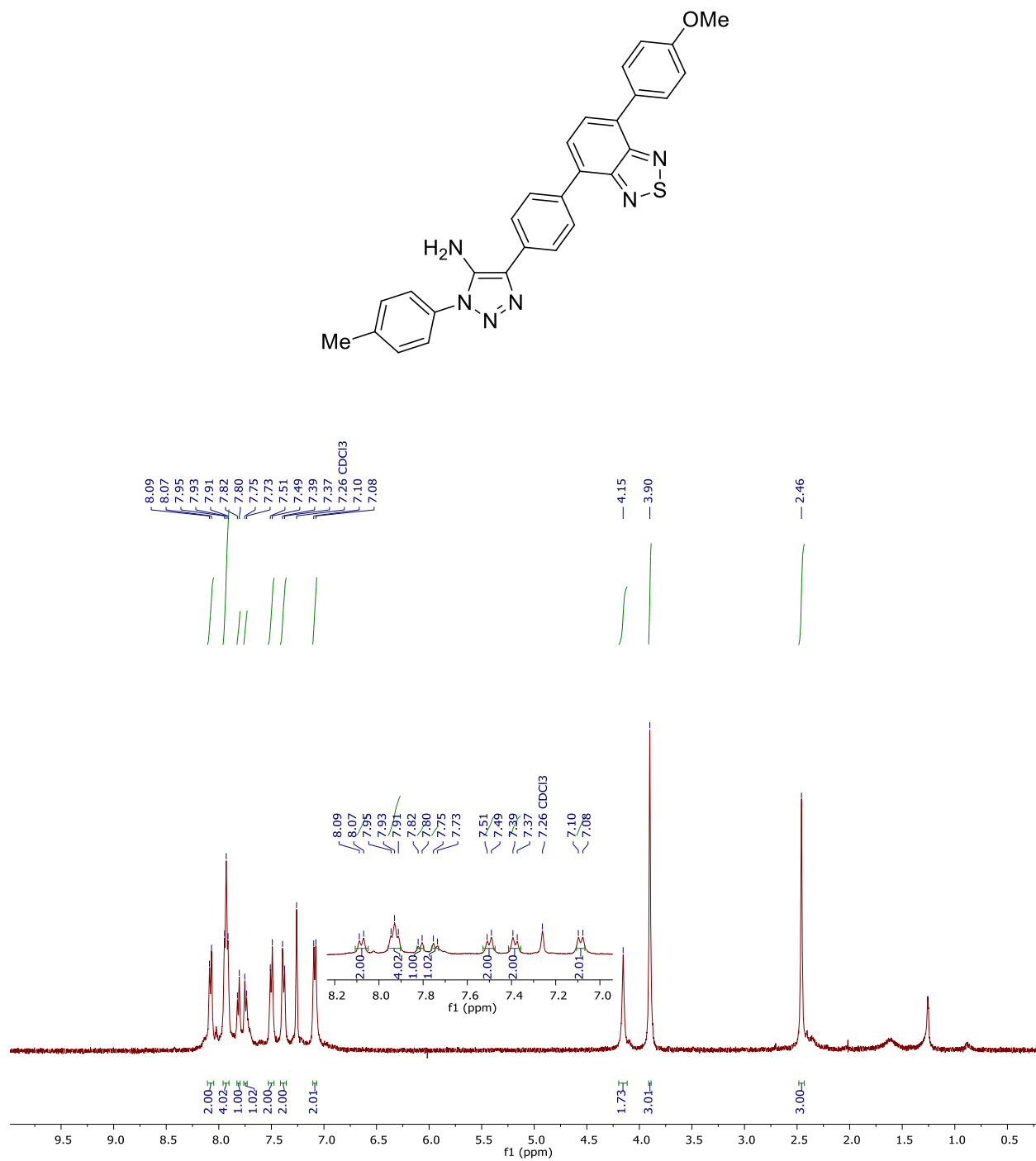


Figure S15. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **4e**

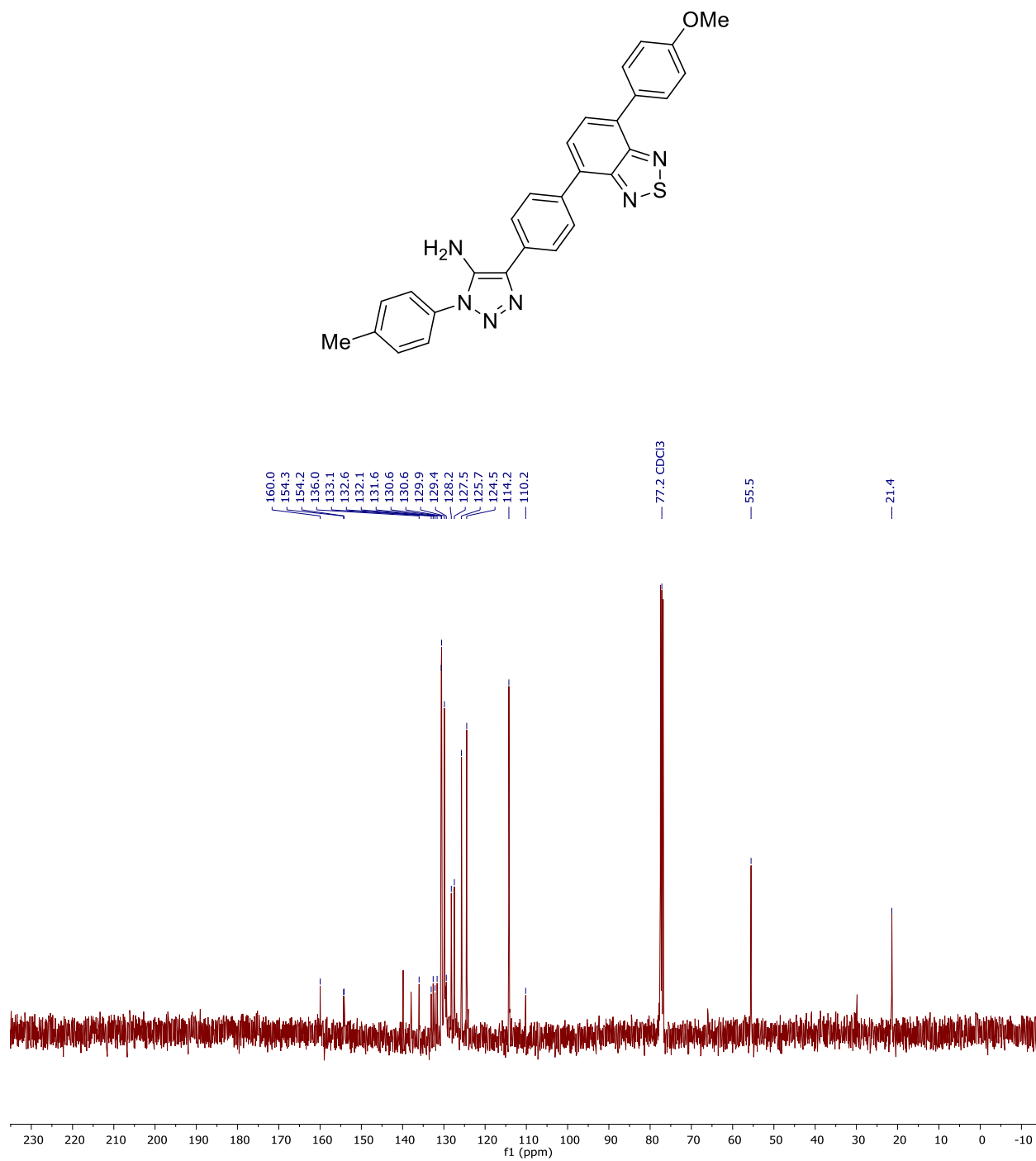


Figure S16. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **4e**

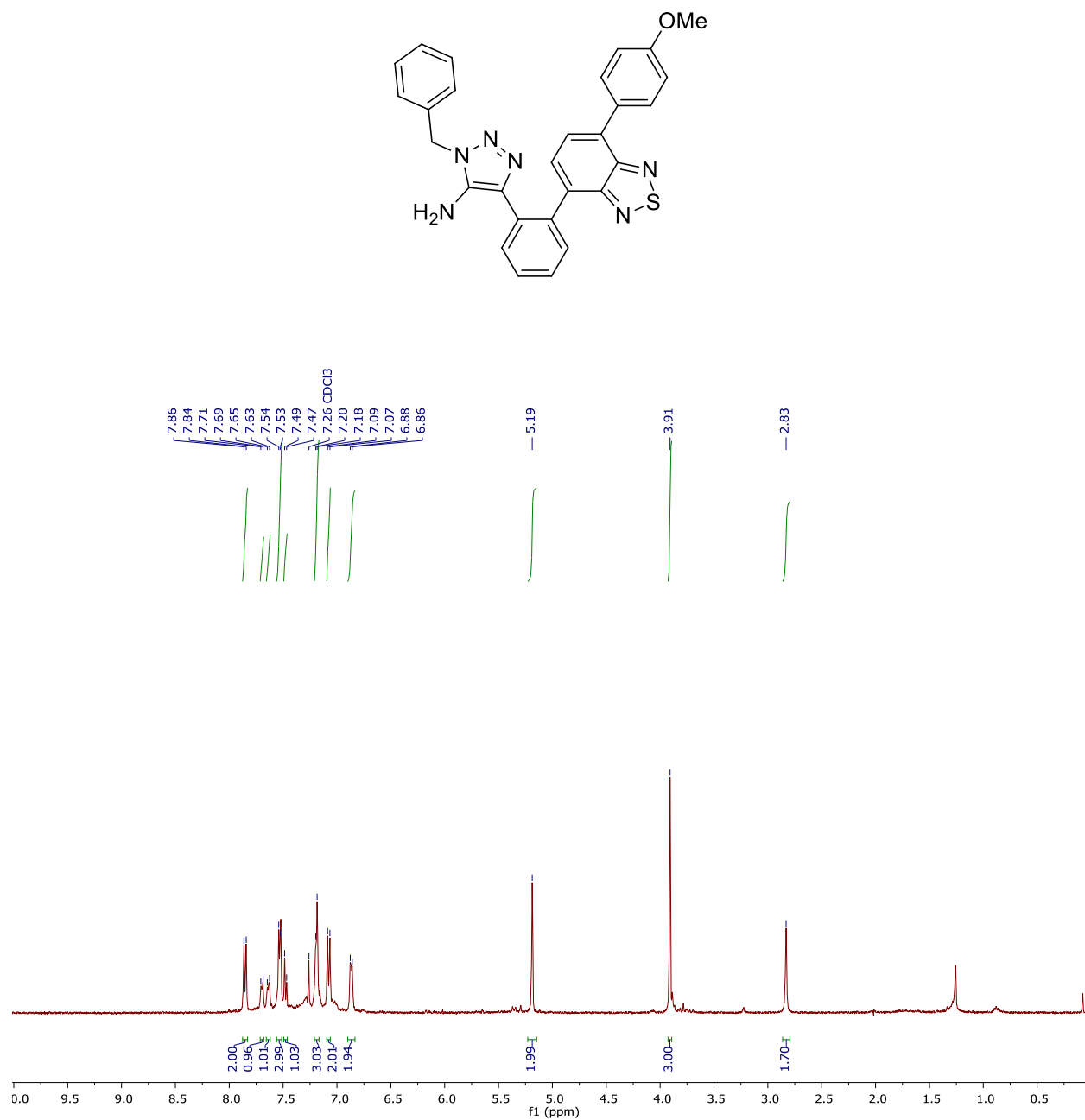


Figure S17. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **4f**

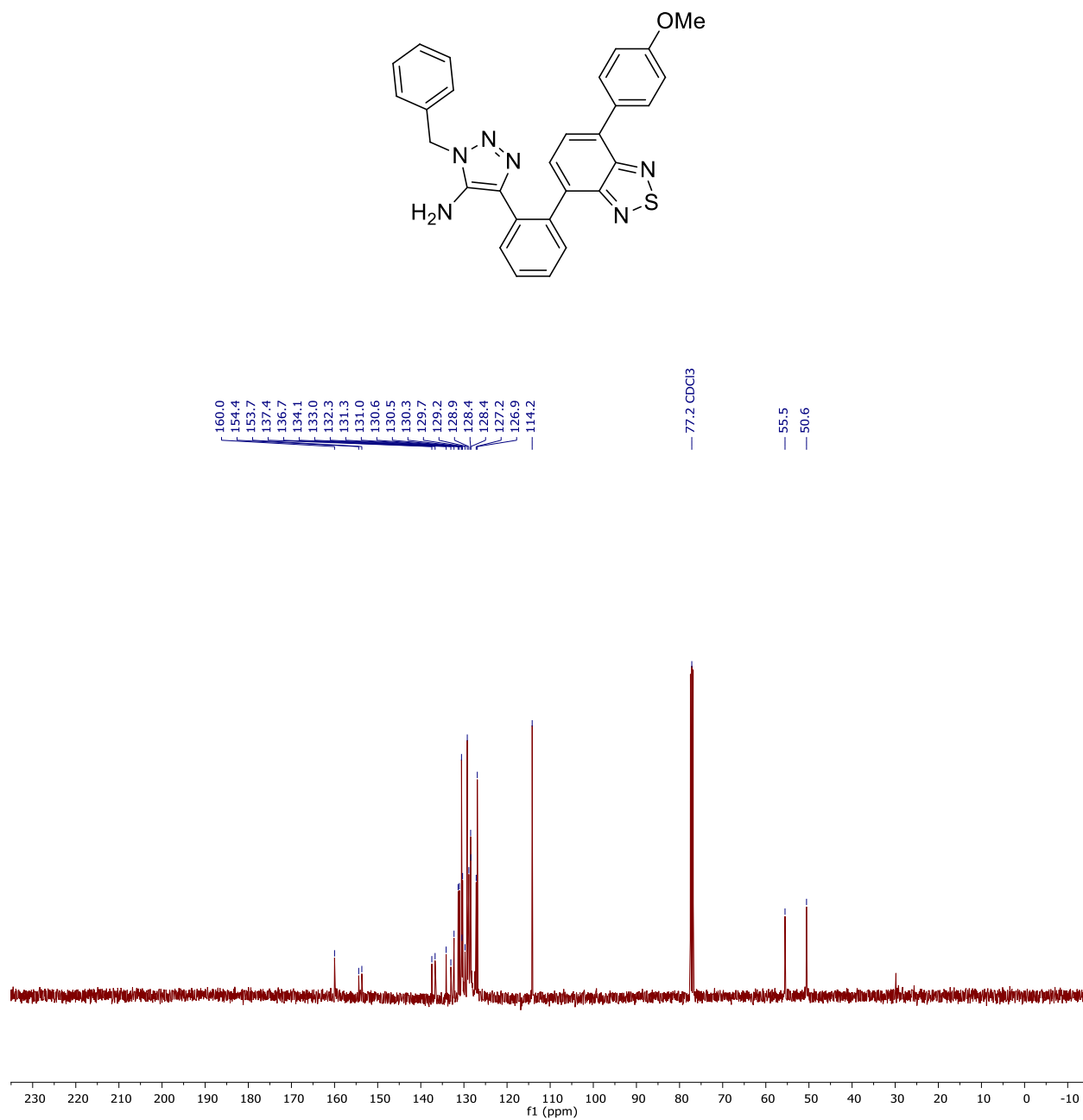


Figure S18. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **4f**

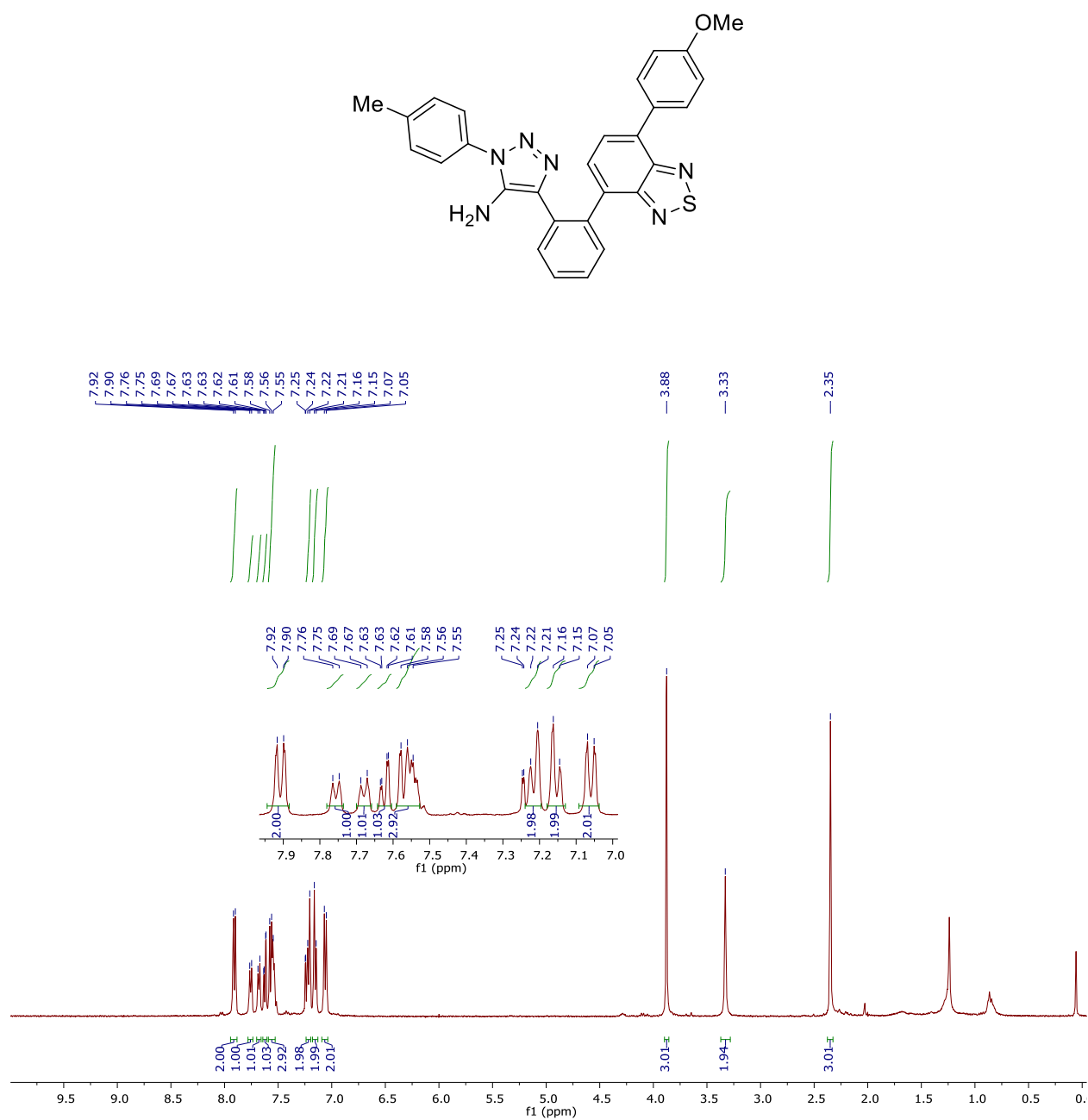


Figure S19. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4g**

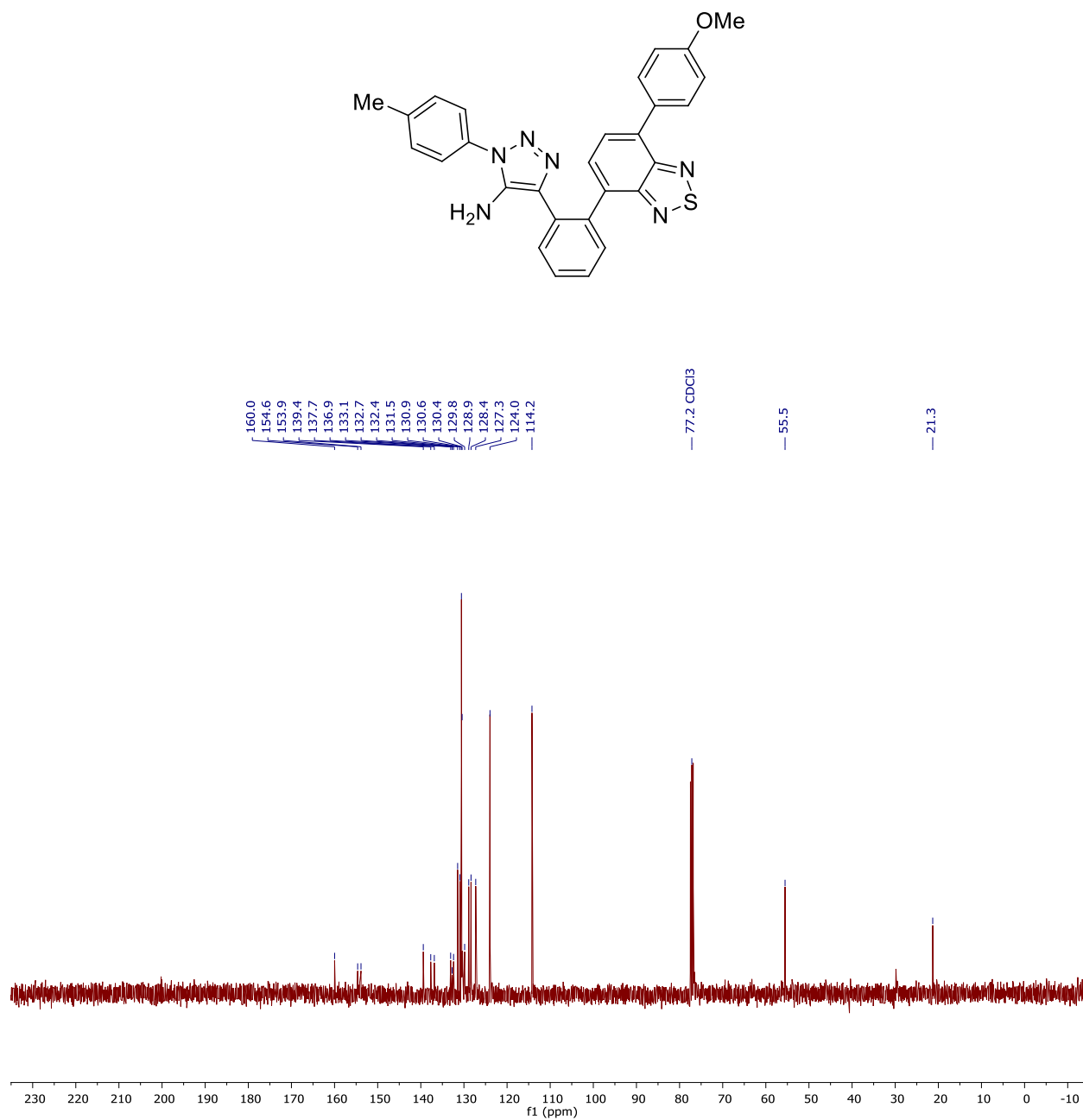


Figure S20. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **4g**

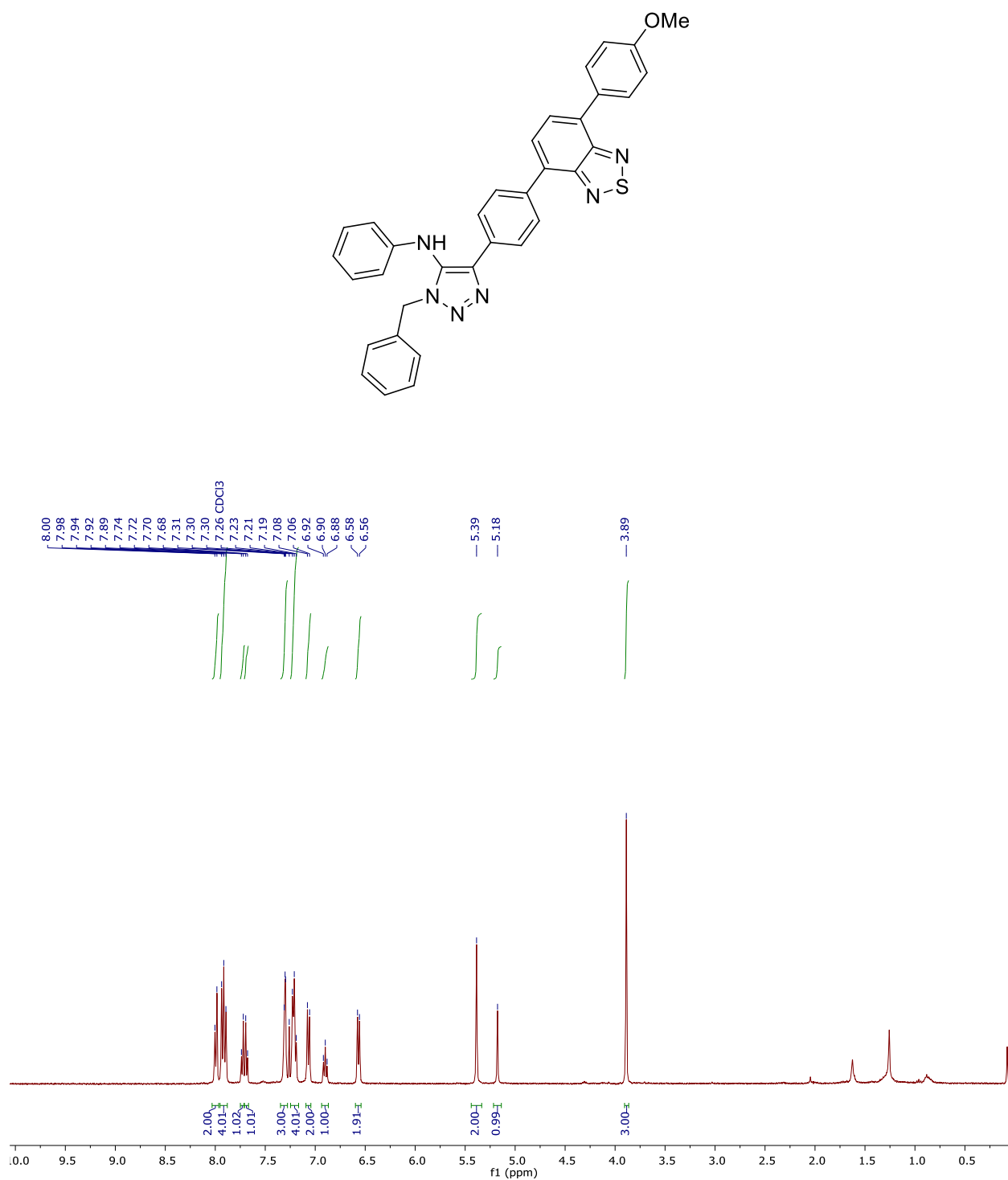


Figure S21. ¹H NMR (400 MHz, chloroform-*d*) spectrum of compound **5a**

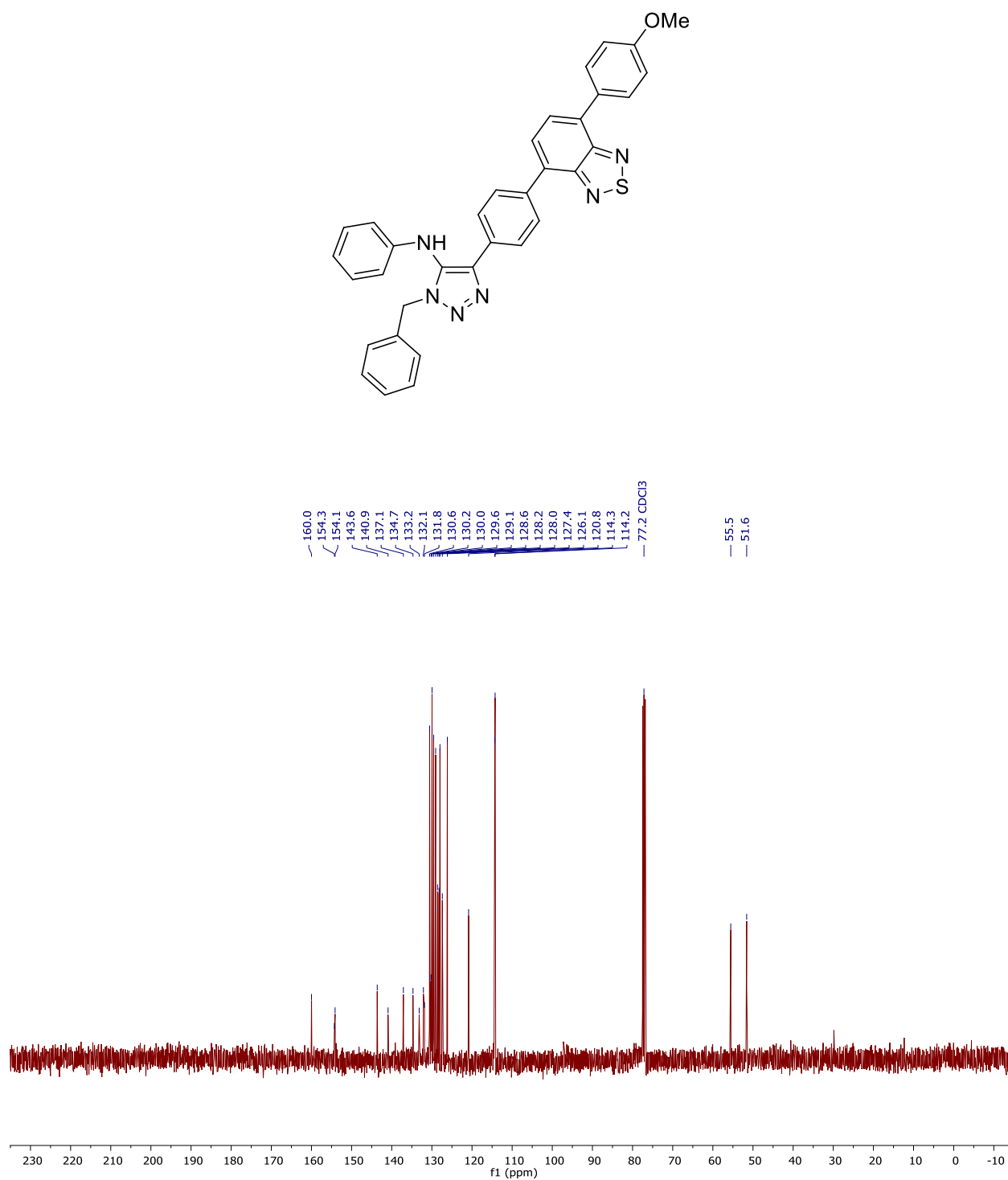


Figure S22. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **5a**

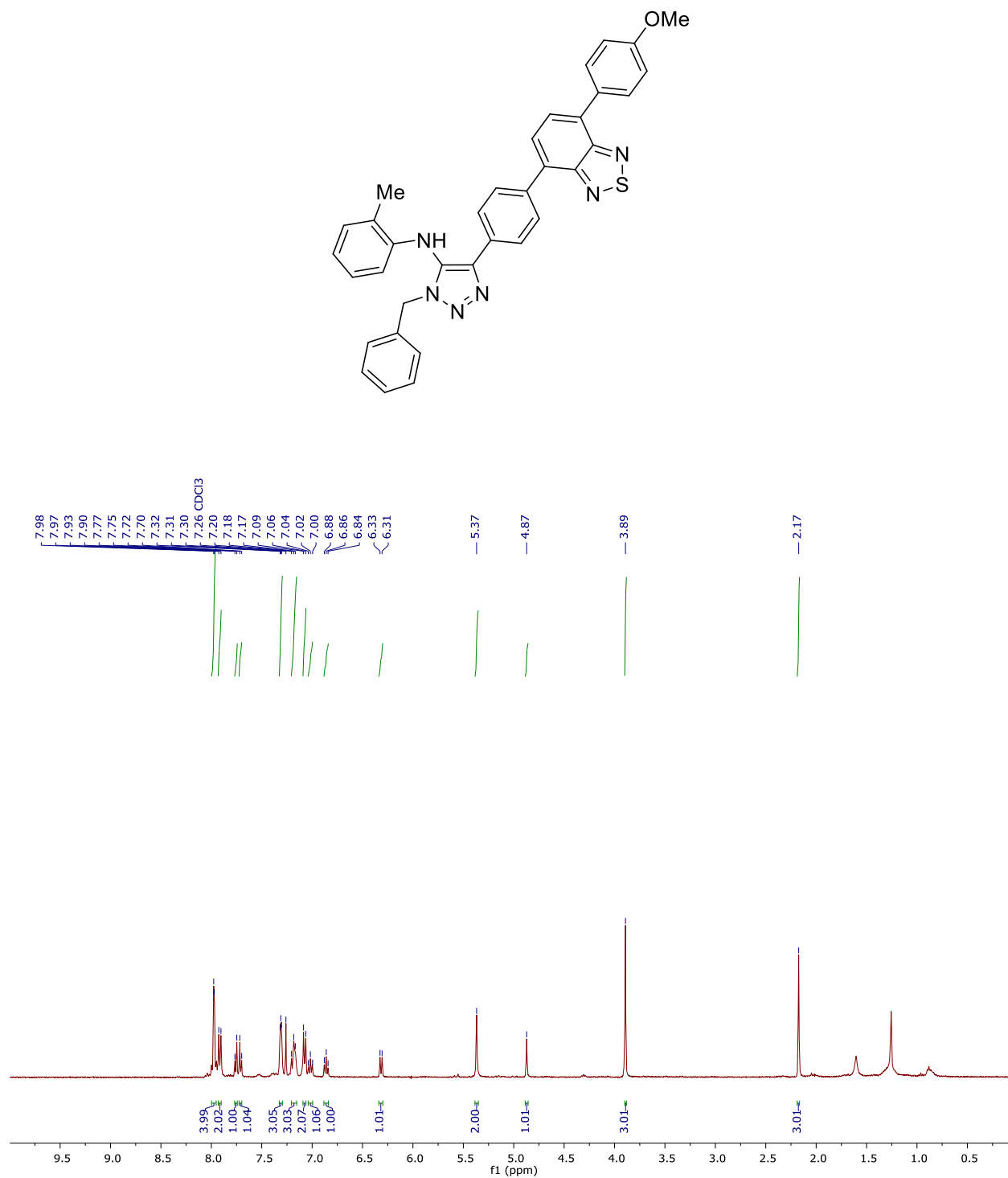


Figure S23. ¹H NMR (400 MHz, chloroform-*d*) spectrum of compound **5b**

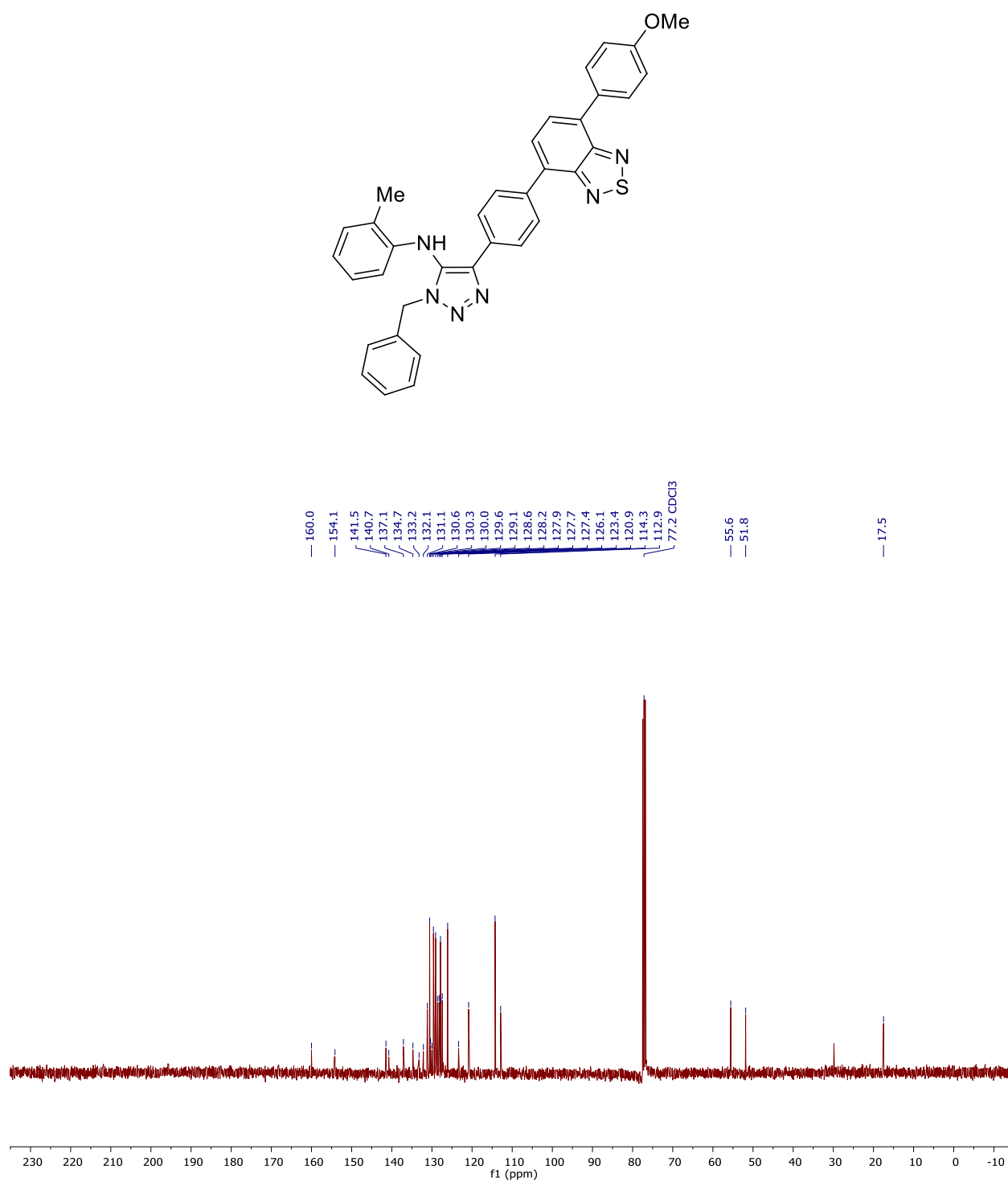


Figure S24. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **5b**

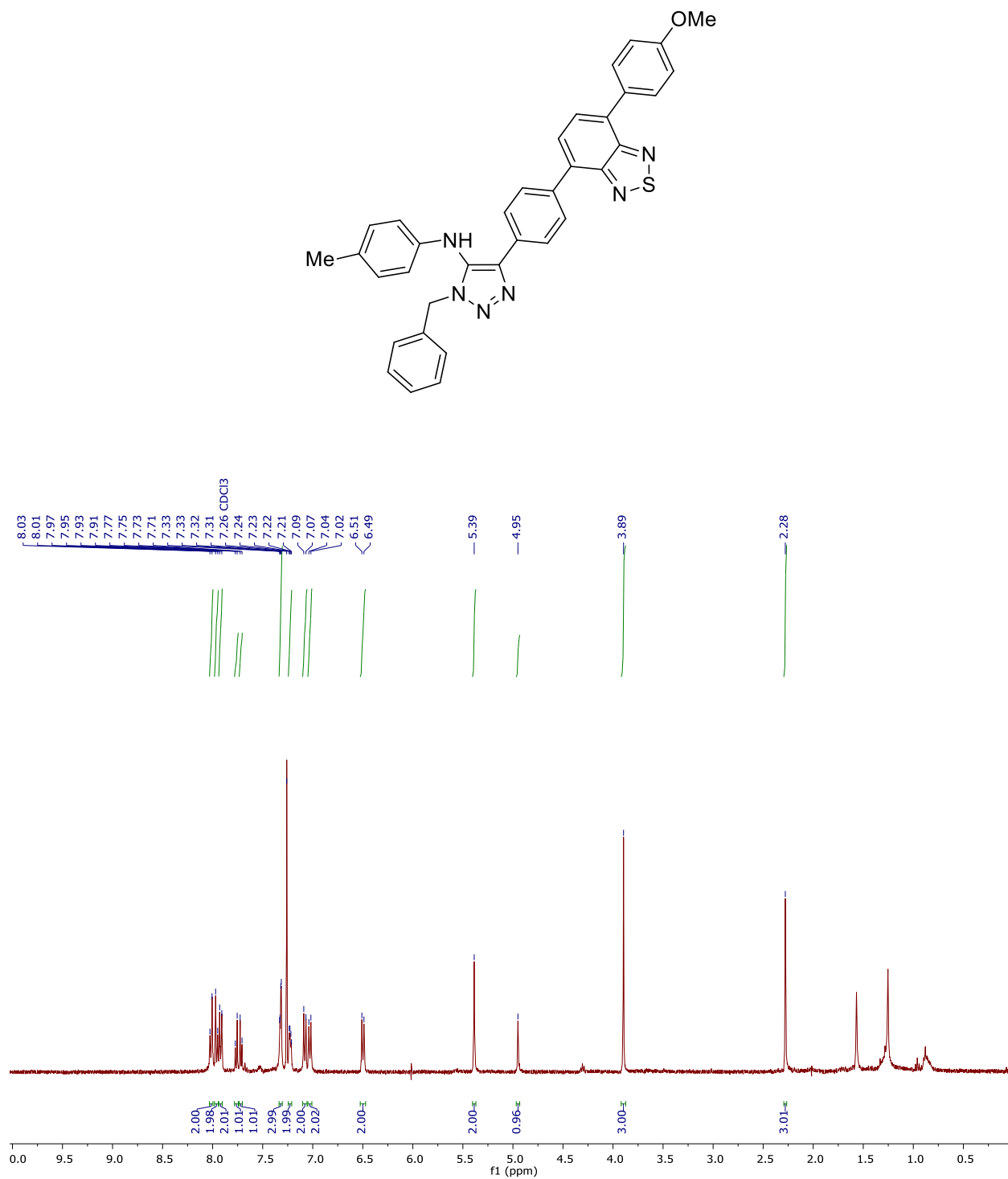


Figure S25. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **5c**

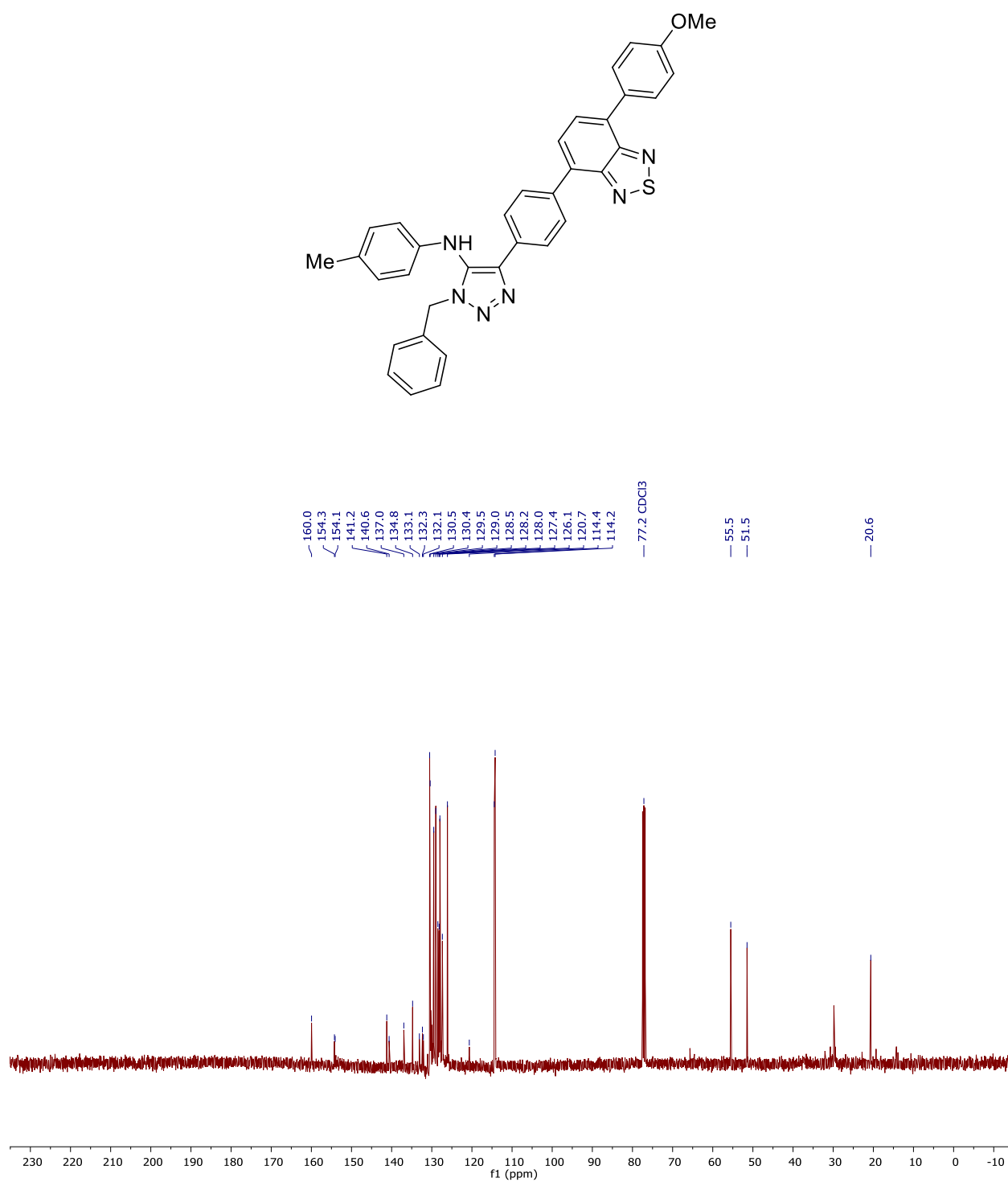


Figure S26. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **5c**

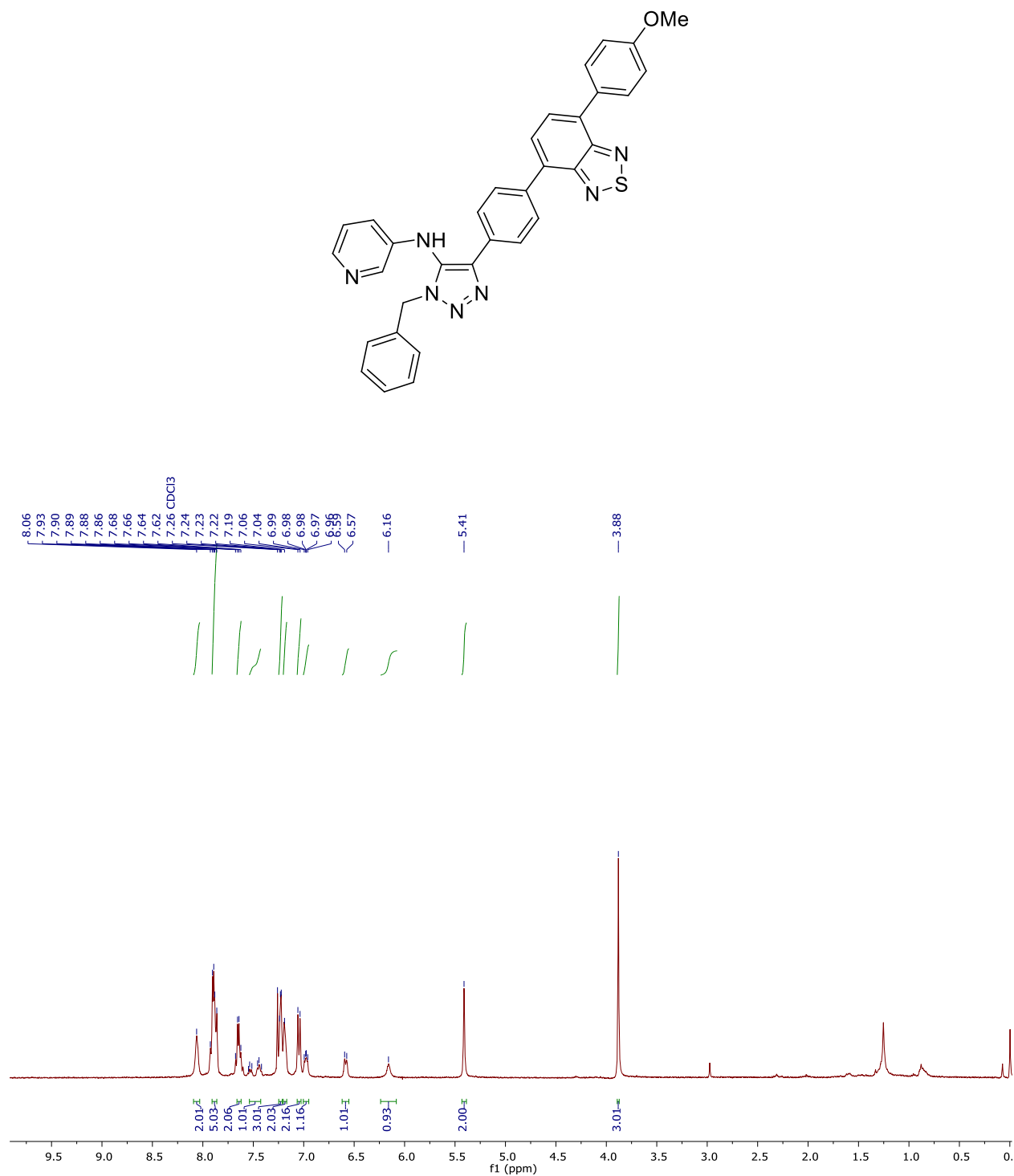


Figure S27. ¹H NMR (400 MHz, chloroform-*d*) spectrum of compound **5d**

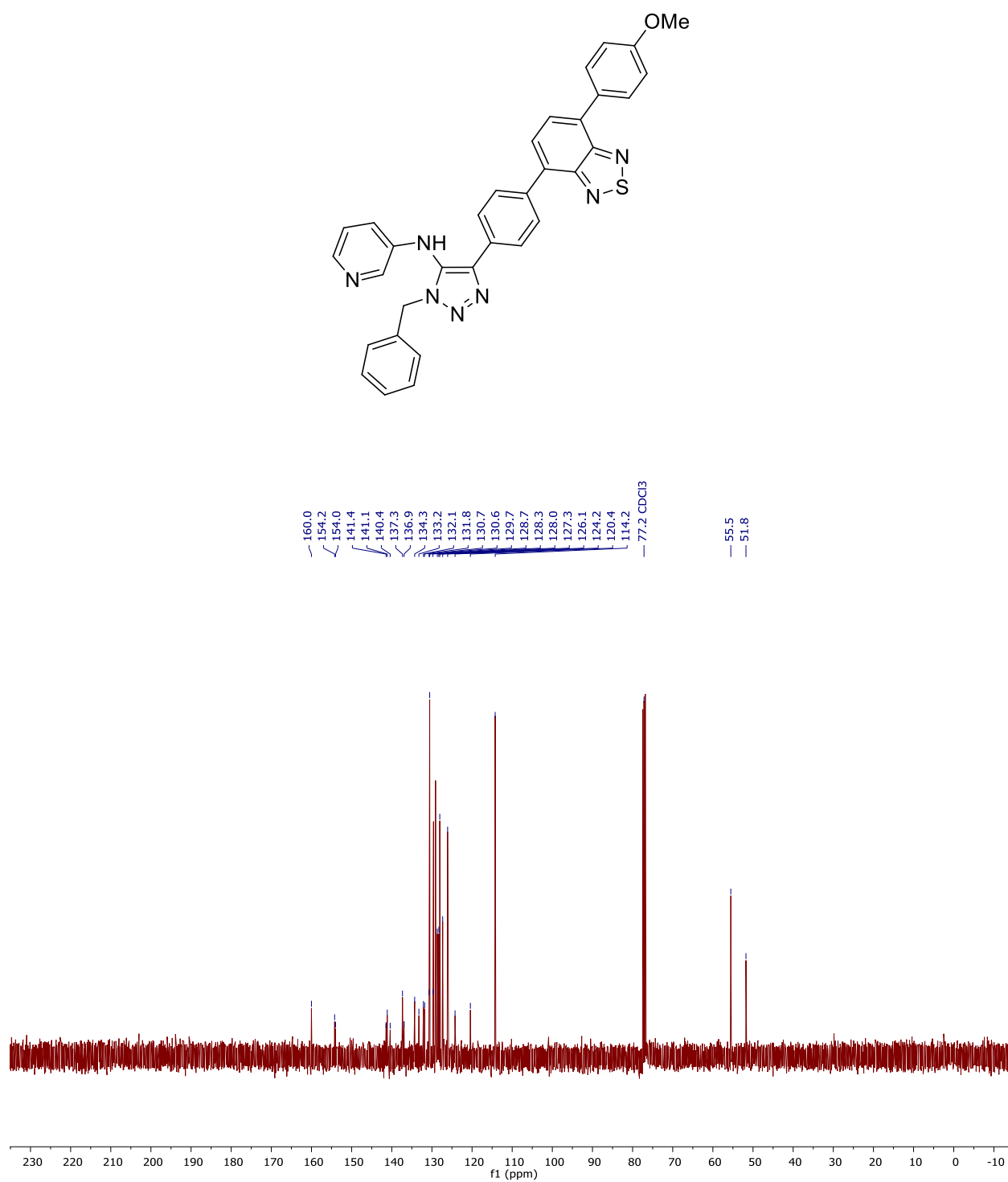


Figure S28. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **5d**

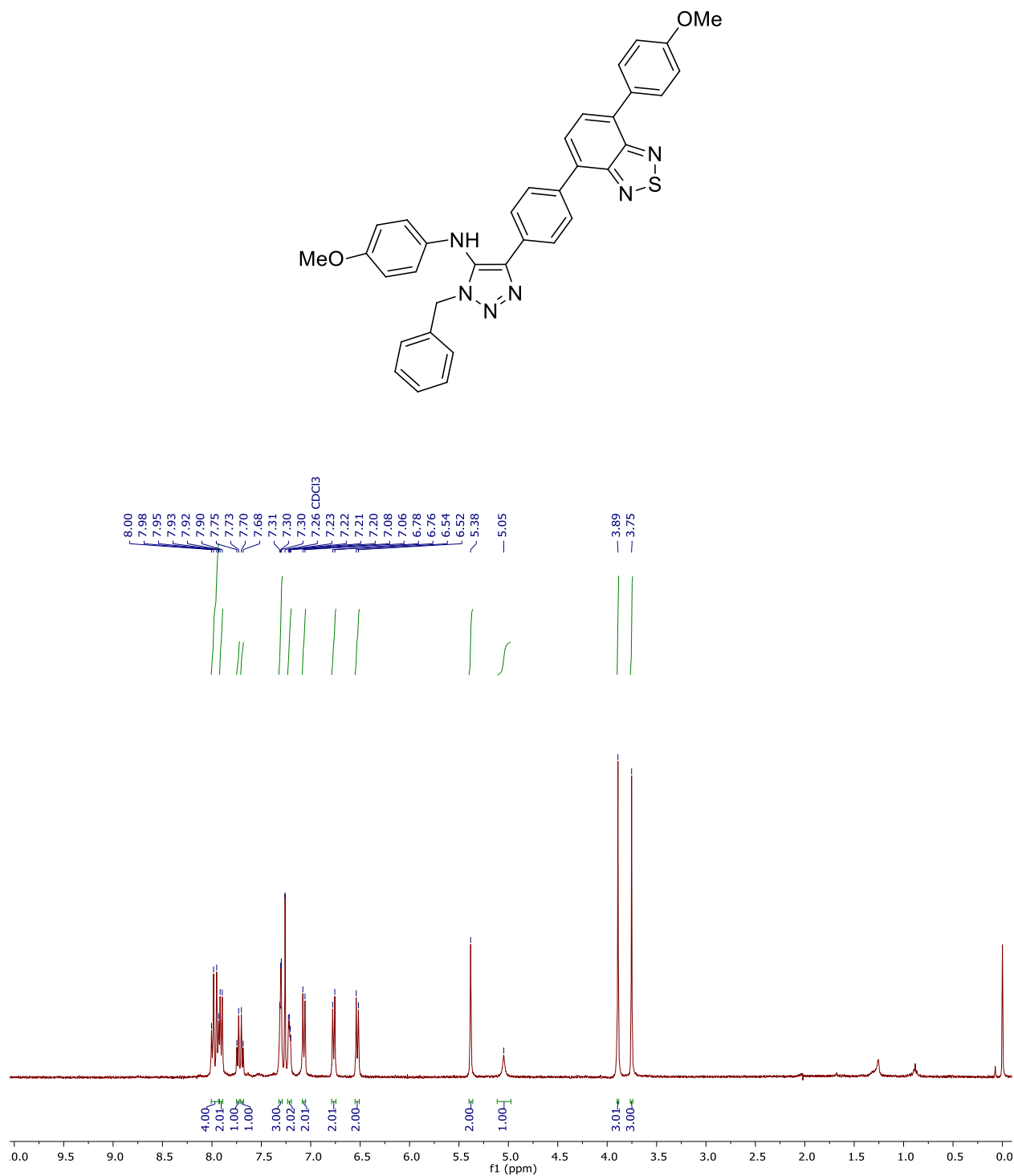


Figure S29. ^1H NMR (400 MHz, chloroform-d) spectrum of compound **5e**

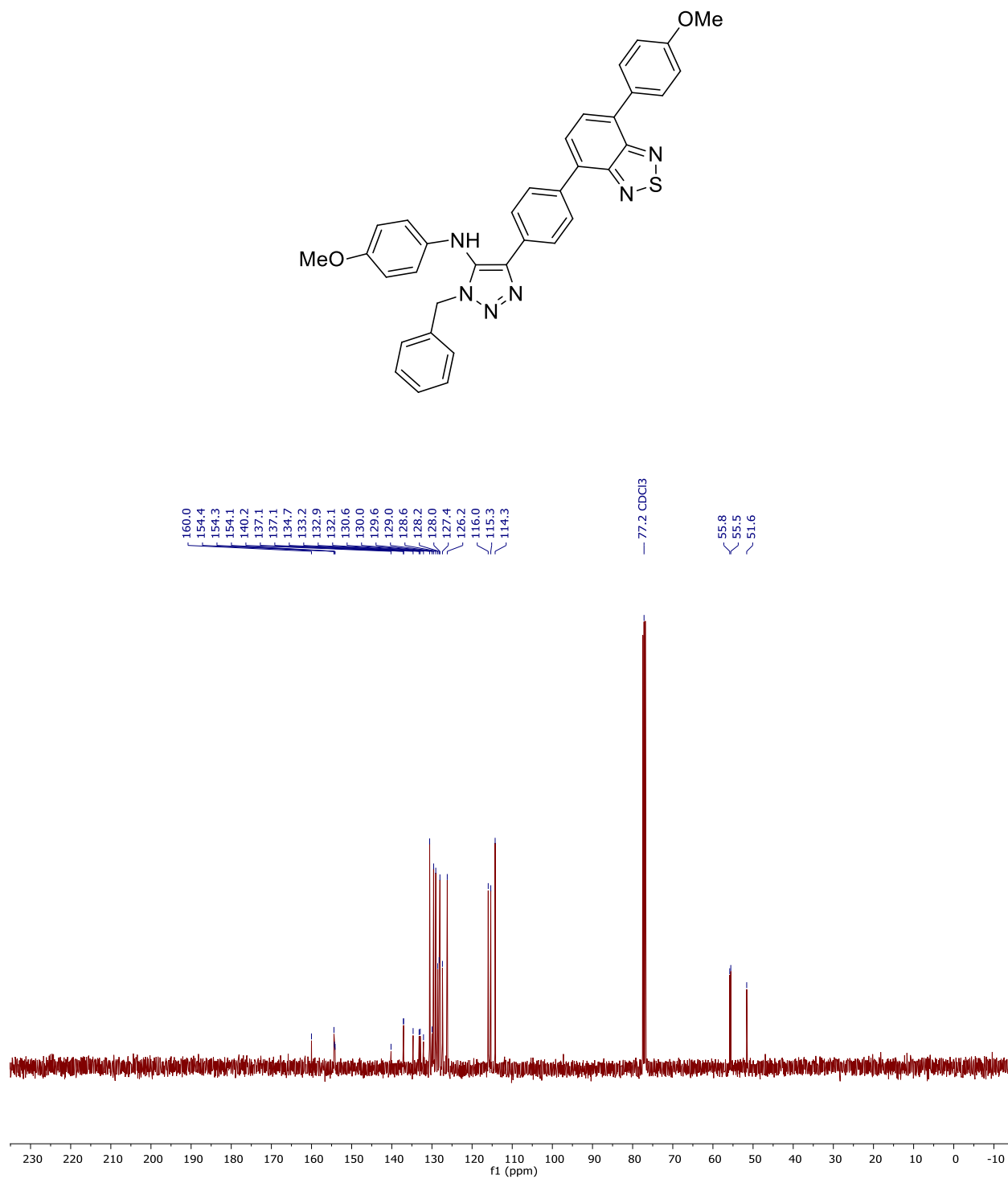


Figure S30. ^{13}C NMR (101 MHz, chloroform-d) spectrum of compound **5e**

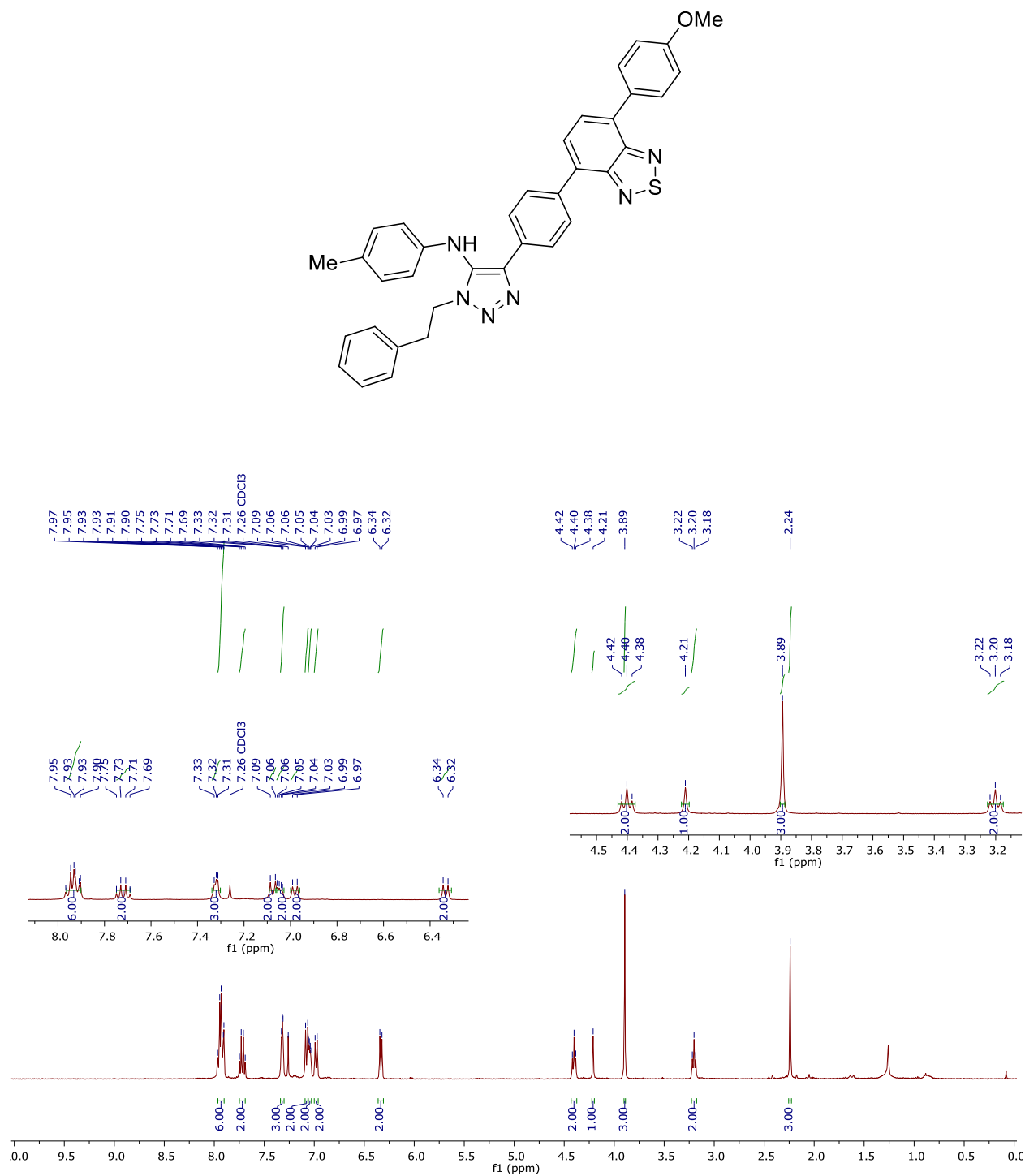


Figure S31. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **5f**

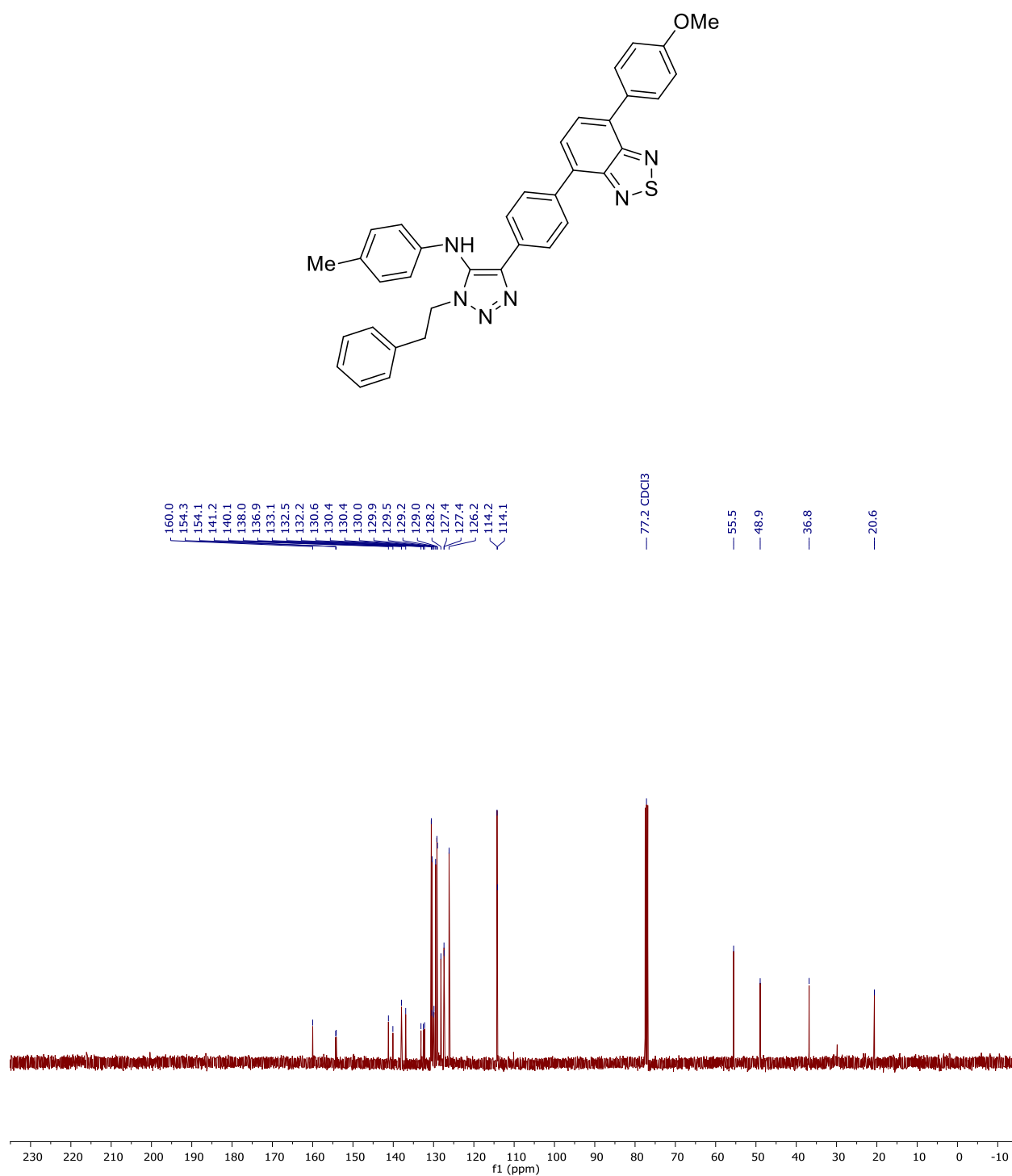


Figure S32. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **5f**

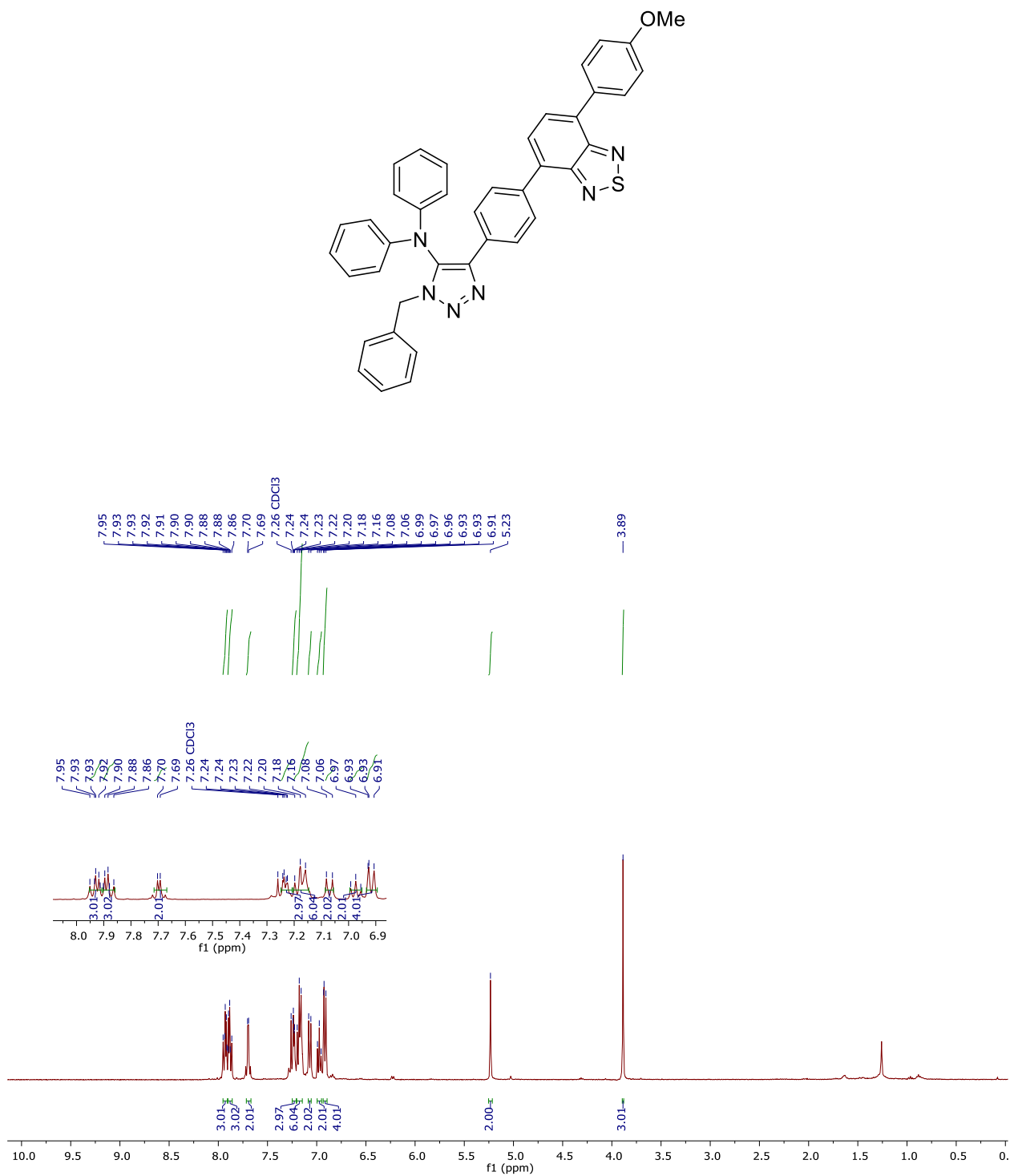


Figure S33. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **6a**

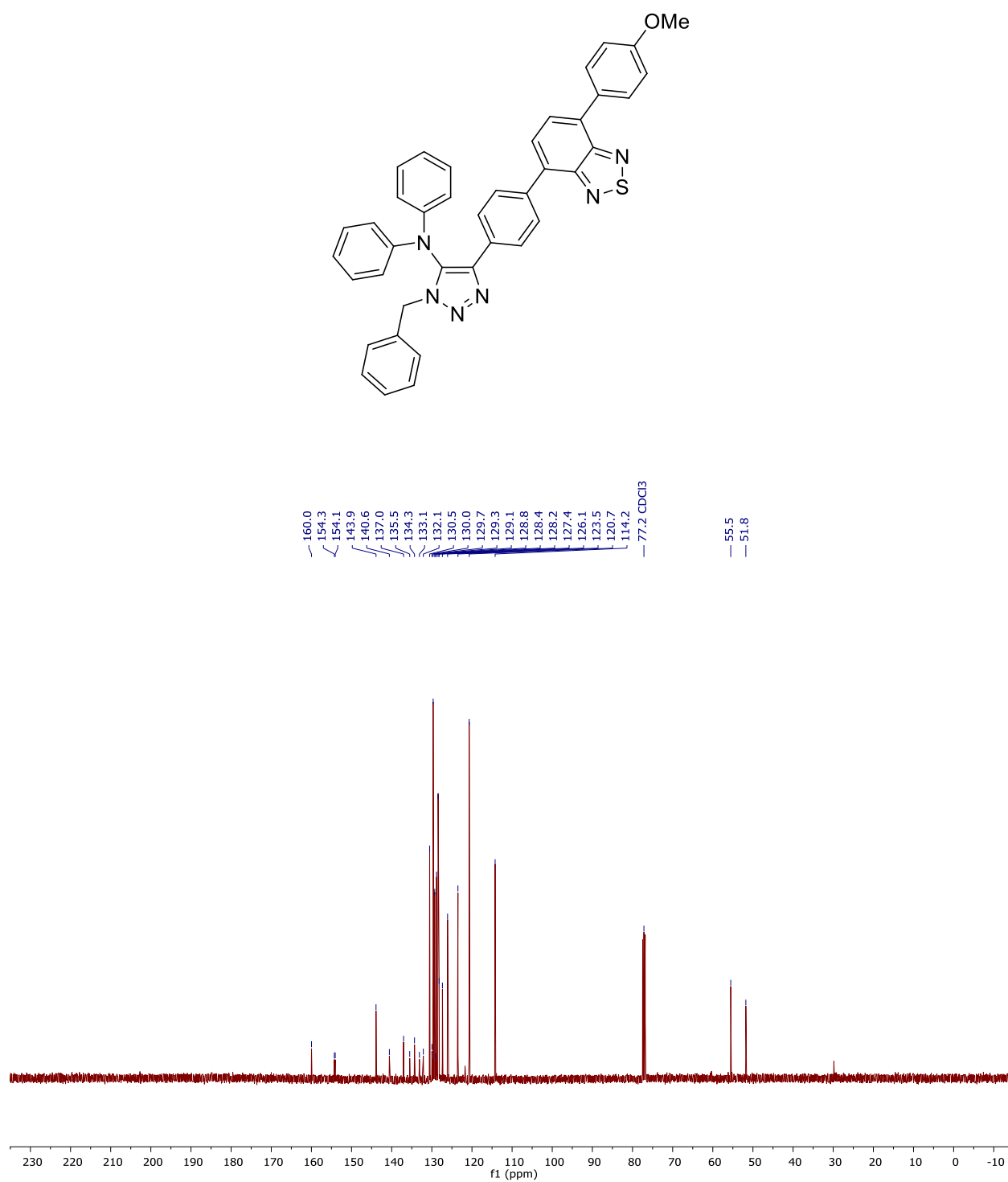


Figure S34. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6a**

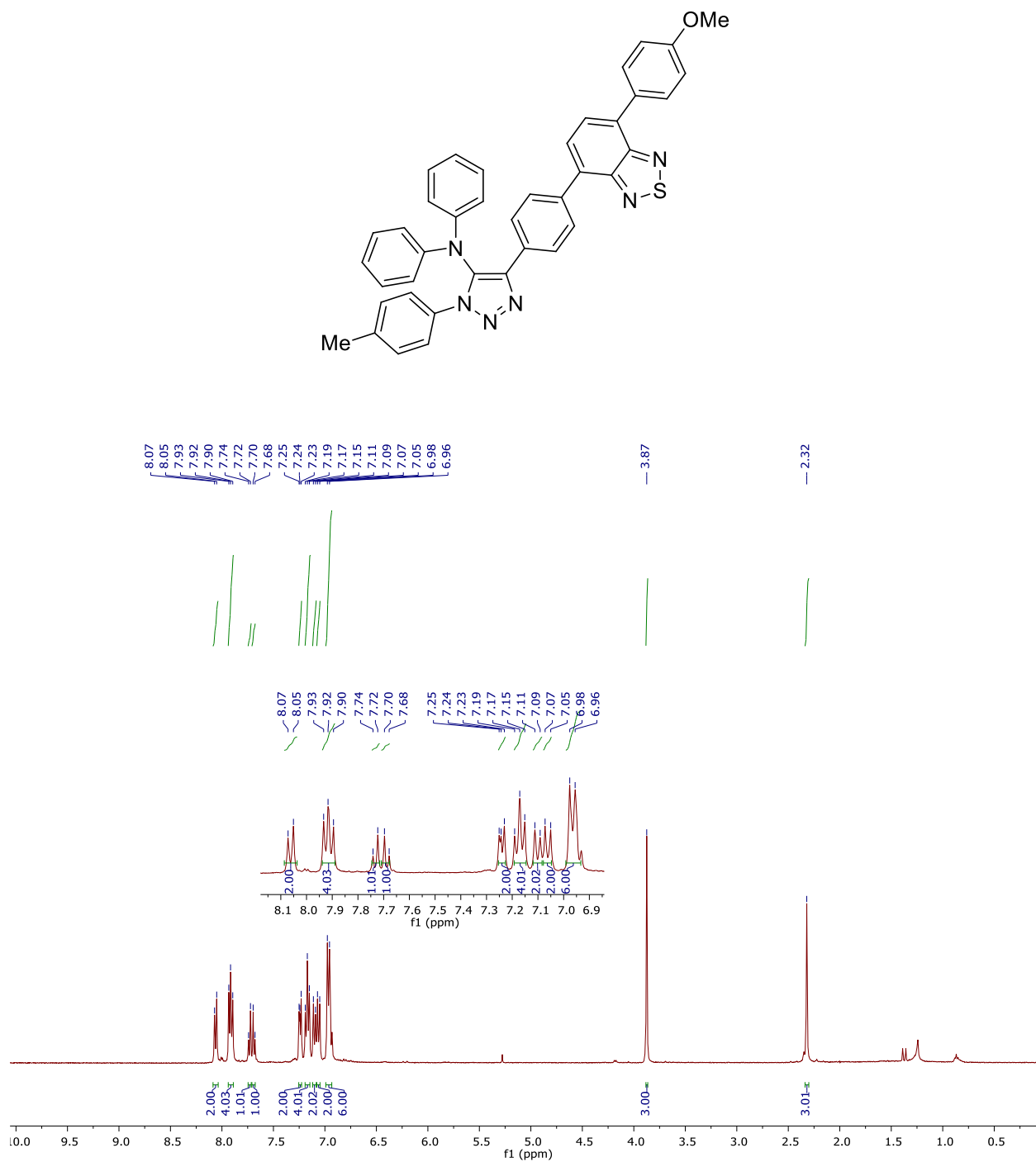


Figure S35. ¹H NMR (400 MHz, chloroform-*d*) spectrum of compound **6b**

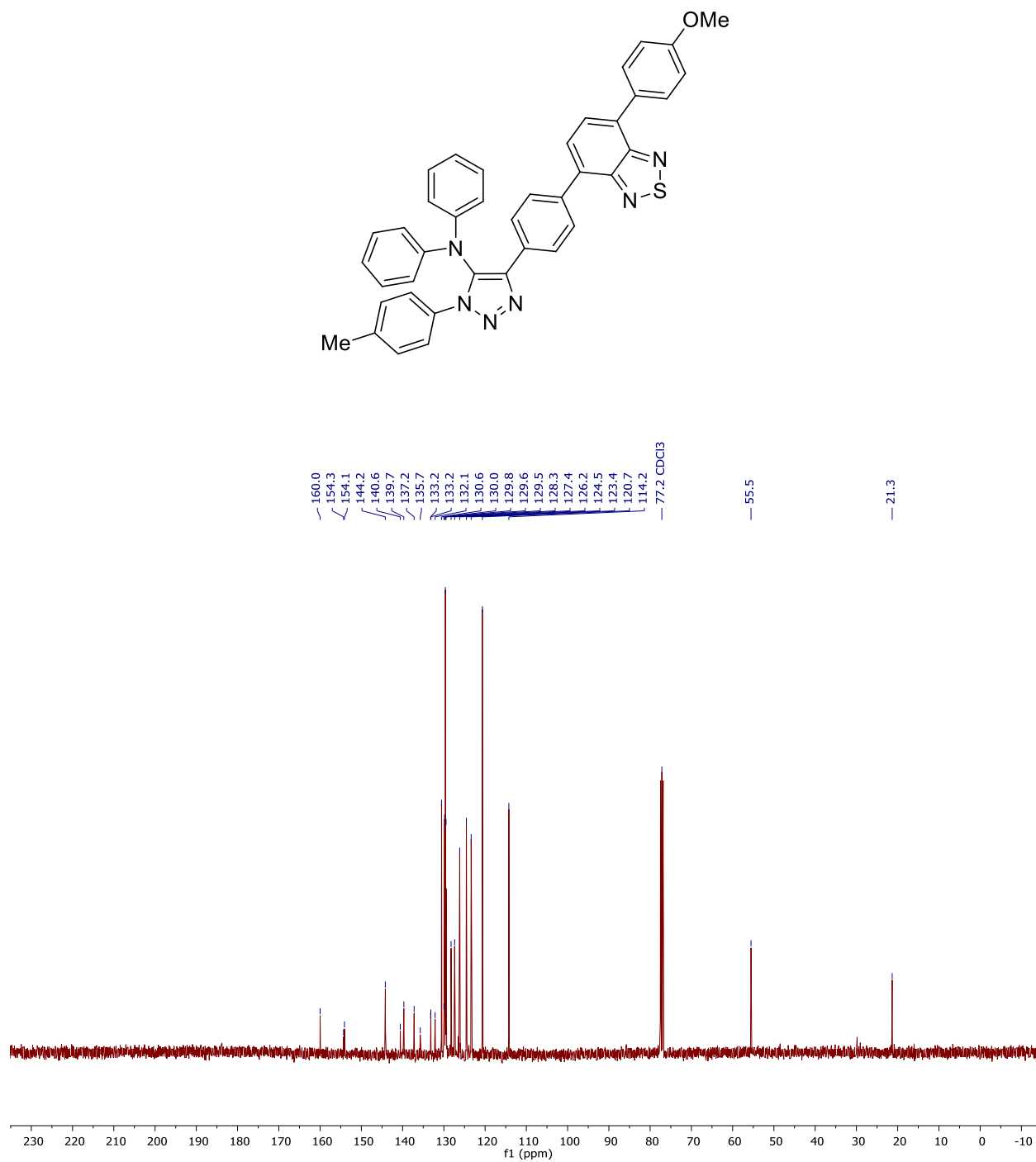


Figure S36. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6b**

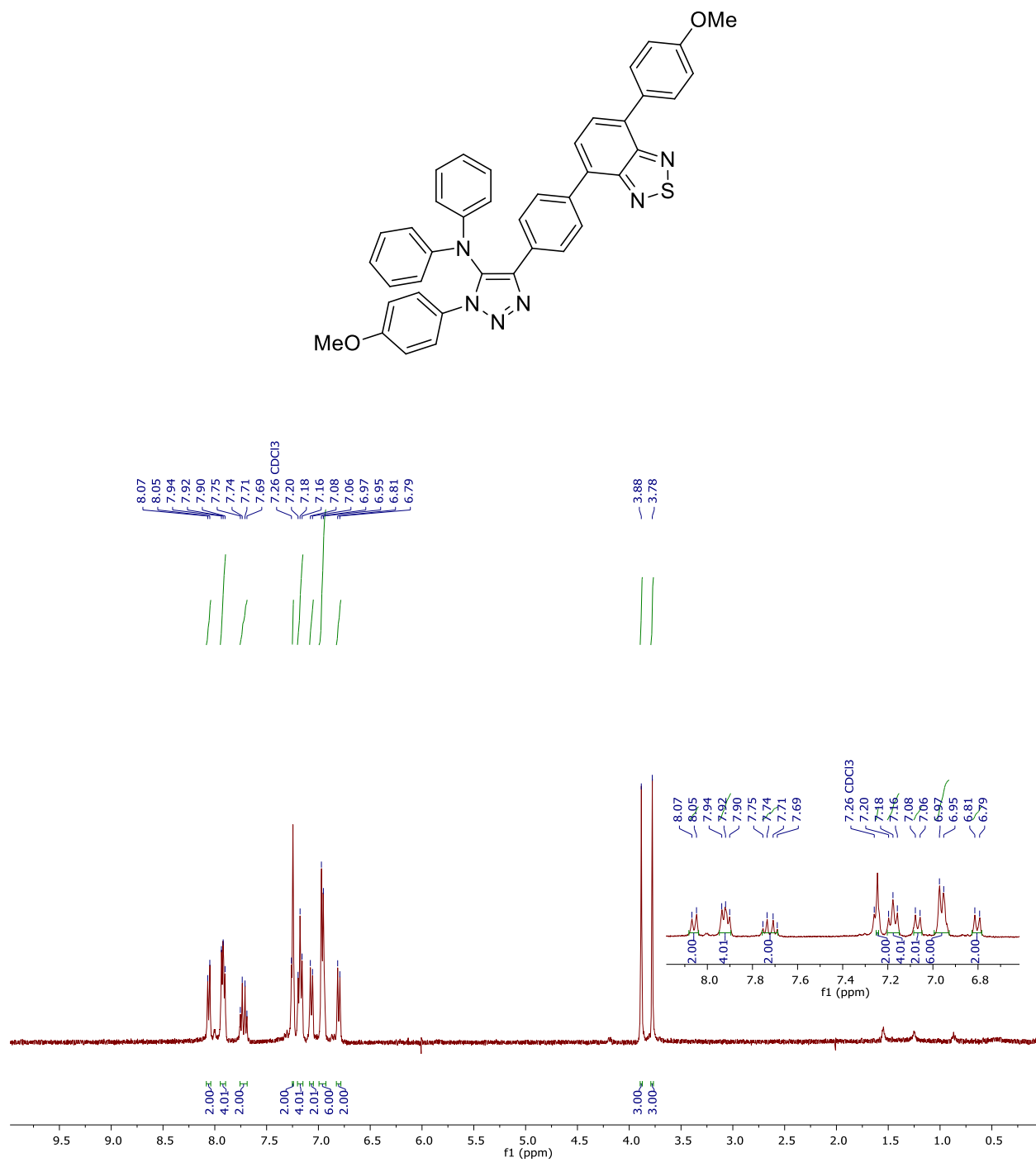


Figure S37. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **6c**

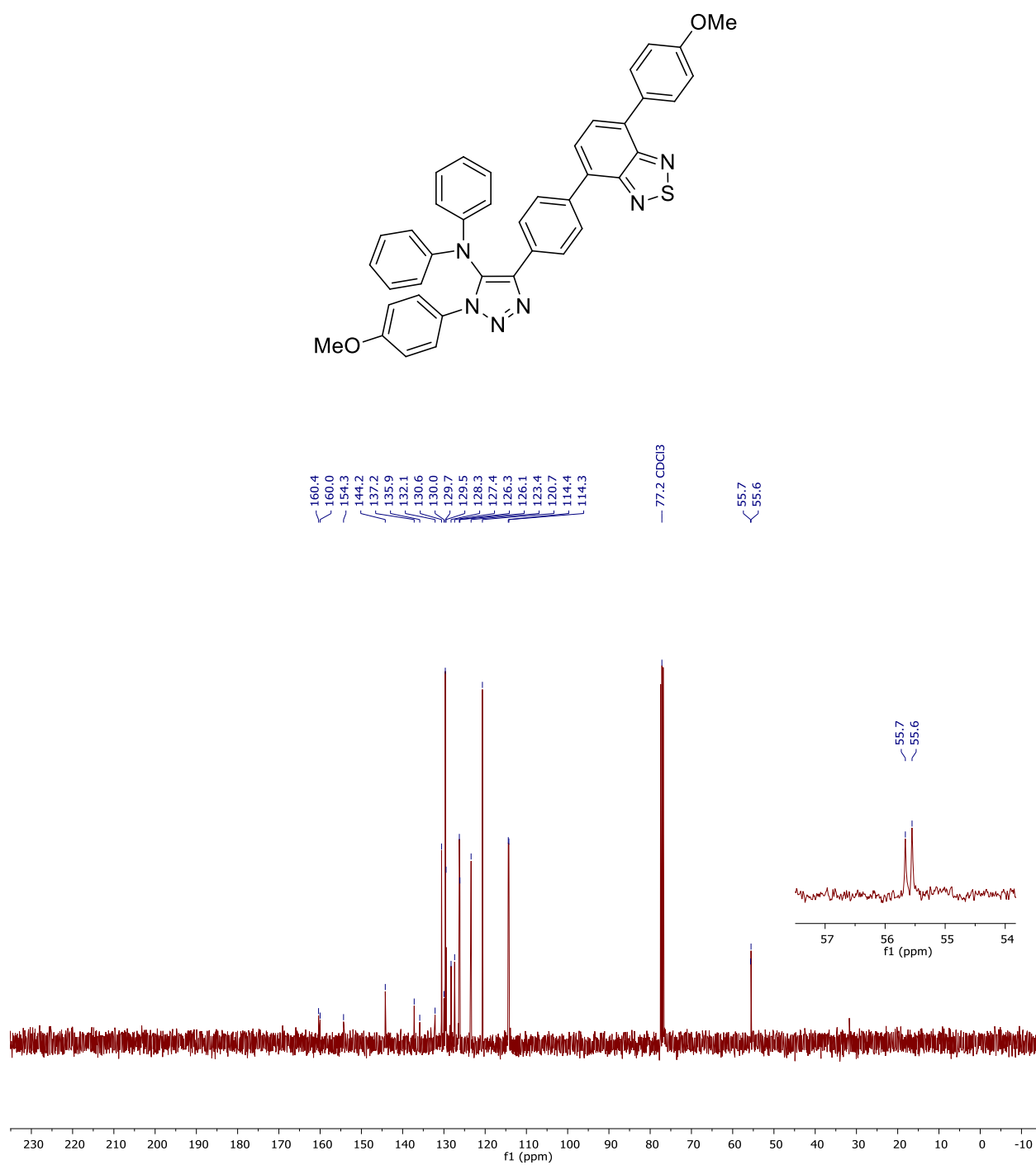


Figure S38. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6c**

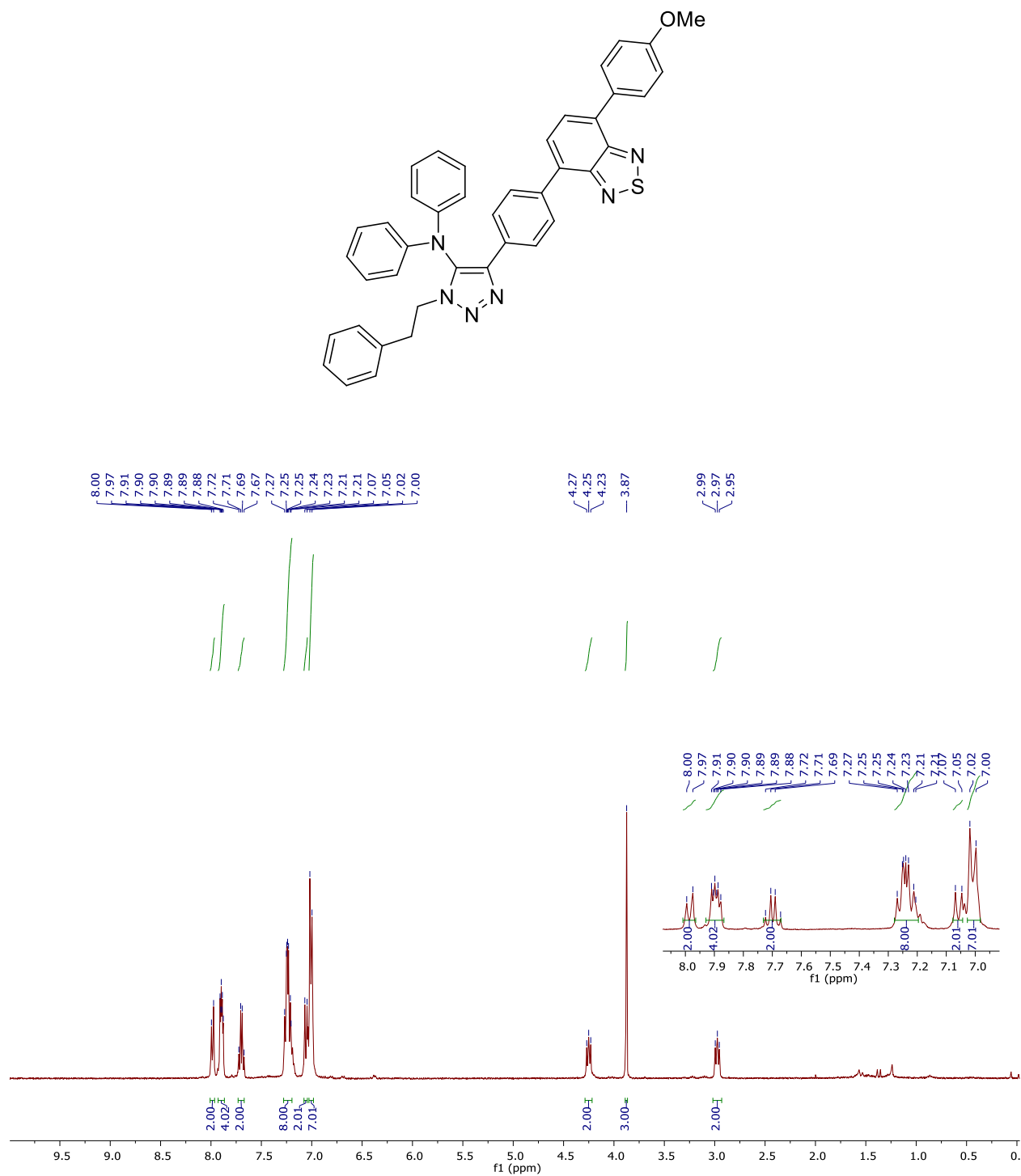


Figure S39. ¹H NMR (400 MHz, chloroform-*d*) spectrum of compound **6d**

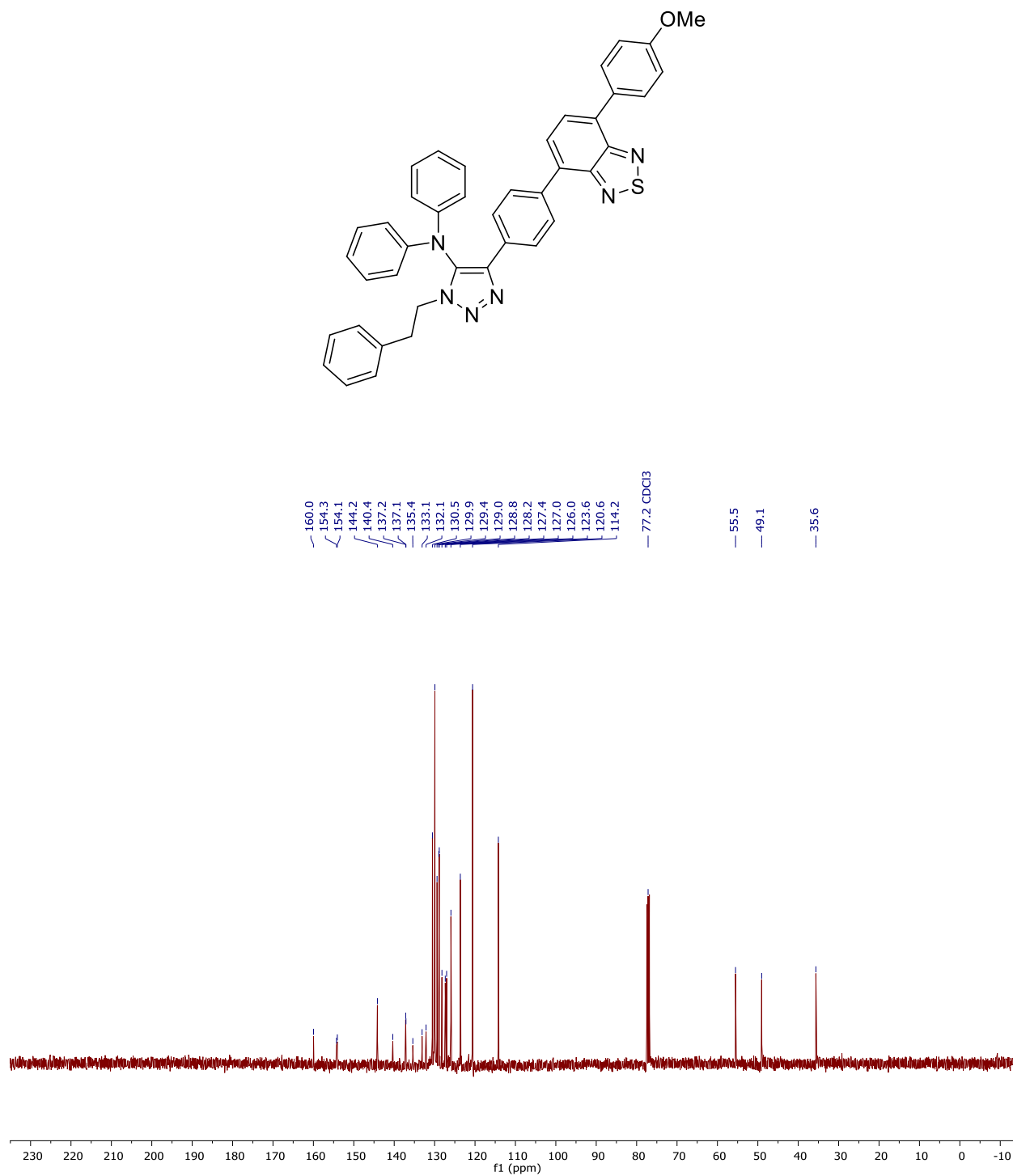


Figure S40. ¹³C NMR (101 MHz, chloroform-*d*) spectrum of compound **6d**

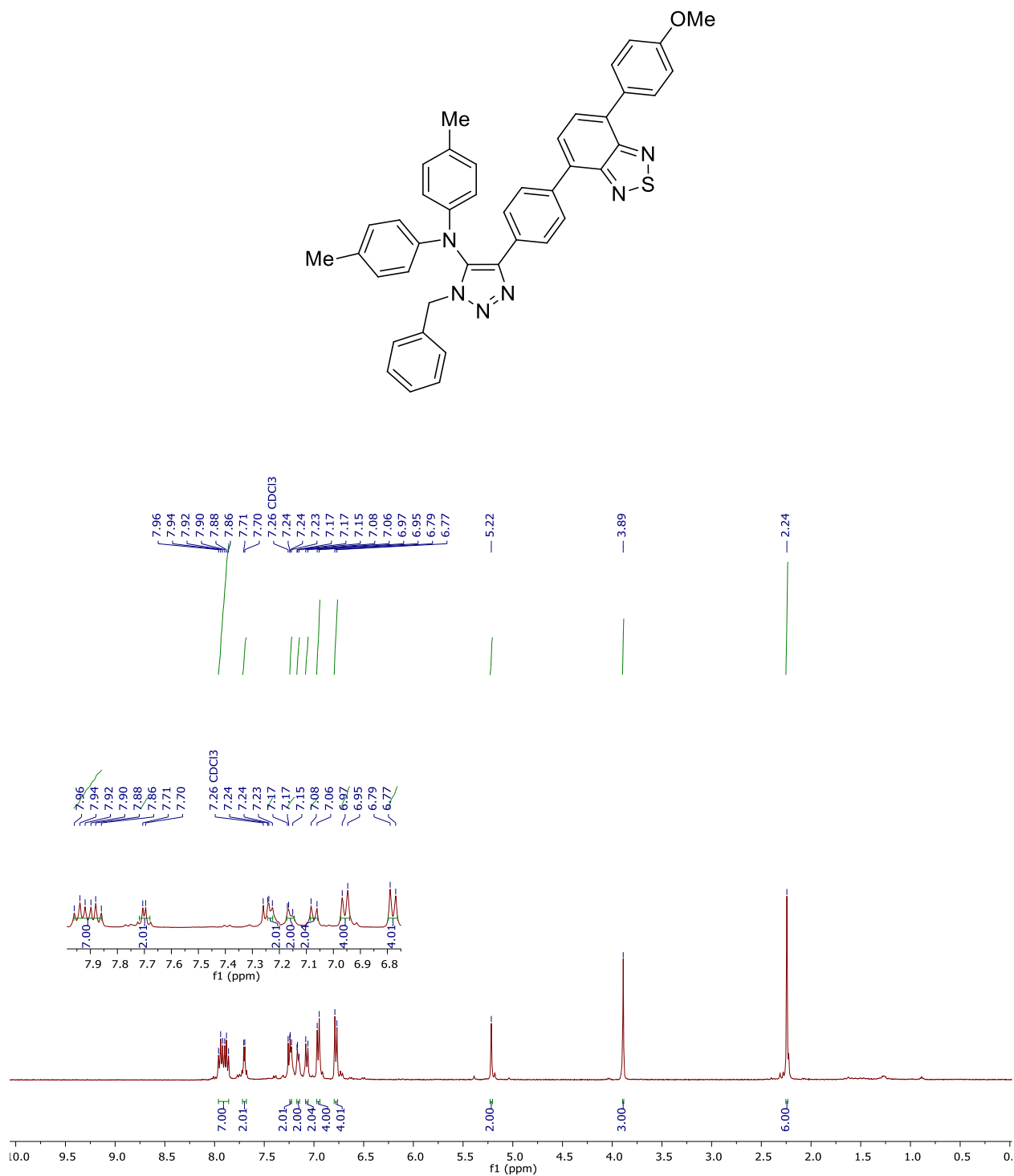


Figure S41. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **6e**

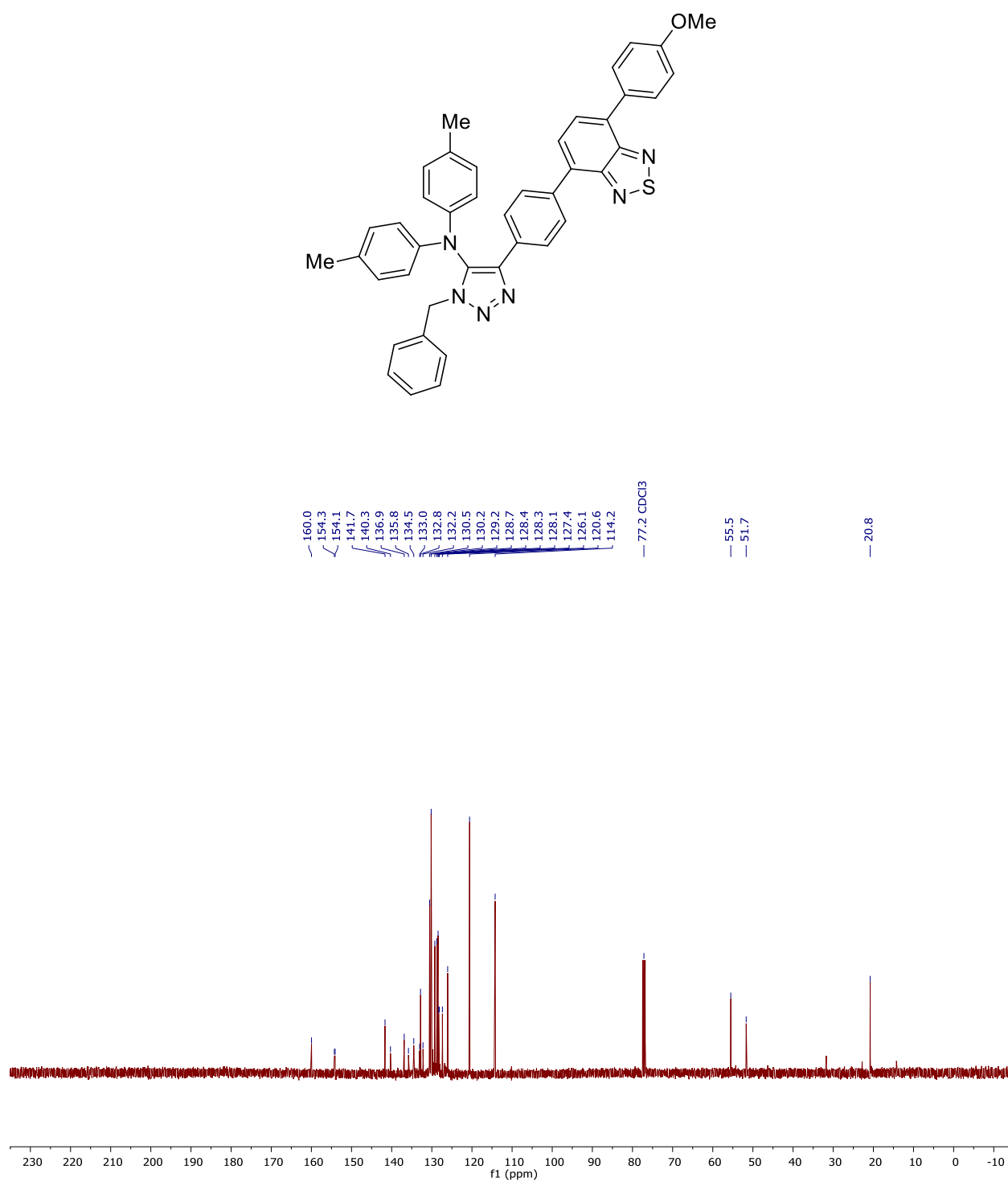


Figure S42. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6e**

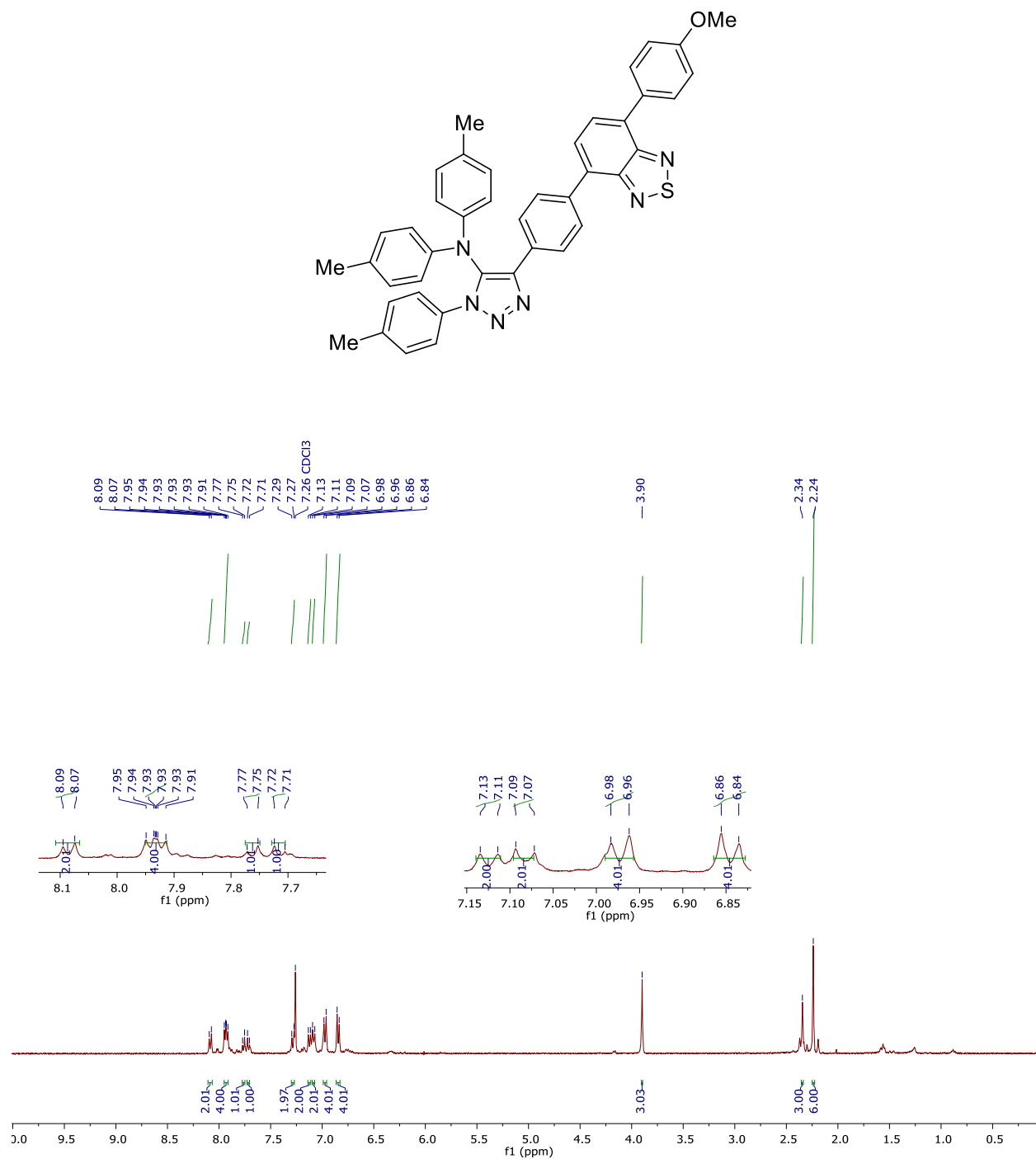


Figure S43. ^1H NMR (400 MHz, chloroform-*d*) spectrum of compound **6f**

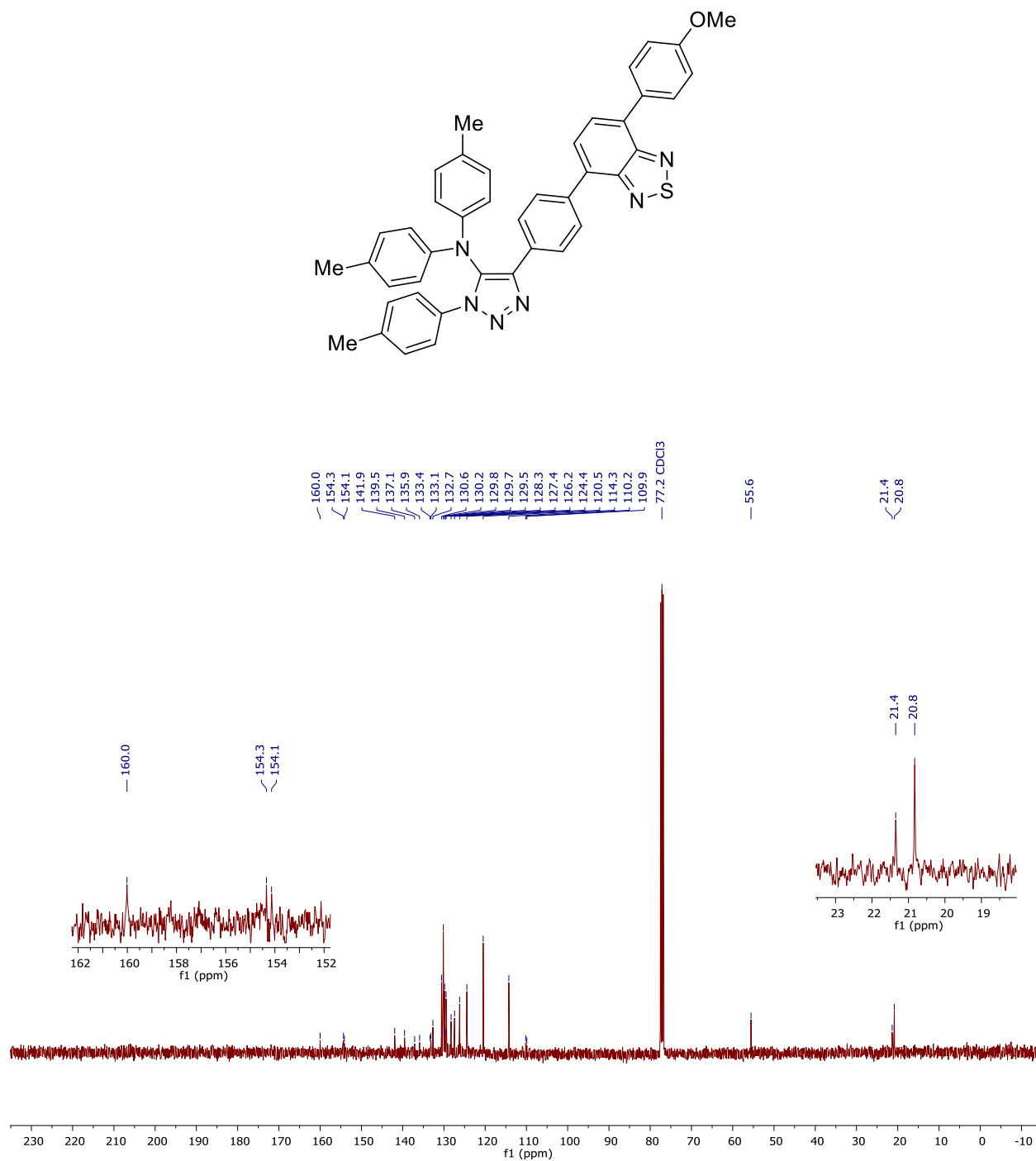


Figure S44. ¹³C NMR (101 MHz, chloroform-*d*) spectrum of compound **6f**

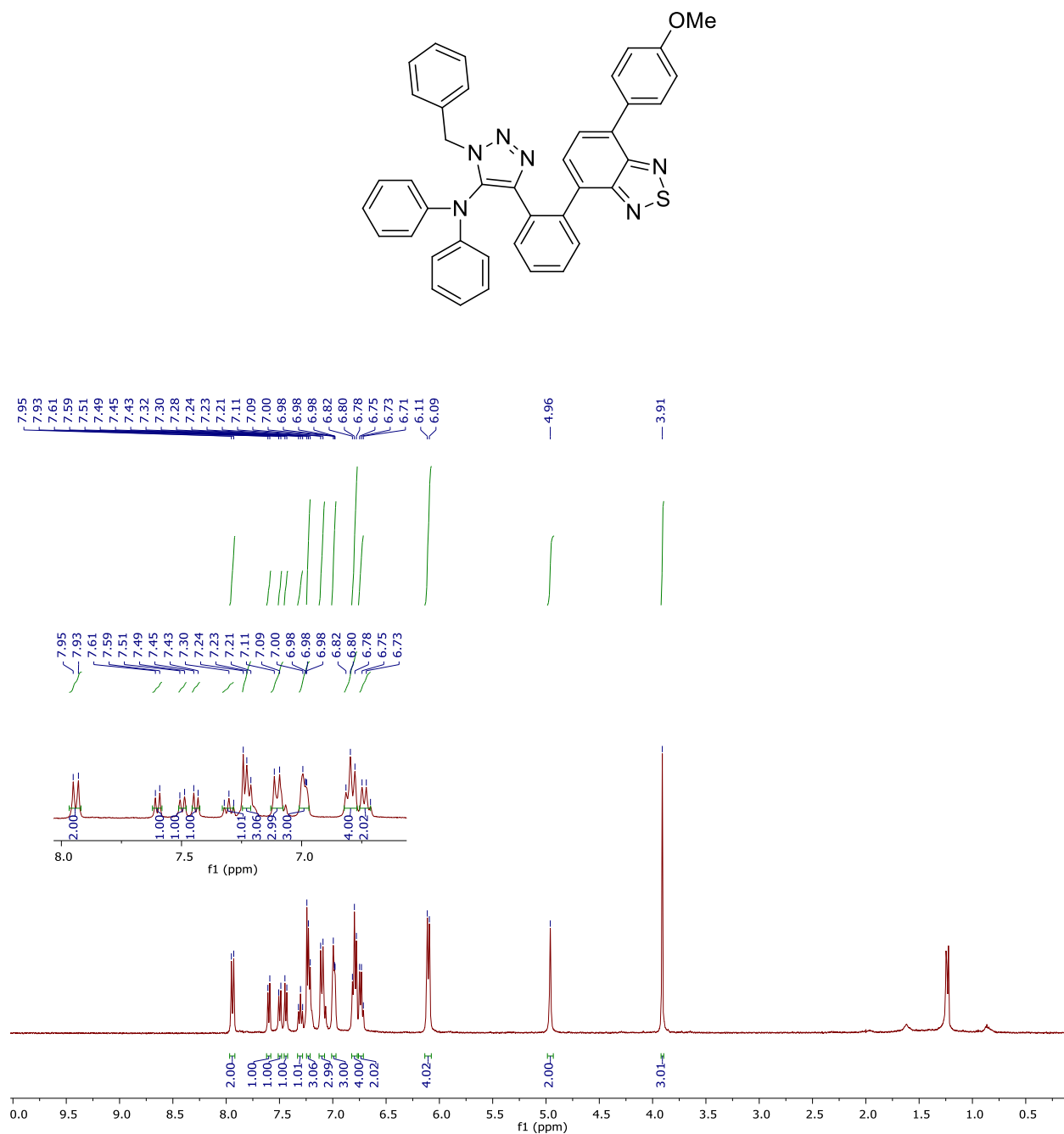


Figure S45. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **6g**

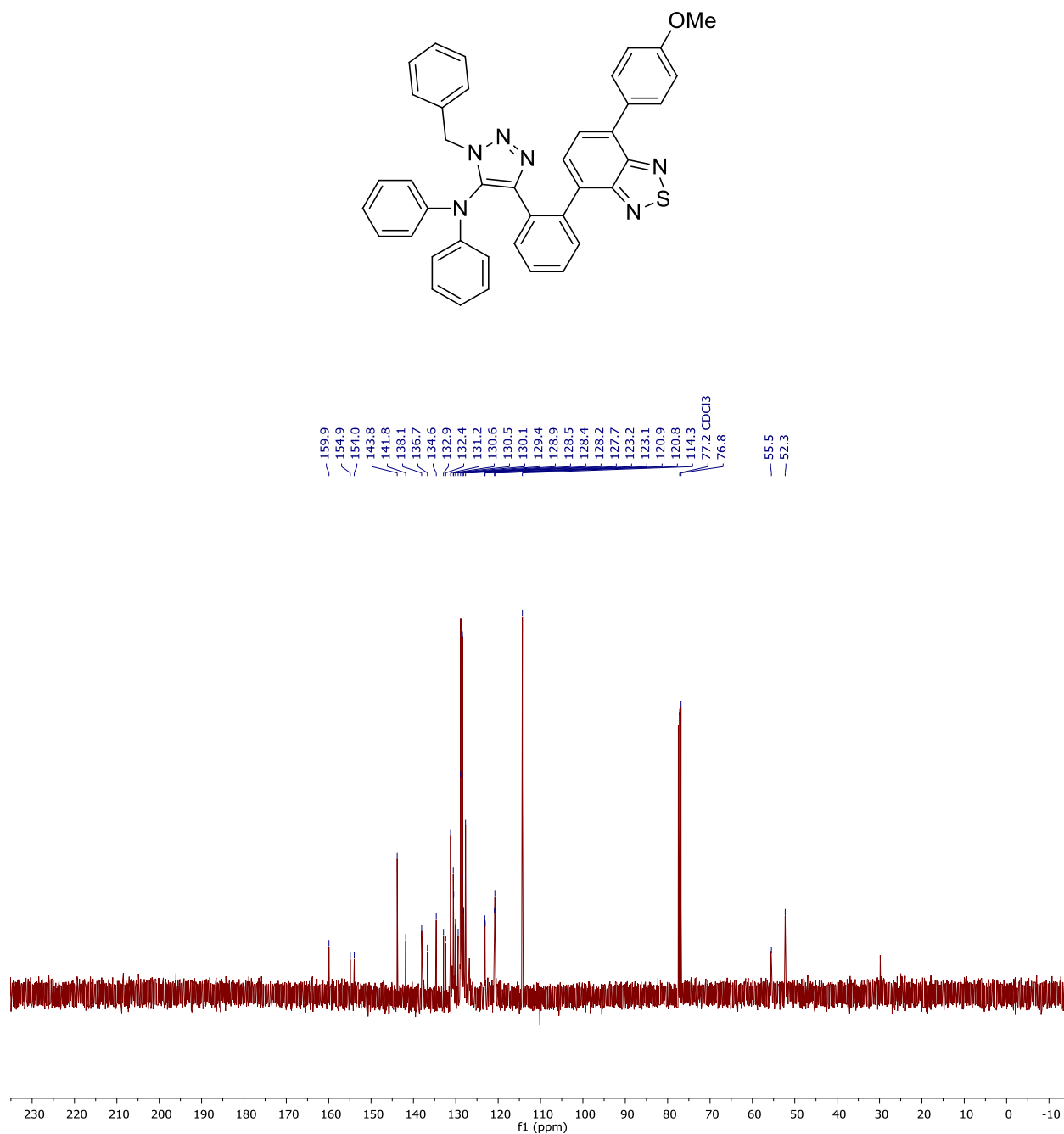


Figure S46. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6g**

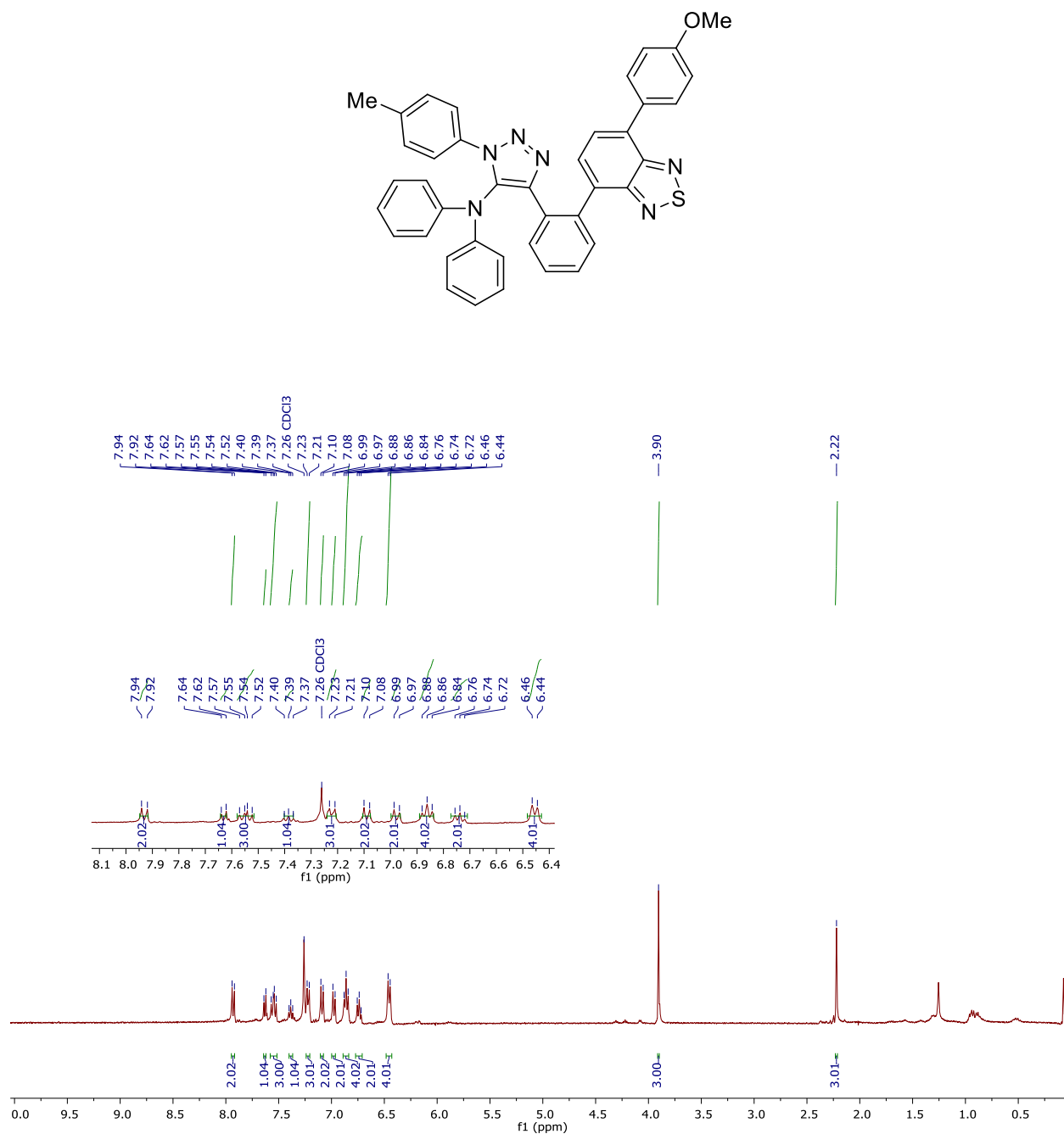


Figure S47. ^1H NMR (400 MHz, chloroform-d) spectrum of compound **6h**

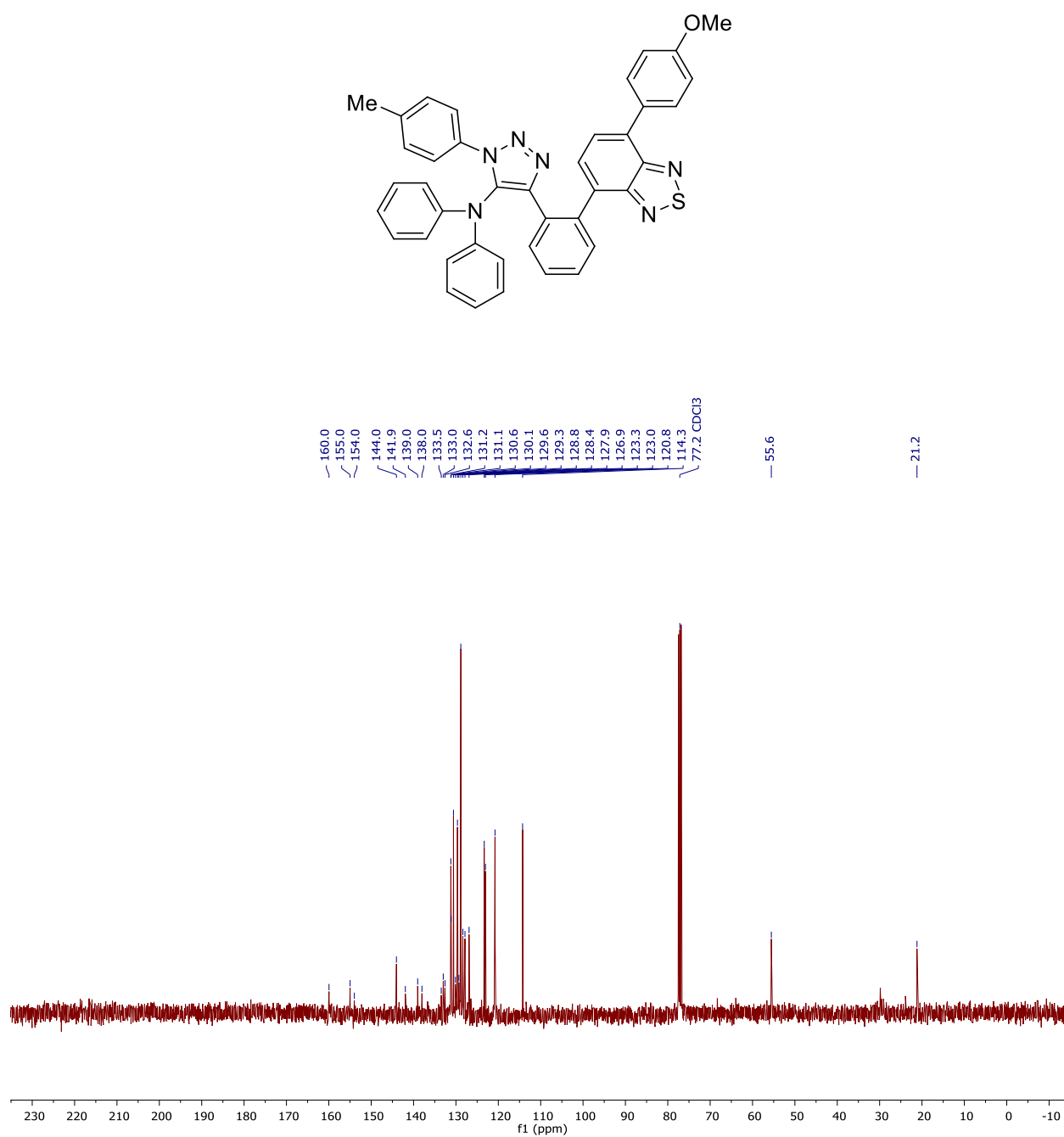


Figure S48. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6h**

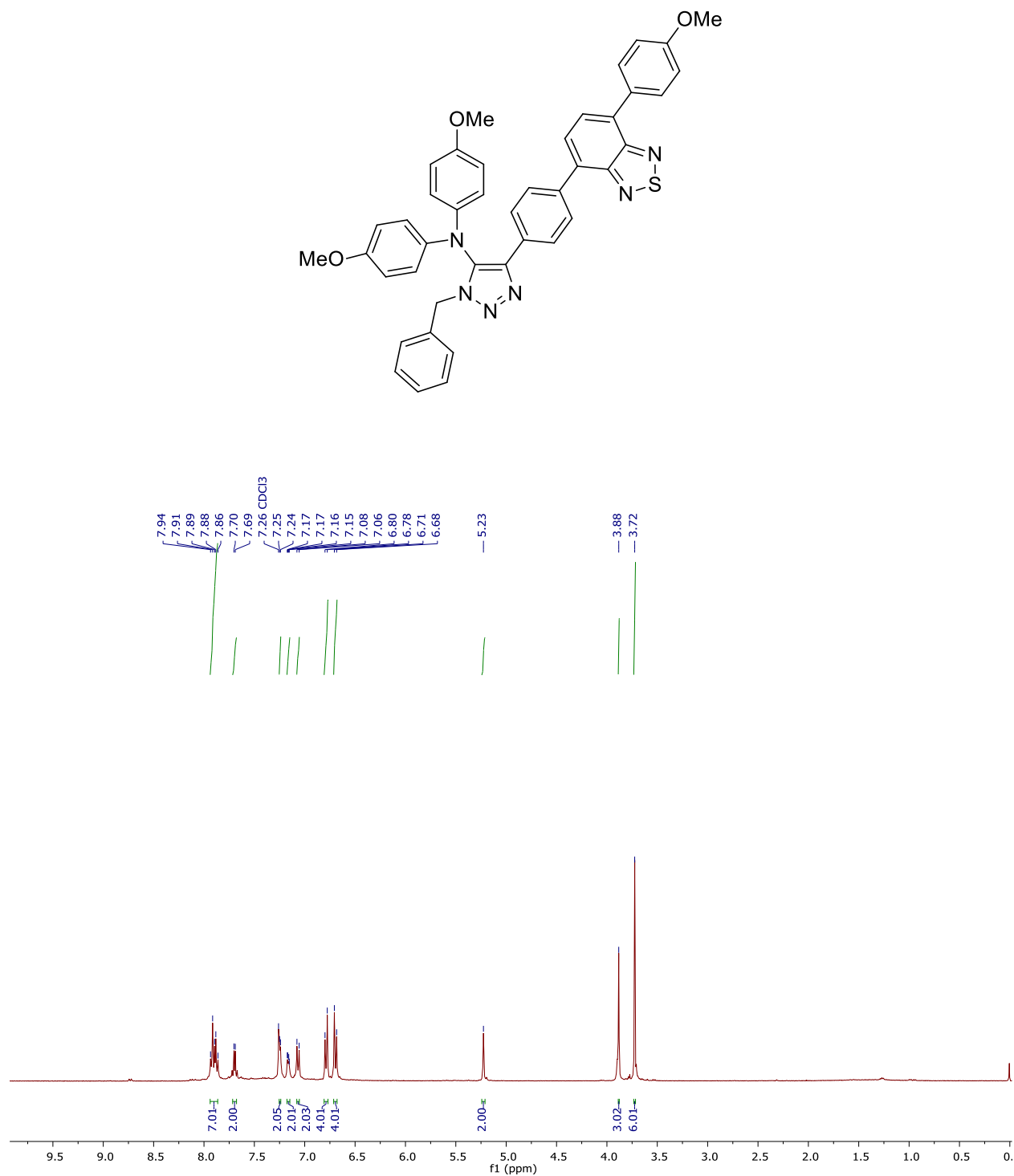


Figure S49. ^1H NMR (400 MHz, chloroform-*d*) spectrum of compound **6i**

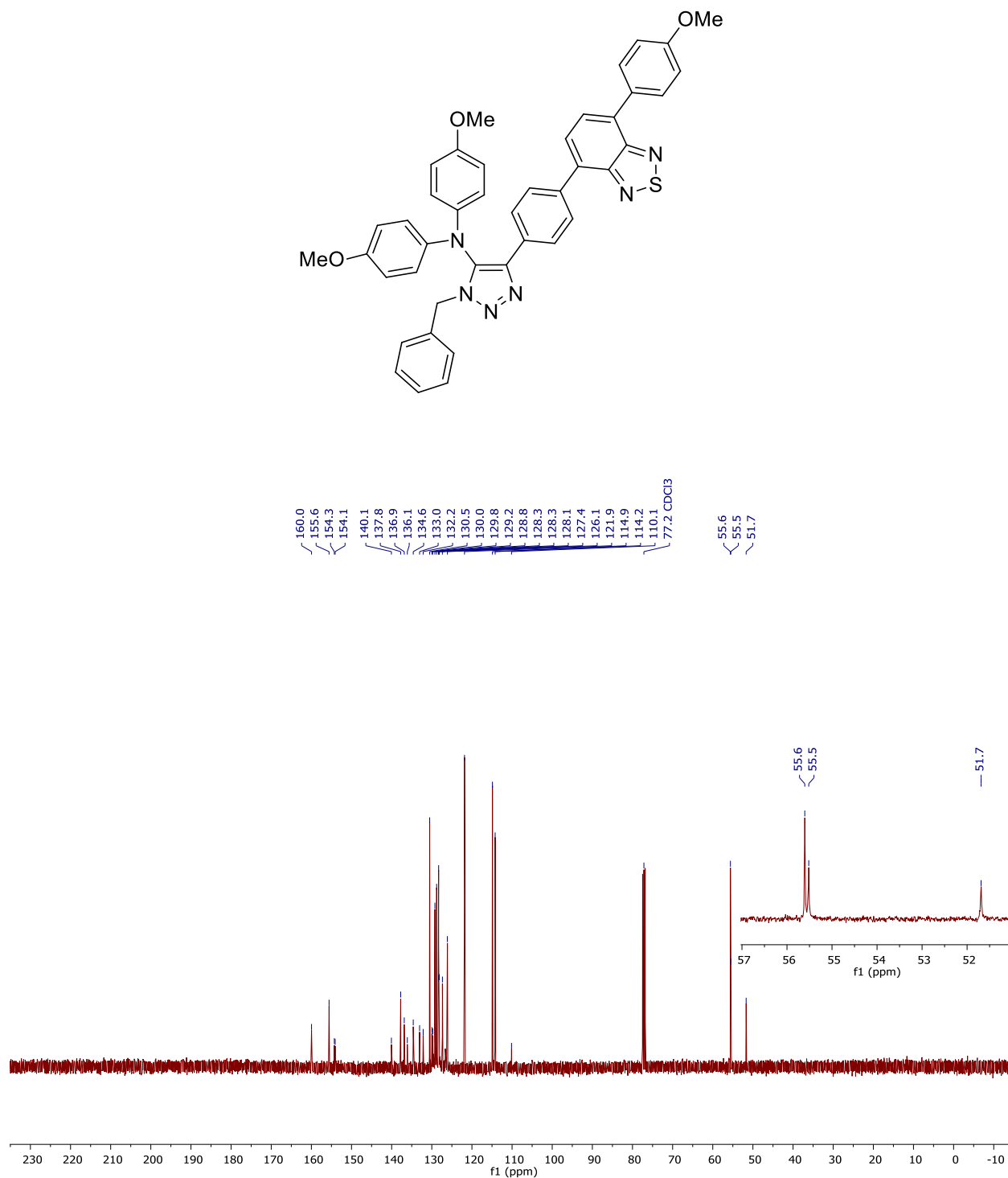


Figure S50. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6i**



Figure S51. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **6j**

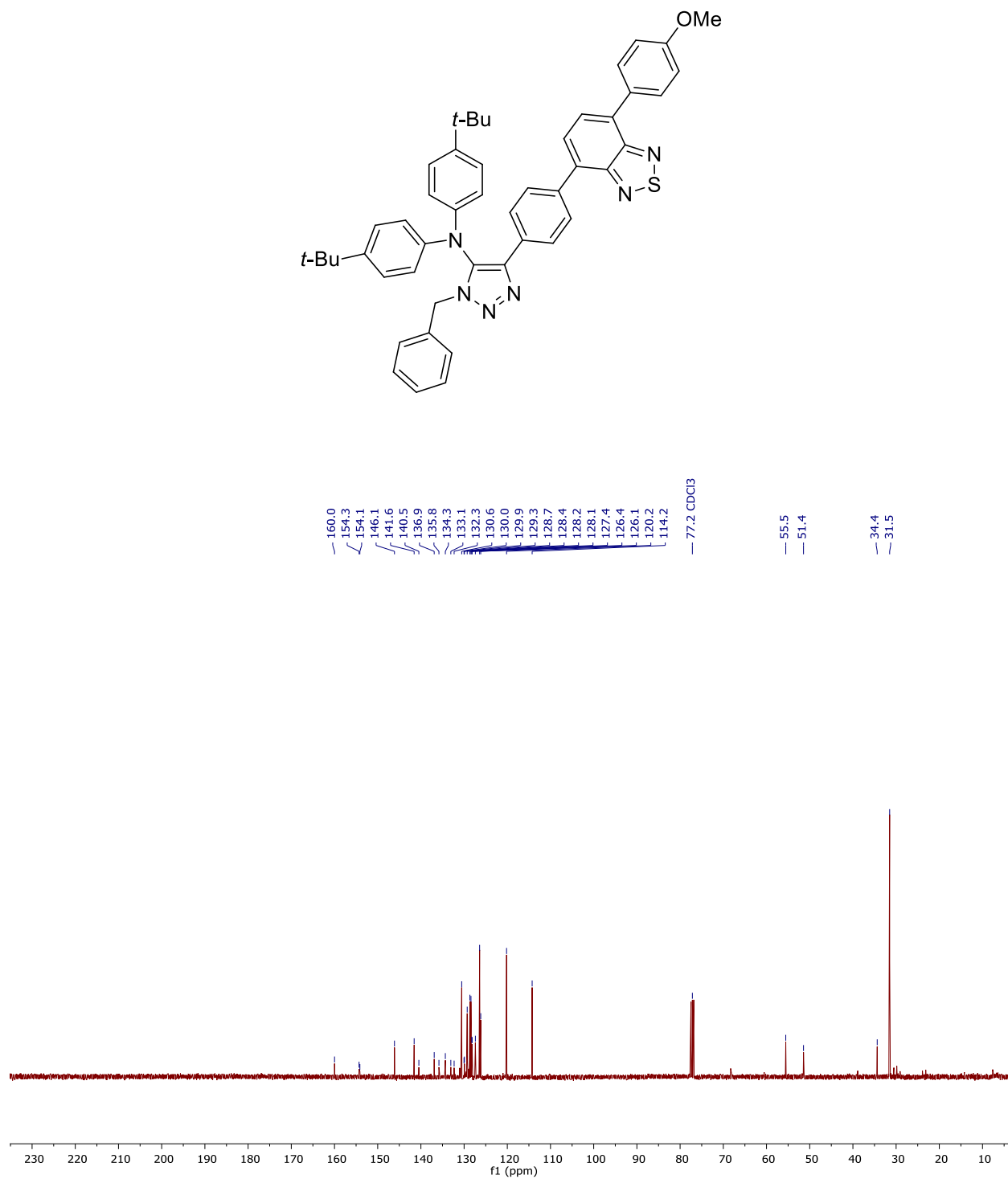


Figure S52. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6j**

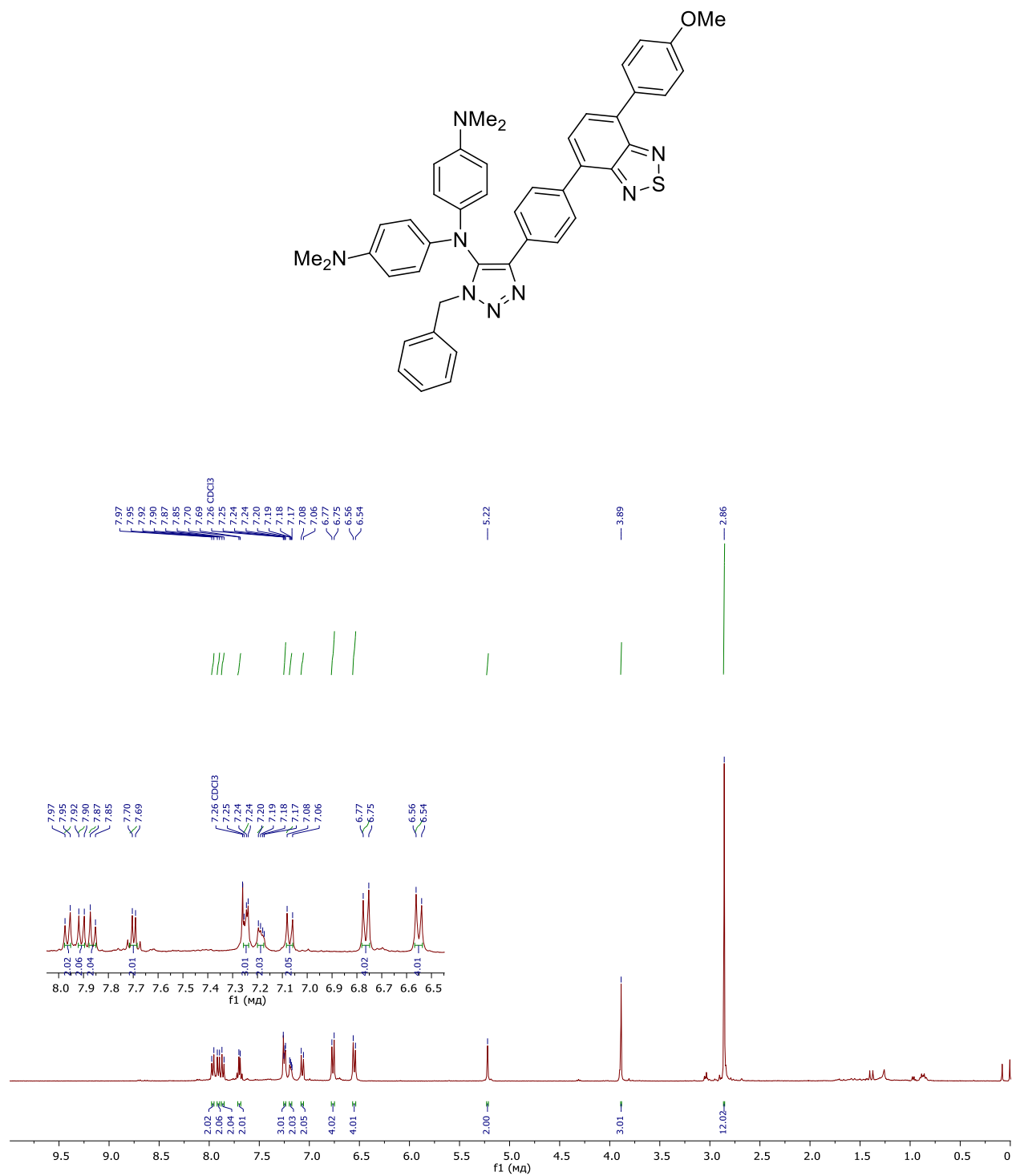


Figure S53. ^1H NMR (400 MHz, $\text{chloroform-}d$) spectrum of compound **6k**

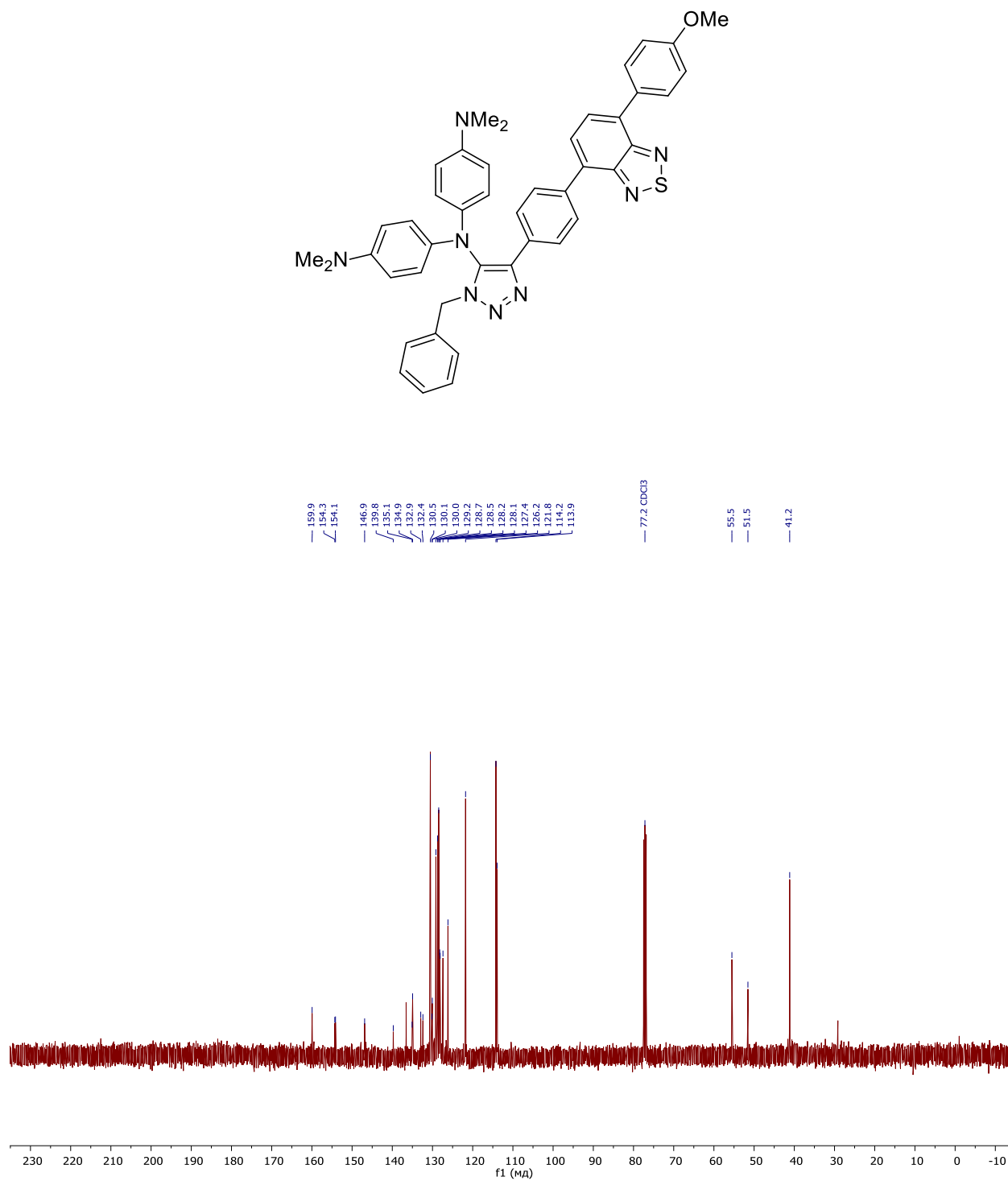


Figure S54. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6k**

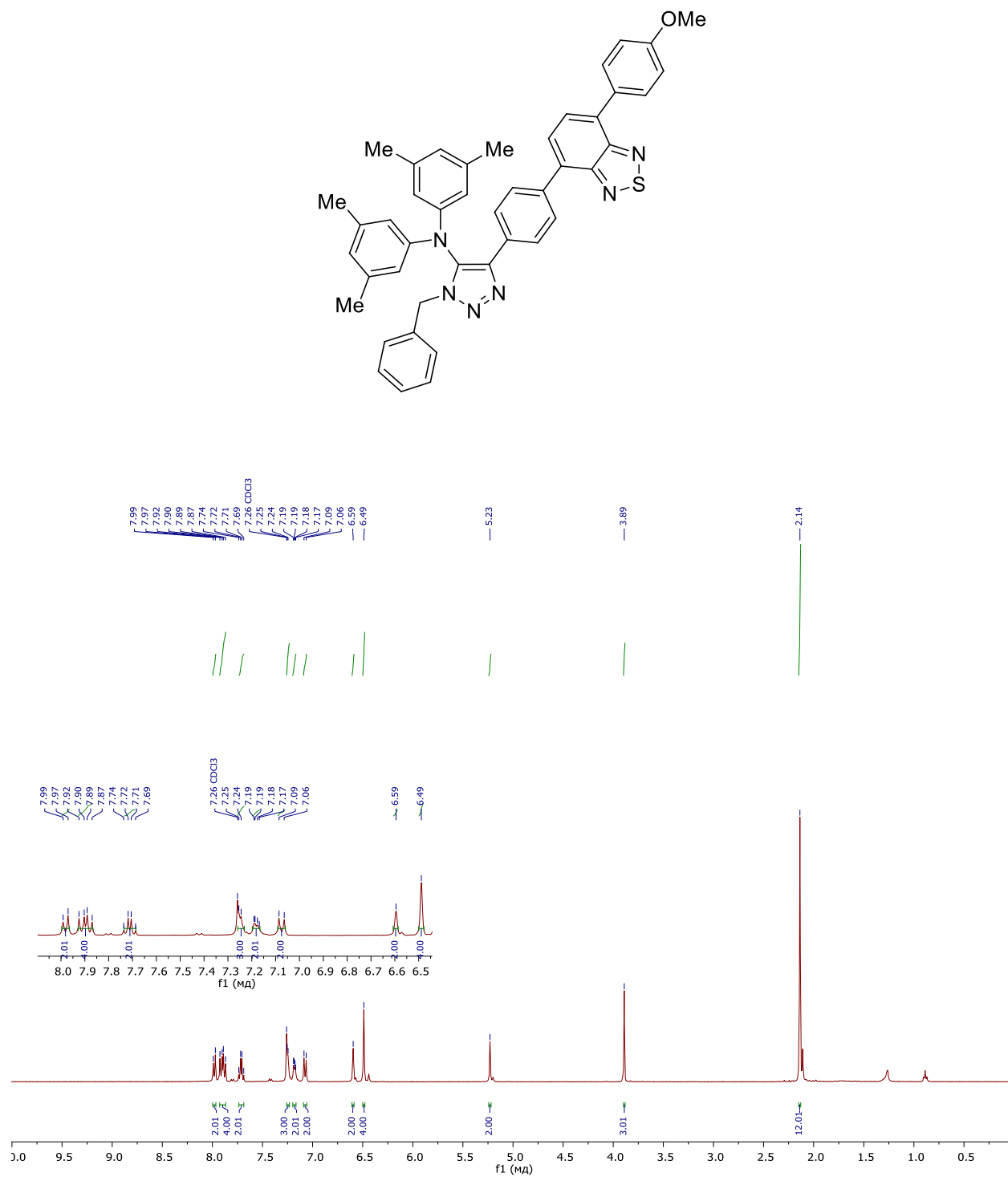


Figure S55. ^1H NMR (400 MHz, chloroform-*d*) spectrum of compound **6l**

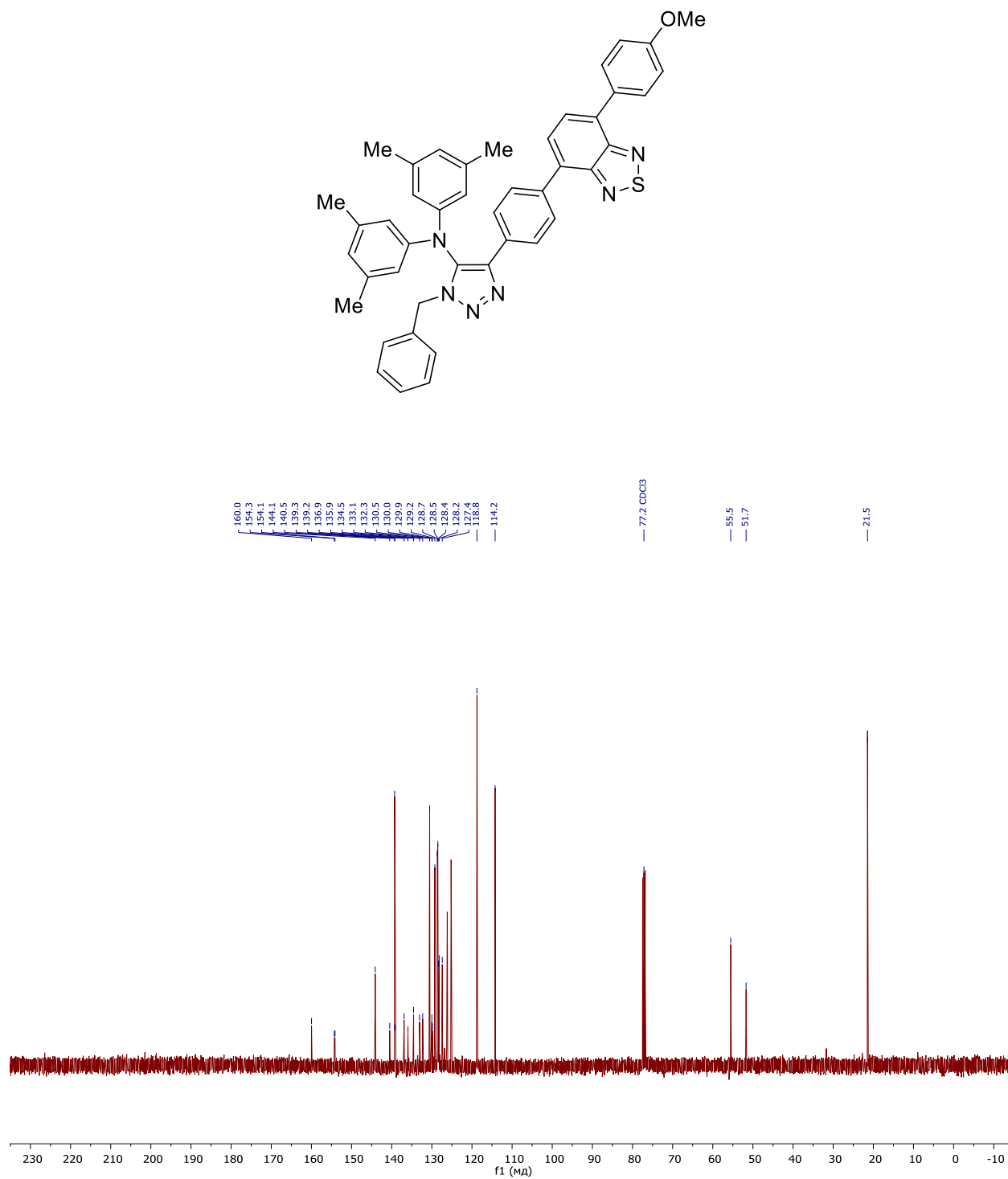


Figure S56. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **6l**

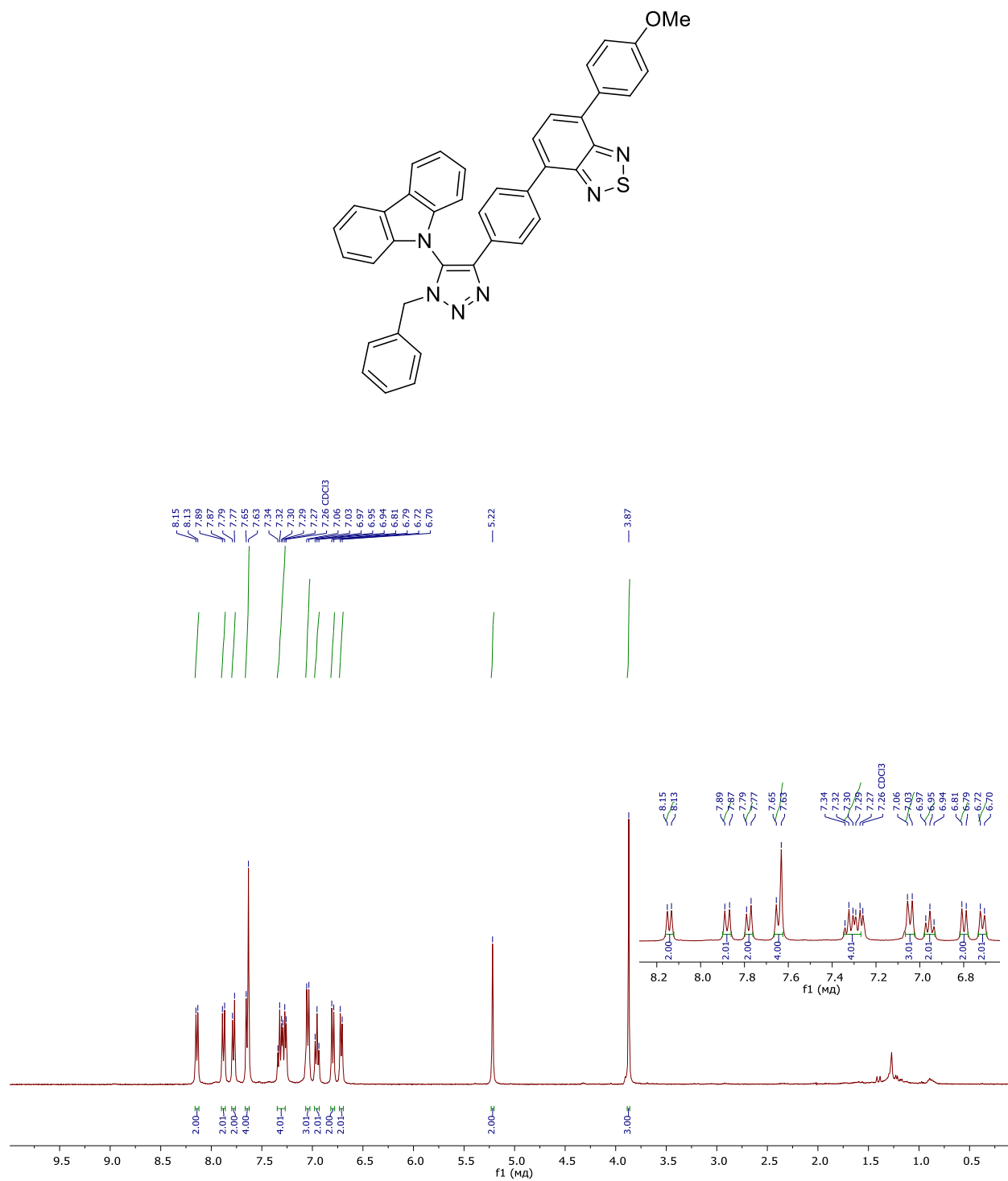


Figure S57. ^1H NMR (400 MHz, chloroform-*d*) spectrum of compound **7a**

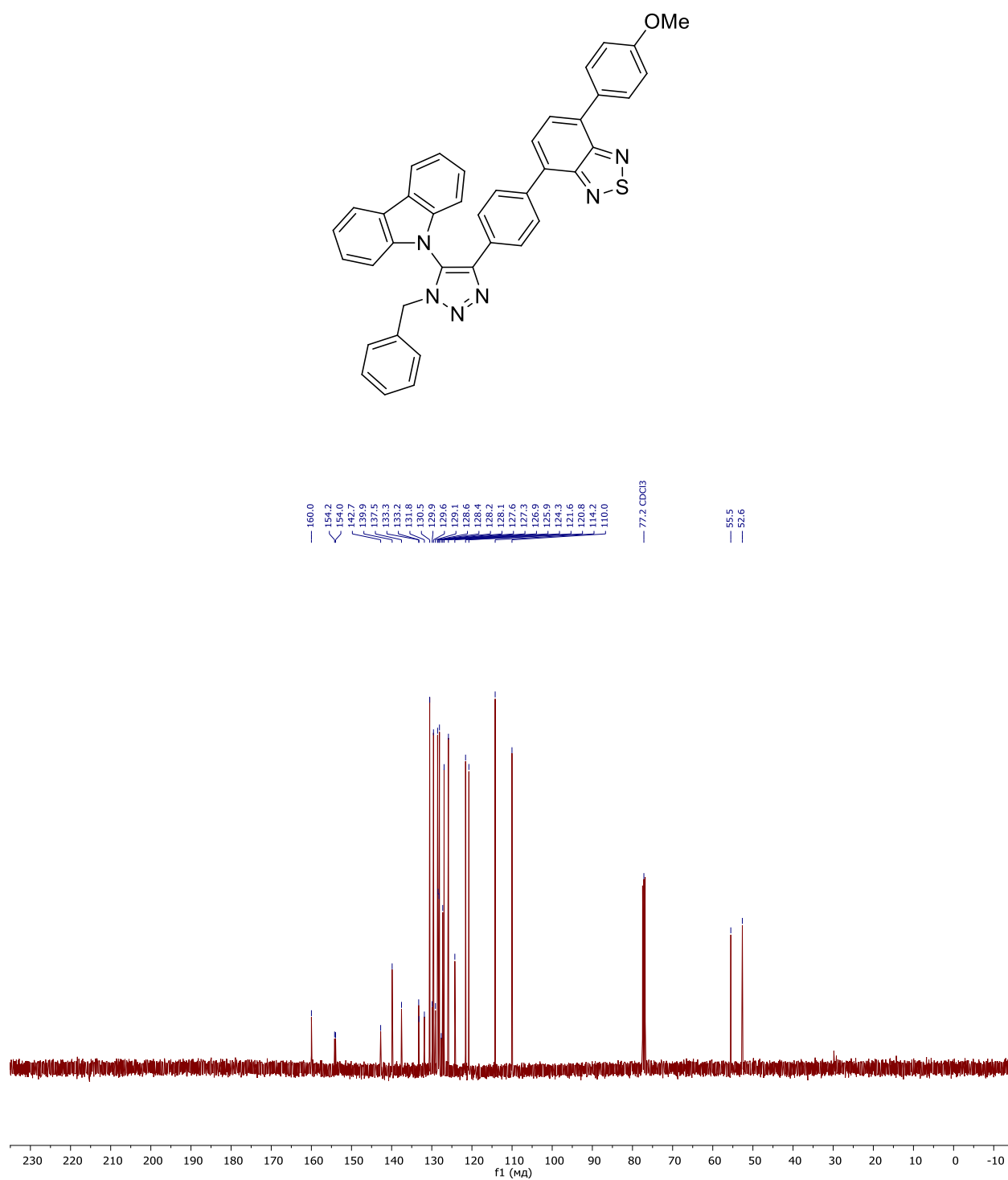


Figure S58. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **7a**

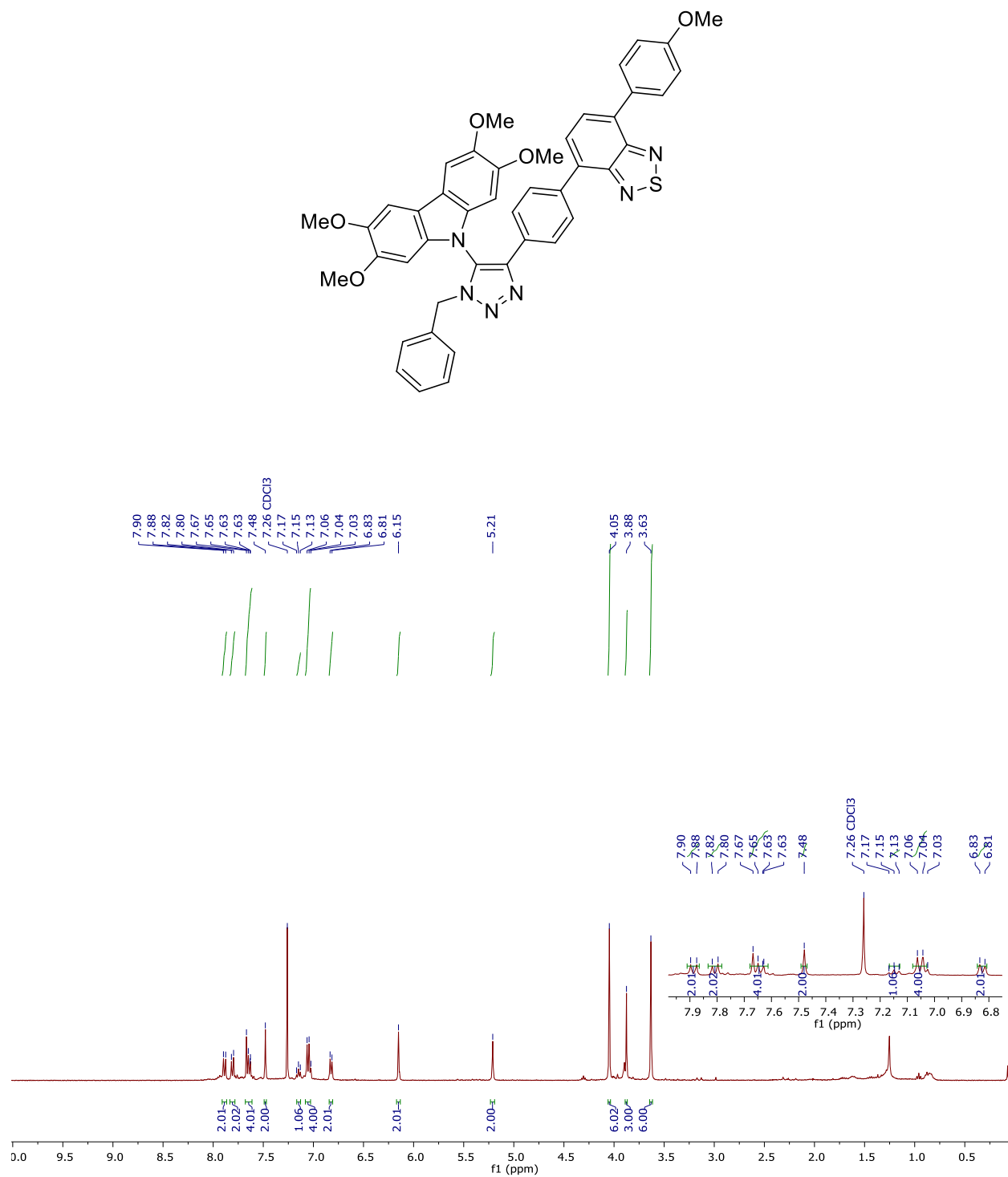


Figure S59. ^1H NMR (400 MHz, chloroform-*d*) spectrum of compound **7b**

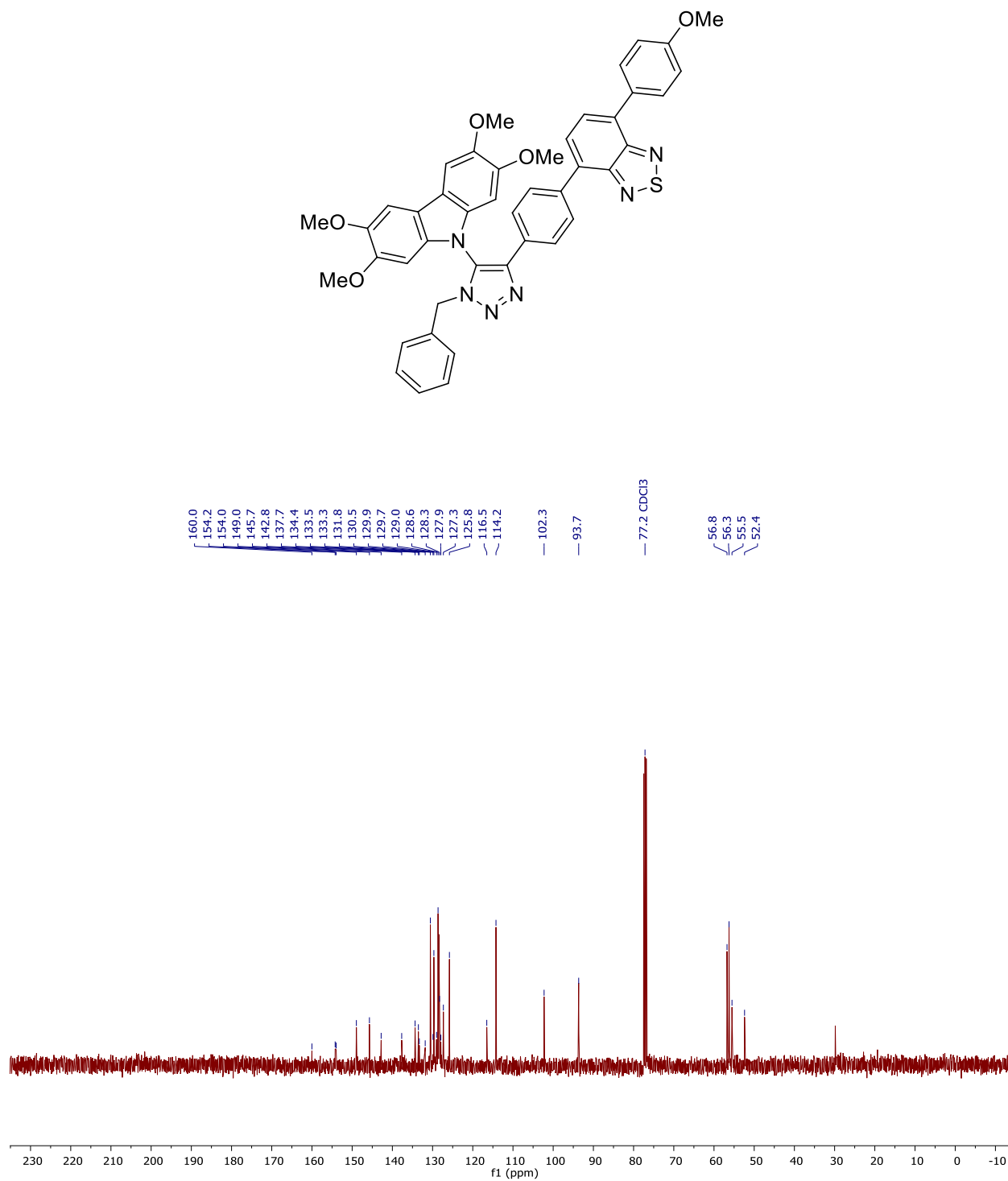


Figure S60. ^{13}C NMR (101 MHz, chloroform-*d*) spectrum of compound **7b**

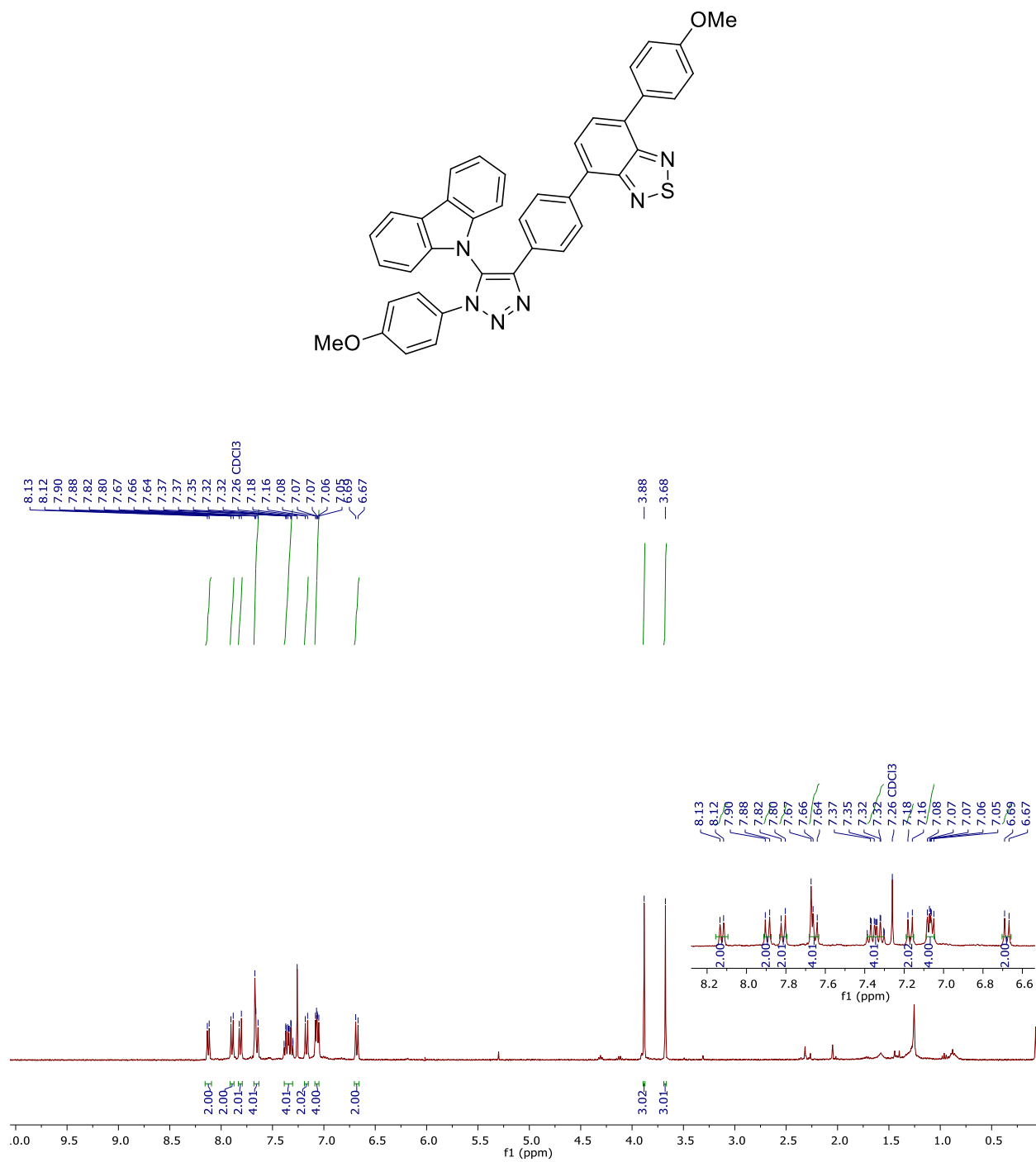


Figure S61. ^1H NMR (400 MHz, chloroform-d) spectrum of compound **7c**

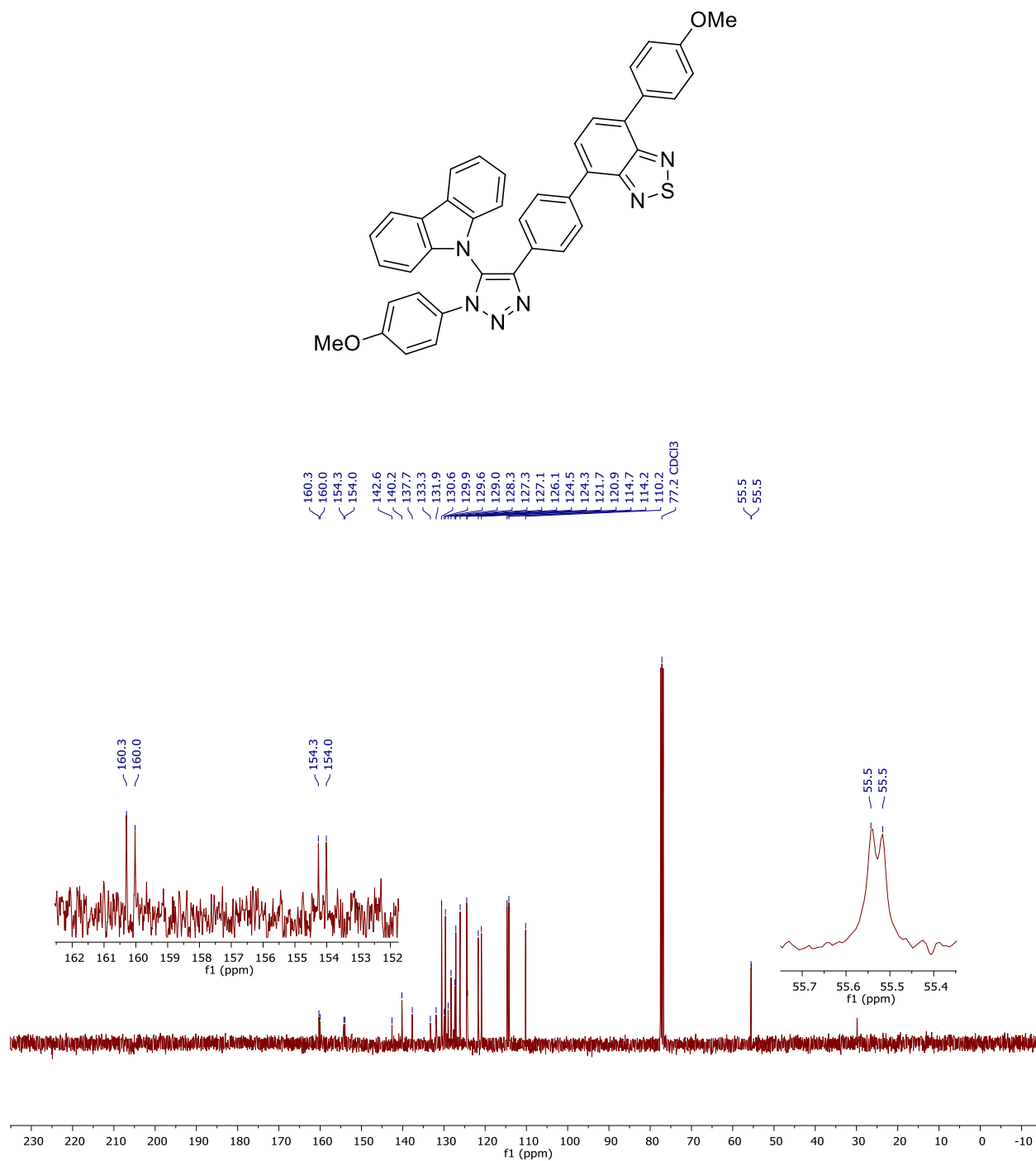


Figure S62. ^{13}C NMR (101 MHz, $\text{chloroform-}d$) spectrum of compound **7c**

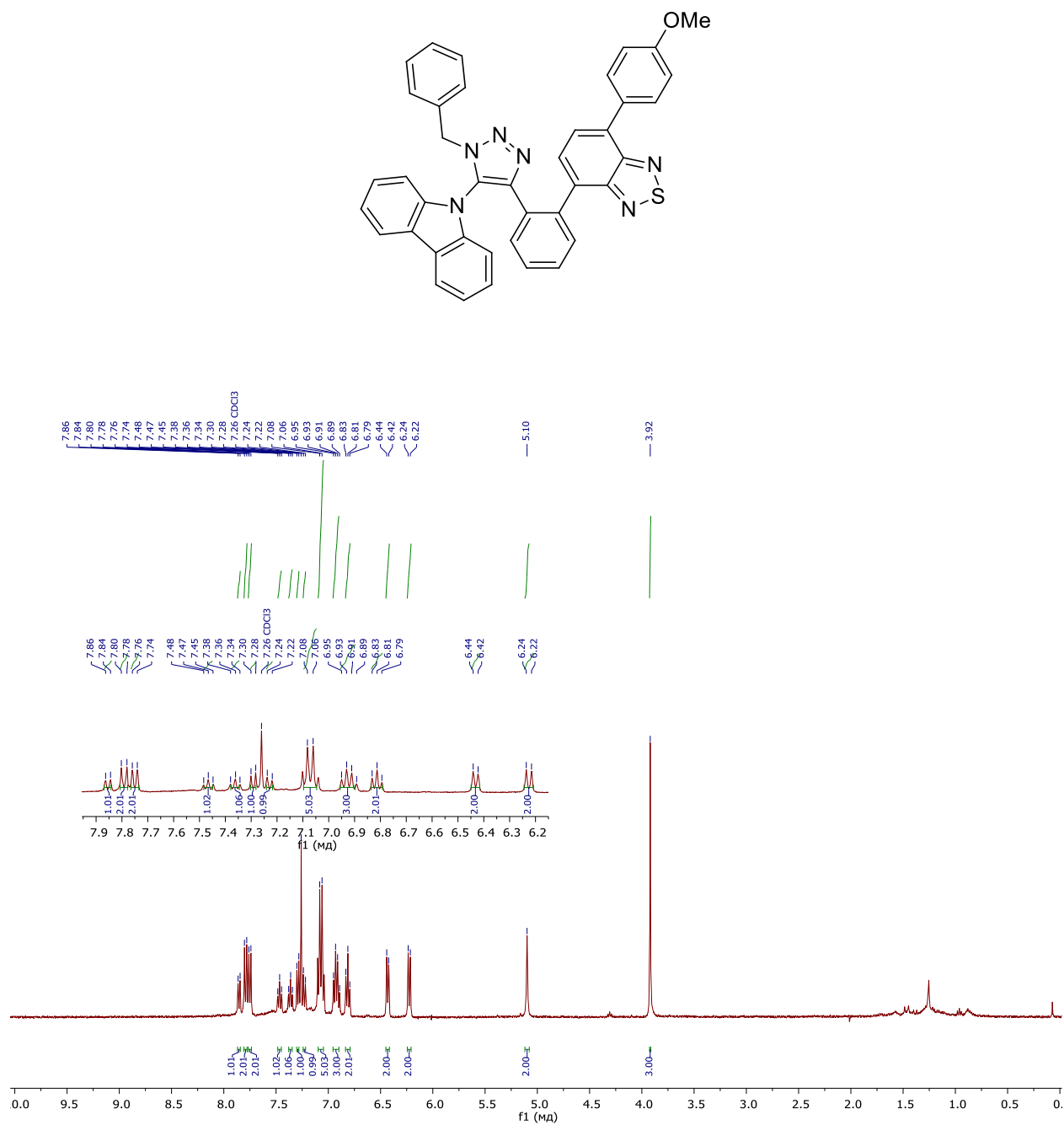


Figure S63. ¹H NMR (400 MHz, chloroform-*d*) spectrum of compound **7d**

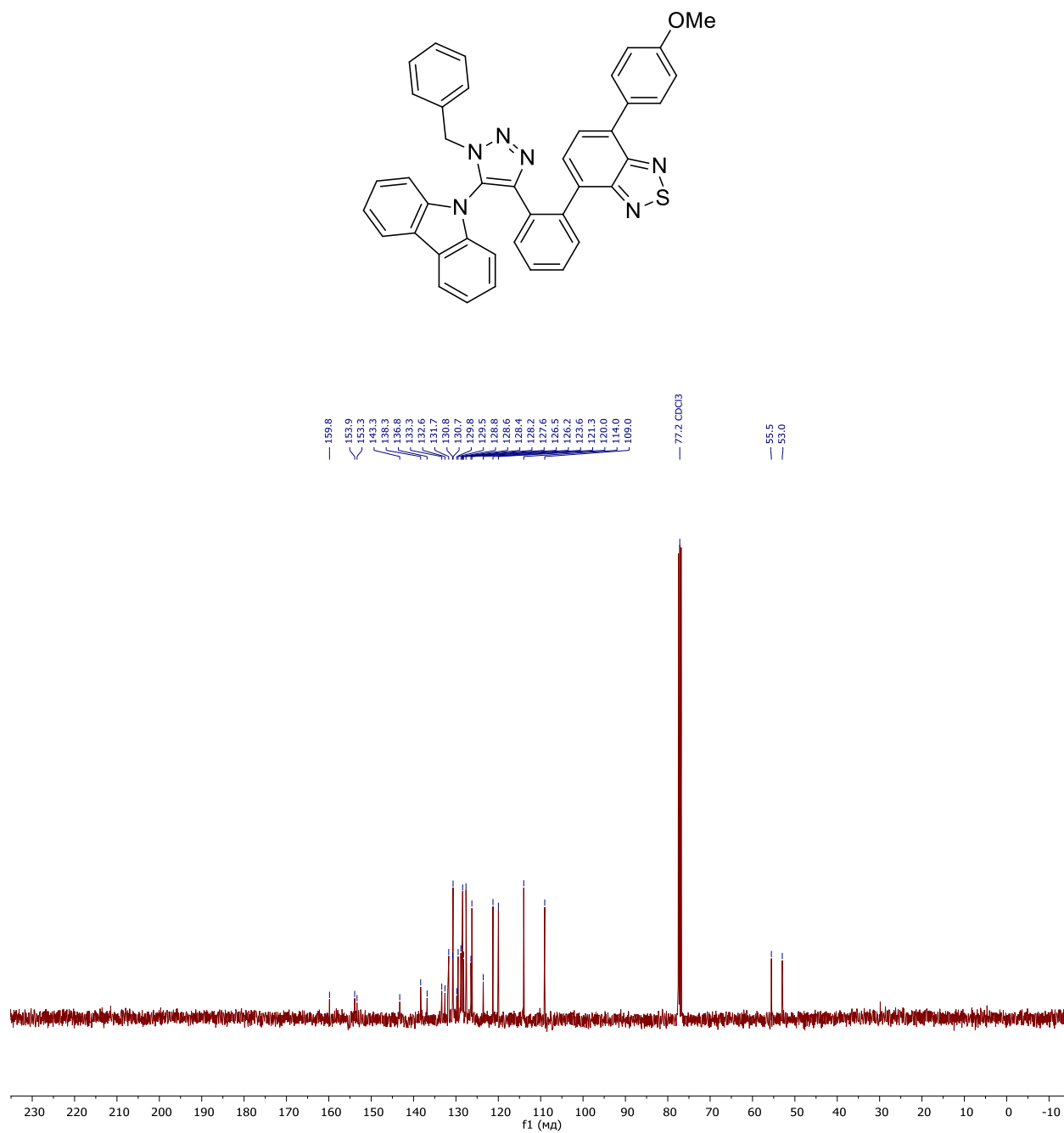


Figure S64. ^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **7d**

Electrochemistry

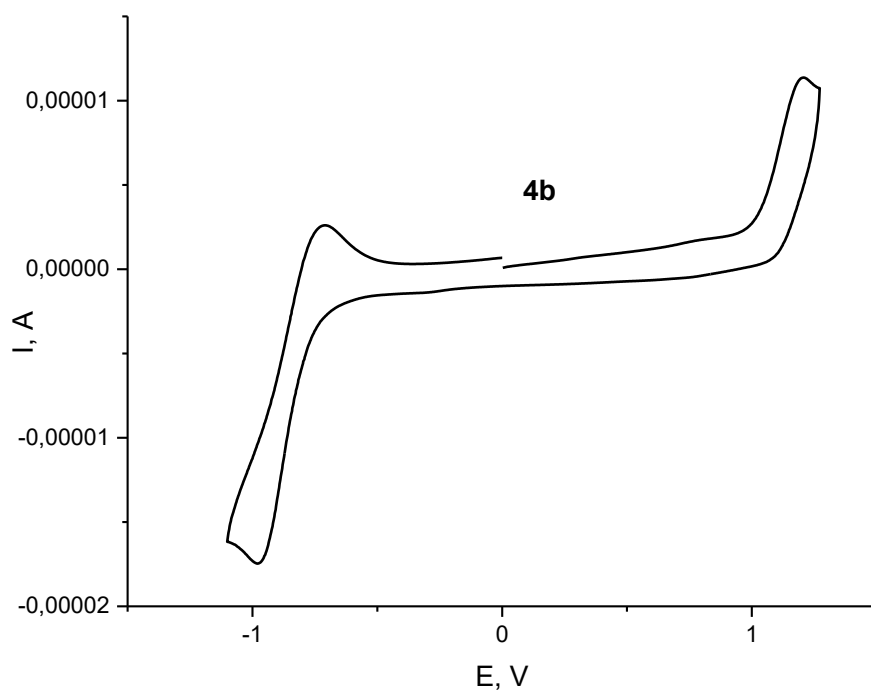


Figure S65. Cyclic voltammogram of **4b**

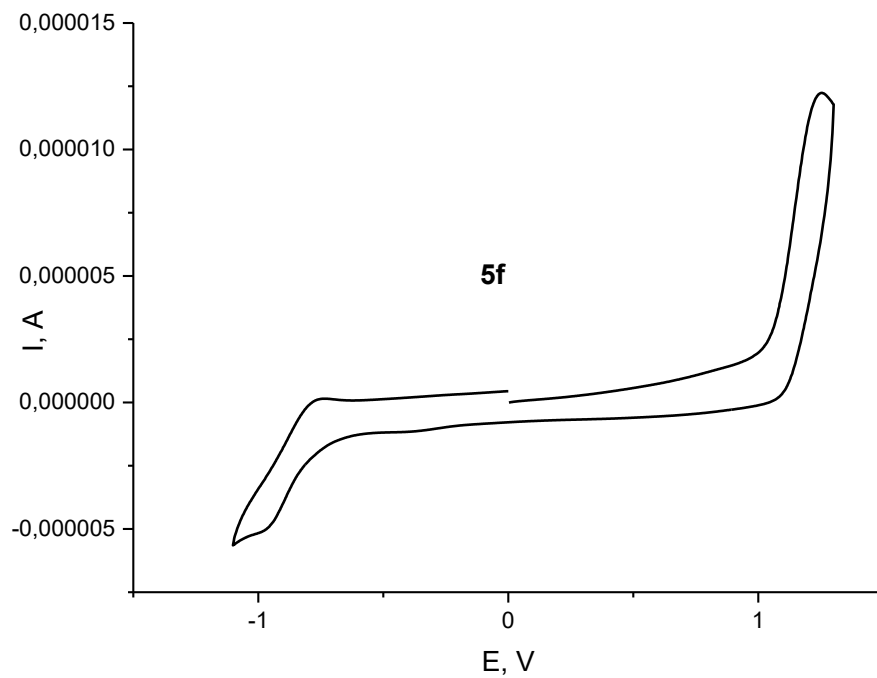


Figure S66. Cyclic voltammogram of **5f**

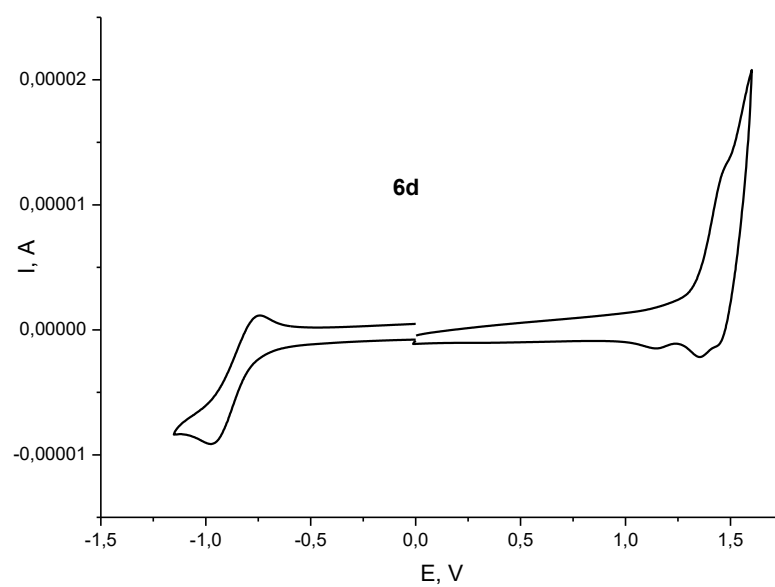


Figure S67. Cyclic voltammogram of **6d**

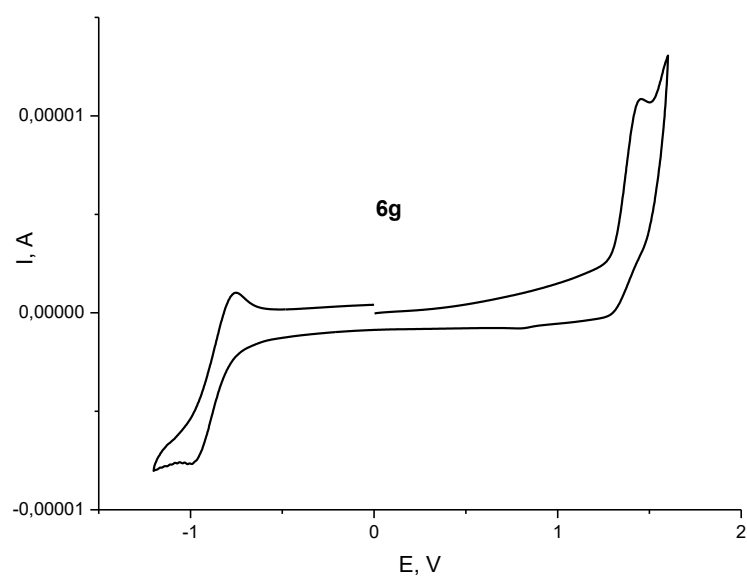


Figure S68. Cyclic voltammogram of **6g**

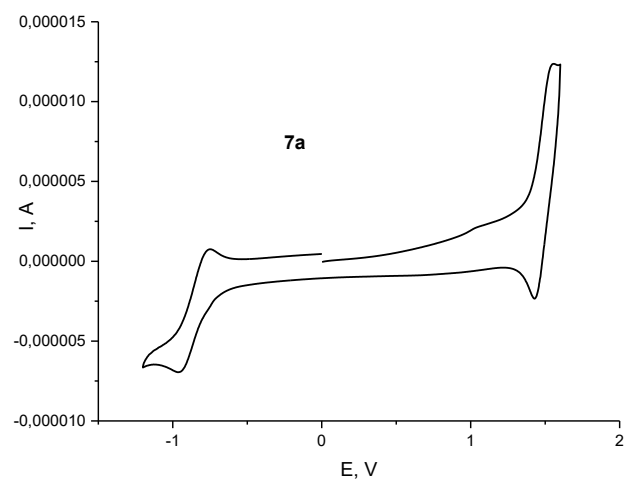


Figure S69. Cyclic voltammogram of **7a**