Electronic Supplementary Information

Reactivity of alkynylindole-2-carboxamides in [Pd]-catalysed C-H activation and phase transfer catalysis: Formation of pyrrolo-diindolones vs β-carbolinones

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(1) Crystal data for the compounds 9a and 10h

X-ray Data. X-ray data for compounds **9a** and **10h**, were collected using MoK_α (λ = 0.71073 Å) radiation. The structures were solved and refined by standard methods as mentioned in the main text. The CCDC numbers are 1453189-1453190.

Compound 9a

Red color needle, $C_{31}H_{202}N_2O_2$, *M* = 454.51, Triclinic, Space group *P-1*, *a* = 9.4276(5), *b* = 11.2761(9), *c* = 11.6981(10) Å, *V* = 1137.32(14) $Å^3$, α = 112.674(8), β = 90.151(5), γ = 96.976(5), *Z* = 2, μ = 0.660 mm^{-1}, data/restraints/parameters: 4333/0/317, R indices (I> 2σ(I)): R1 = 0.0449, *w*R2 (all data) = 0.1166, CCDC No. 1453189.

Compound 10h

Colorless block, $C_{26}H_{22}N_2O_2$, *M* = 394.46, Triclinic, Space group *P-1*, *a* = 11.5059(4), *b* = 12.8459(6), *c* = 15.6020(8) Å, α = 106.081(4), β = 93.226(4), γ = 109.728(4), *V* = 2056.95(16) $Å^3$, *Z* = 4, μ = 0.643 mm^{-1}, data/restraints/parameters: 7879/0/547, R indices (I> 2σ(I)): R1 = 0.0488, *w*R2 (all data) = 0.1277, CCDC No. 1453190.

(2) Copies of ^{1}H/ ^{13}C NMR spectra for starting precursors

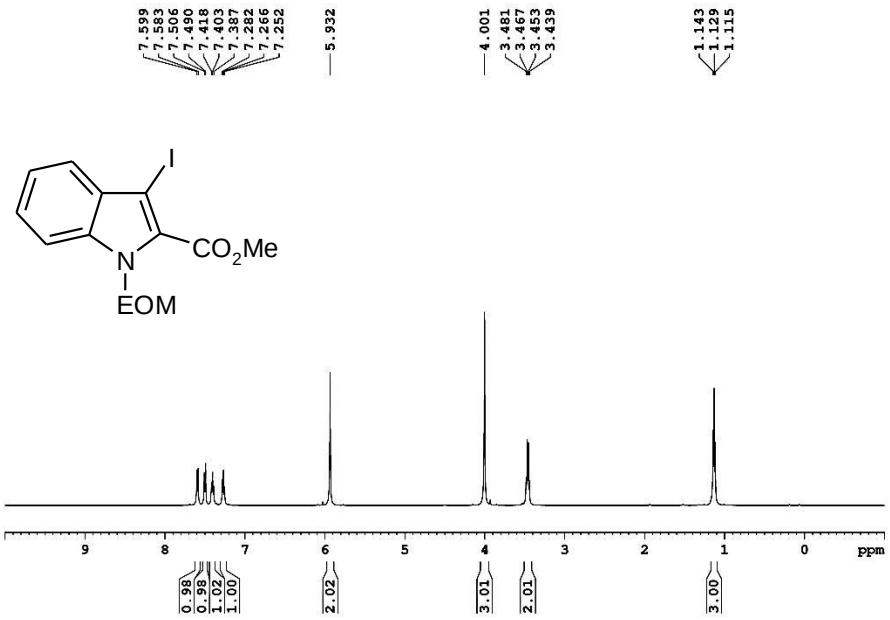

Figure S1. ^{1}H NMR spectrum of compound **5d**

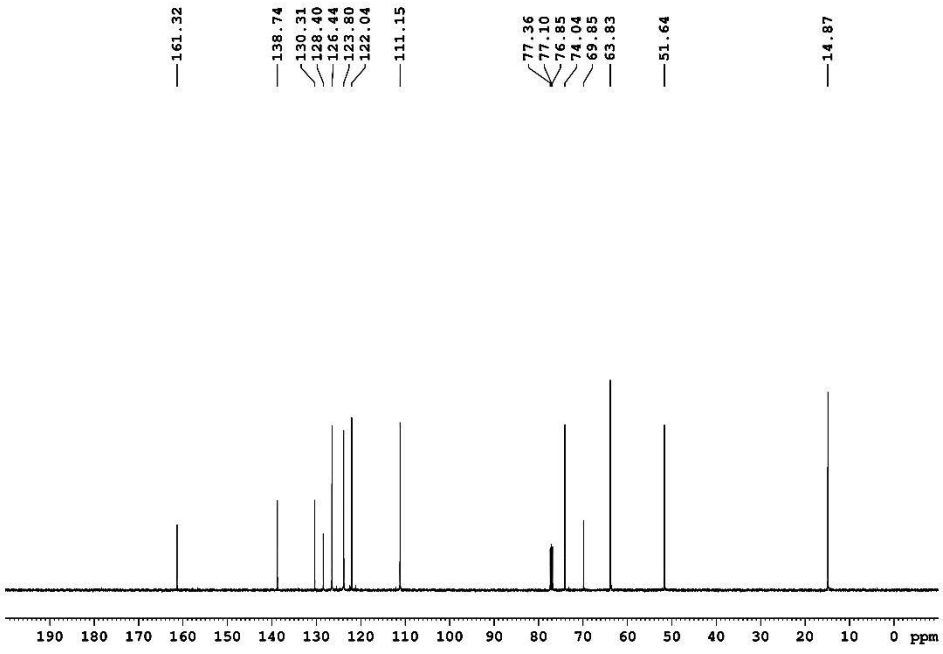

Figure S2. ^{13}C NMR spectrum of compound **5d**

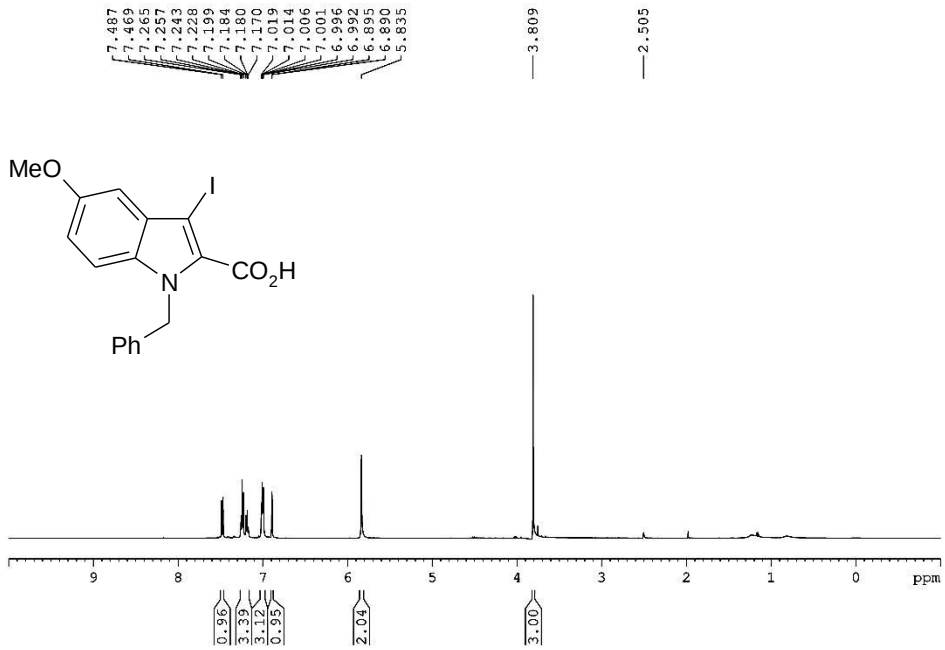

Figure S3. ^{1}H NMR spectrum of compound **6b**

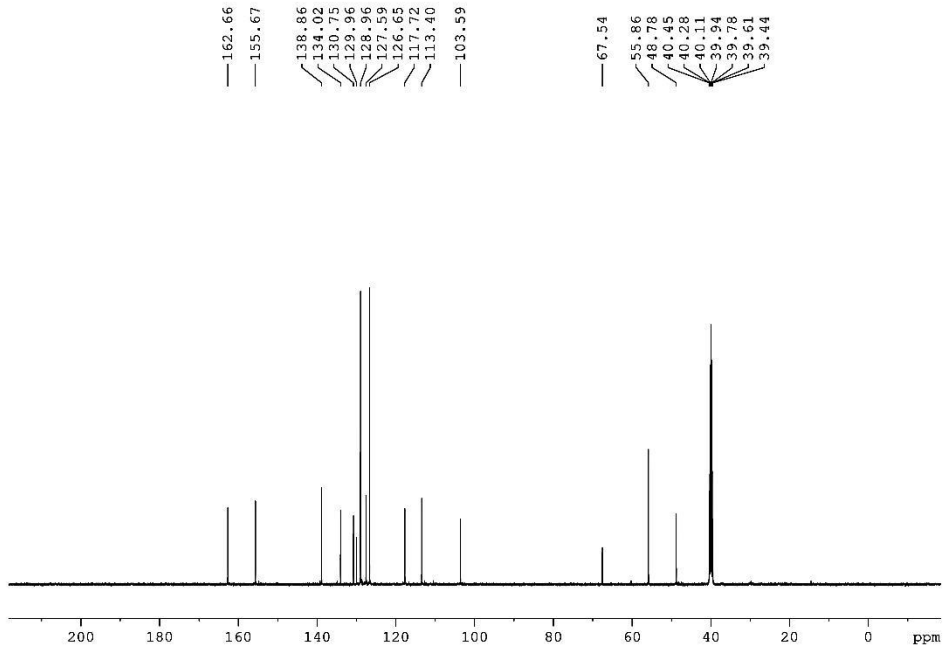

Figure S4. ^{13}C NMR spectrum of compound **6b**

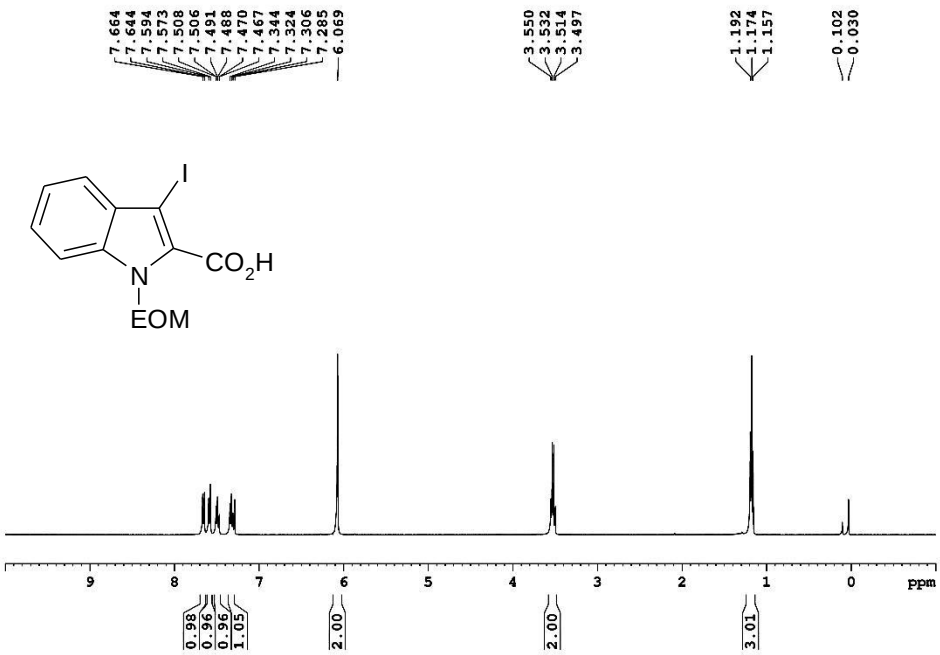

Figure S5. ^{1}H NMR spectrum of compound **6d**

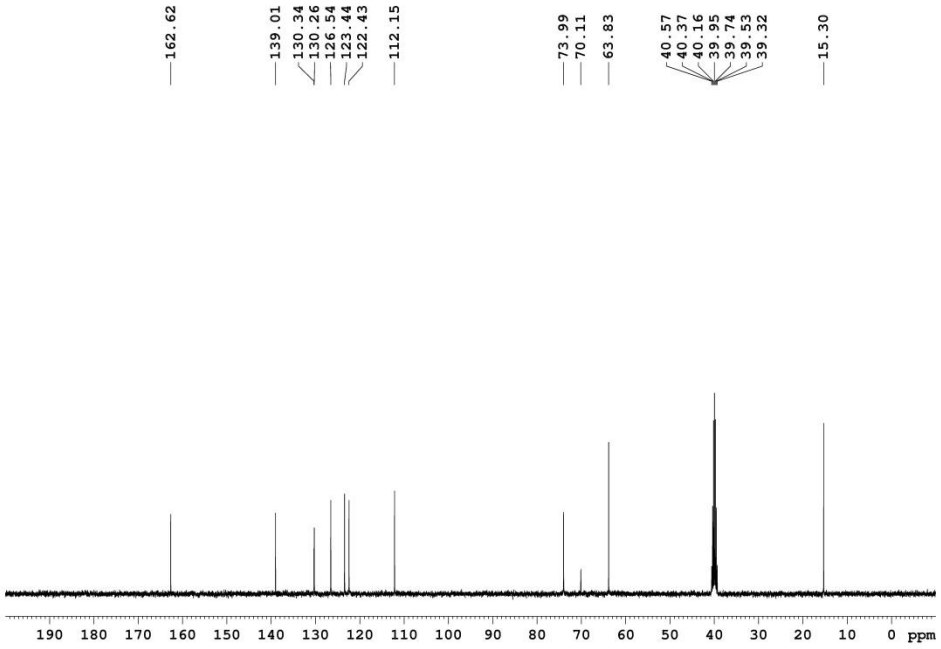

Figure S6. ^{13}C NMR spectrum of compound **6d**

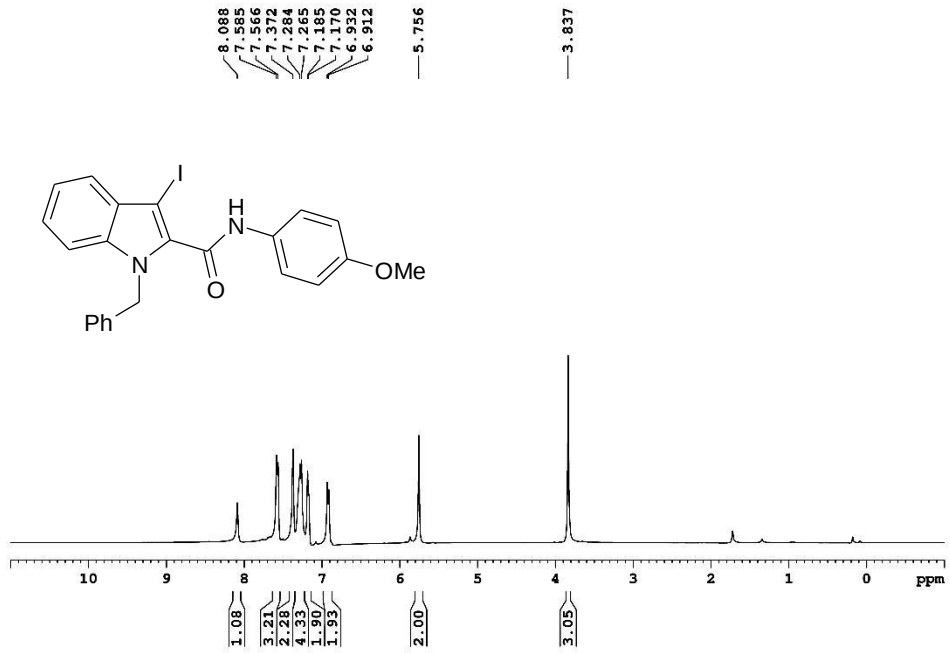

Figure S7. ^{1}H NMR spectrum of compound **7a**

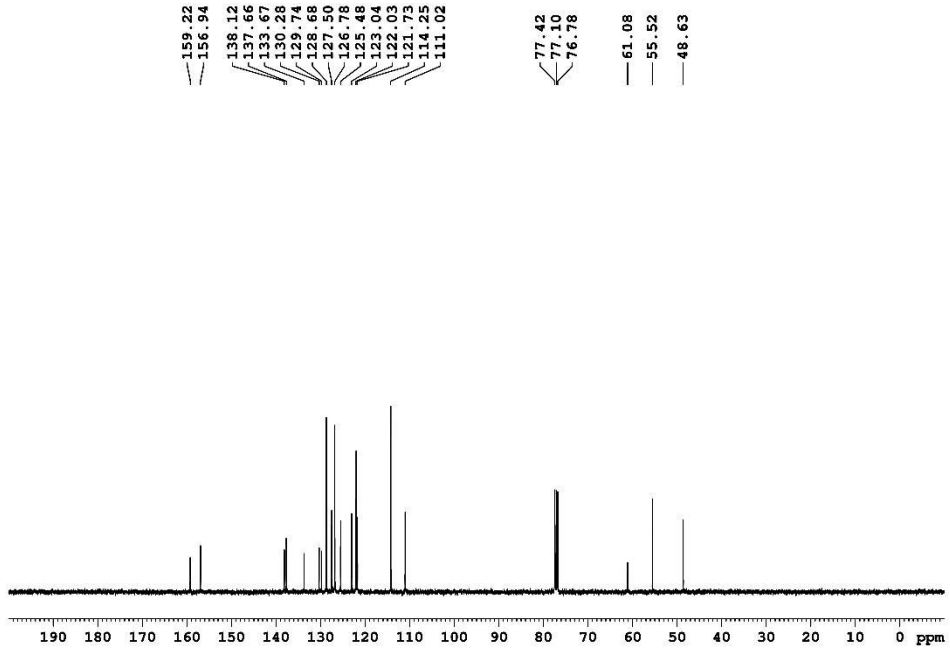

Figure S8. ^{13}C NMR spectrum of compound **7a**

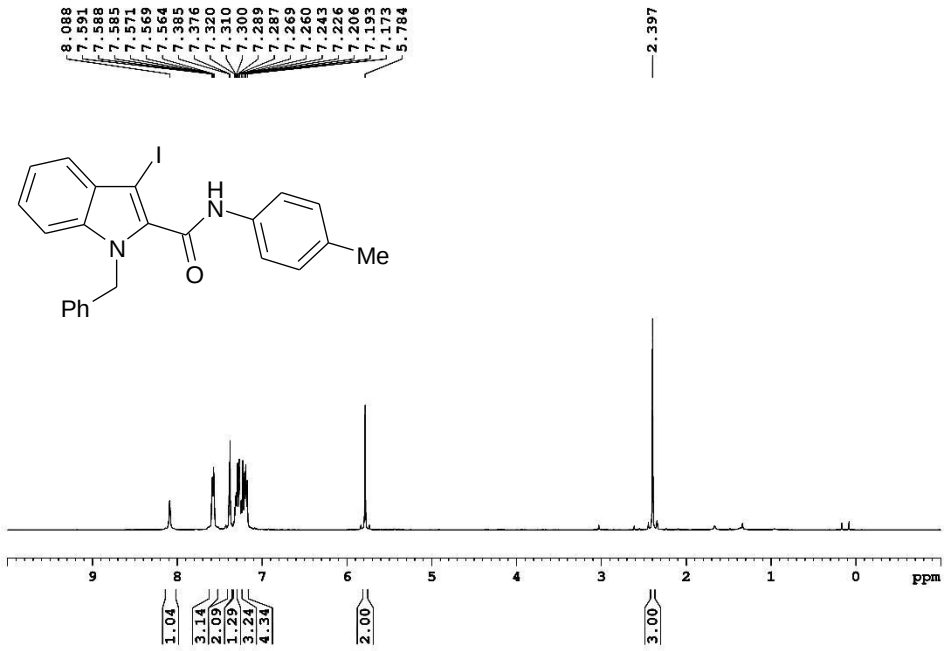

Figure S9. ^{1}H NMR spectrum of compound **7b**

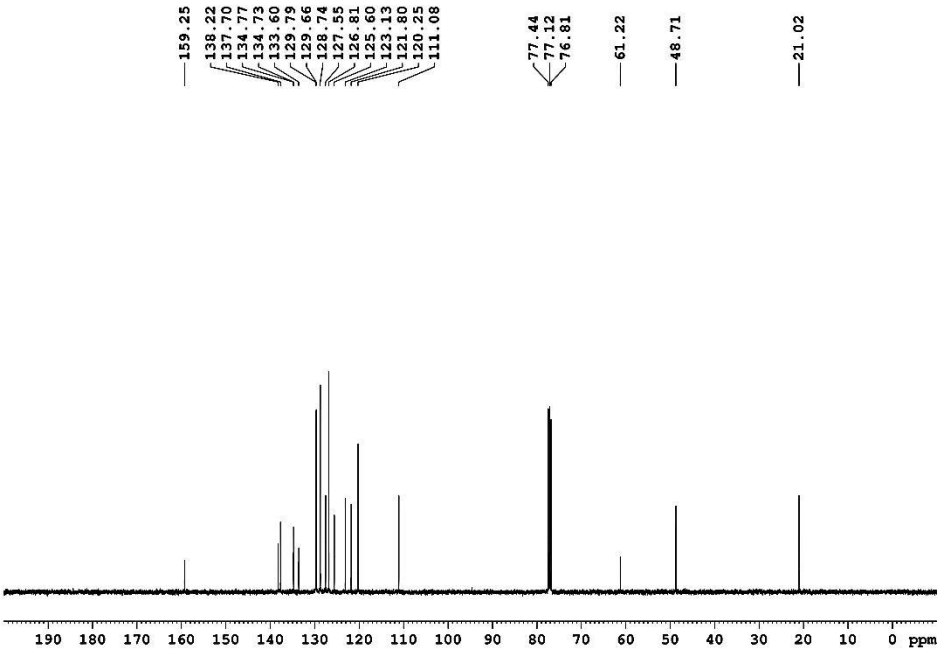

Figure S10. ^{13}C NMR spectrum of compound **7b**

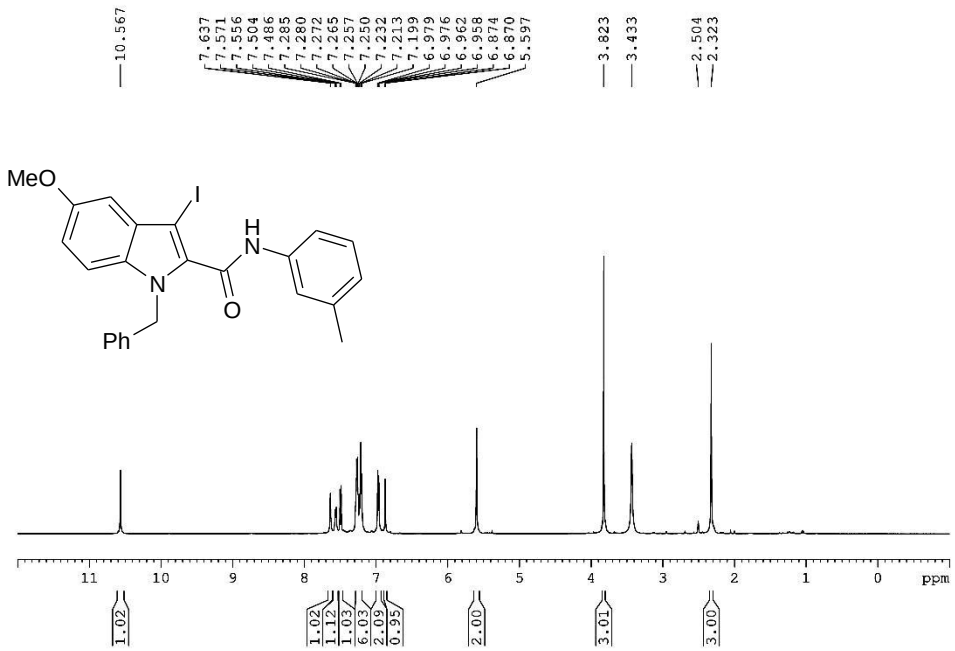

Figure S11. ^{1}H NMR spectrum of compound **7c**

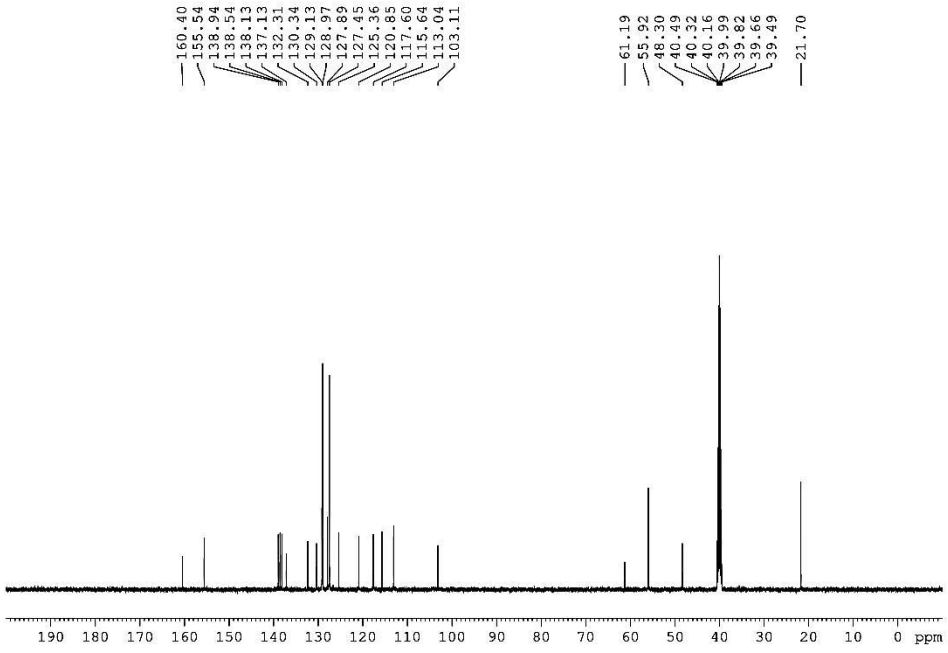

Figure S12. ^{13}C NMR spectrum of compound **7c**

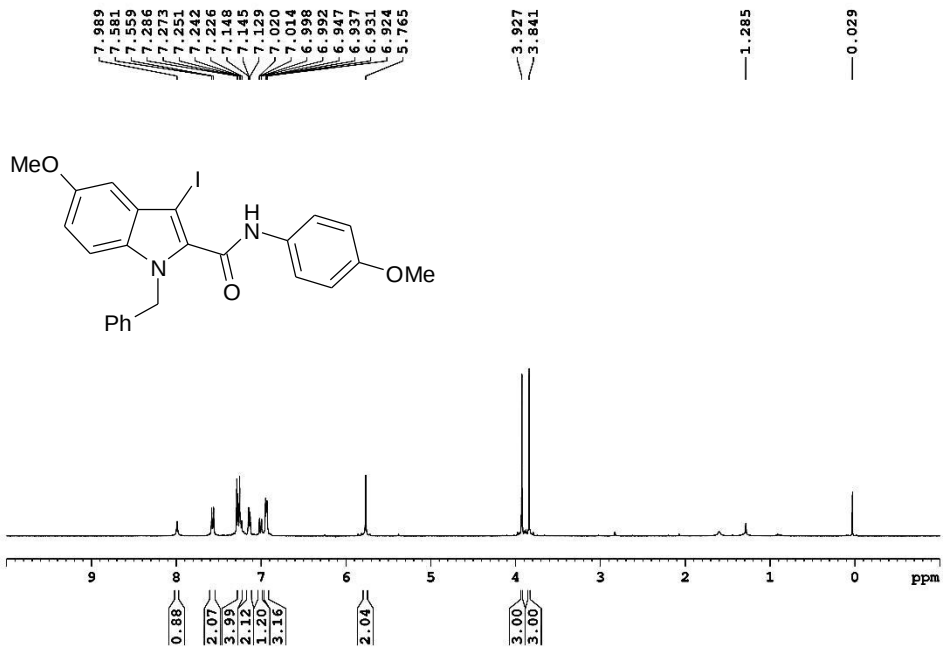

Figure S13. ^{1}H NMR spectrum of compound **7d**

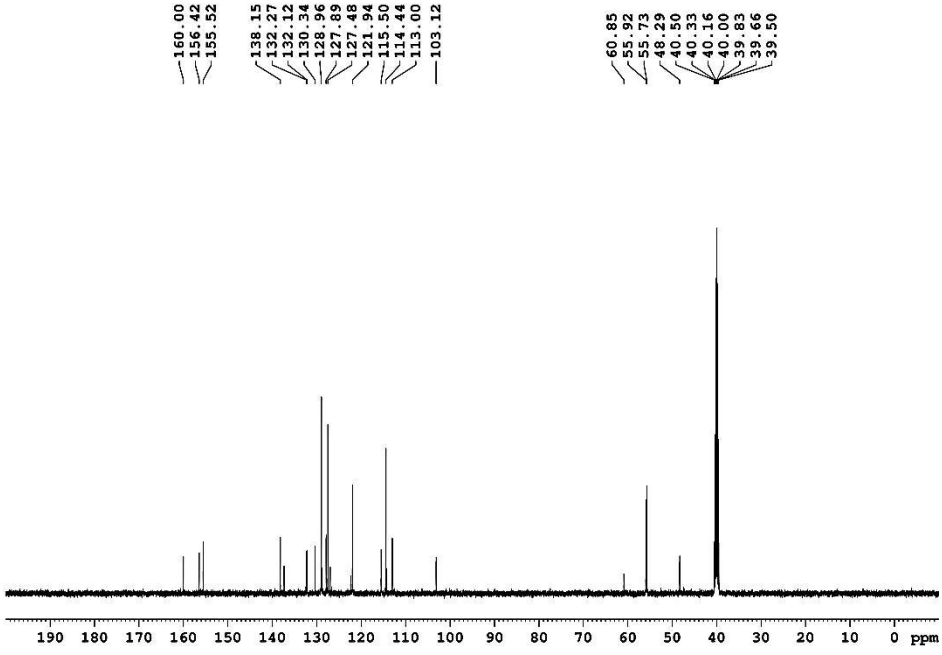

Figure S14. ^{13}C NMR spectrum of compound **7d**

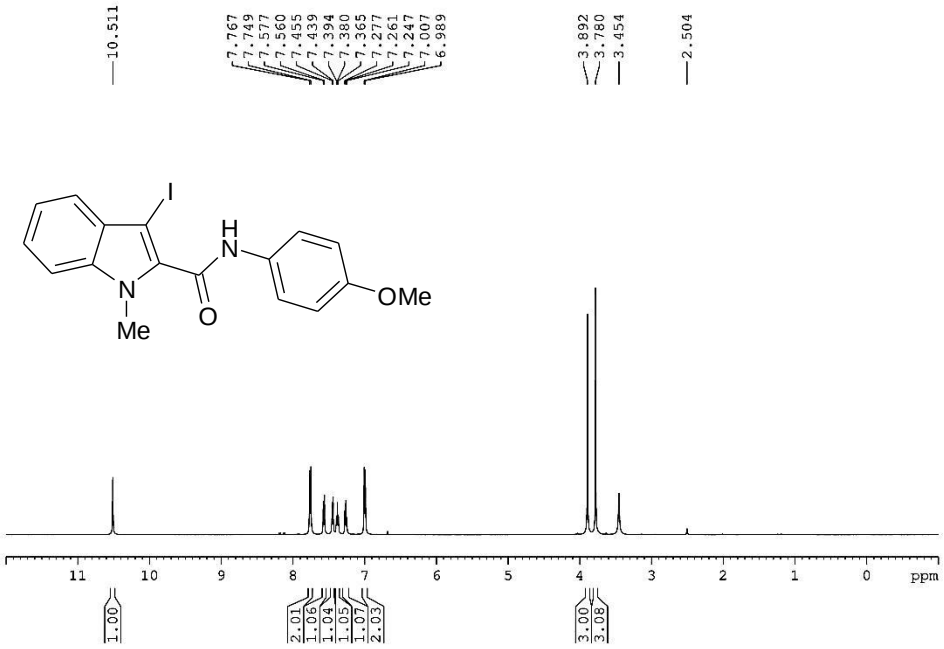

Figure S15. ^{1}H NMR spectrum of compound **7e**

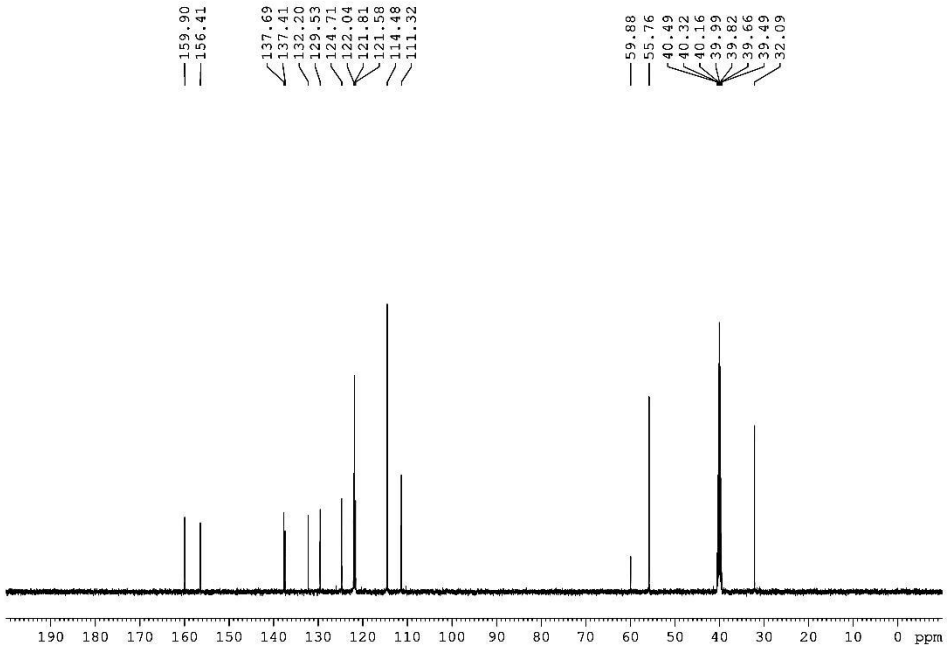

Figure S16. ^{13}C NMR spectrum of compound **7e**

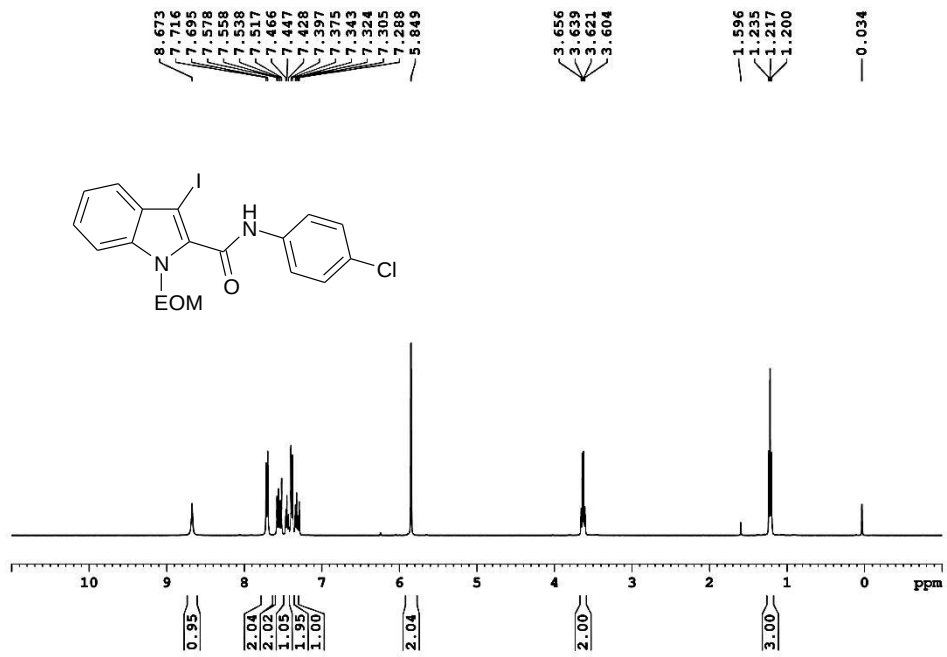

Figure S17. ^{1}H NMR spectrum of compound **7f**

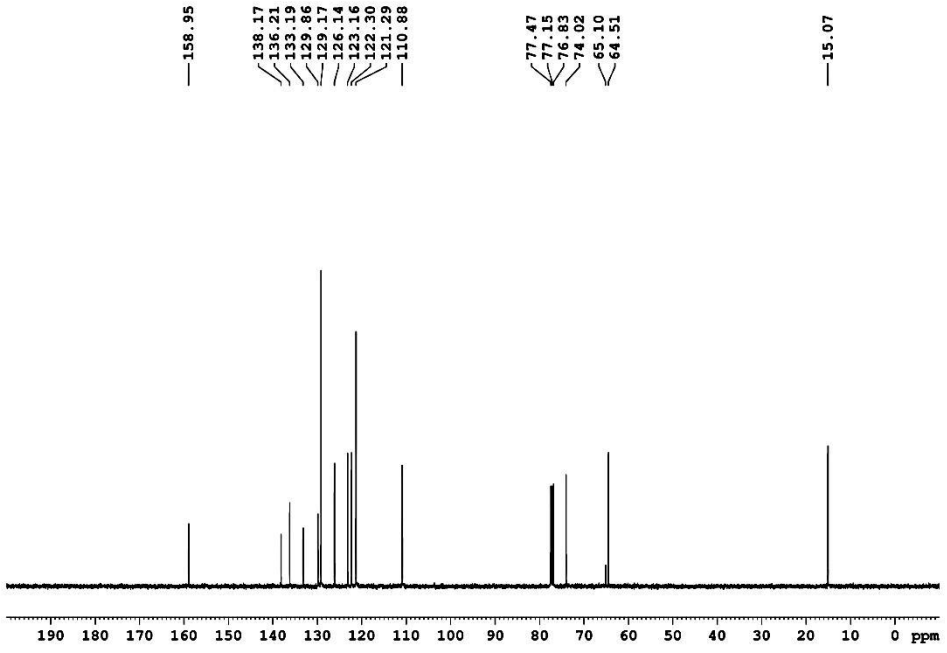

Figure S18. ^{13}C NMR spectrum of compound **7f**

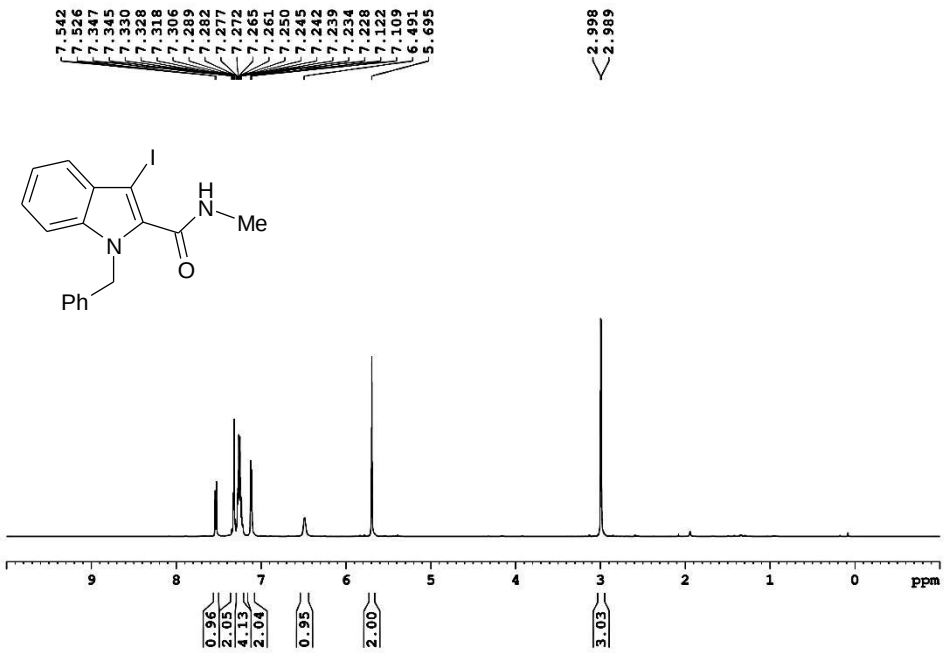

Figure S19. ^{1}H NMR spectrum of compound **7g**

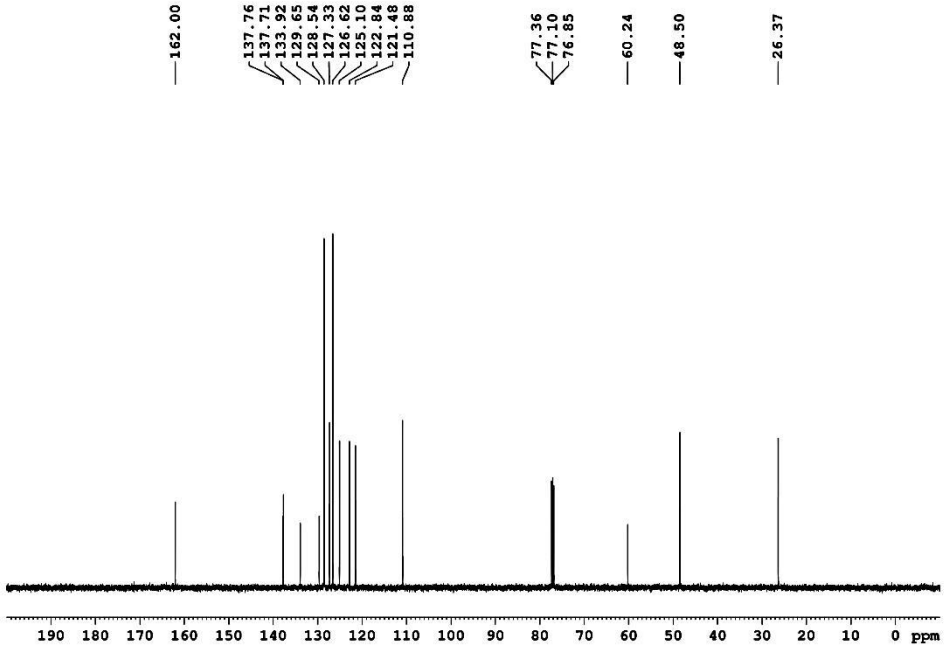

Figure S20. ^{13}C NMR spectrum of compound **7g**

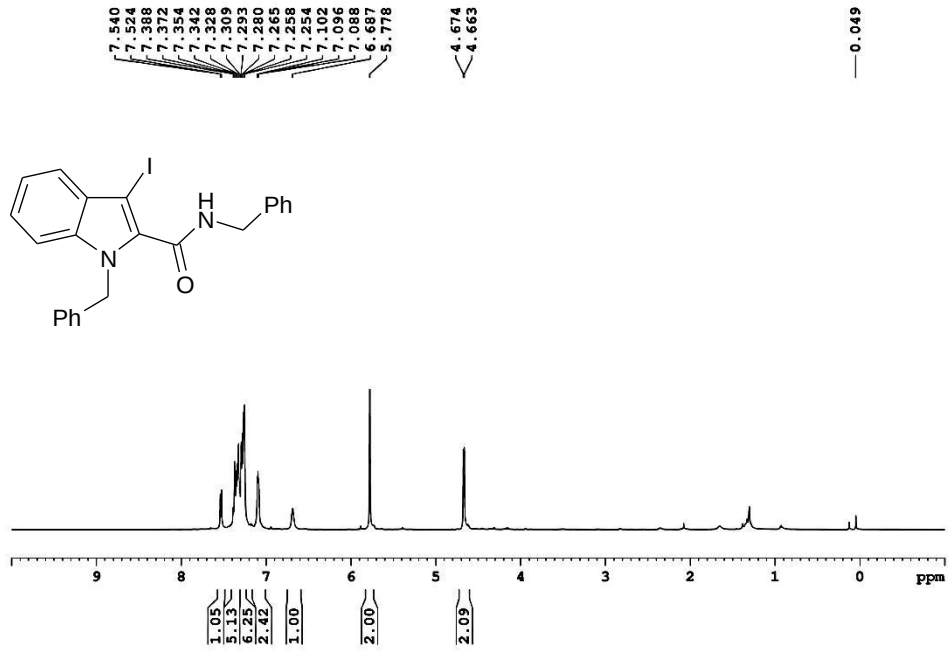

Figure S21. ^{1}H NMR spectrum of compound **7h**

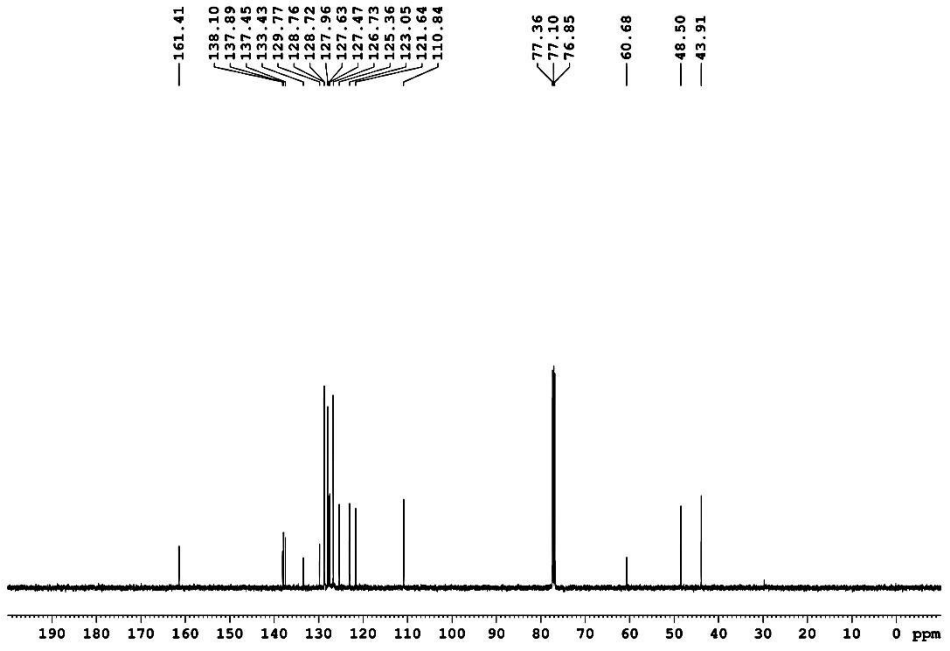

Figure S22. ^{13}C NMR spectrum of compound **7h**

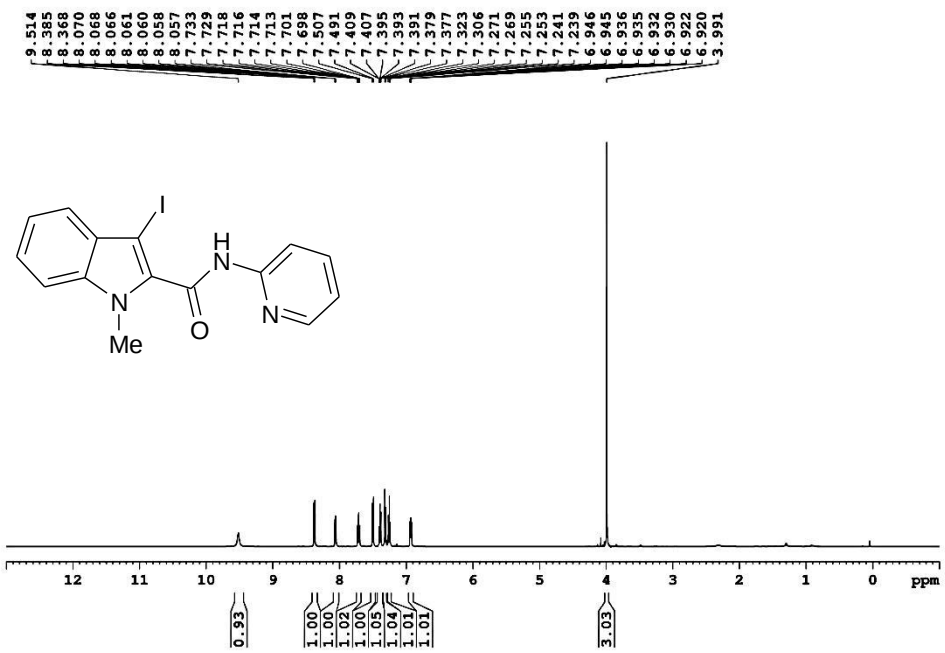

Figure S23. ^{1}H NMR spectrum of compound **7i**

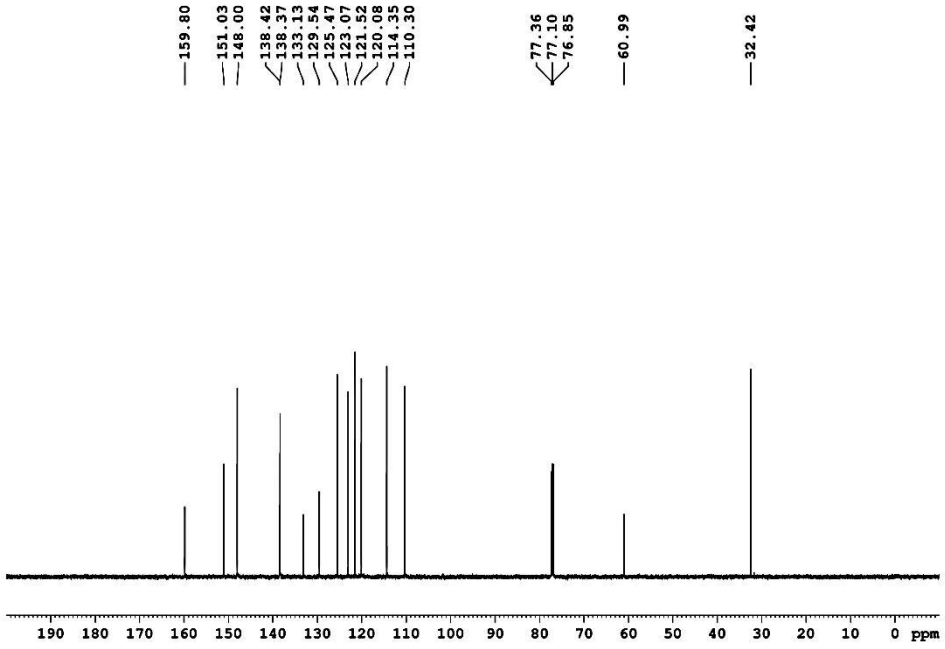

Figure S24. ^{13}C NMR spectrum of compound **7i**

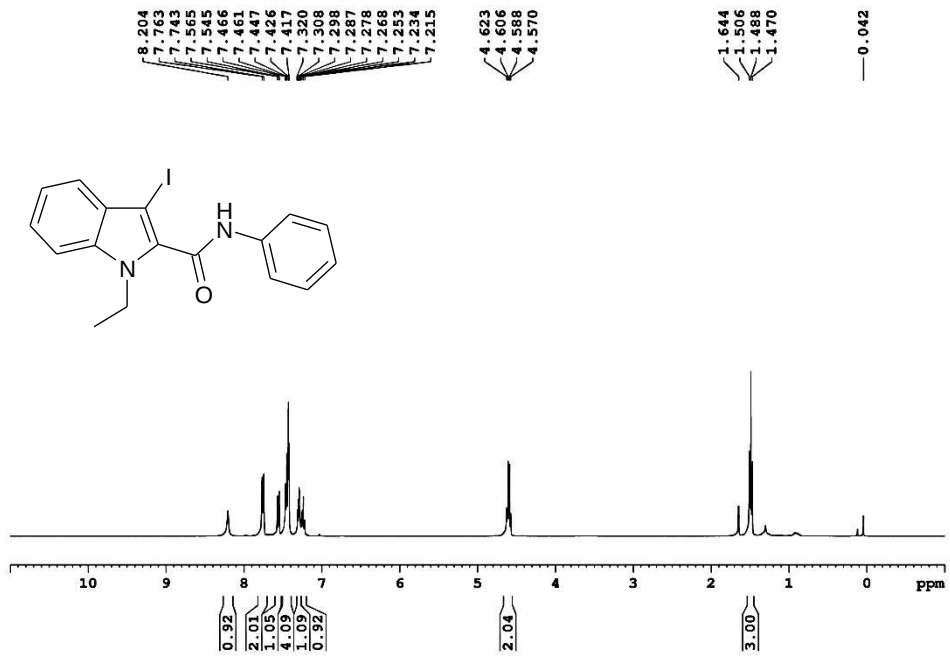

Figure S25. ^{1}H NMR spectrum of compound **7j**

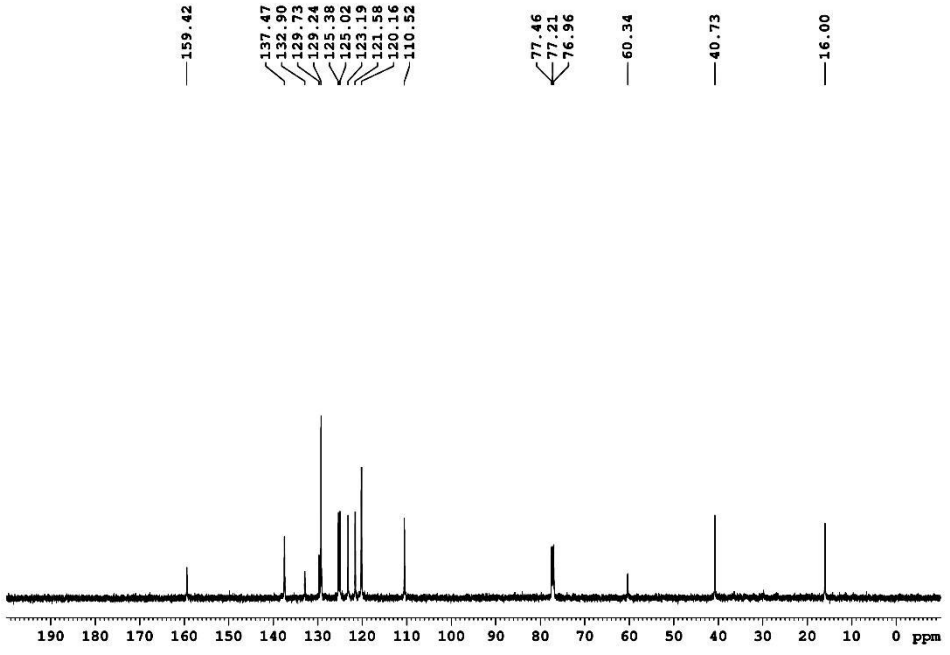

Figure S26. ^{13}C NMR spectrum of compound **7j**

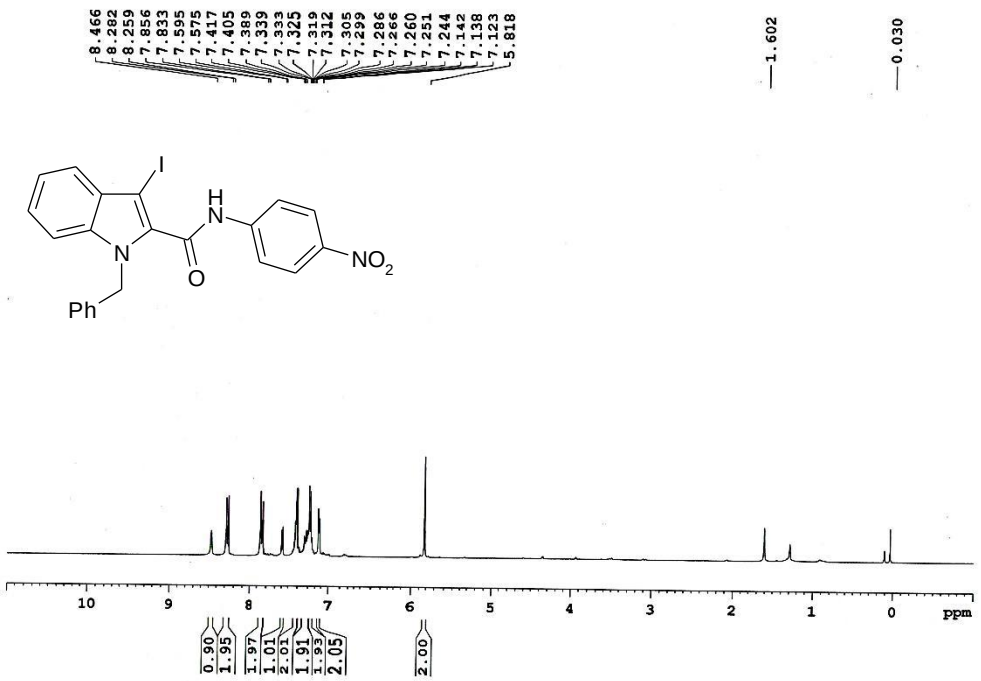

Figure S27. ^{1}H NMR spectrum of compound **7k**

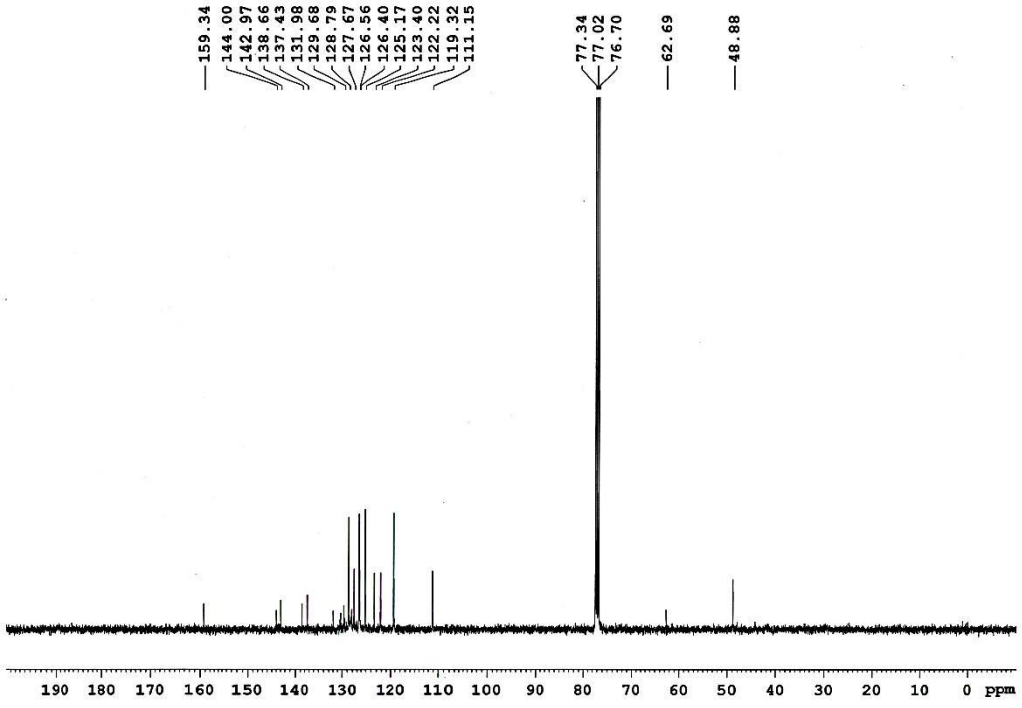

Figure S28. ^{13}C NMR spectrum of compound **7k**

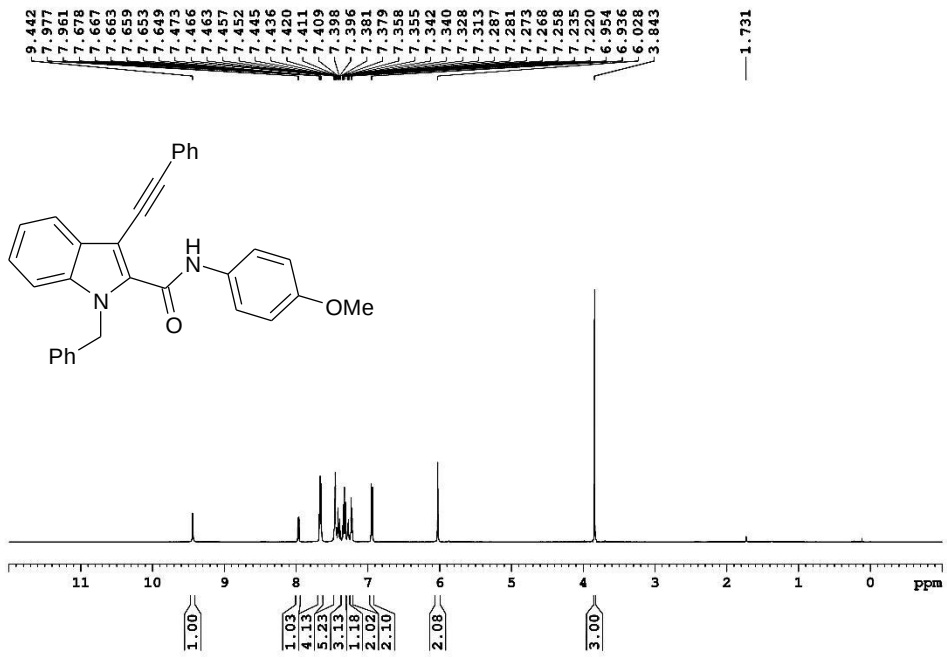

Figure S29. ^{1}H NMR spectrum of compound **8a**

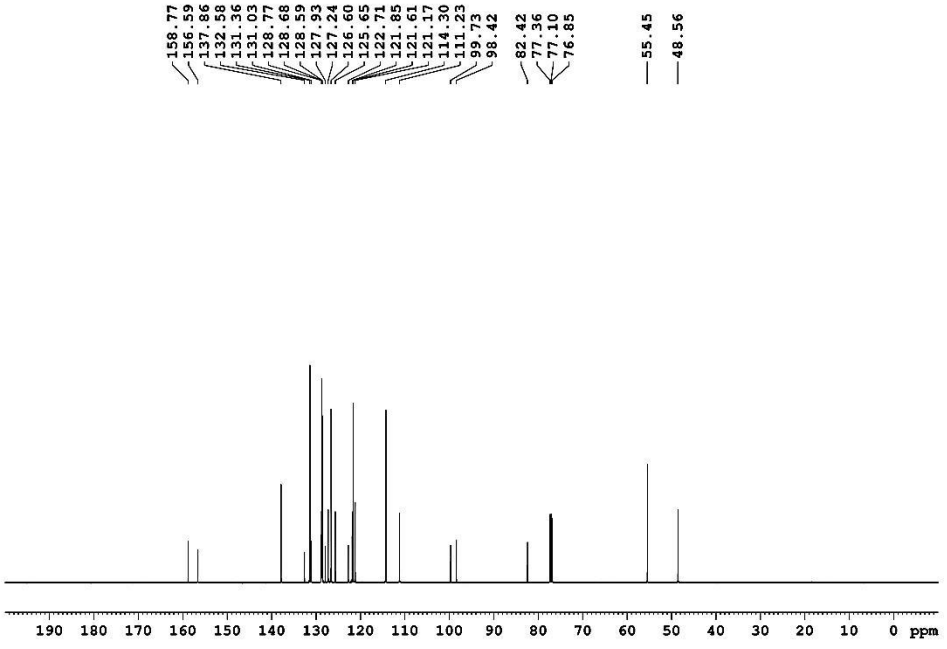

Figure S30. ^{13}C NMR spectrum of compound **8a**

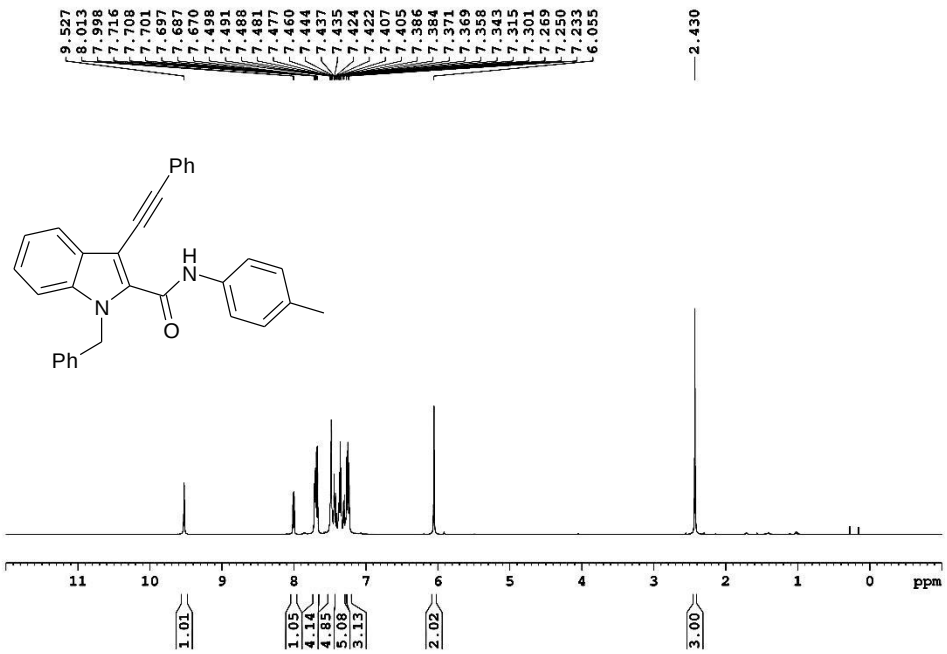

Figure S31. ^{1}H NMR spectrum of compound **8b**

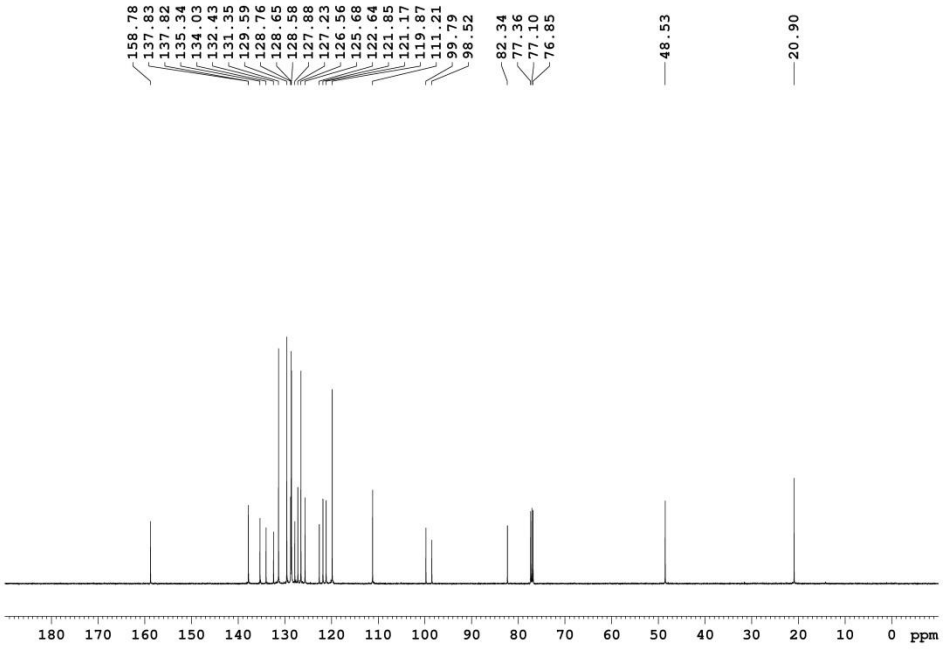

Figure S32. ^{13}C NMR spectrum of compound **8b**

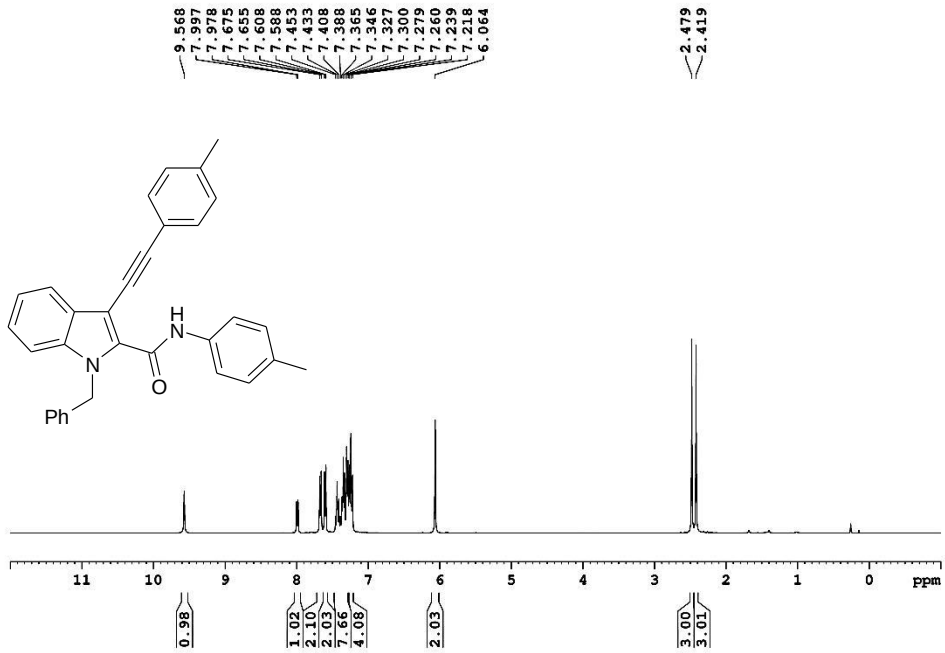

Figure S33. ^{1}H NMR spectrum of compound **8c**

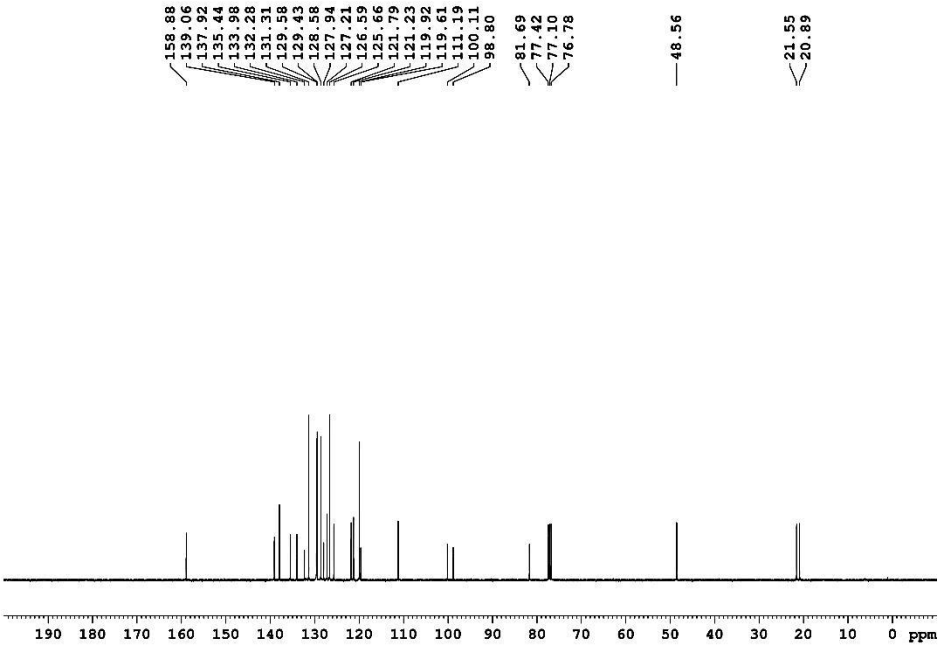

Figure S34. ^{13}C NMR spectrum of compound **8c**

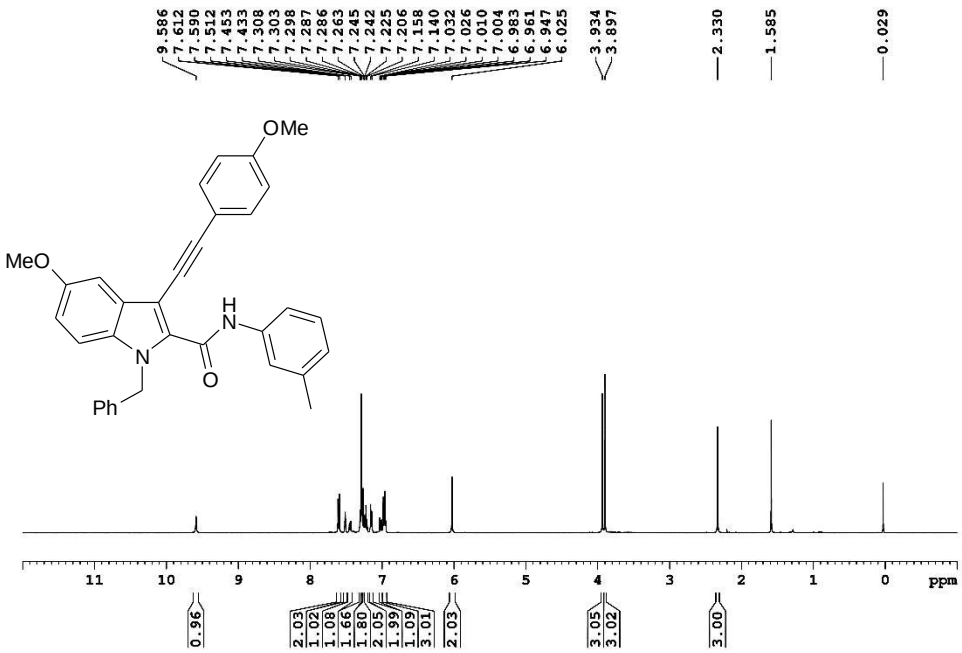

Figure S35. ^{1}H NMR spectrum of compound **8d**

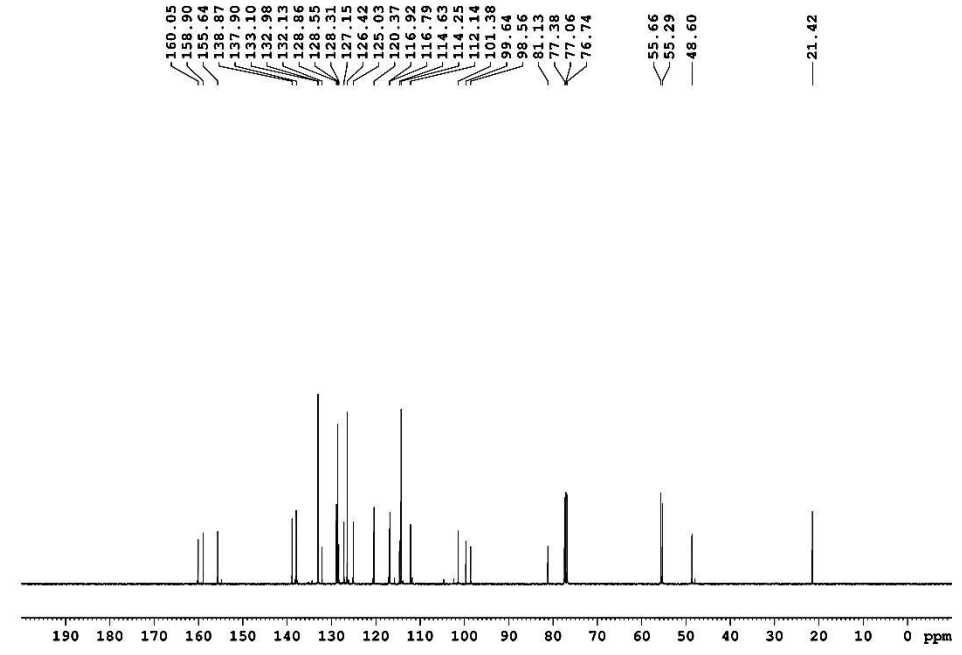

Figure S36. ^{13}C NMR spectrum of compound **8d**

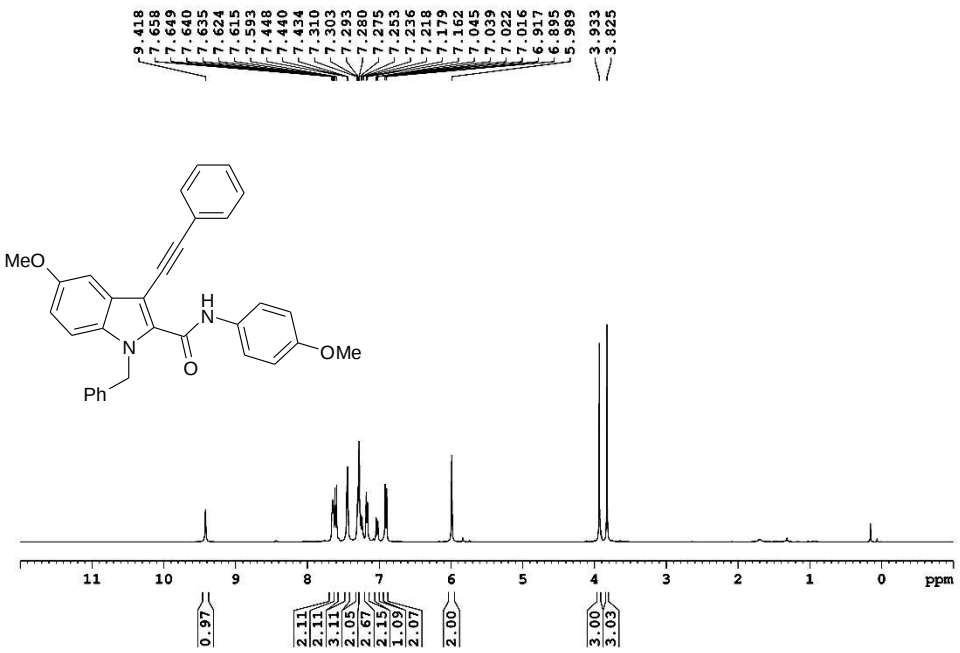

Figure S37. ^{1}H NMR spectrum of compound **8e**

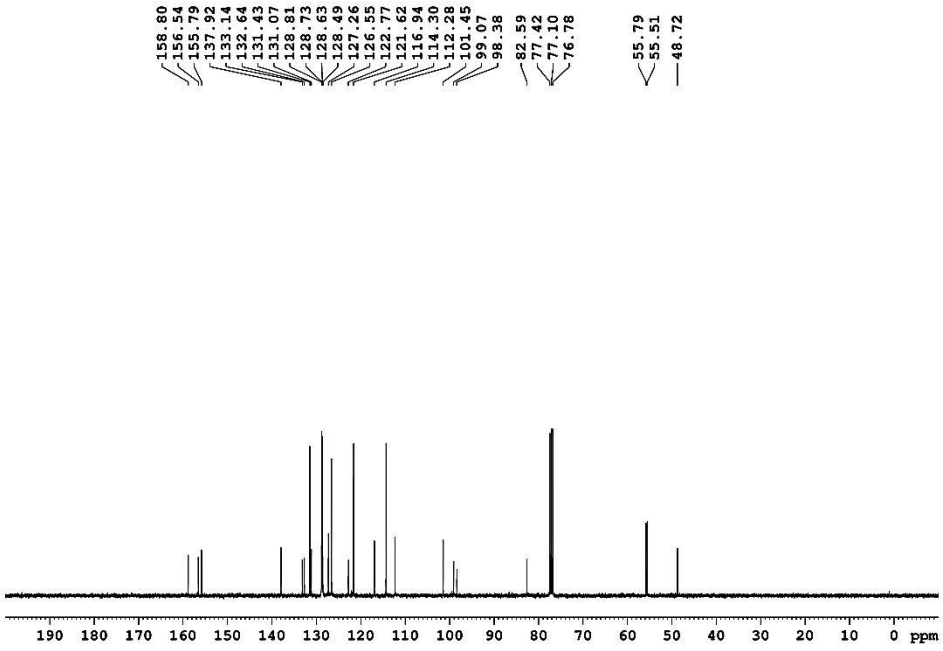

Figure S38. ^{13}C NMR spectrum of compound **8e**

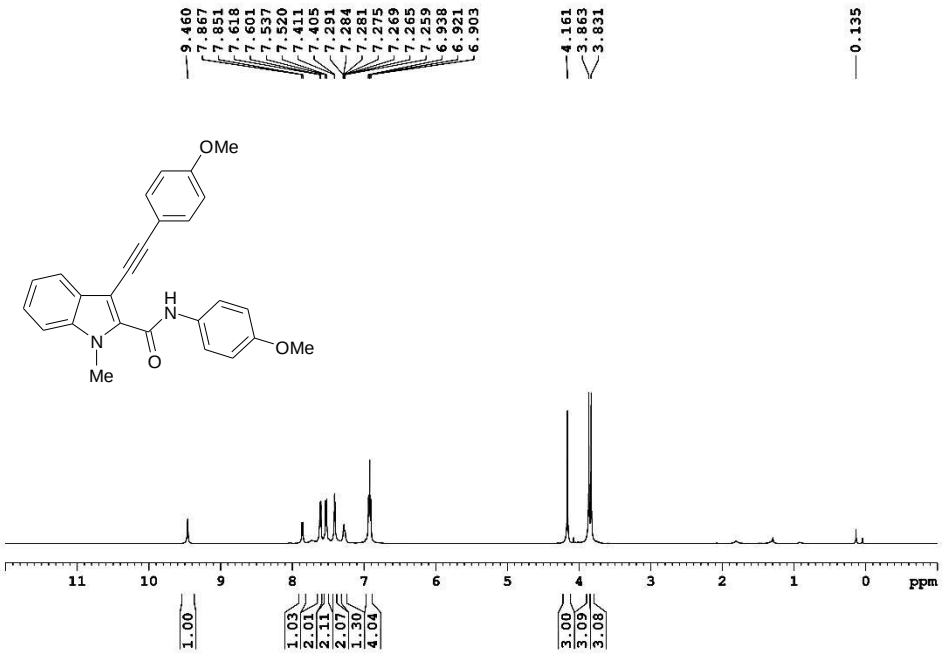

Figure S39. ^{1}H NMR spectrum of compound **8f**

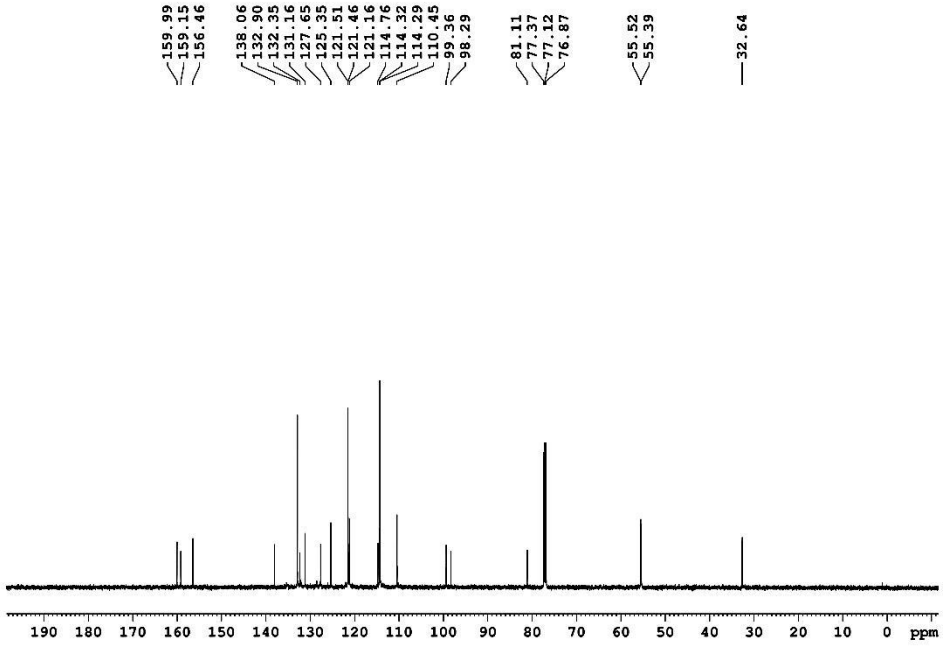

Figure S40. ^{13}C NMR spectrum of compound **8f**

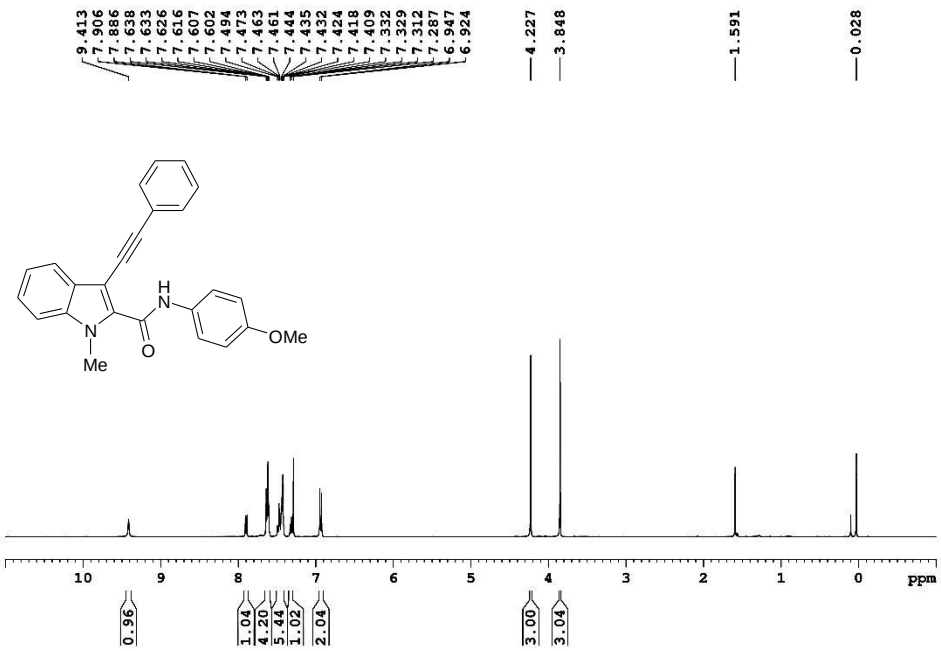

Figure S41. ^{1}H NMR spectrum of compound **8g**

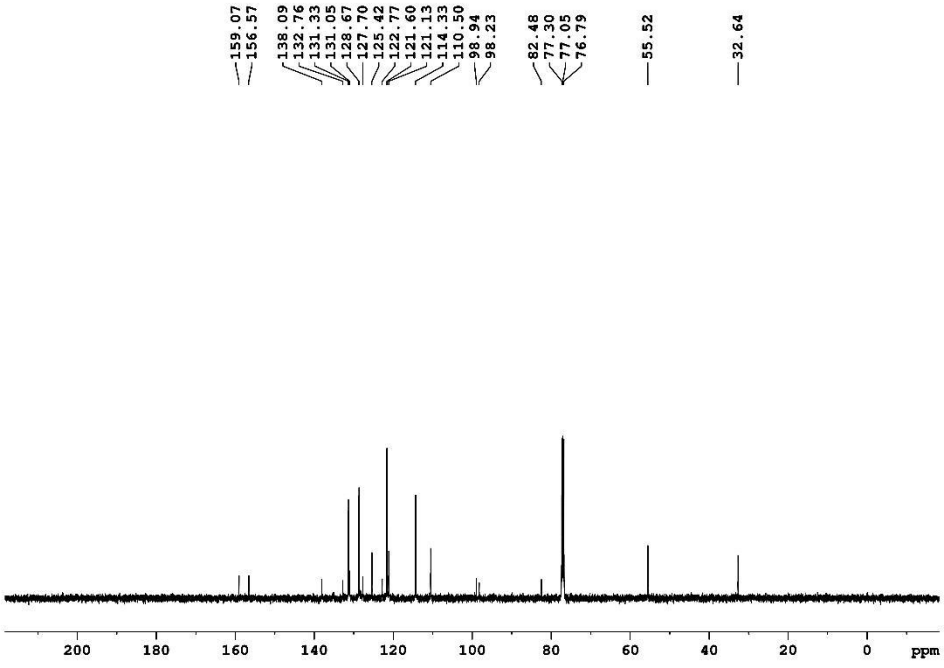

Figure S42. ^{13}C NMR spectrum of compound **8g**

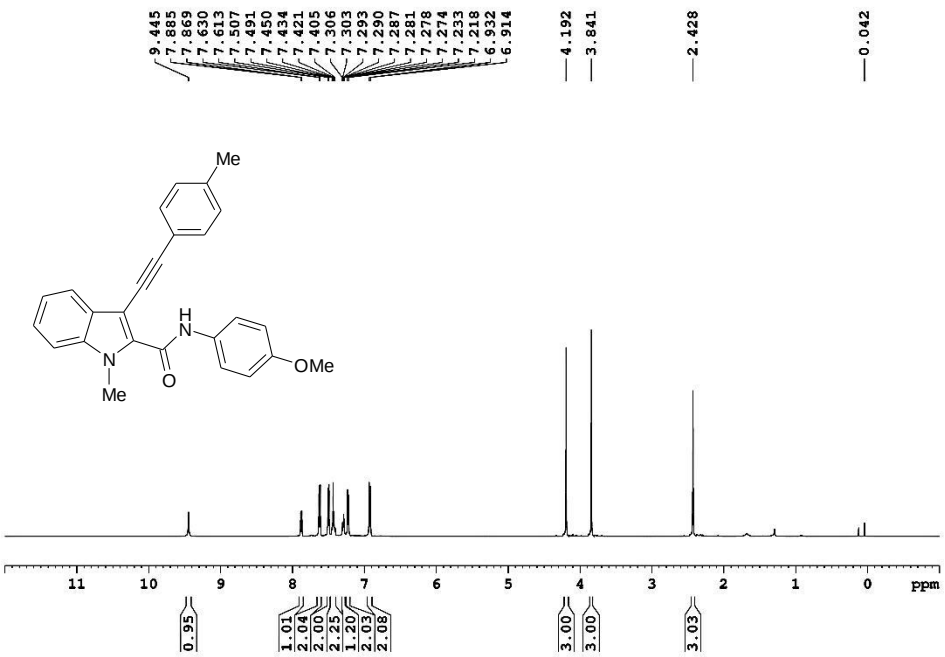

Figure S43. ^{1}H NMR spectrum of compound **8h**

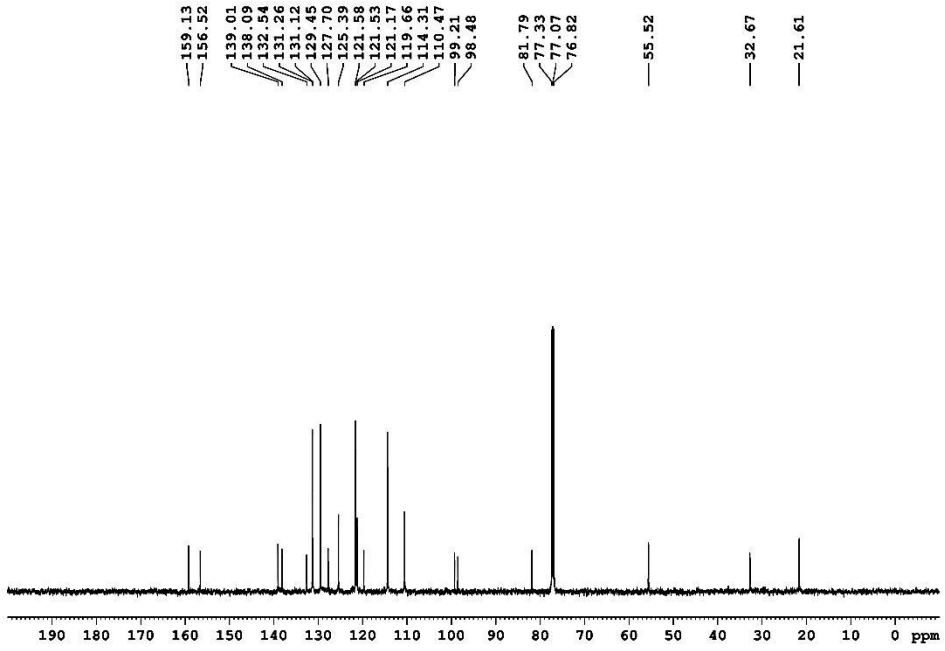

Figure S44. ^{13}C NMR spectrum of compound **8h**

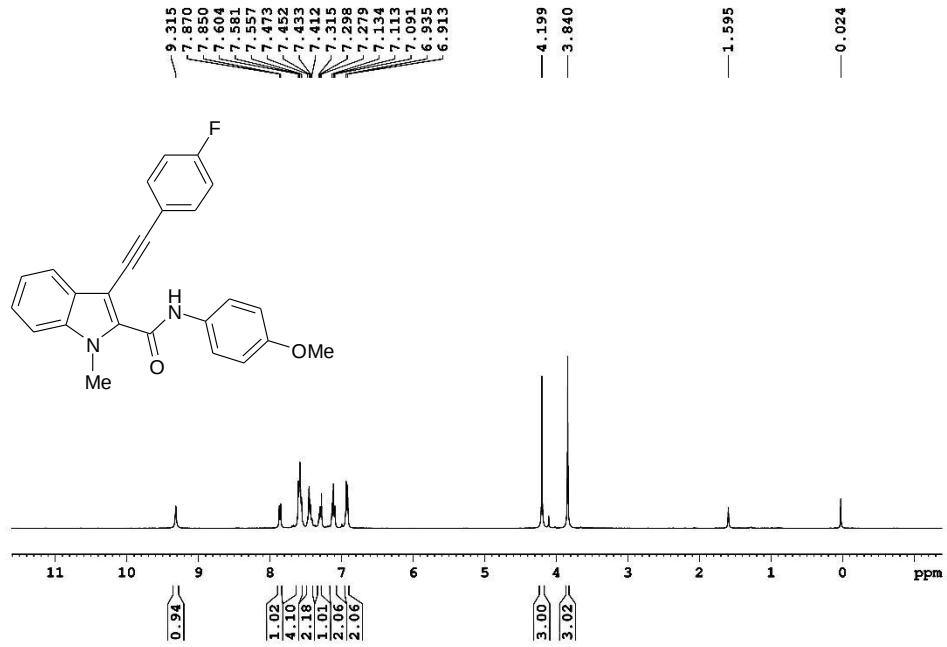

Figure S45. ^{1}H NMR spectrum of compound **8i**

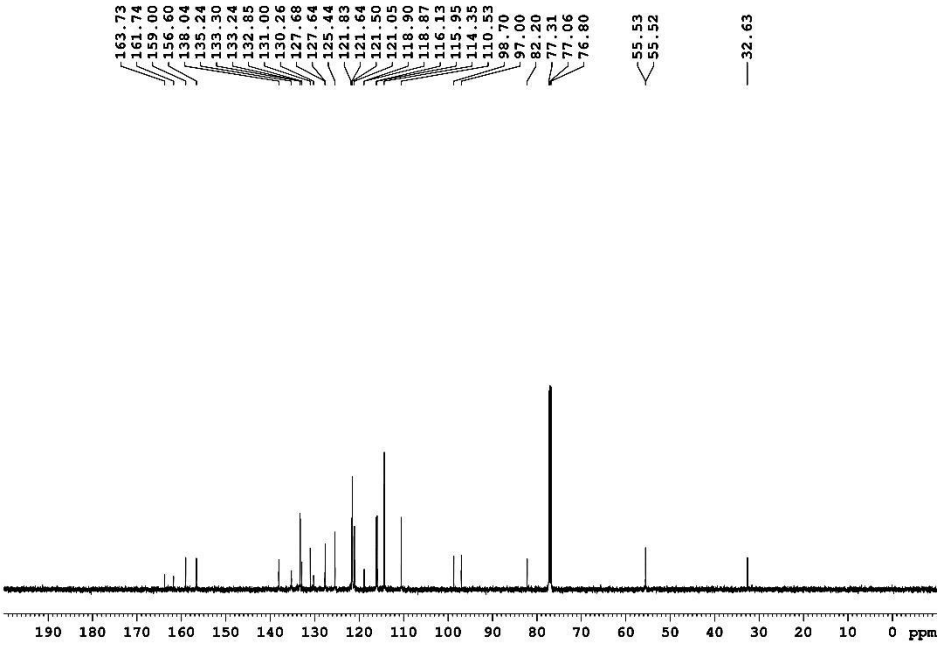

Figure S46. ^{13}C NMR spectrum of compound **8i**

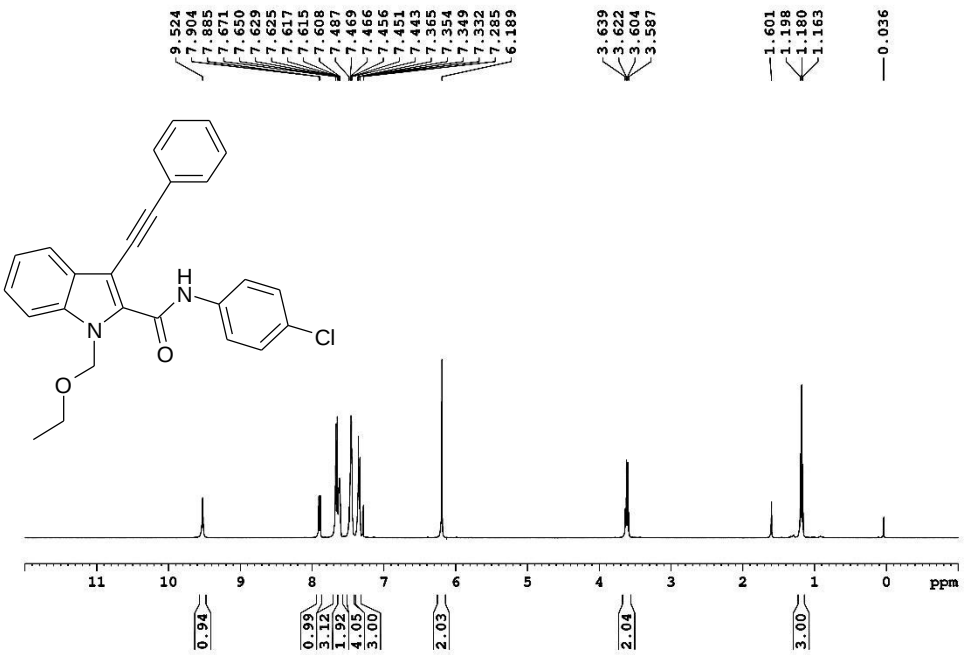

Figure S47. ^{1}H NMR spectrum of compound **8j**

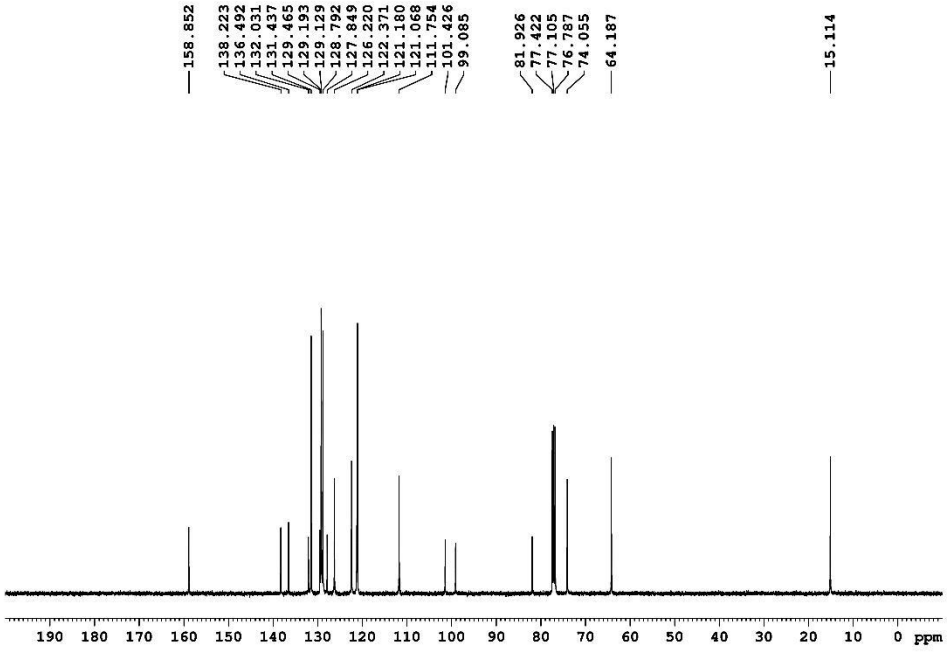

Figure S48. ^{13}C NMR spectrum of compound **8j**

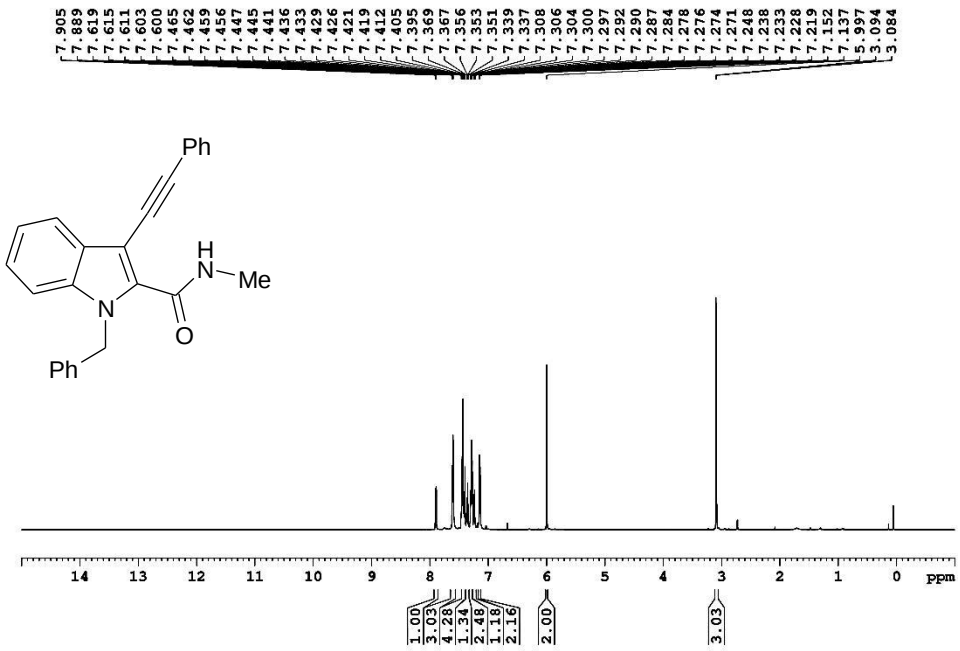

Figure S49. ^{1}H NMR spectrum of compound **8k**

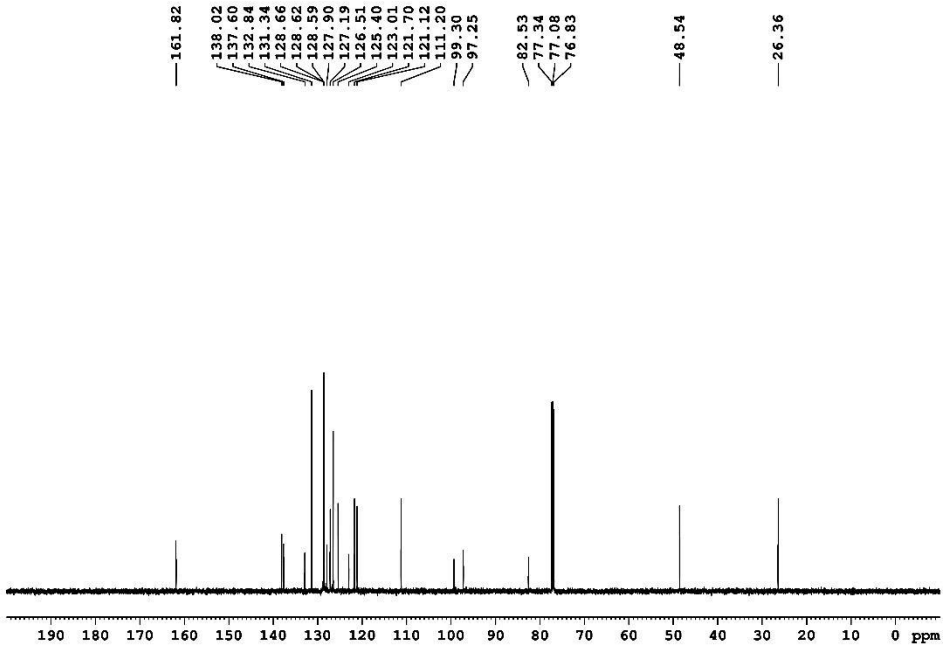

Figure S50. ^{13}C NMR spectrum of compound **8k**

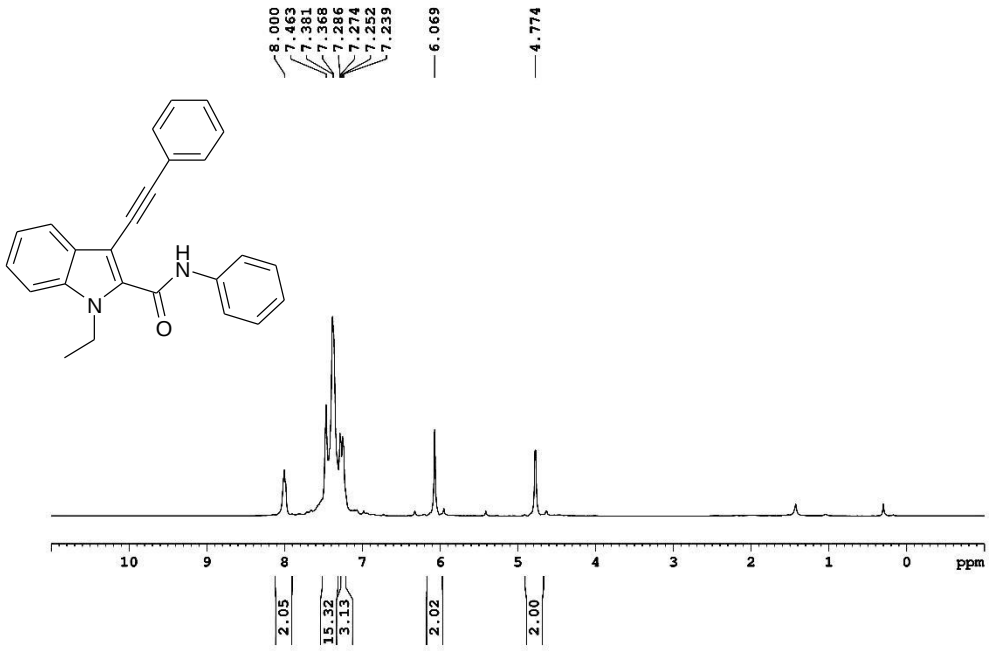

Figure S51. ^{1}H NMR spectrum of compound **8l**

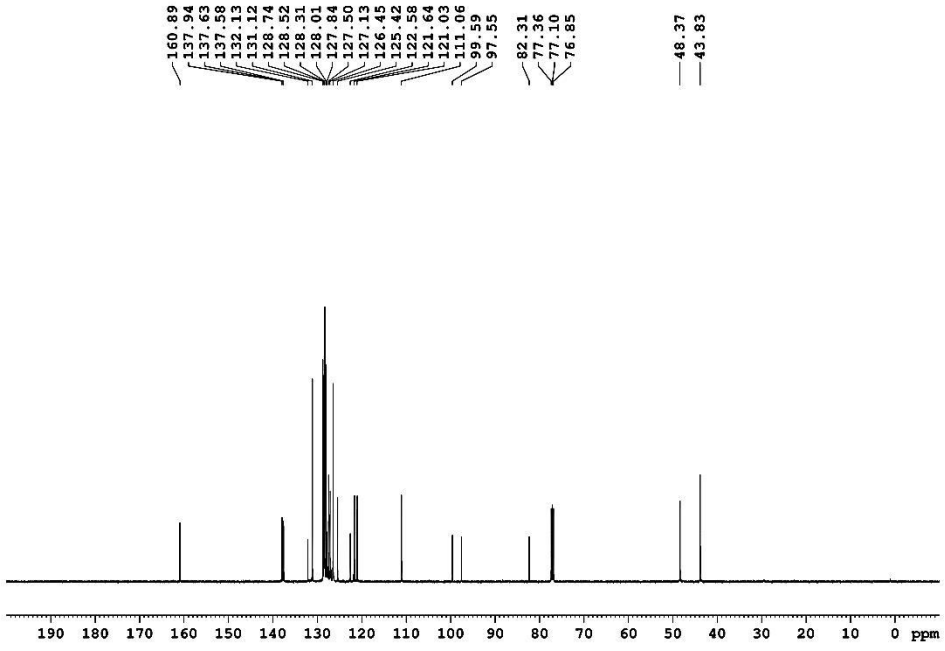

Figure S52. ^{13}C NMR spectrum of compound **8l**

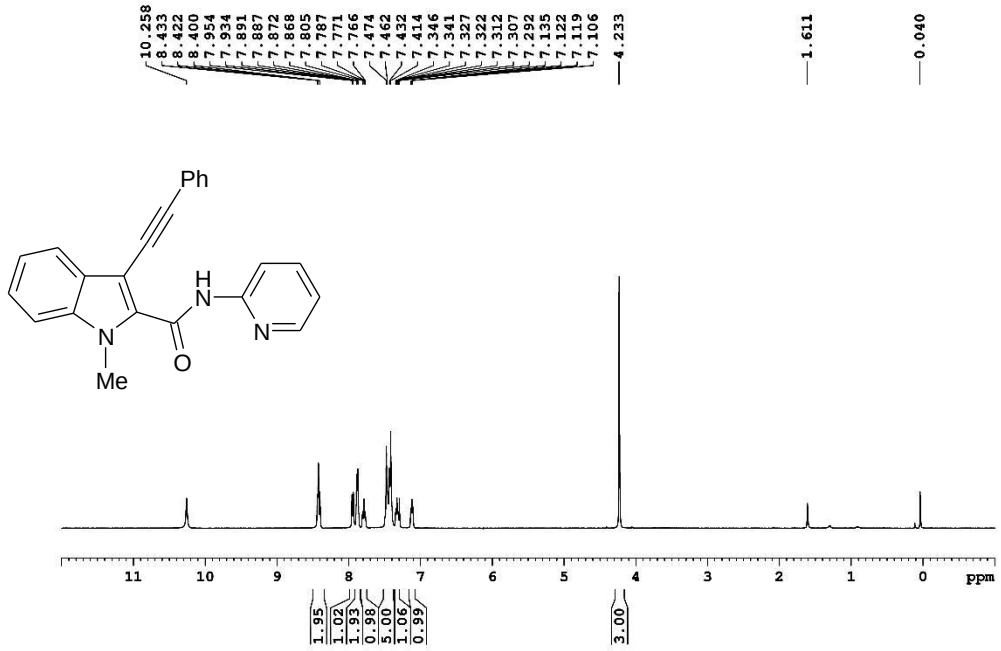

Figure S53. ^{1}H NMR spectrum of compound **8m**

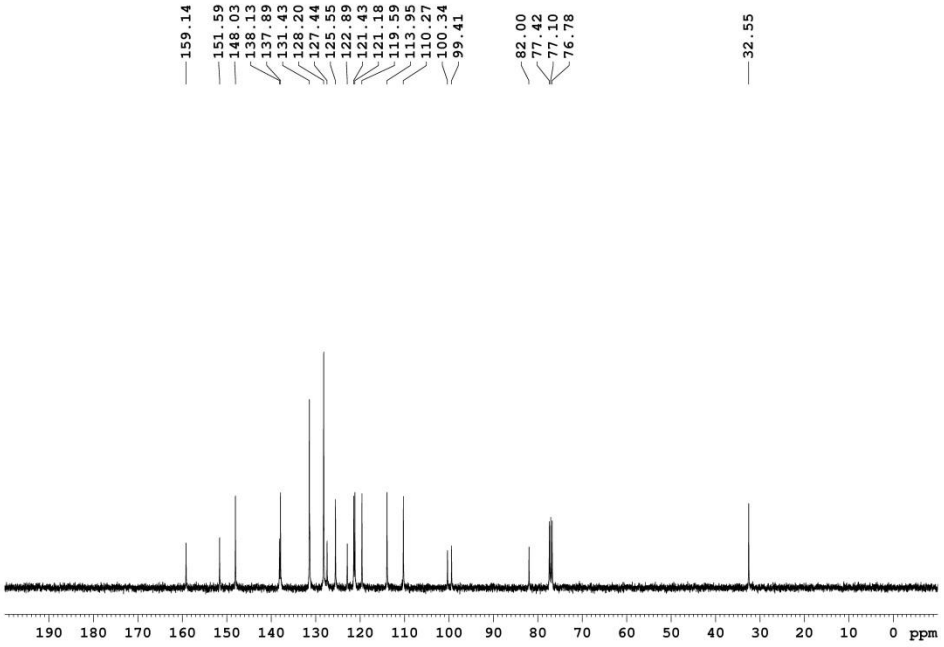

Figure S54. ^{13}C NMR spectrum of compound **8m**

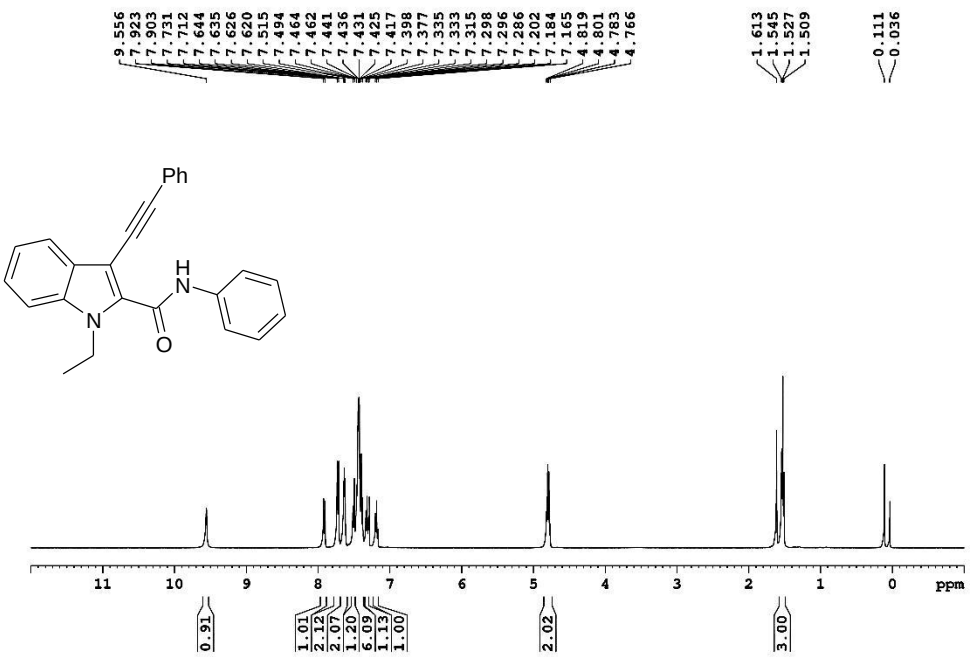

Figure S55. ^{1}H NMR spectrum of compound **8n**

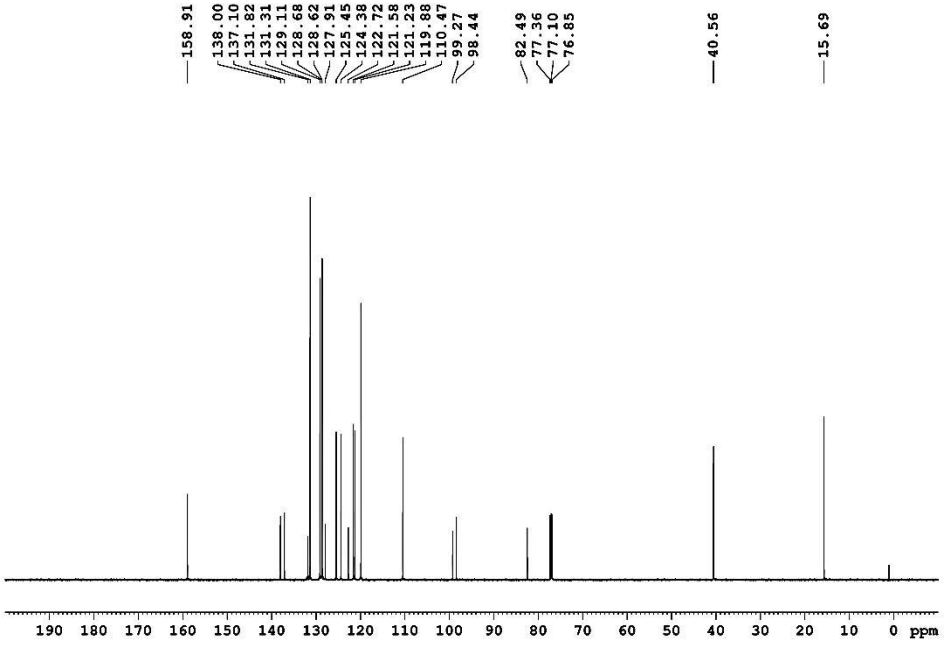

Figure S56. ^{13}C NMR spectrum of compound **8n**

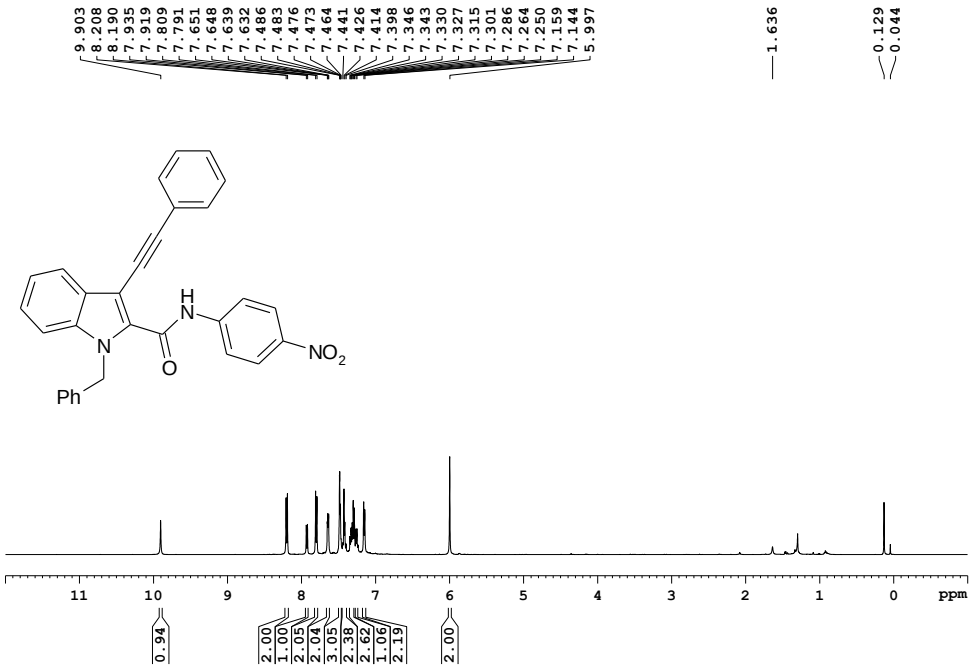

Figure S57. ^{1}H NMR spectrum of compound **8o**

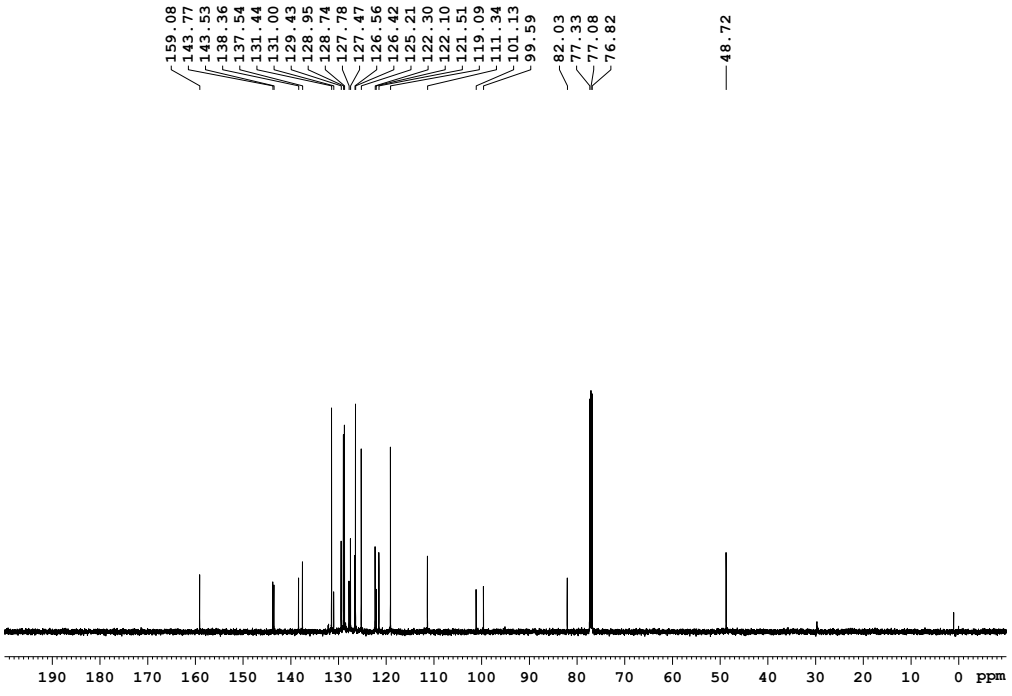

Figure S58. ^{13}C NMR spectrum of compound **8o**

(2) Copies of $^{1}H/\ ^{13}C$ NMR spectra for pyrrolo diindolones 9a-j and β-Carbolinones 10a-o.

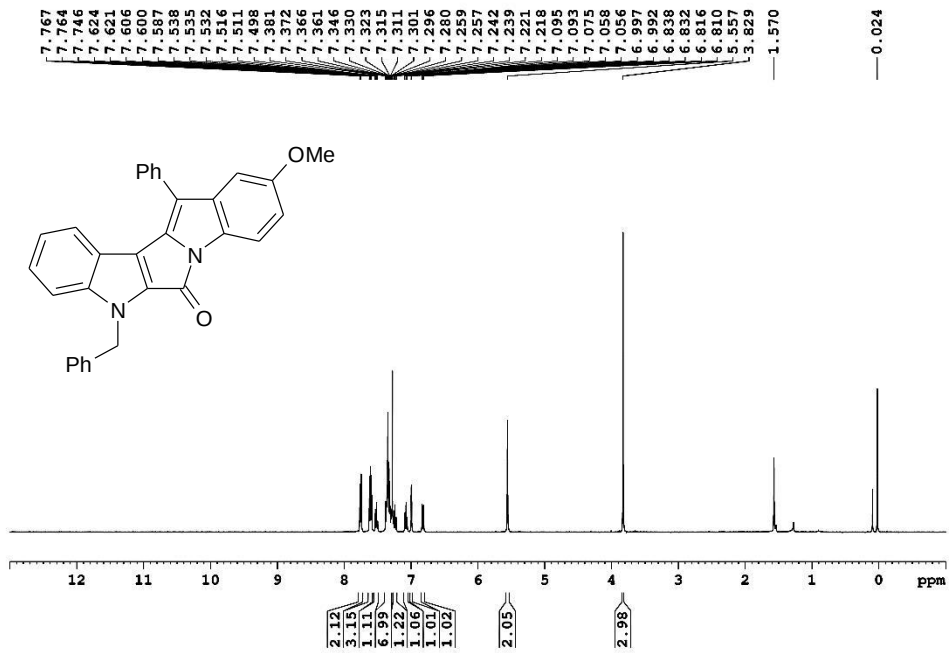

Figure S59. ^{1}H NMR spectrum of compound **9a**

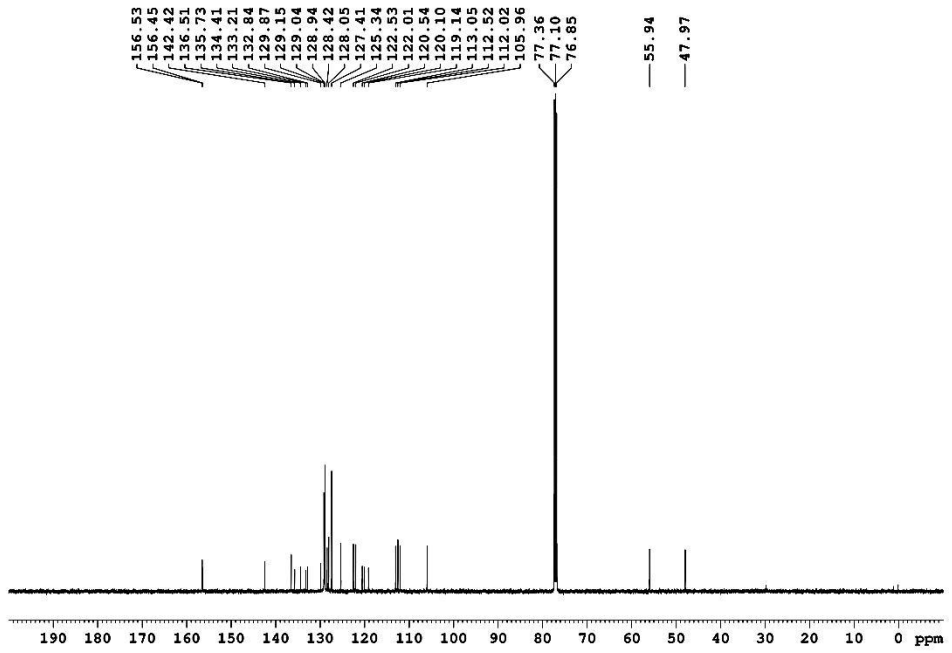

Figure S60. ^{13}C NMR spectrum of compound **9a**

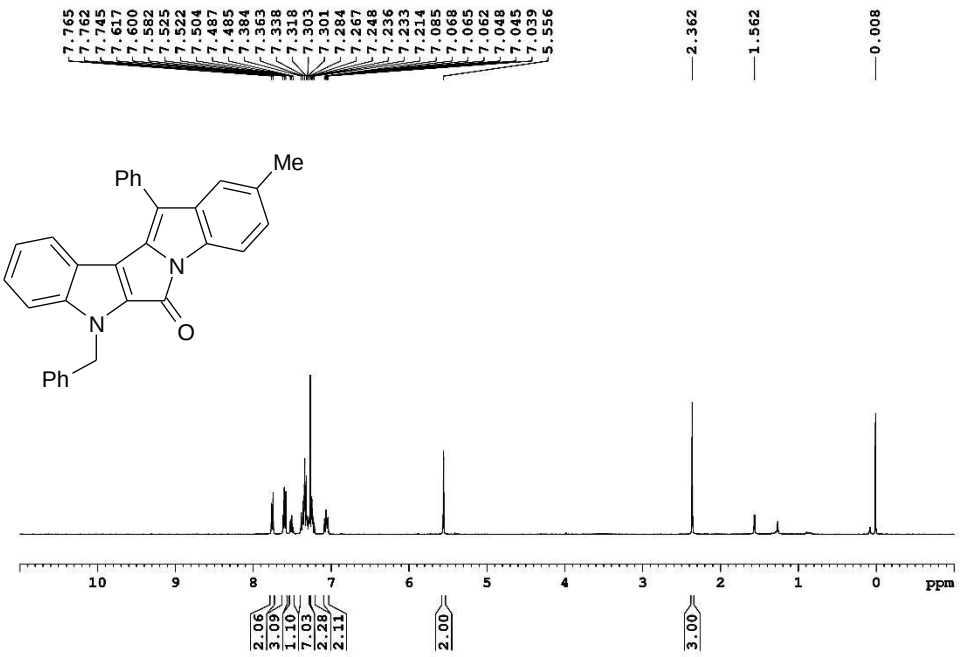

Figure S61. ^{1}H NMR spectrum of compound **9b**

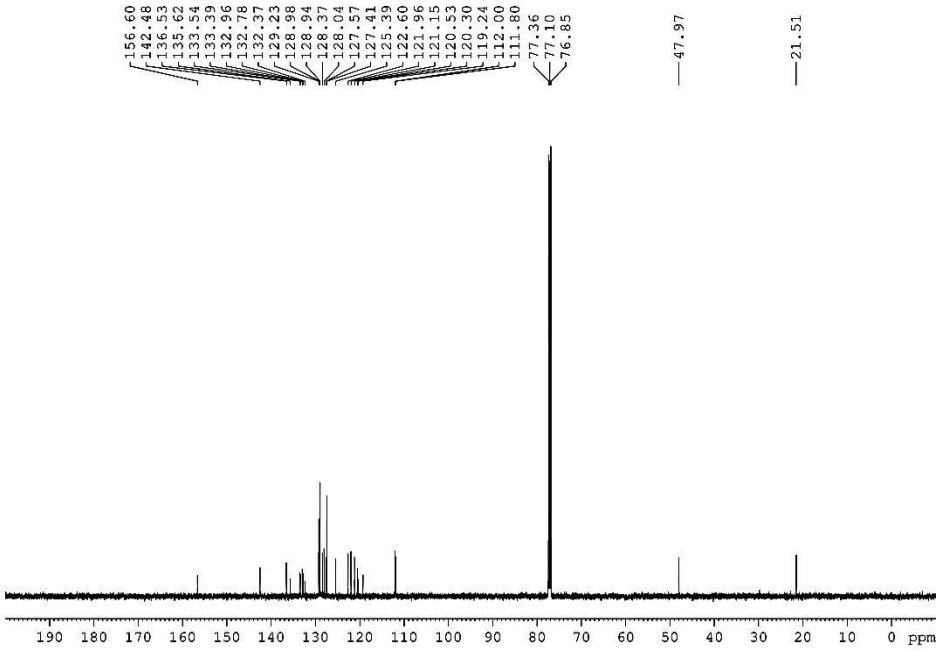

Figure S62. ^{13}C NMR spectrum of compound **9b**

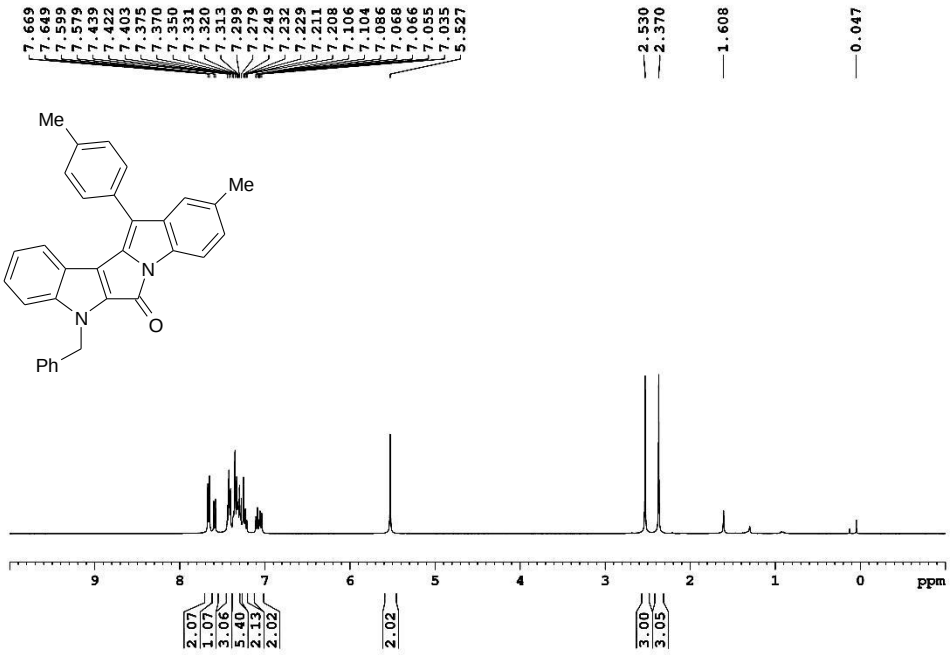

Figure S63. ^{1}H NMR spectrum of compound **9c**

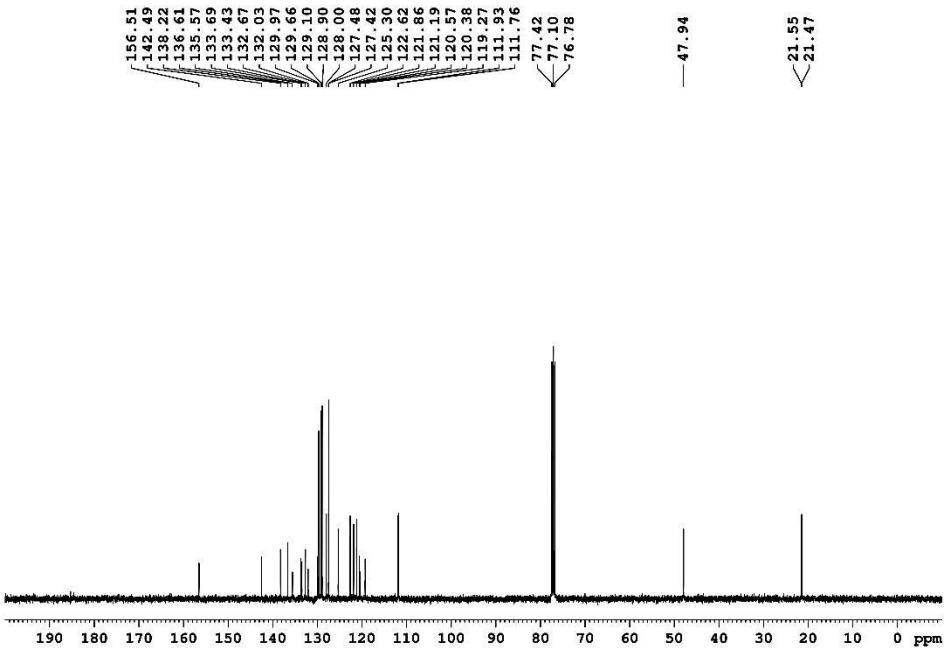

Figure S64. ^{13}C NMR spectrum of compound **9c**

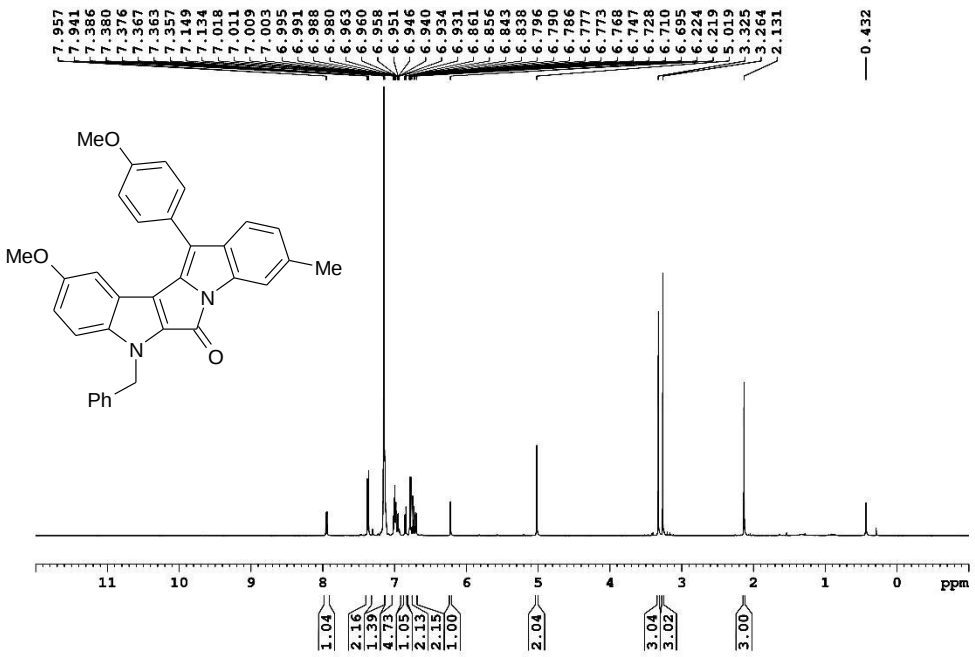

Figure S65. ^{1}H NMR spectrum of compound **9d**

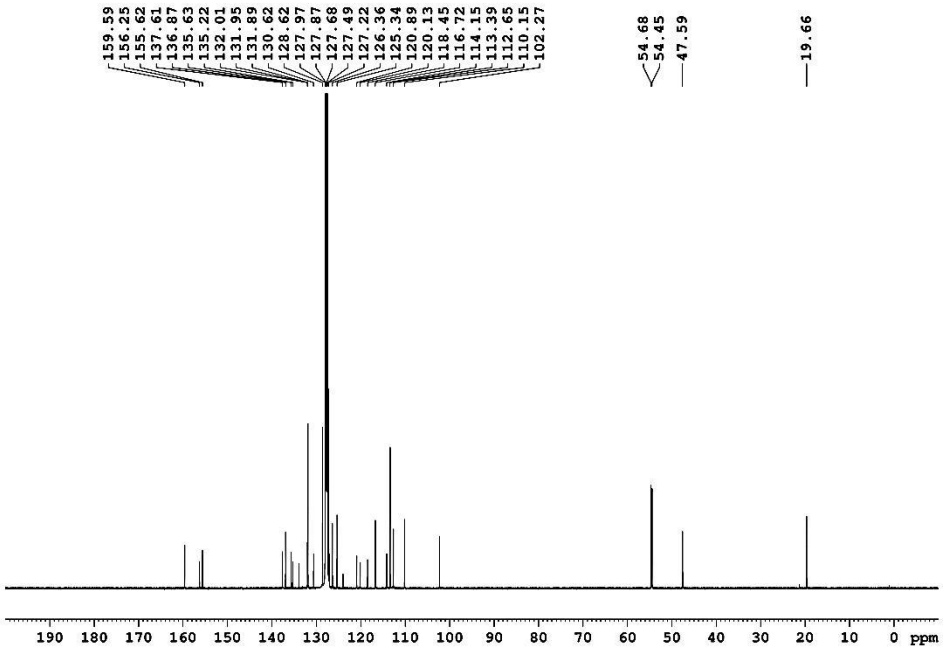

Figure S66. ^{13}C NMR spectrum of compound **9d**

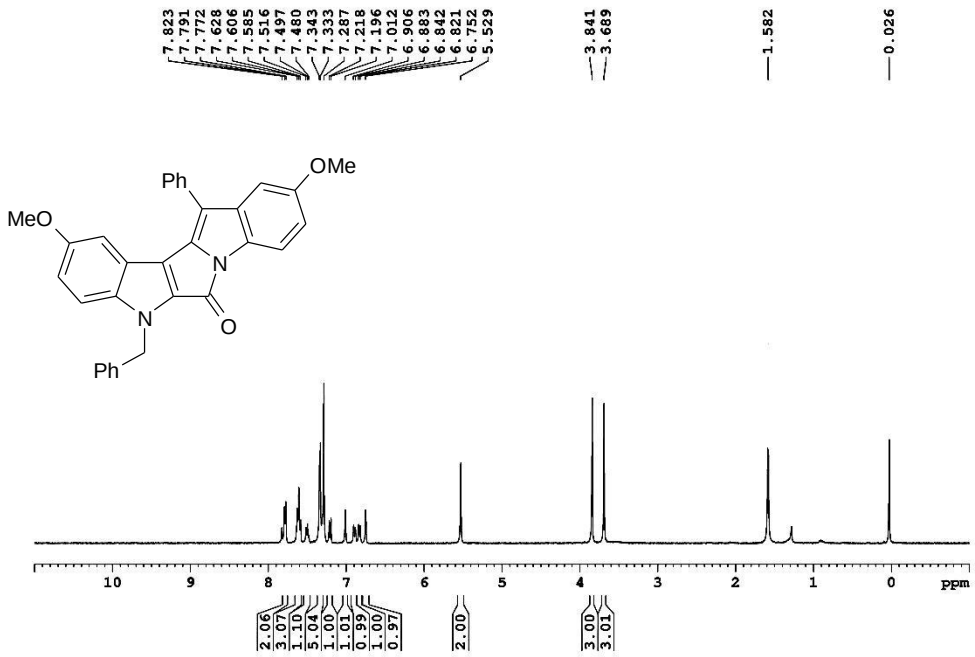

Figure S67. ^{1}H NMR spectrum of compound **9e**

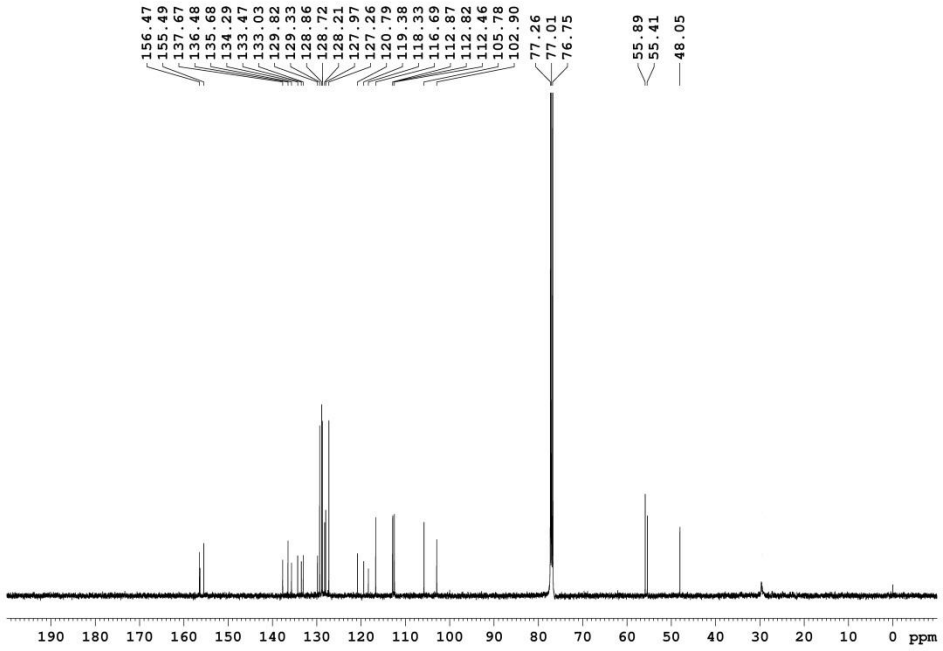

Figure S68. ^{13}C NMR spectrum of compound **9e**

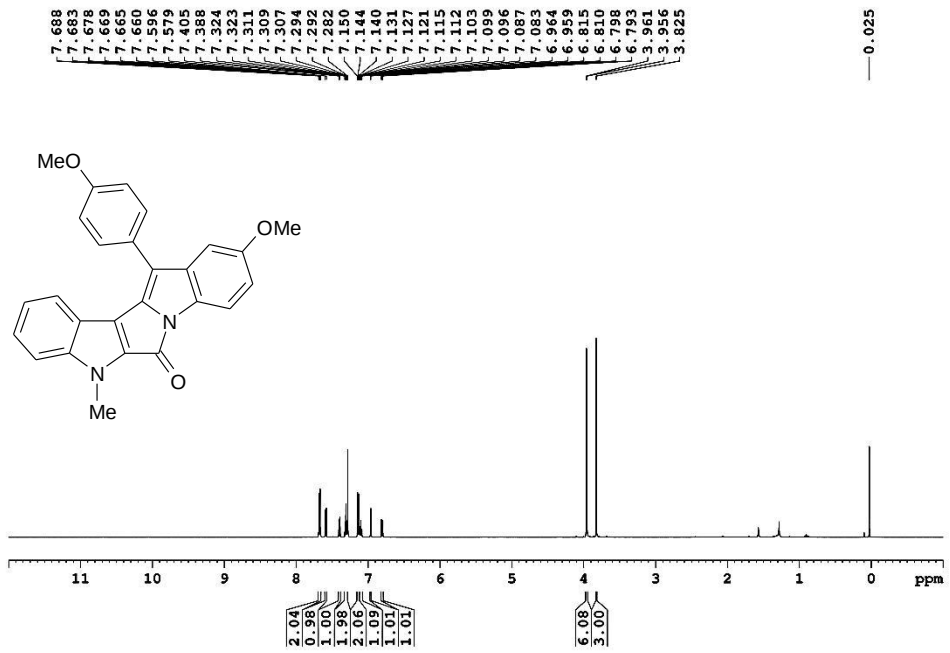

Figure S69. ^{1}H NMR spectrum of compound **9f**

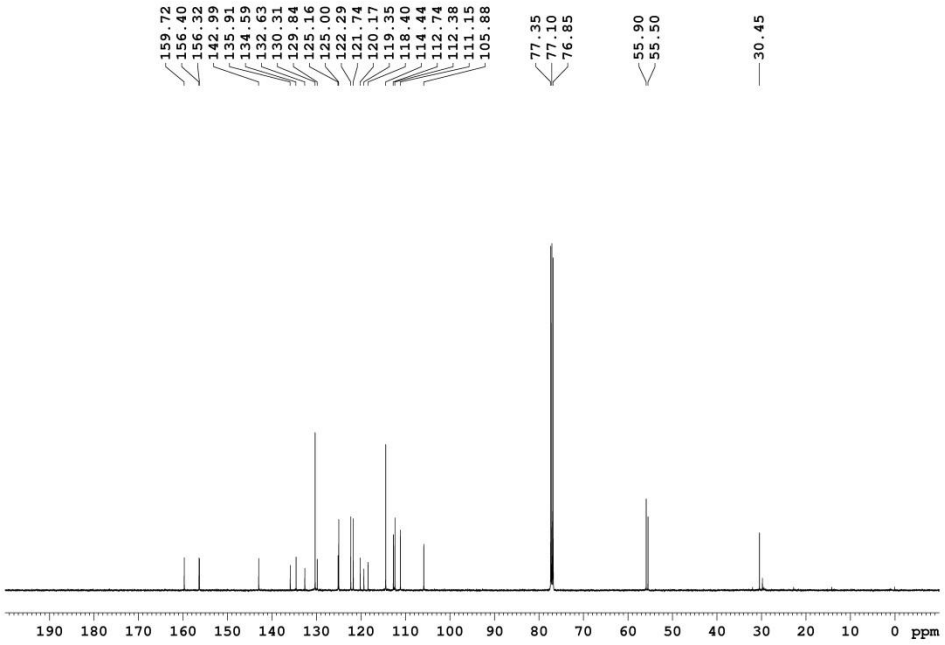

Figure S70. ^{13}C NMR spectrum of compound **9f**

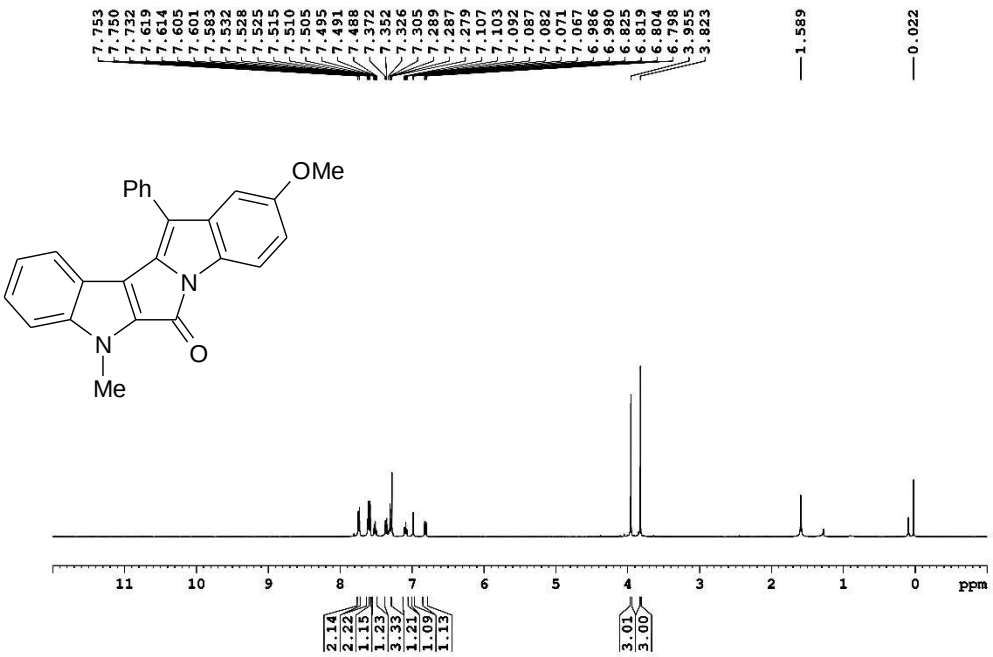

Figure S71. ^{1}H NMR spectrum of compound **9g**

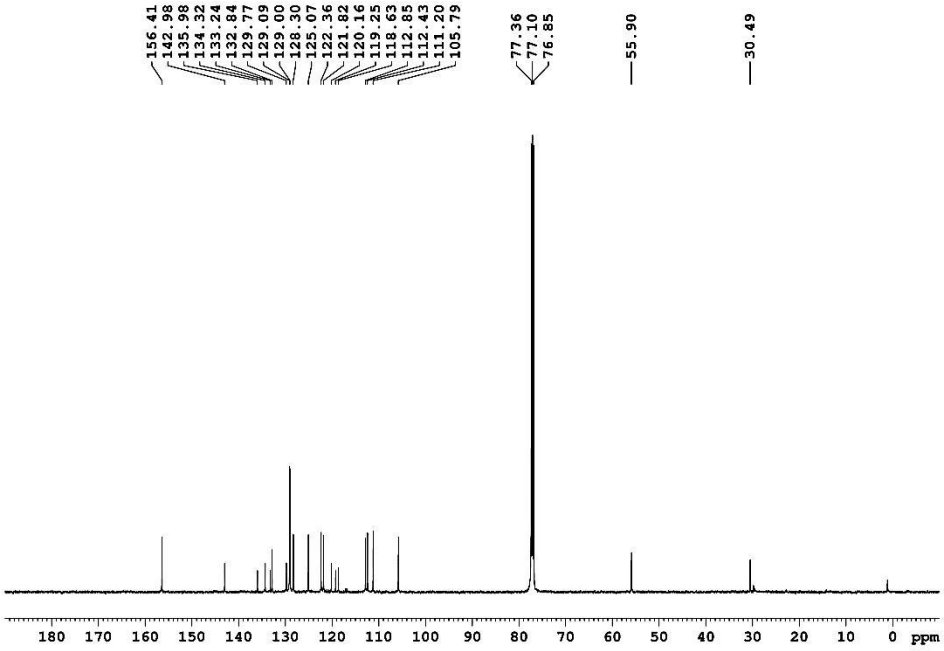

Figure S72. ^{13}C NMR spectrum of compound **9g**

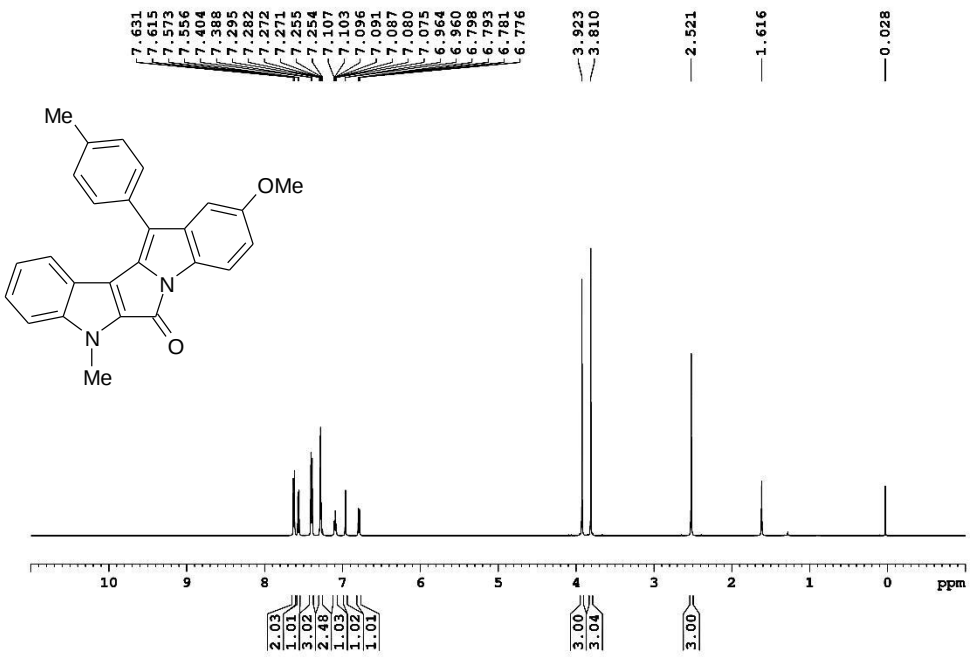

Figure S73. ^{1}H NMR spectrum of compound **9h**

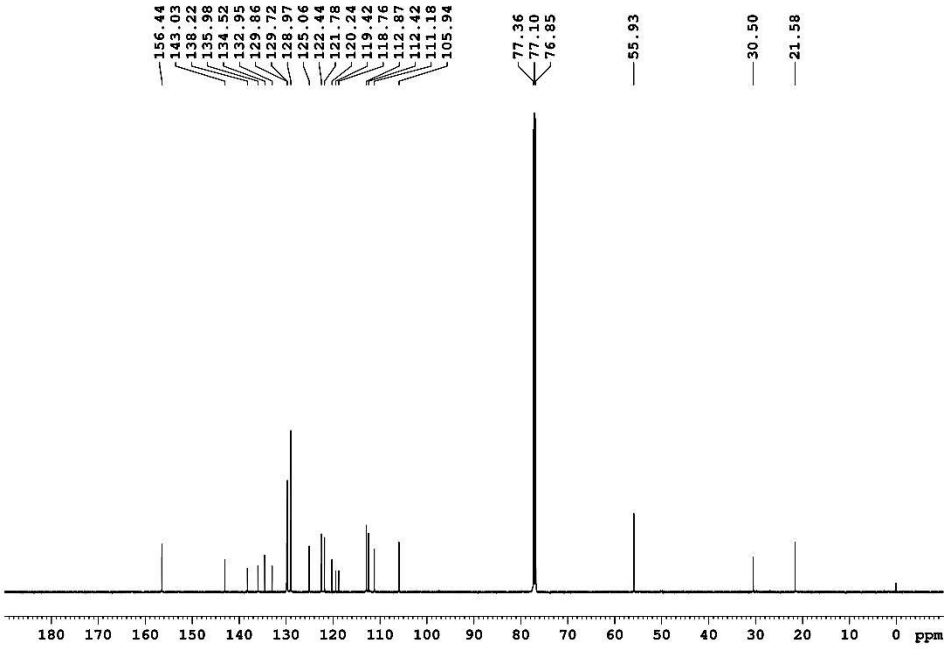

Figure S74. ^{13}C NMR spectrum of compound **9h**

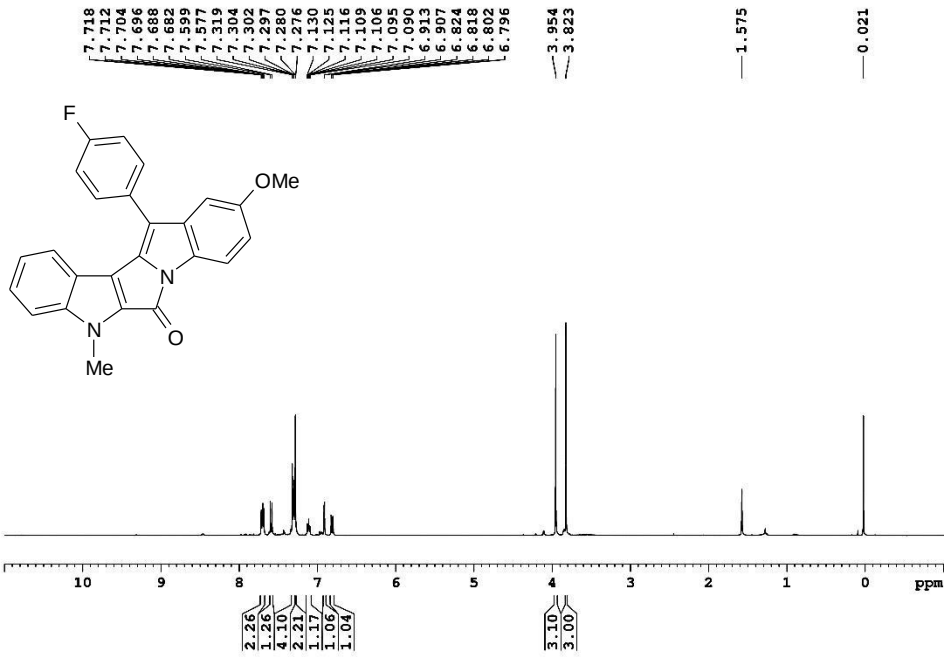

Figure S75. ^{1}H NMR spectrum of compound **9i**

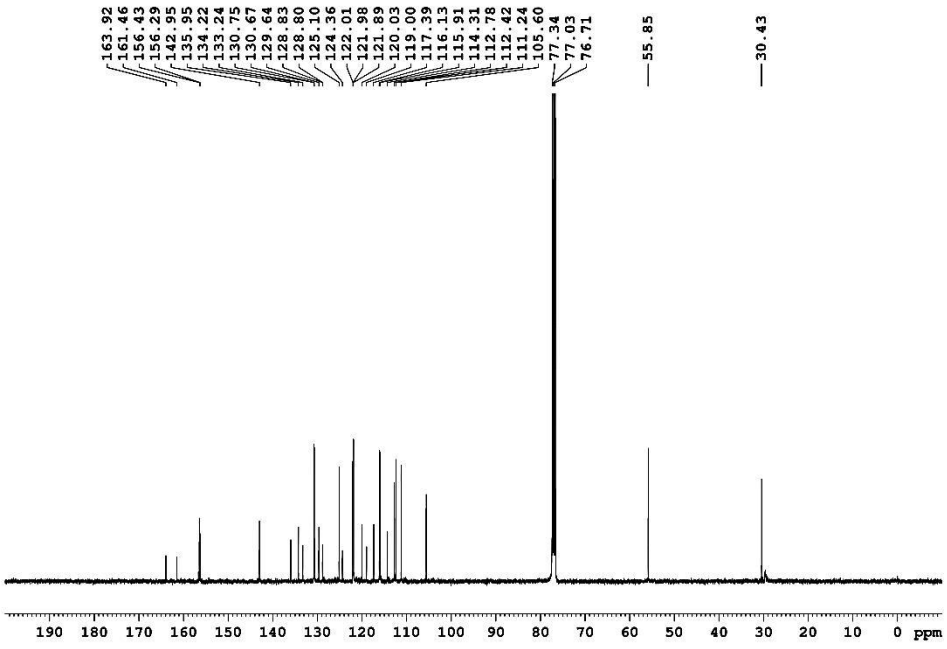

Figure S76. ^{13}C NMR spectrum of compound **9i**

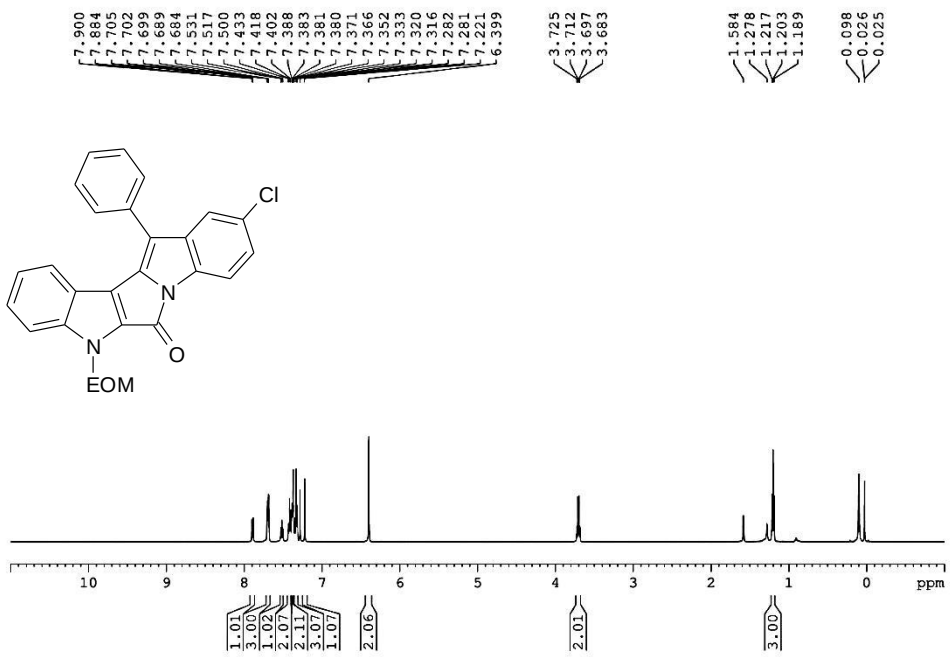

Figure S77. ^{1}H NMR spectrum of compound **9j**

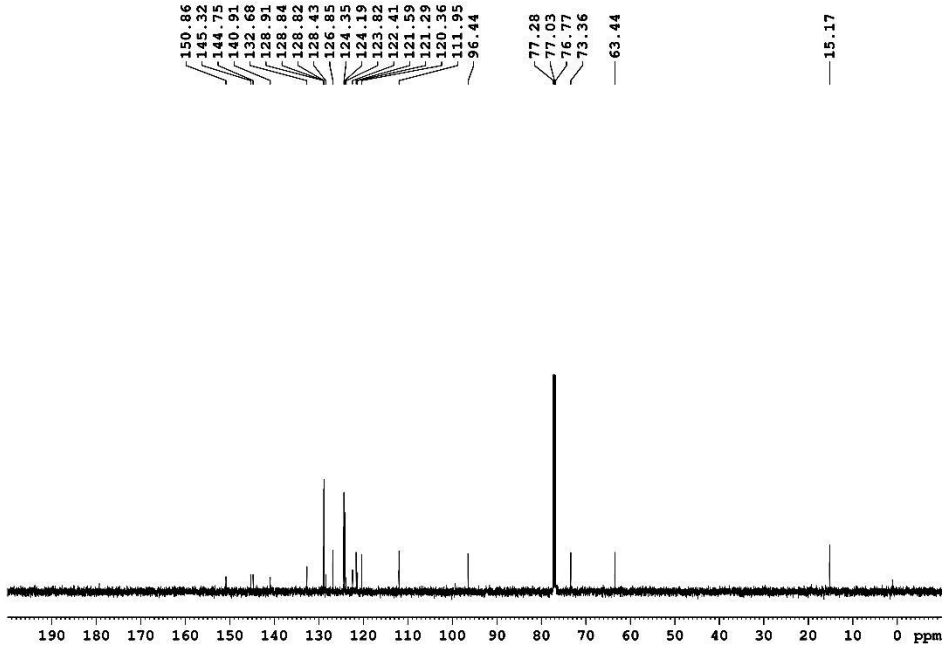

Figure S78. ^{13}C NMR spectrum of compound **9j**

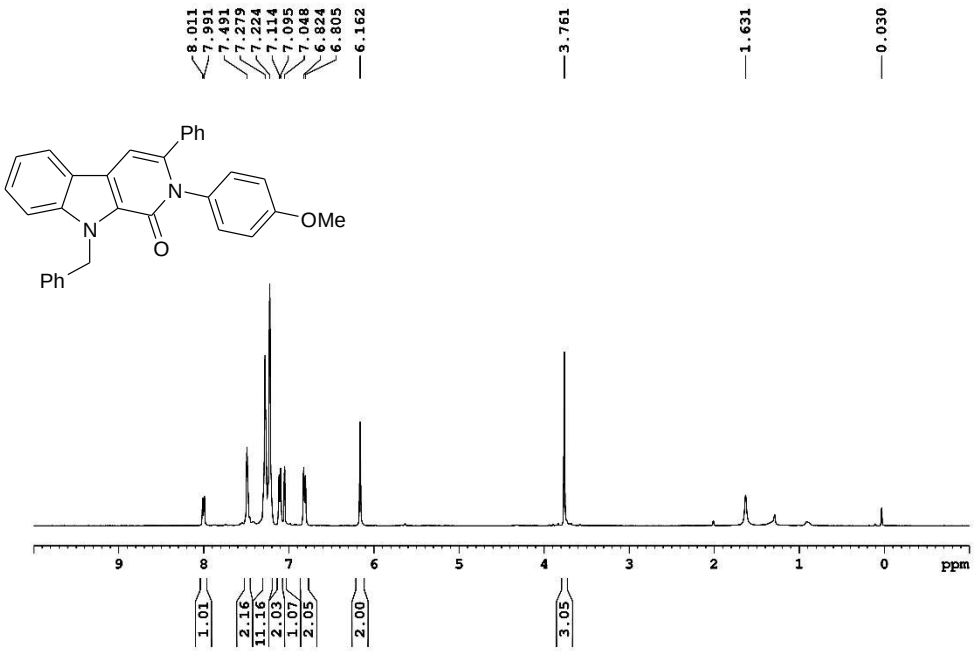

Figure S79. ^{1}H NMR spectrum of compound **10a**

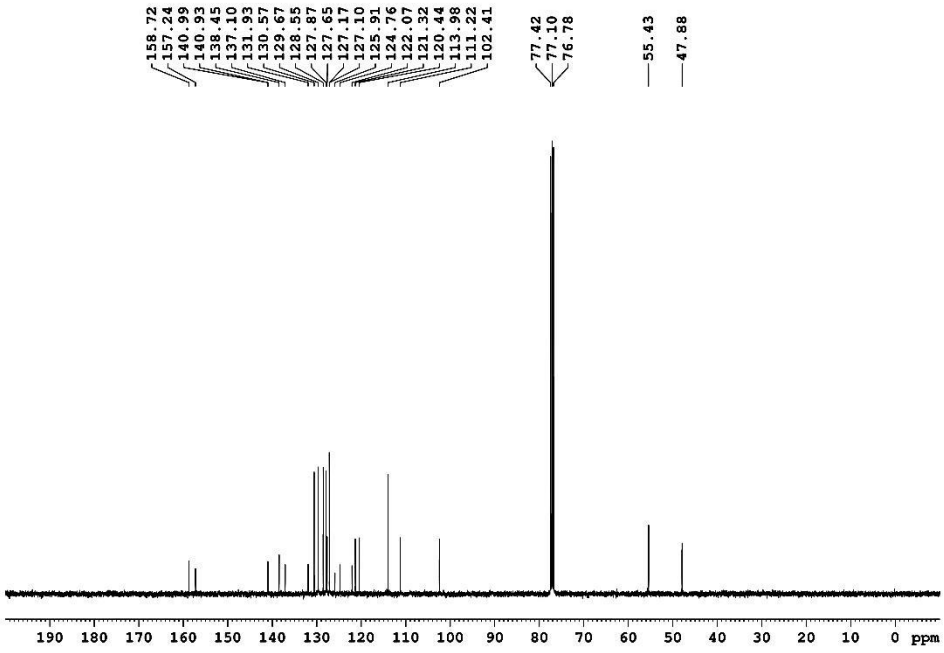

Figure S80. ^{13}C NMR spectrum of compound **10a**

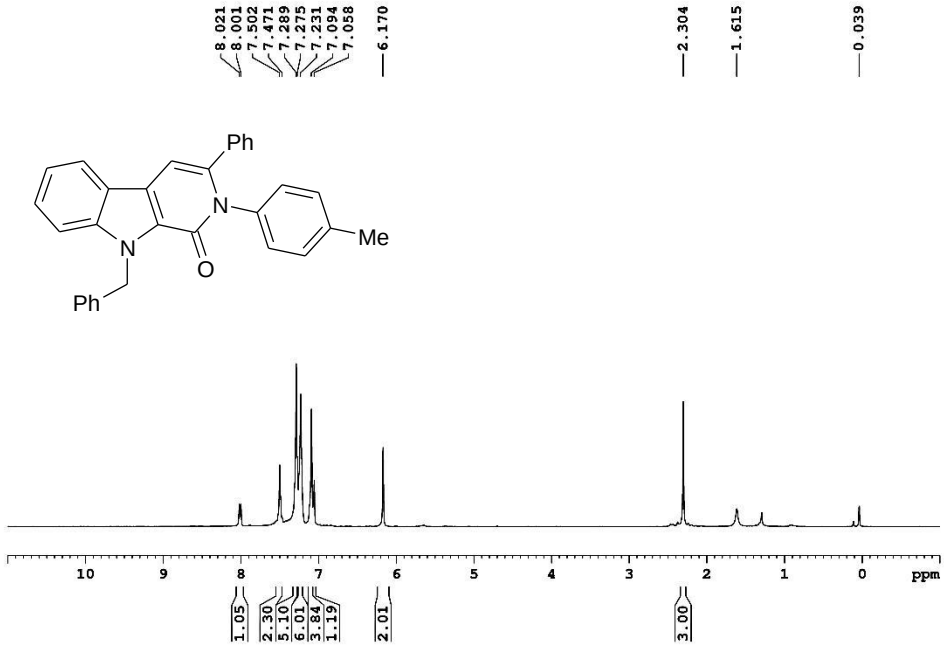

Figure S81. ^{1}H NMR spectrum of compound **10b**

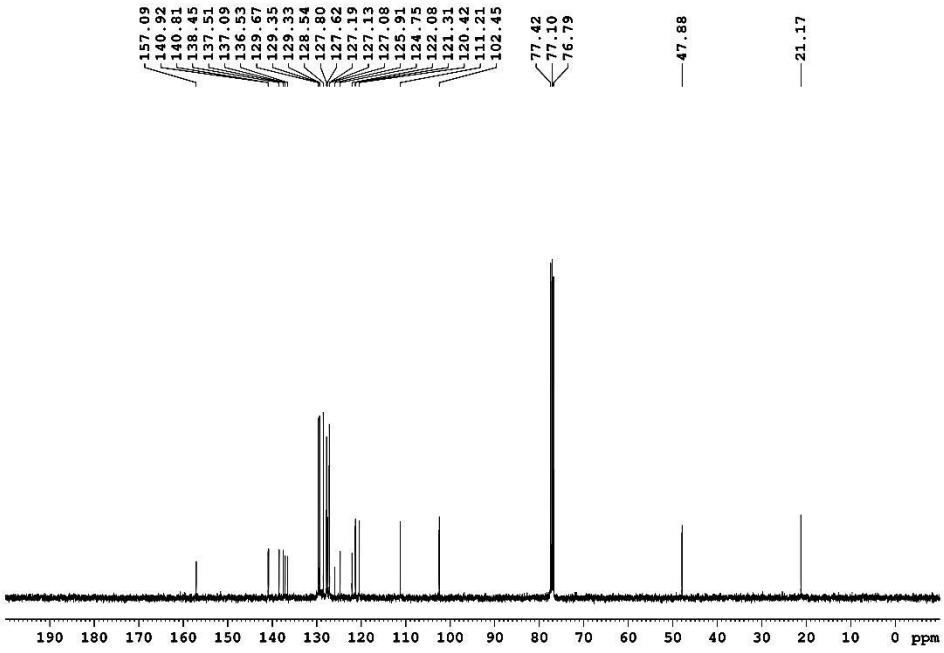

Figure S82. ^{13}C NMR spectrum of compound **10b**

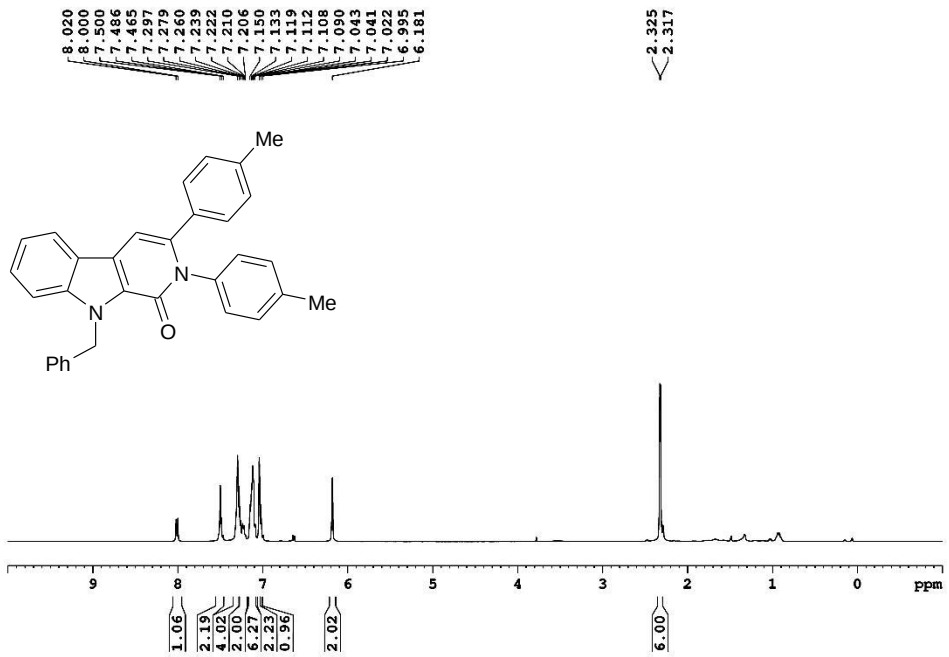

Figure S83. ^{1}H NMR spectrum of compound **10c**

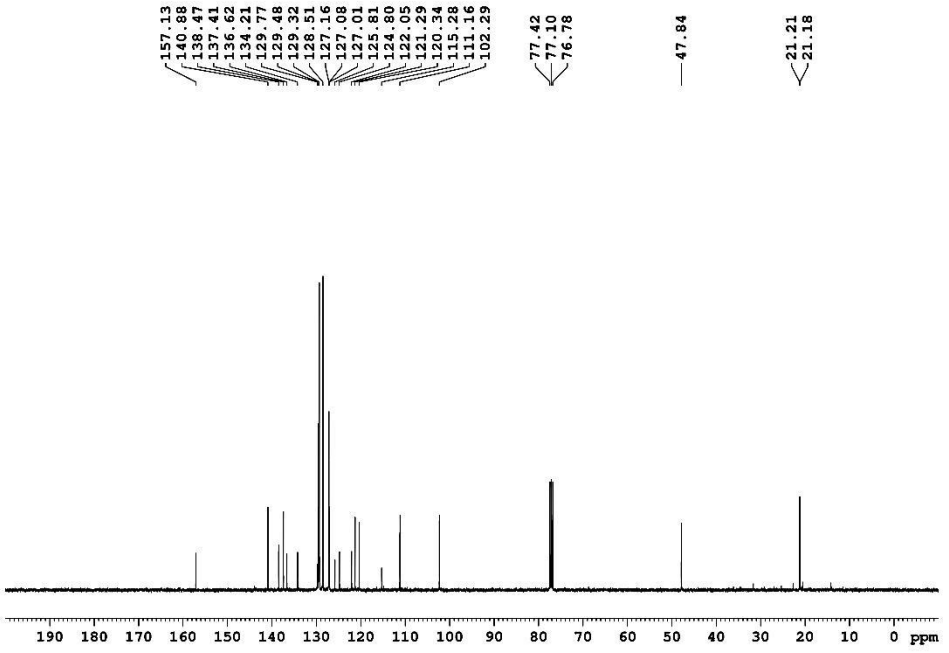

Figure S84. ^{13}C NMR spectrum of compound **10c**

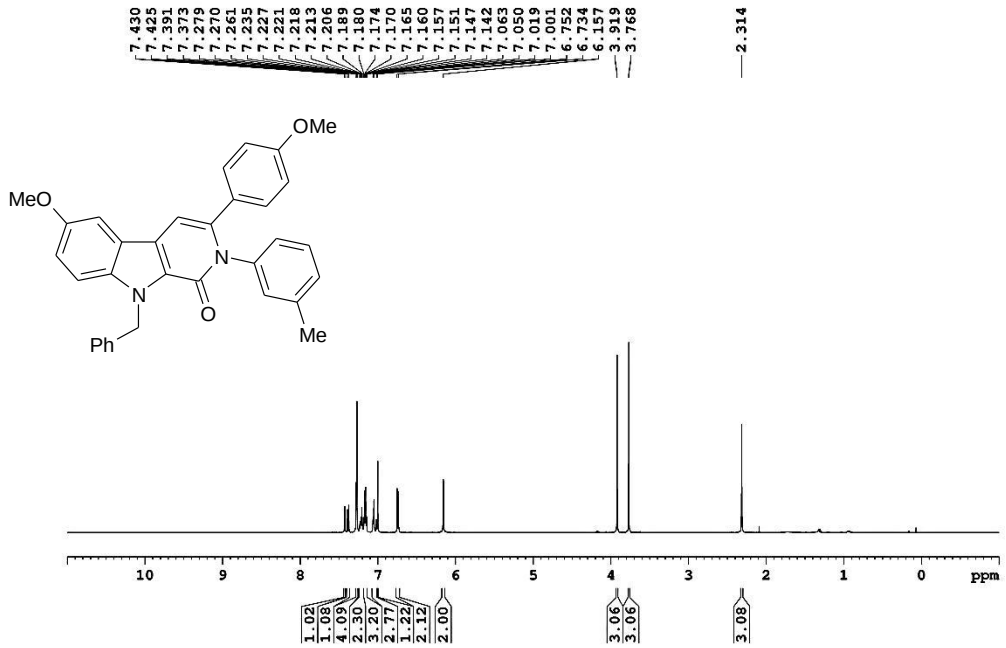

Figure S85. ^{1}H NMR spectrum of compound **10d**

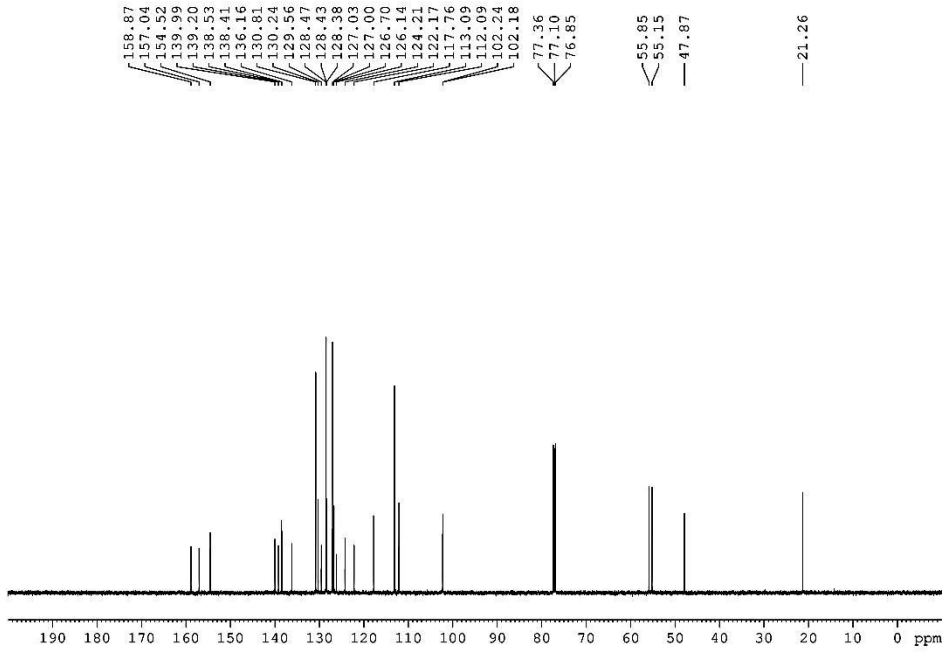

Figure S86. ^{13}C NMR spectrum of compound **10d**

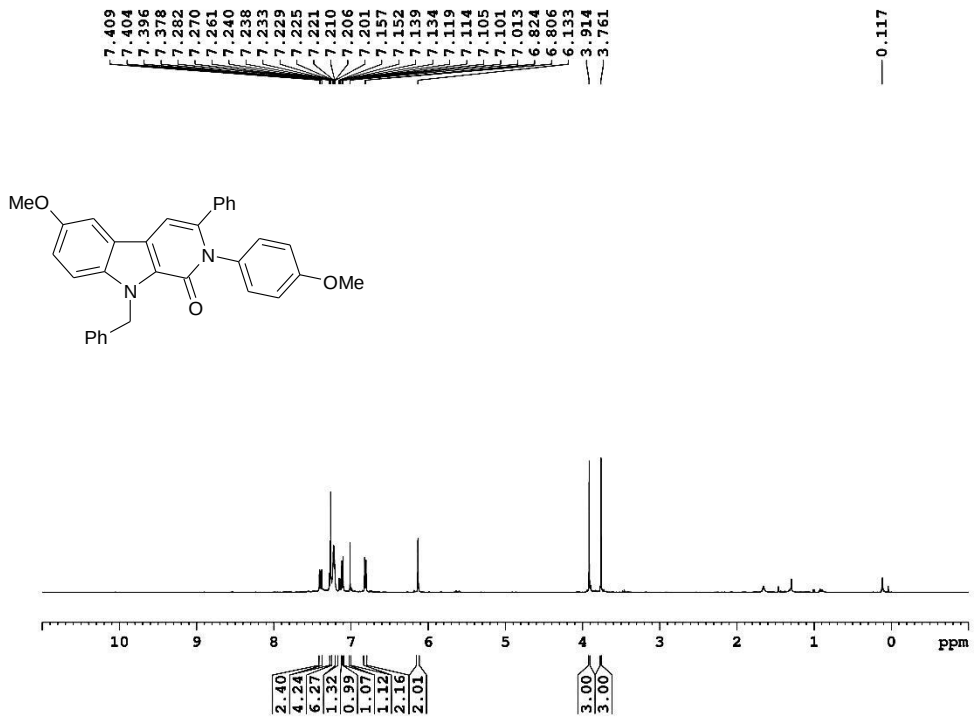

Figure S87. ^{1}H NMR spectrum of compound **10e**

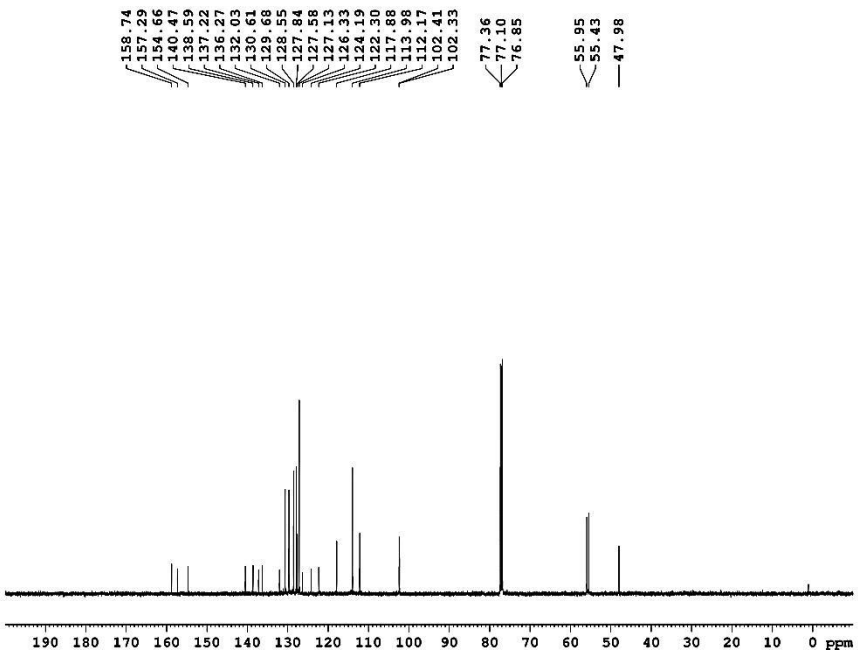

Figure S88. ^{13}C NMR spectrum of compound **10e**

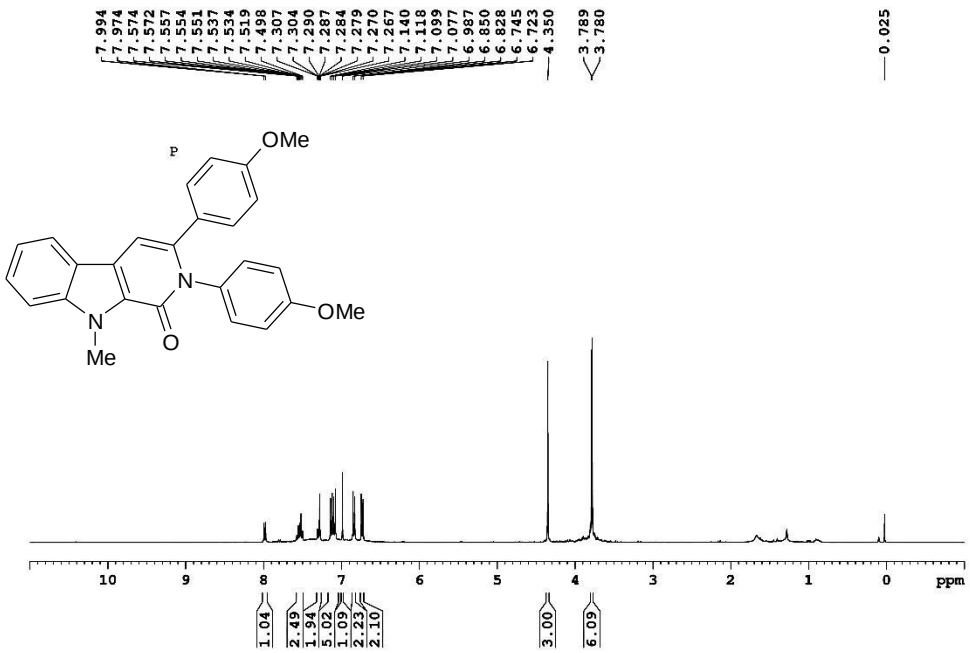

Figure S89. ^{1}H NMR spectrum of compound **10f**

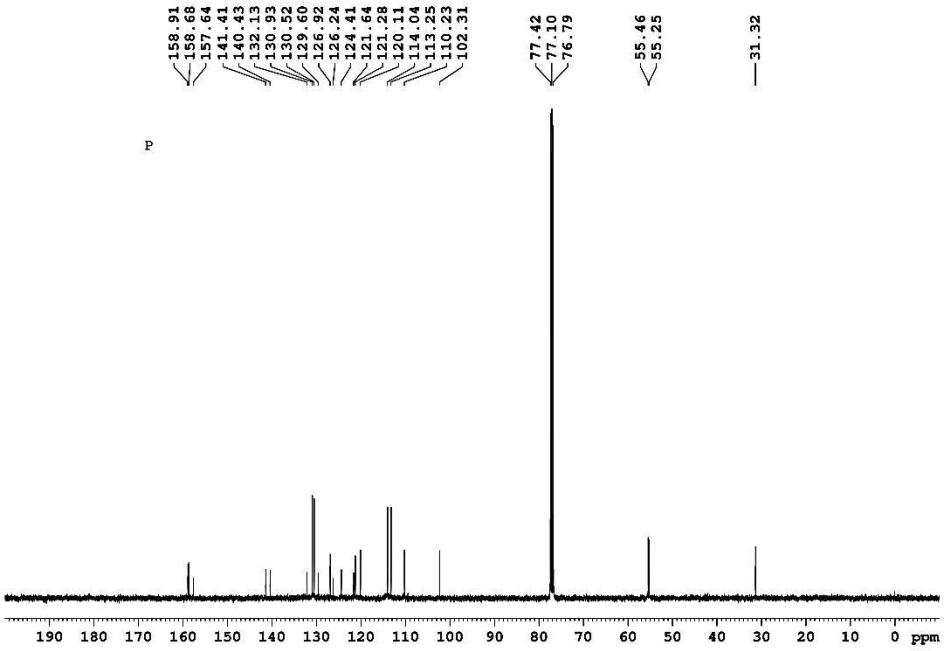

Figure S90. ^{13}C NMR spectrum of compound **10f**

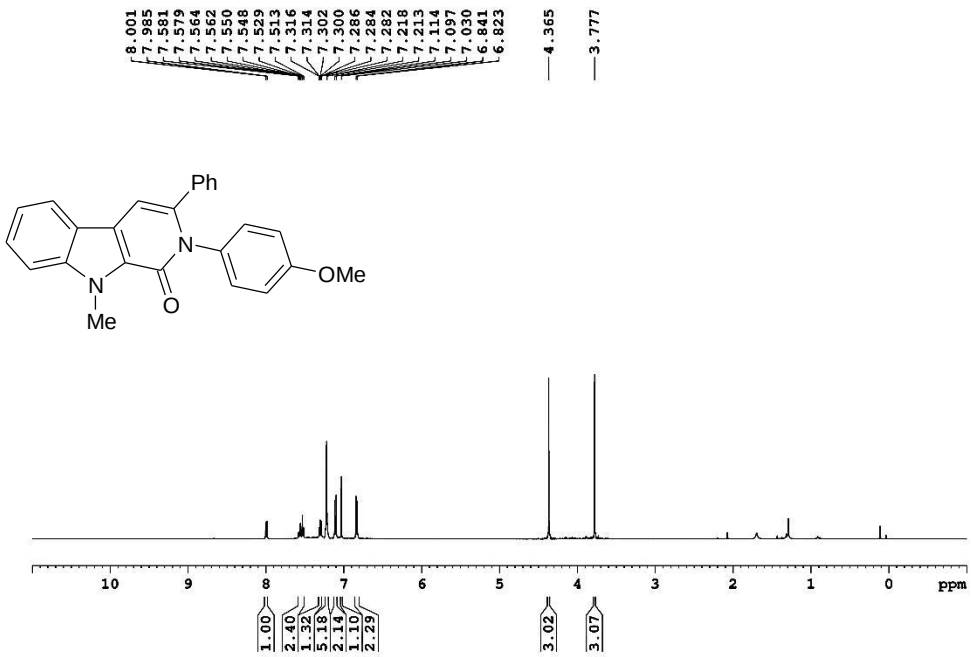

Figure S91. ^{1}H NMR spectrum of compound **10g**

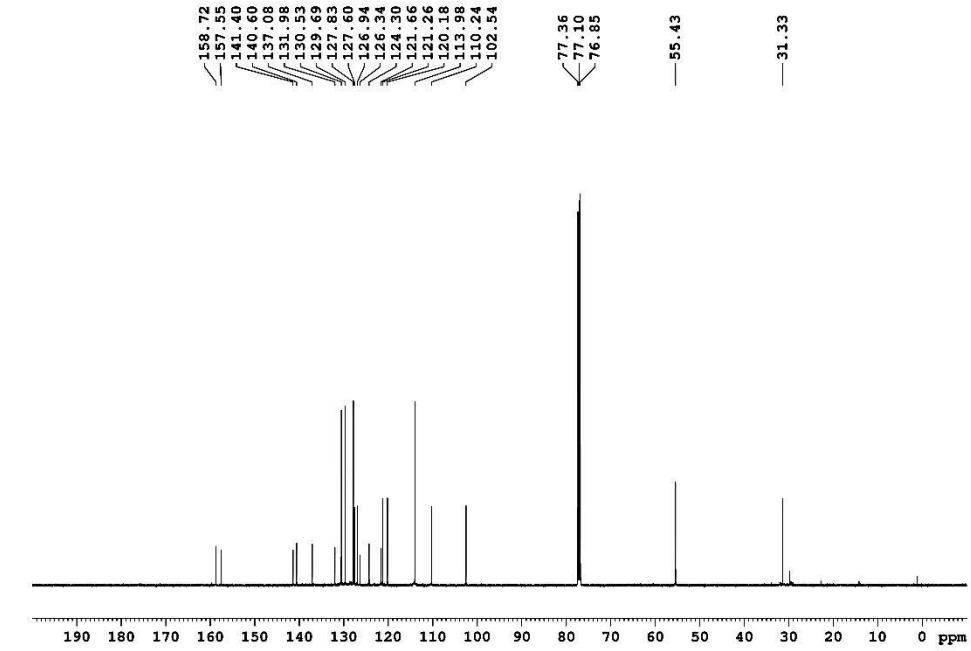

Figure S92. ^{13}C NMR spectrum of compound **10g**

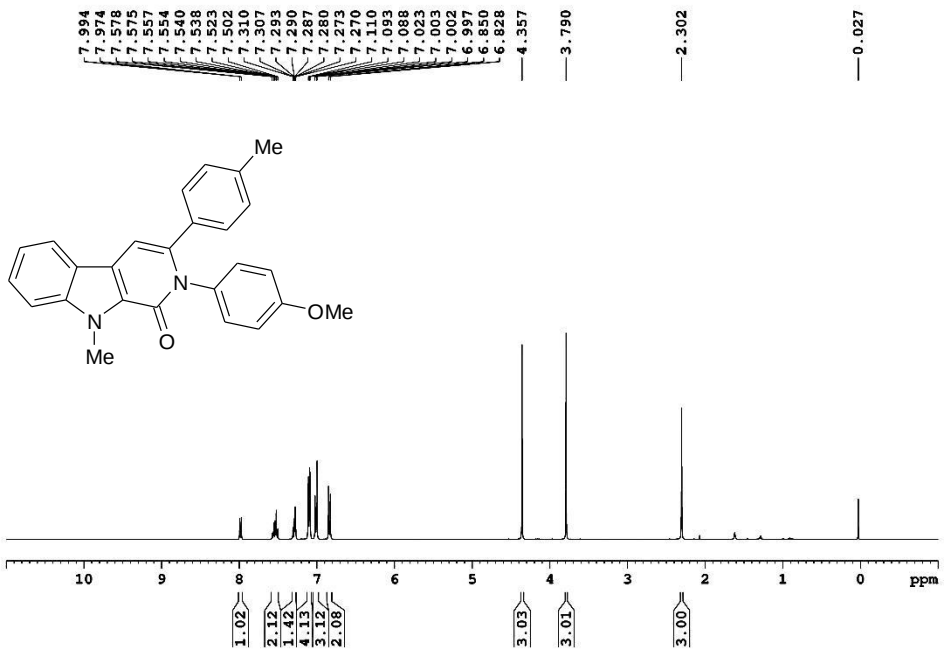

Figure S93. ^{1}H NMR spectrum of compound **10h**

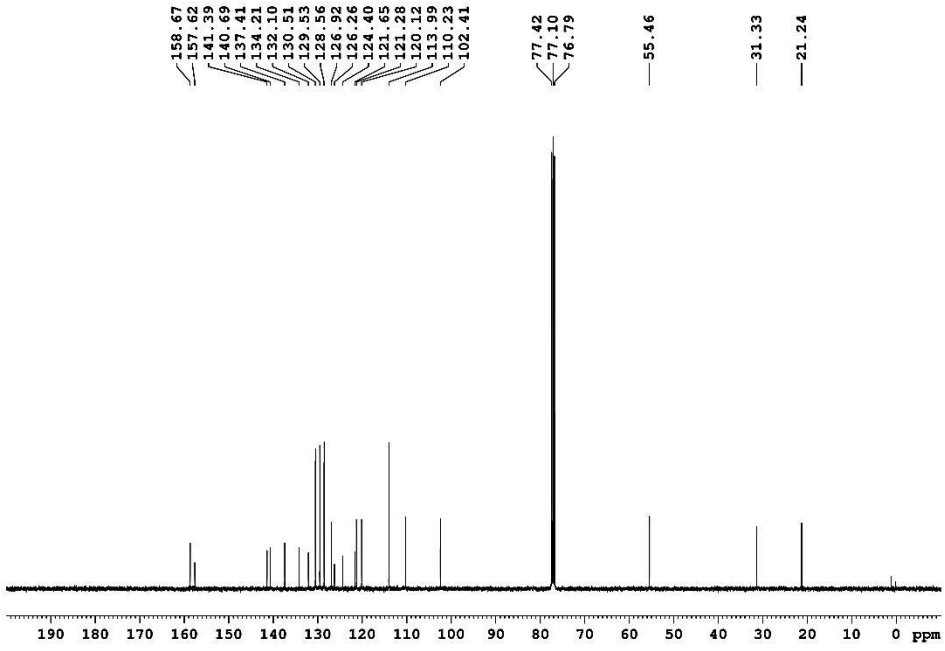

Figure S94. ^{13}C NMR spectrum of compound **10h**

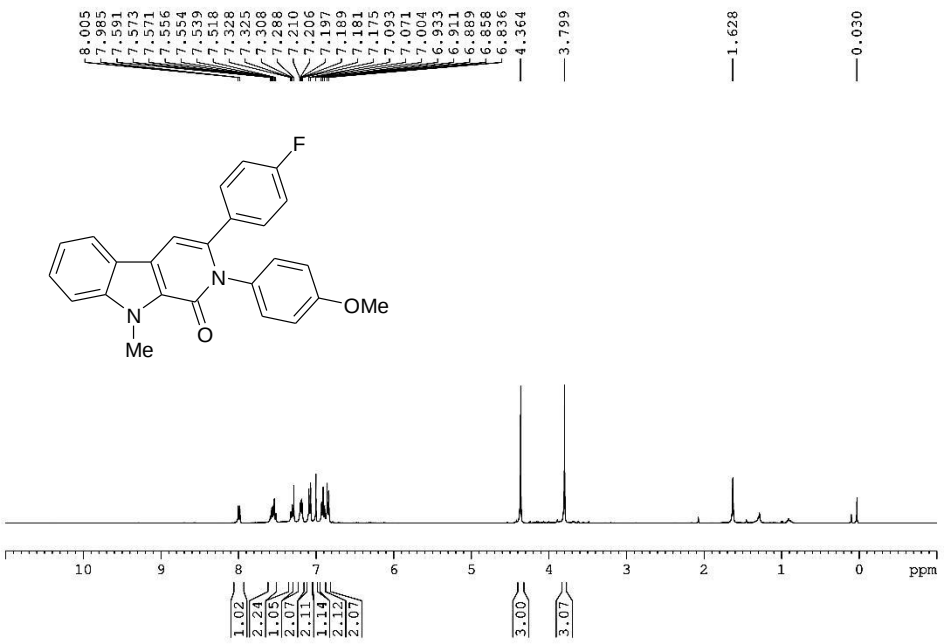

Figure S95. ^{1}H NMR spectrum of compound **10i**

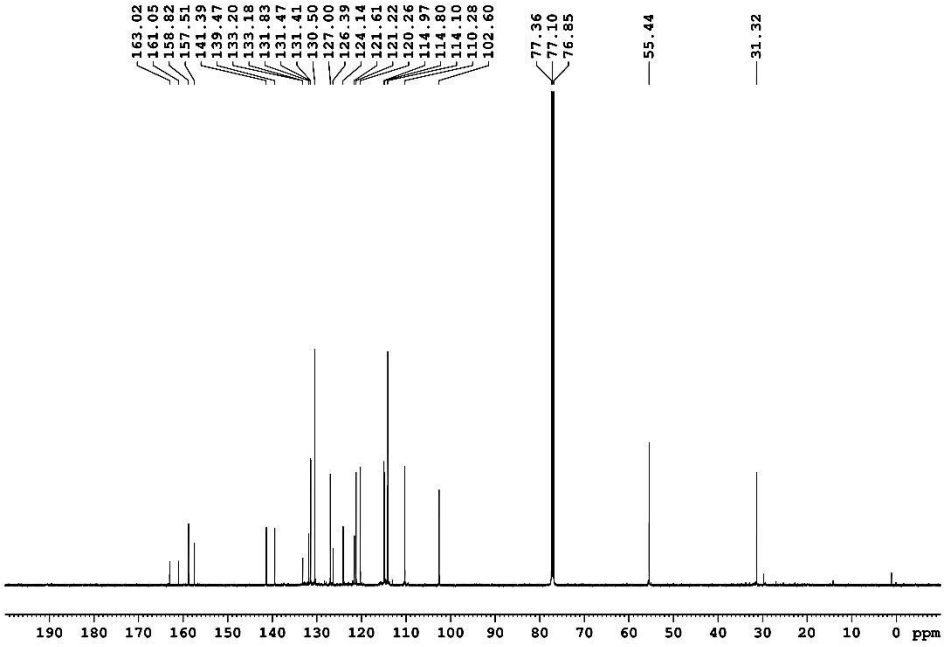

Figure S96. ^{13}C NMR spectrum of compound **10i**

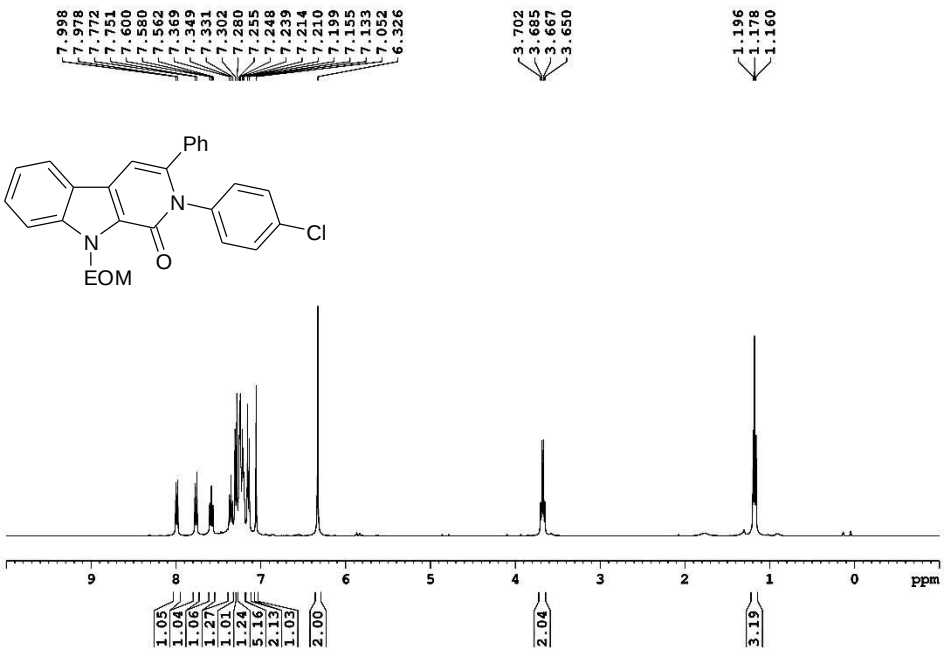

Figure S97. ^{1}H NMR spectrum of compound **10j**

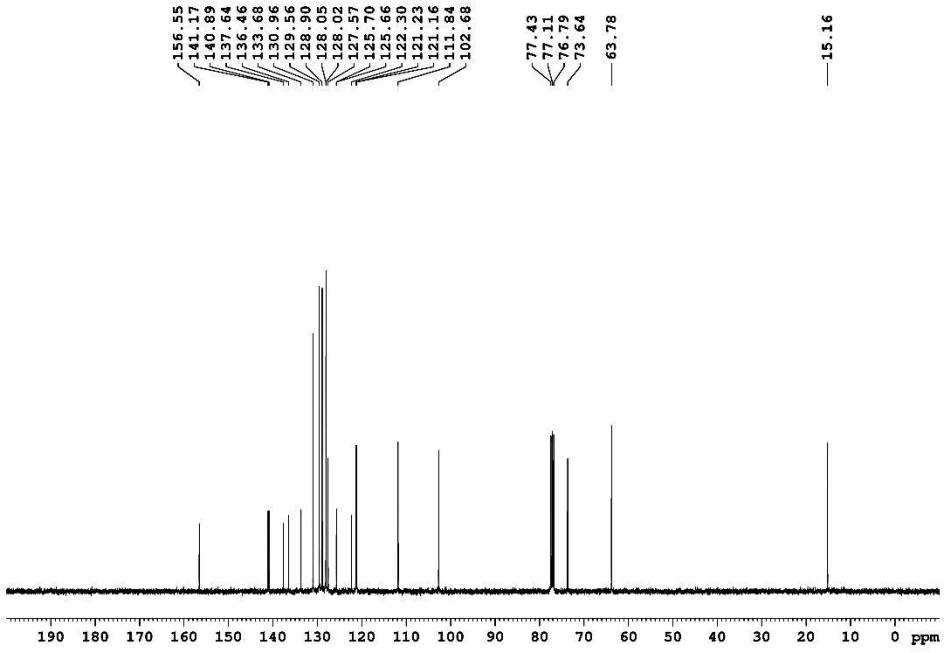

Figure S98. ^{13}C NMR spectrum of compound **10j**

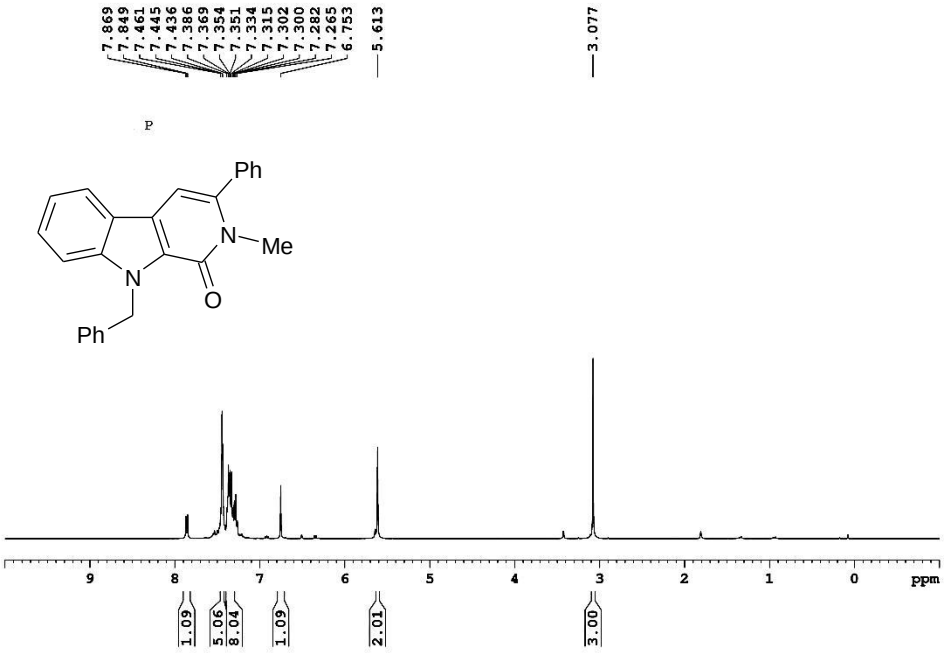

Figure S99. ^{1}H NMR spectrum of compound **10k**

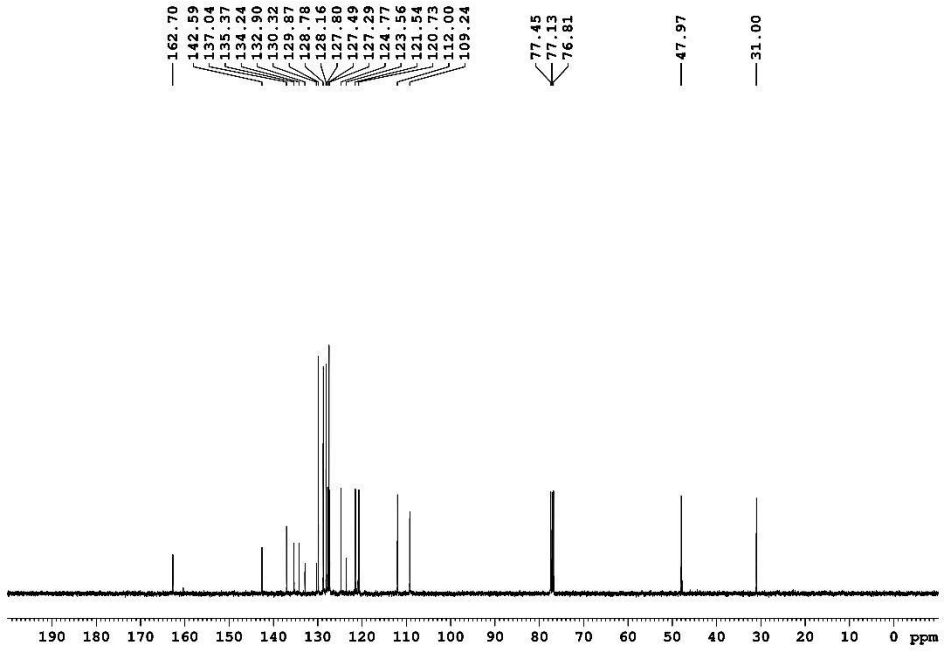

Figure S100. ^{13}C NMR spectrum of compound **10k**

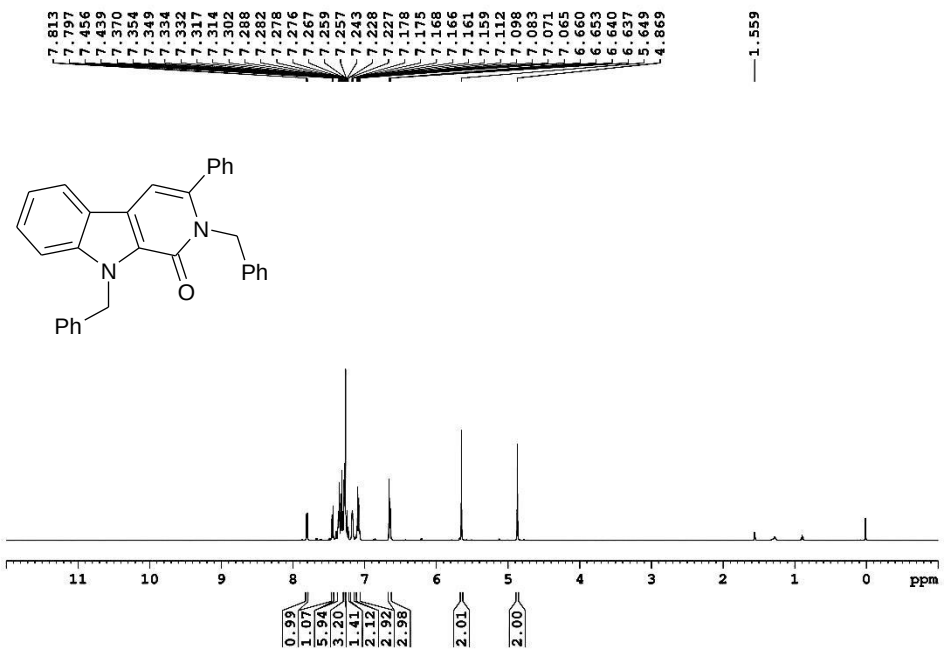

Figure S101. ^{1}H NMR spectrum of compound **10l**

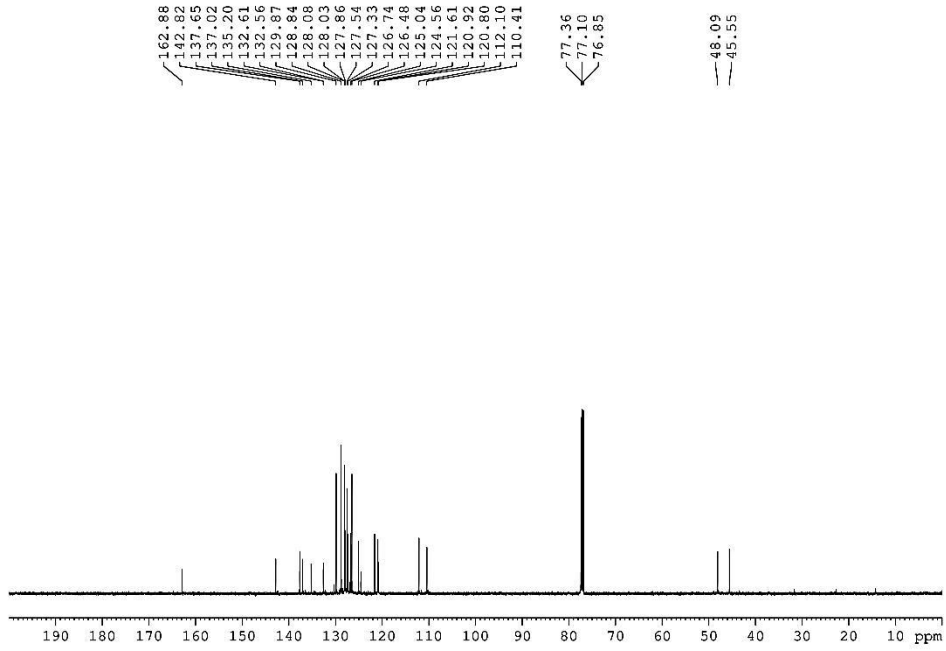

Figure S102. ^{13}C NMR spectrum of compound **10l**

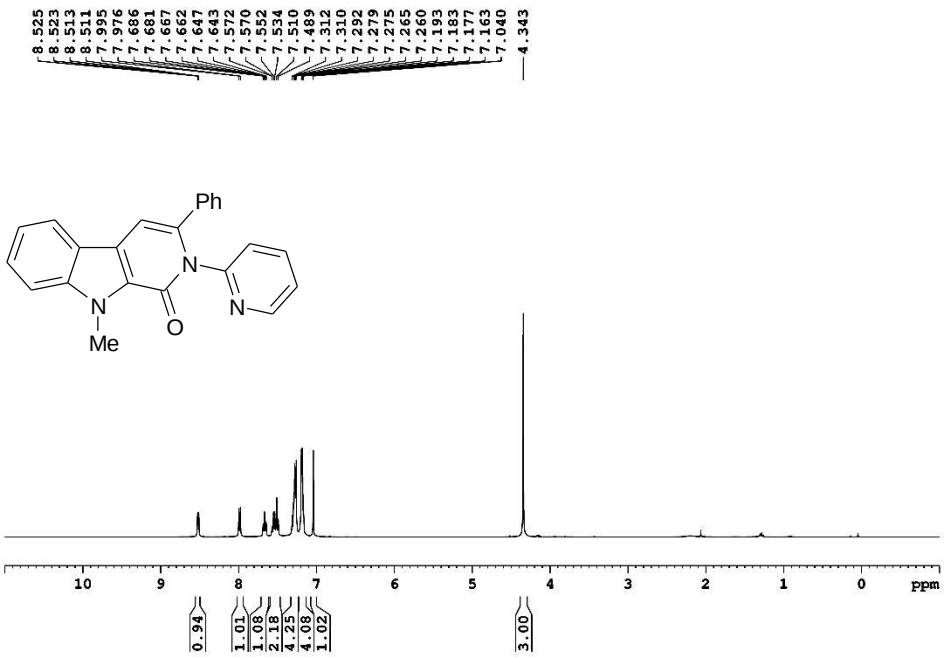

Figure S103. ^{1}H NMR spectrum of compound **10m**

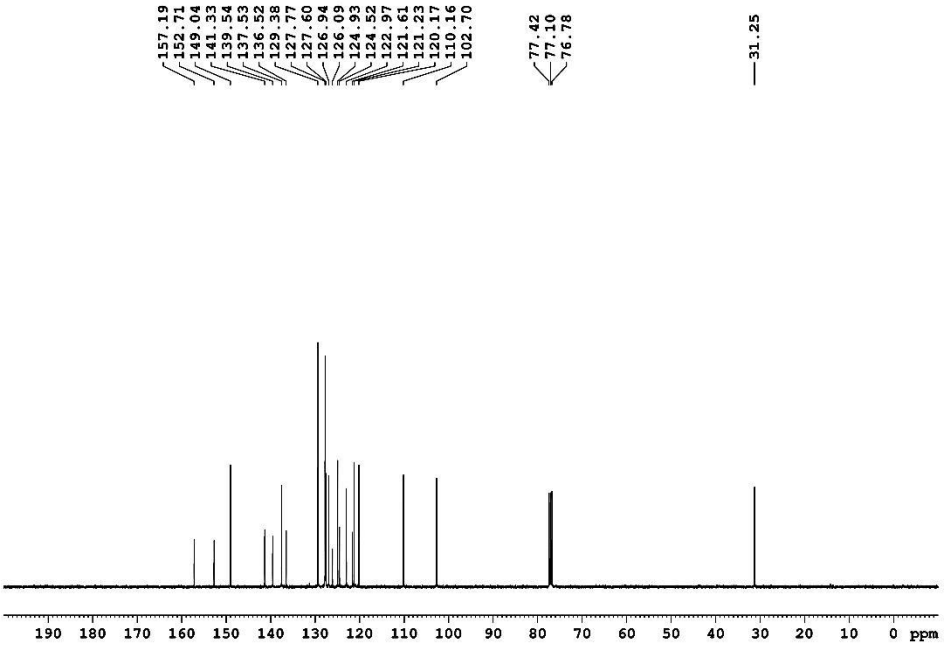

Figure S104. ^{13}C NMR spectrum of compound **10m**

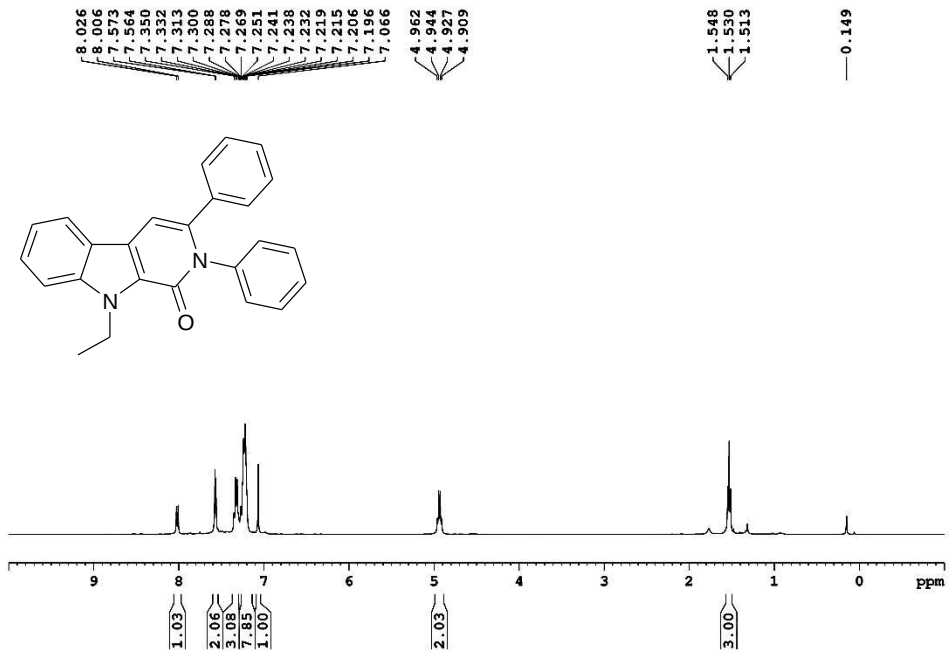

Figure S105. ^{1}H NMR spectrum of compound **10n**

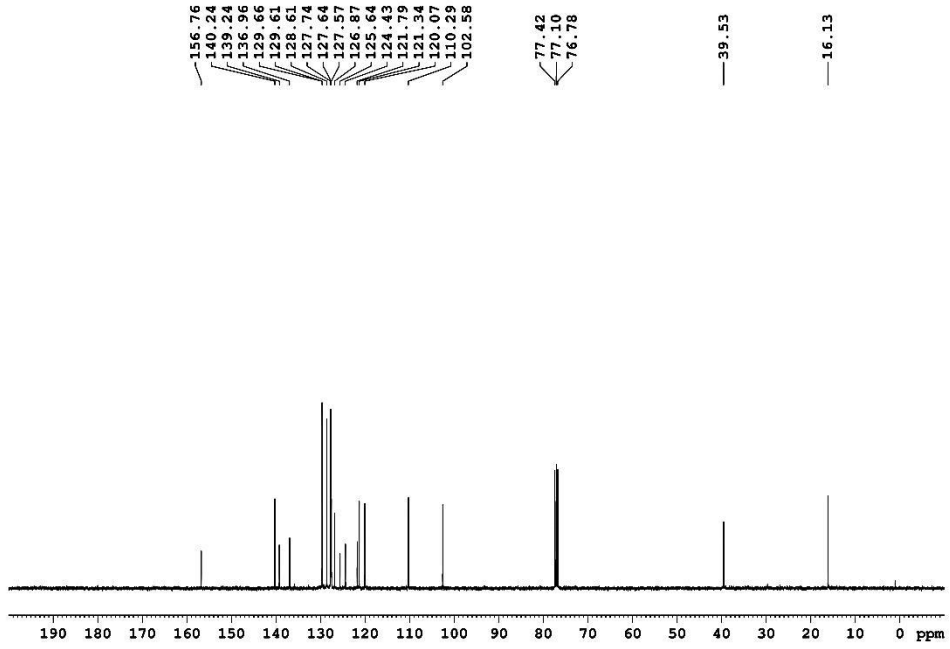

Figure S106. ^{13}C NMR spectrum of compound **10n**

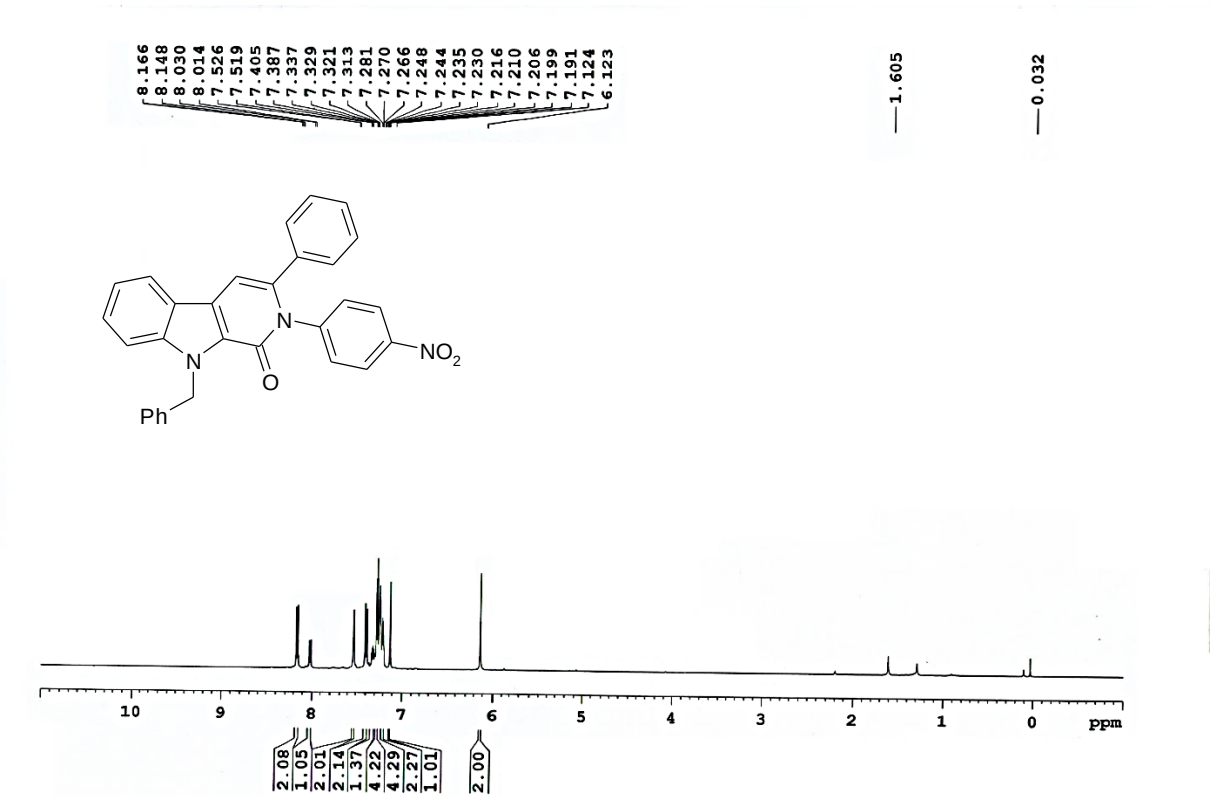

Figure S107. ^{1}H NMR spectrum of compound **10o**

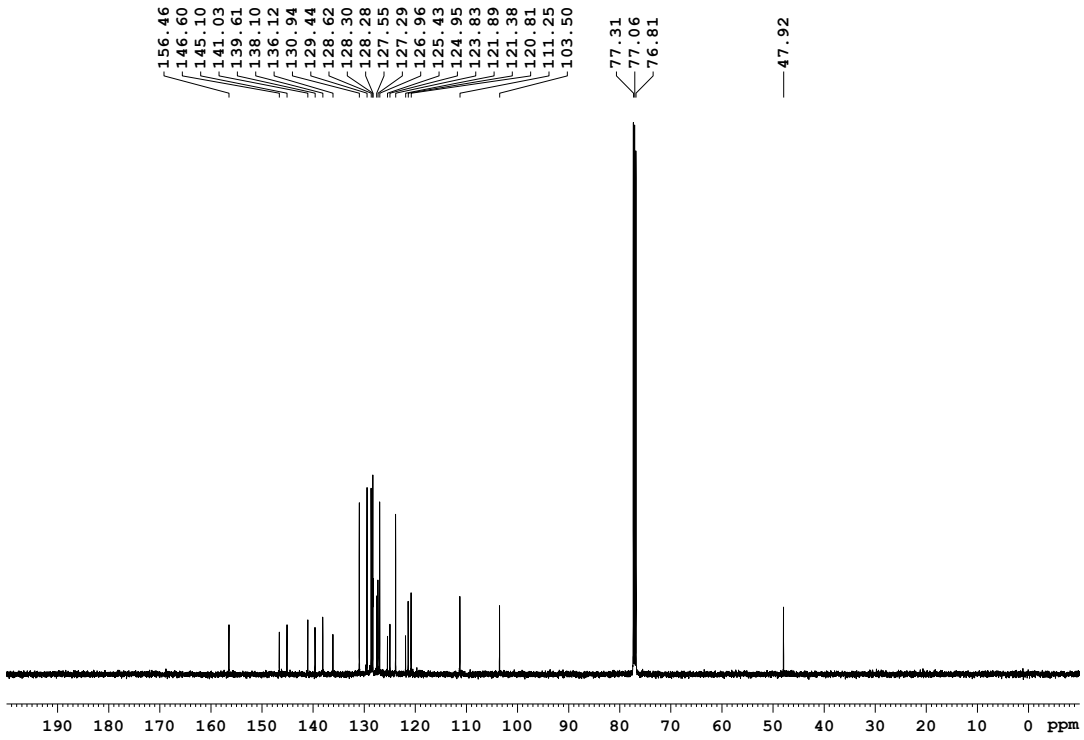

Figure S108. ^{13}C NMR spectrum of compound **10o**