

One-pot synthesis of spiropyrroloquinoline-isoindolinone and their aza-analogs via Ugi-4CR/ metal-free intramolecular bis-annulation process

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Supporting Information

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1. Copies of ^1H and ^{13}C NMR spectra for compounds 8a-o

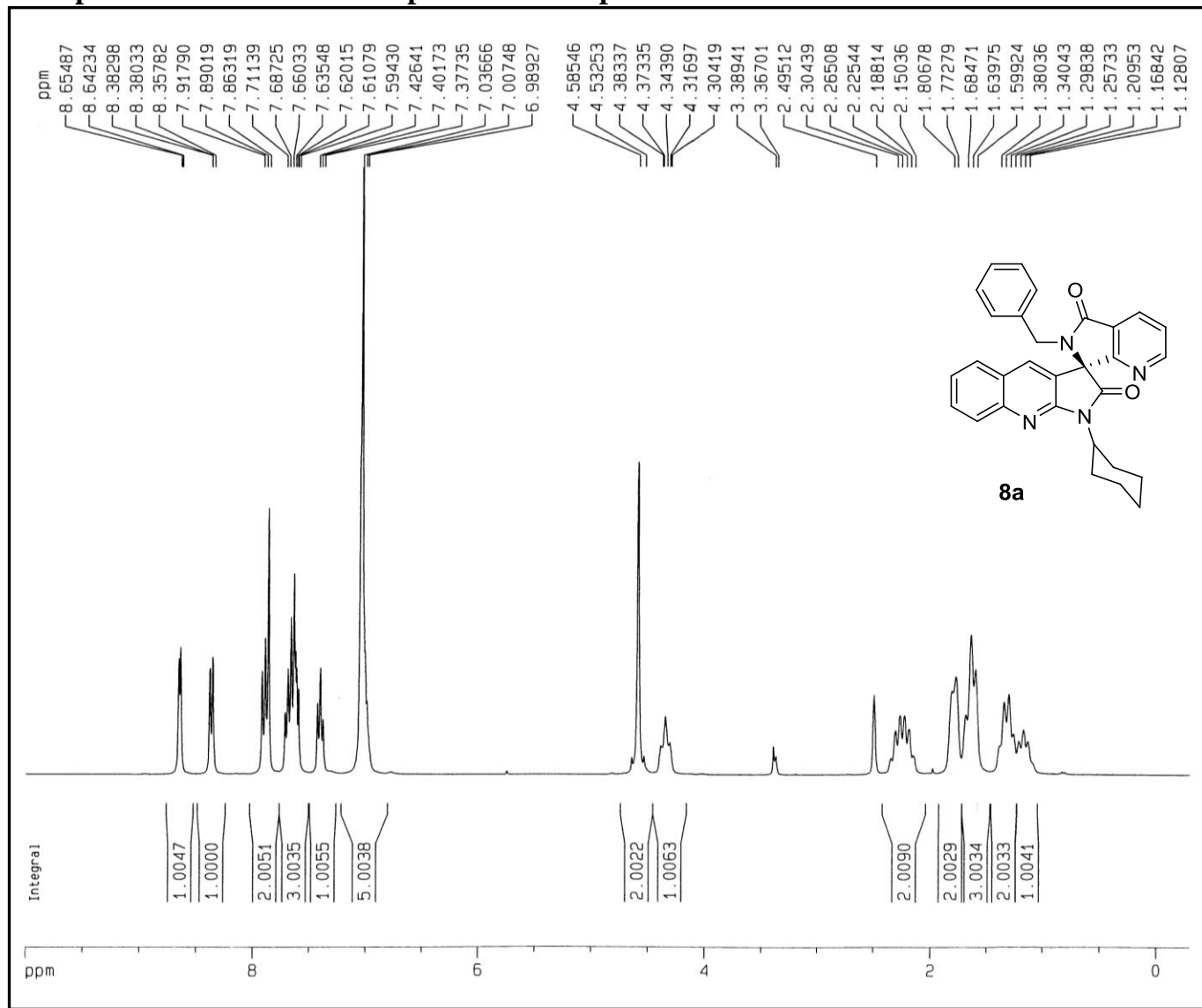
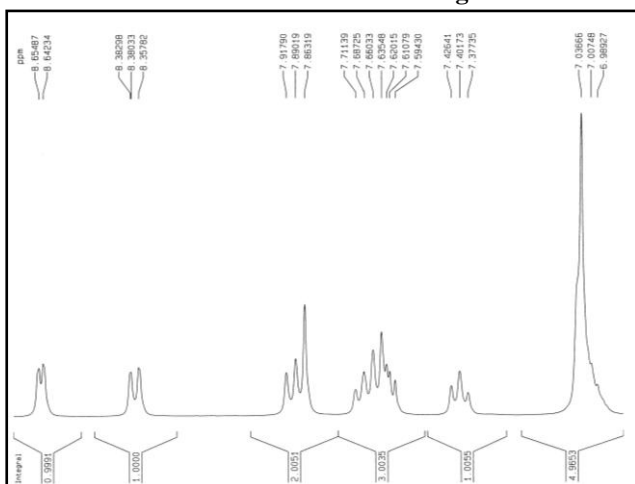


Figure 1. ^1H NMR (300 MHz, $\text{DMSO-}d_6$) (**8a**).



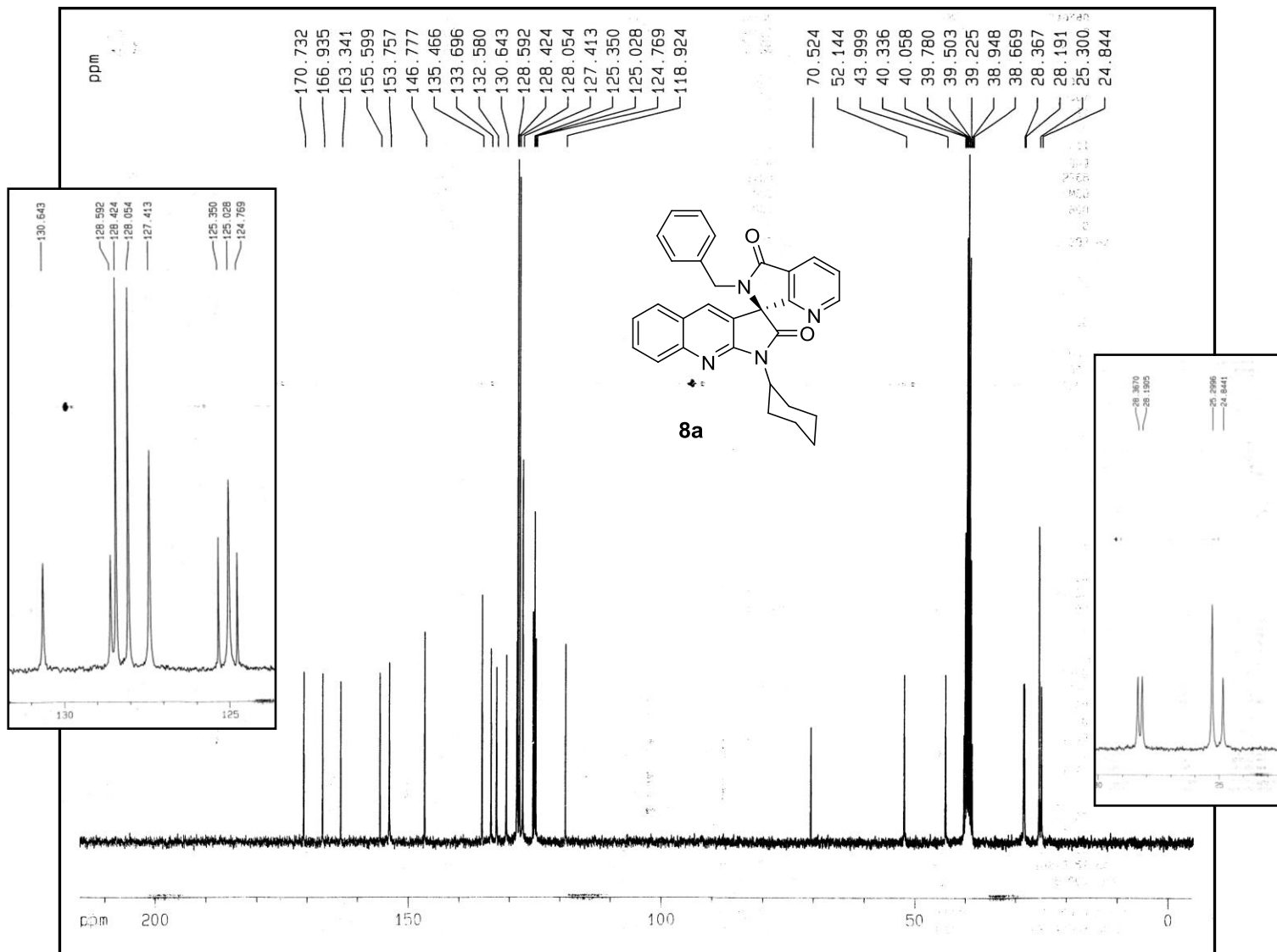


Figure 2. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**8a**).

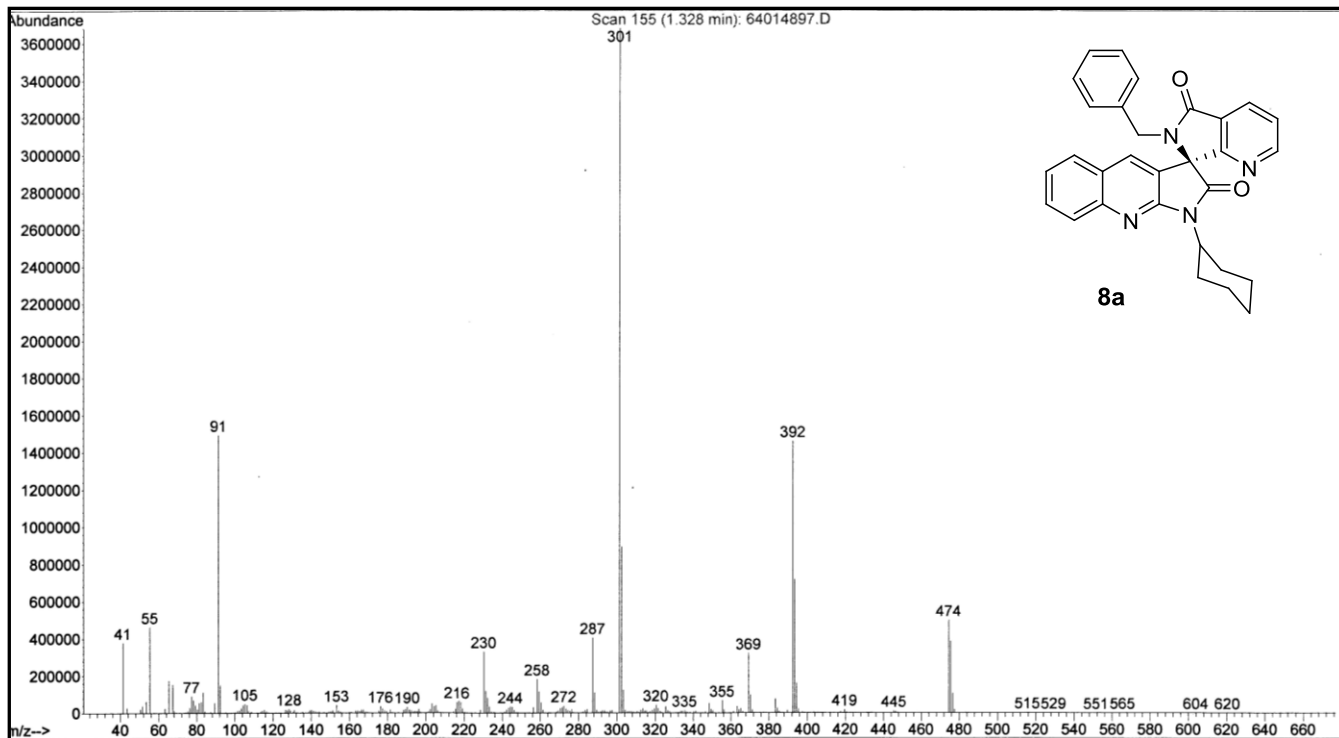


Figure 3. Mass (**8a**).

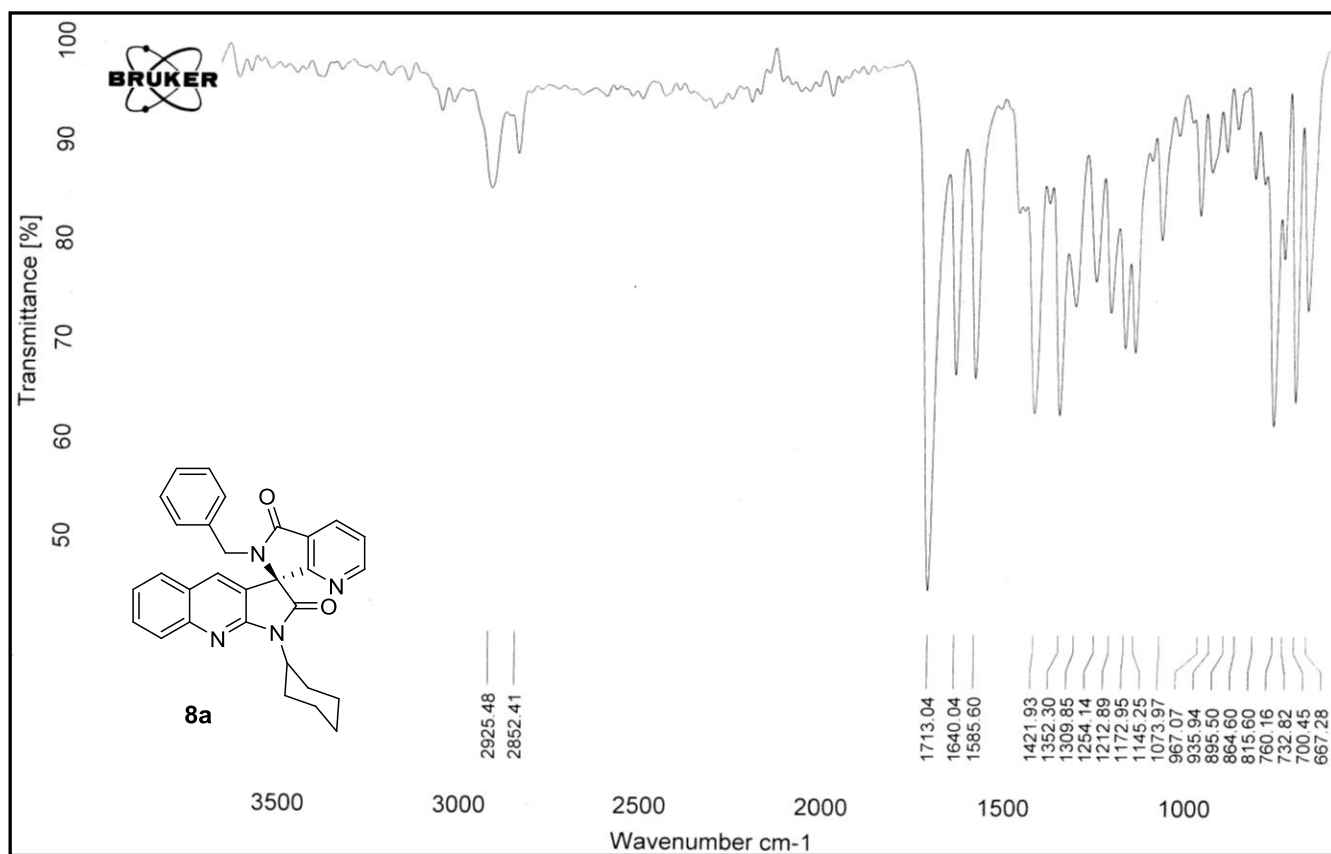


Figure 4. IR (8a).

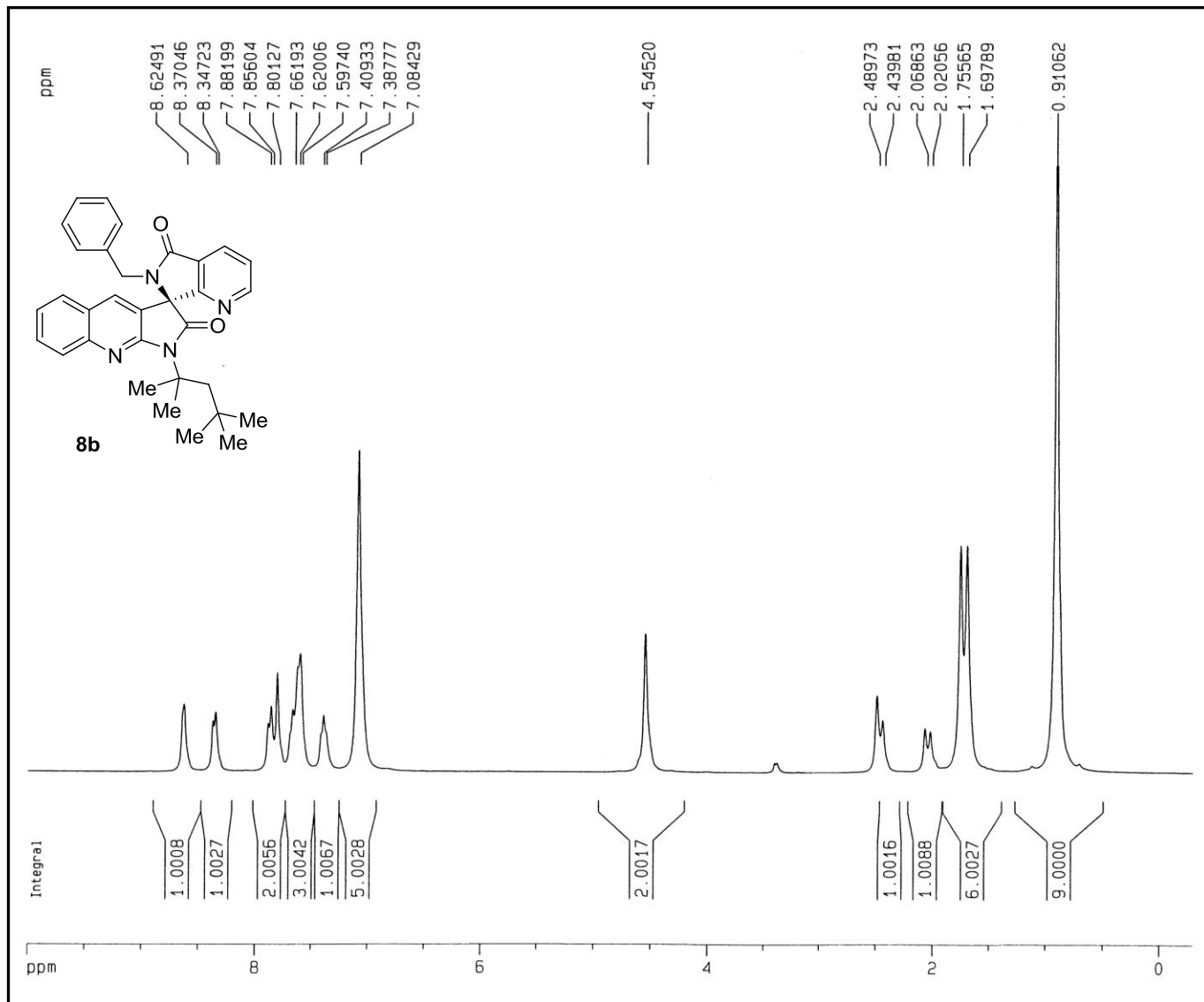
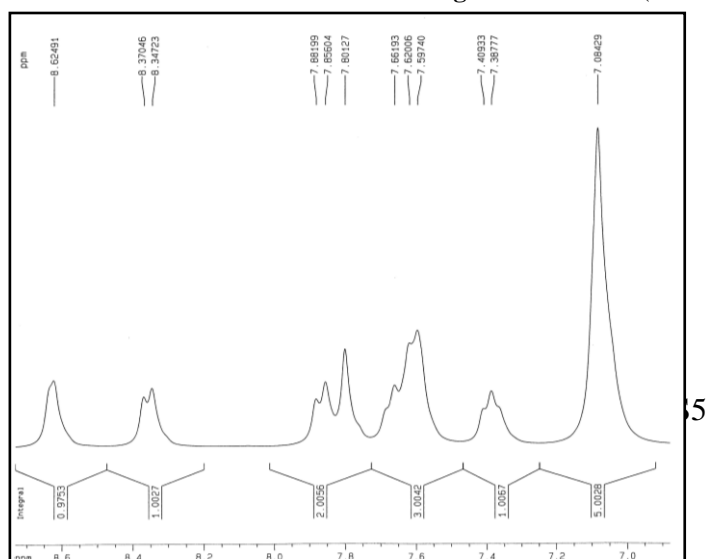


Figure 5. ¹H NMR (300 MHz, DMSO-d₆) (**8b**).



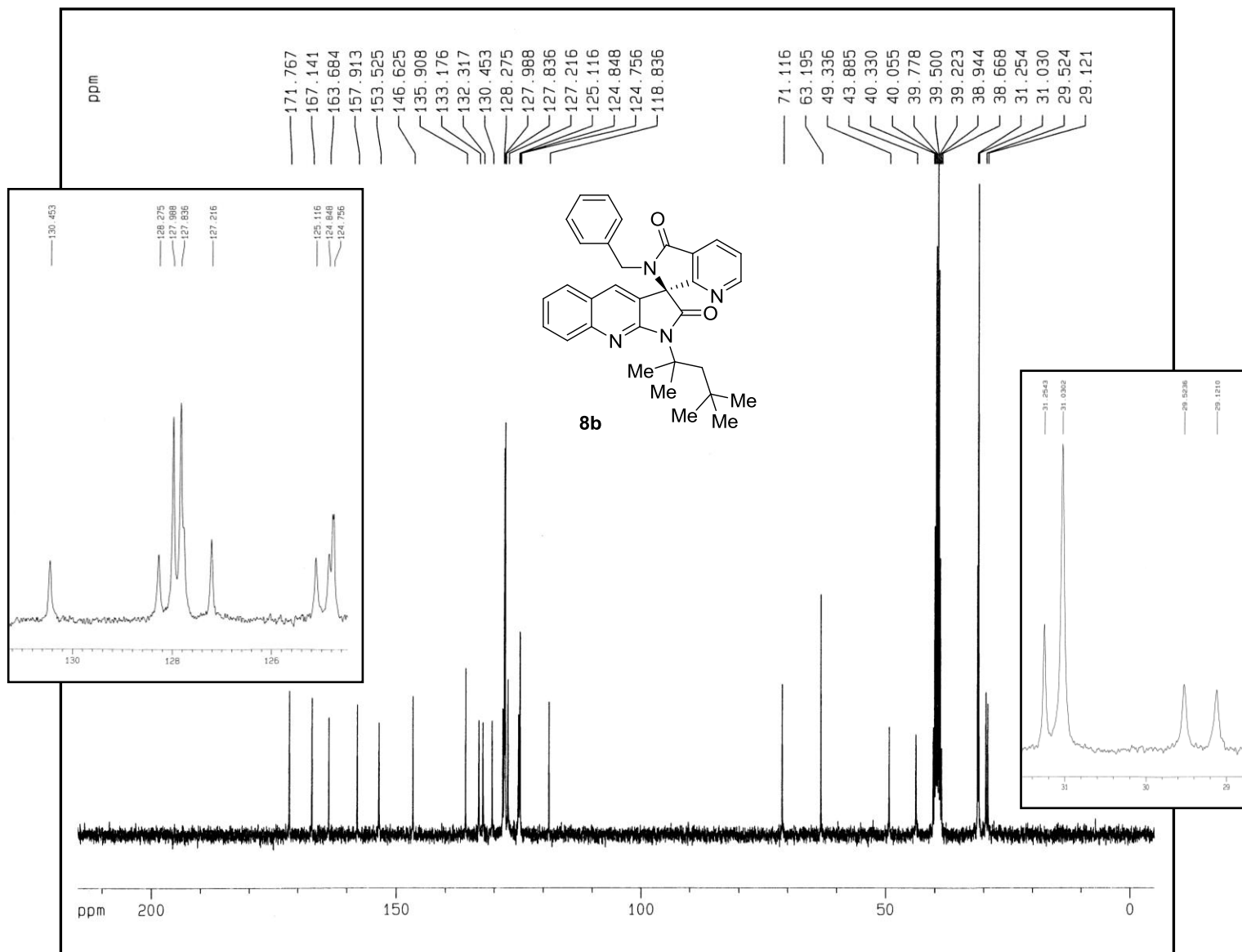


Figure 6. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**8b**).

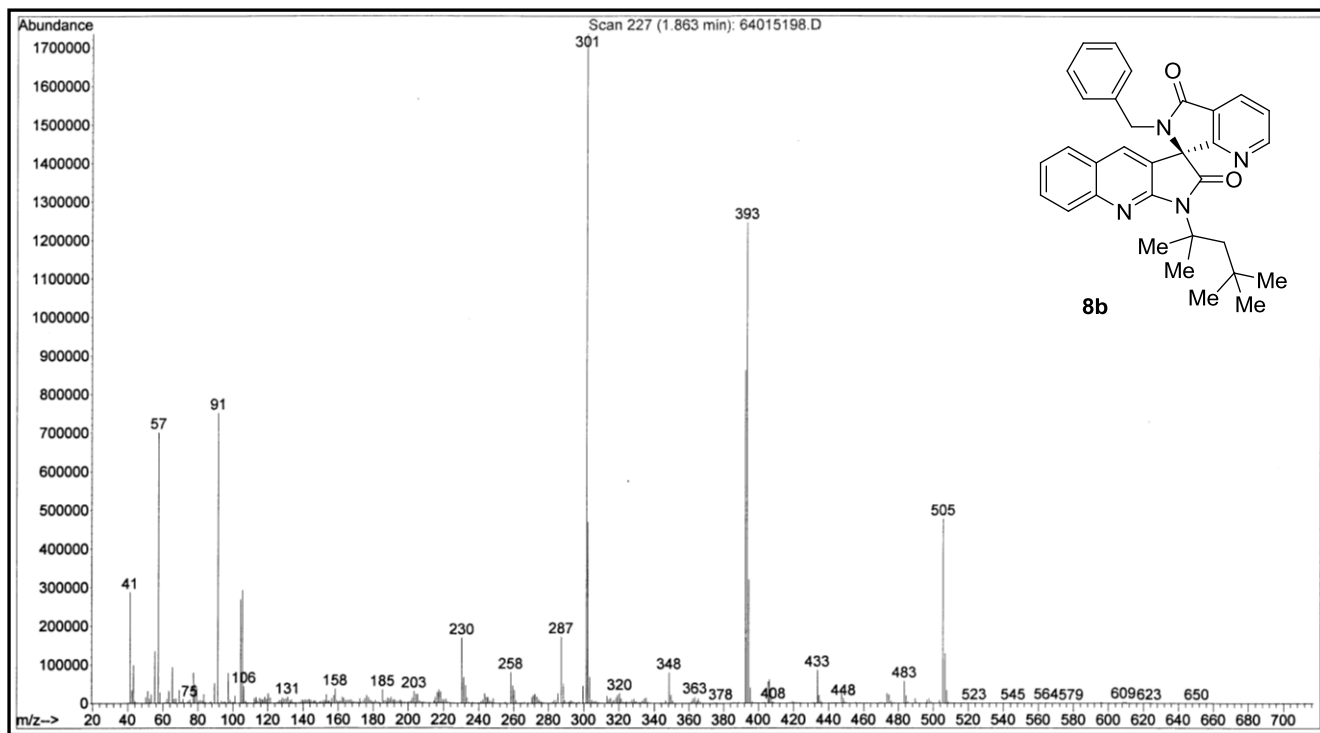


Figure 7. Mass (8b).

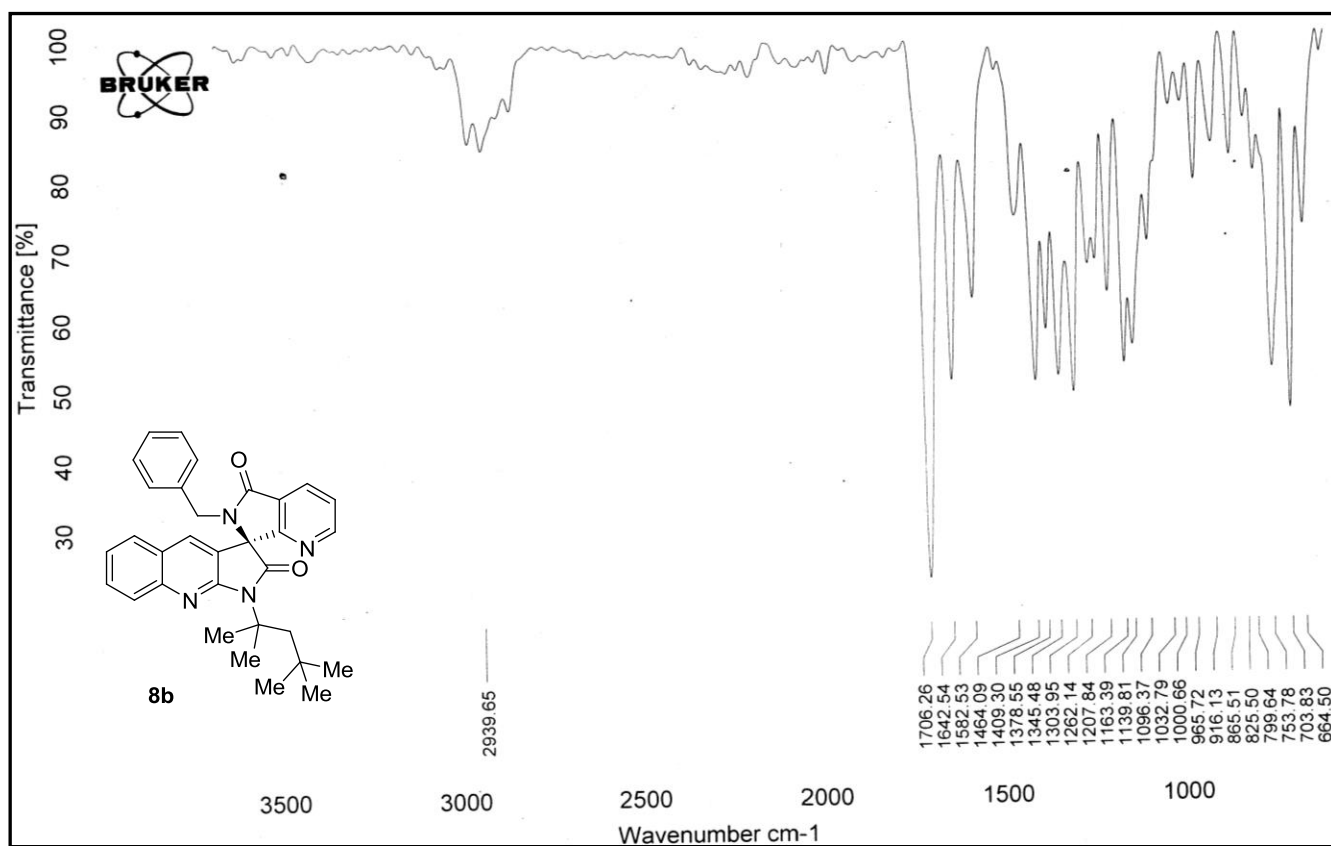


Figure 8. IR (8b).

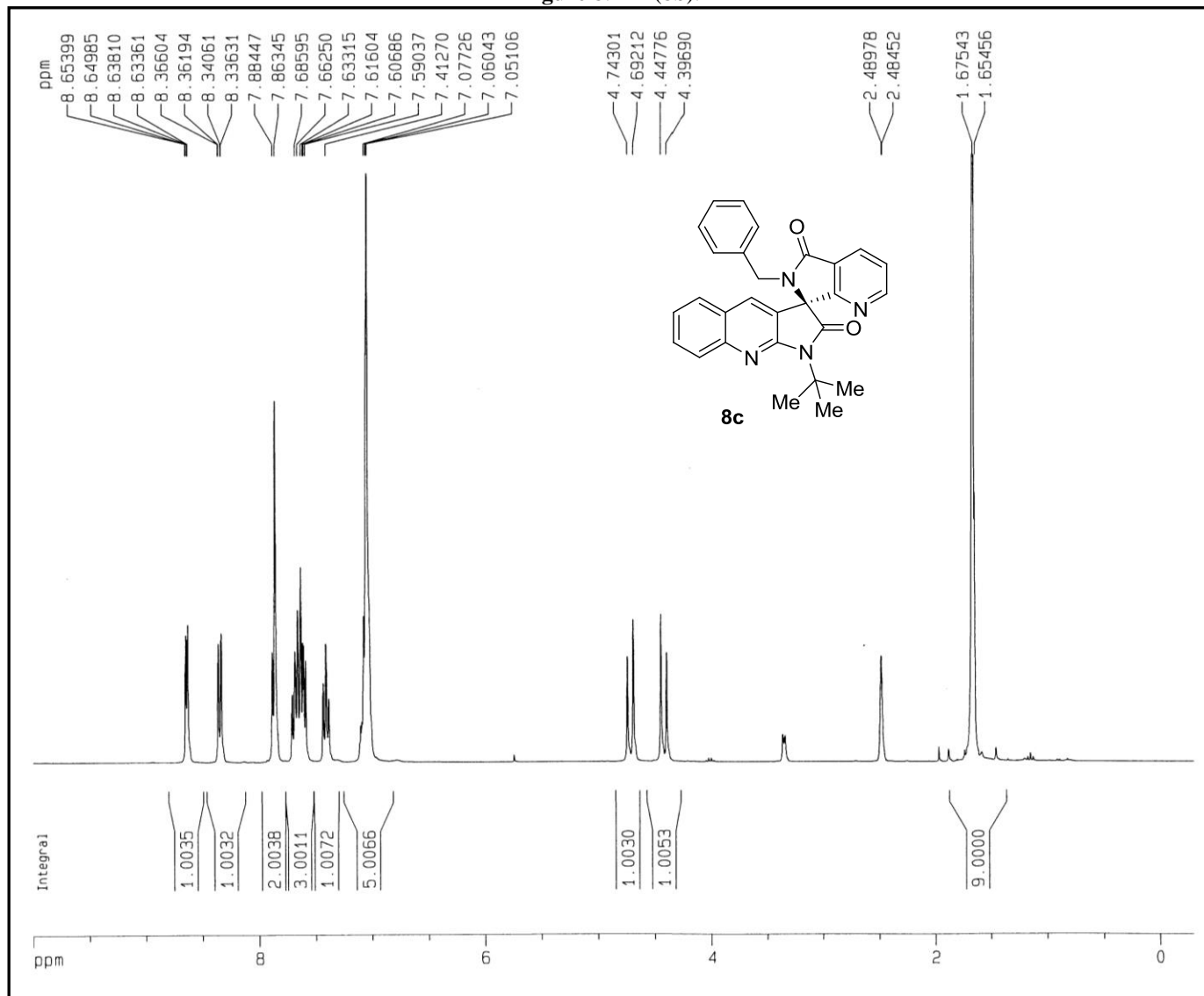
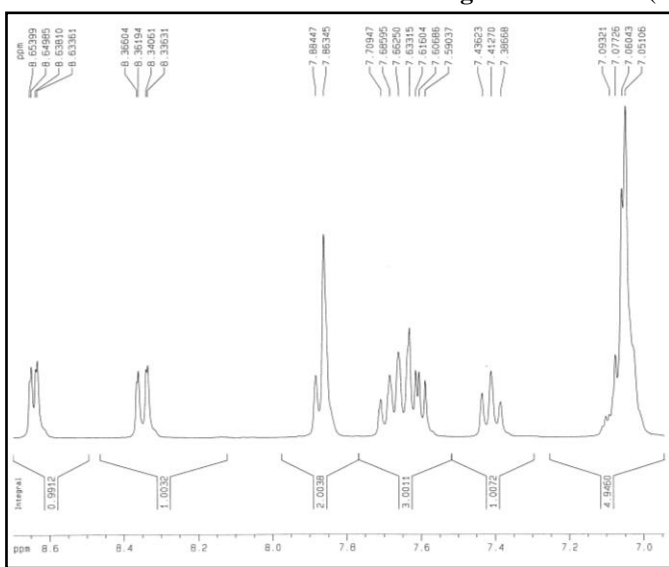


Figure 9. ¹H NMR (300 MHz, DMSO-d₆) (8c).



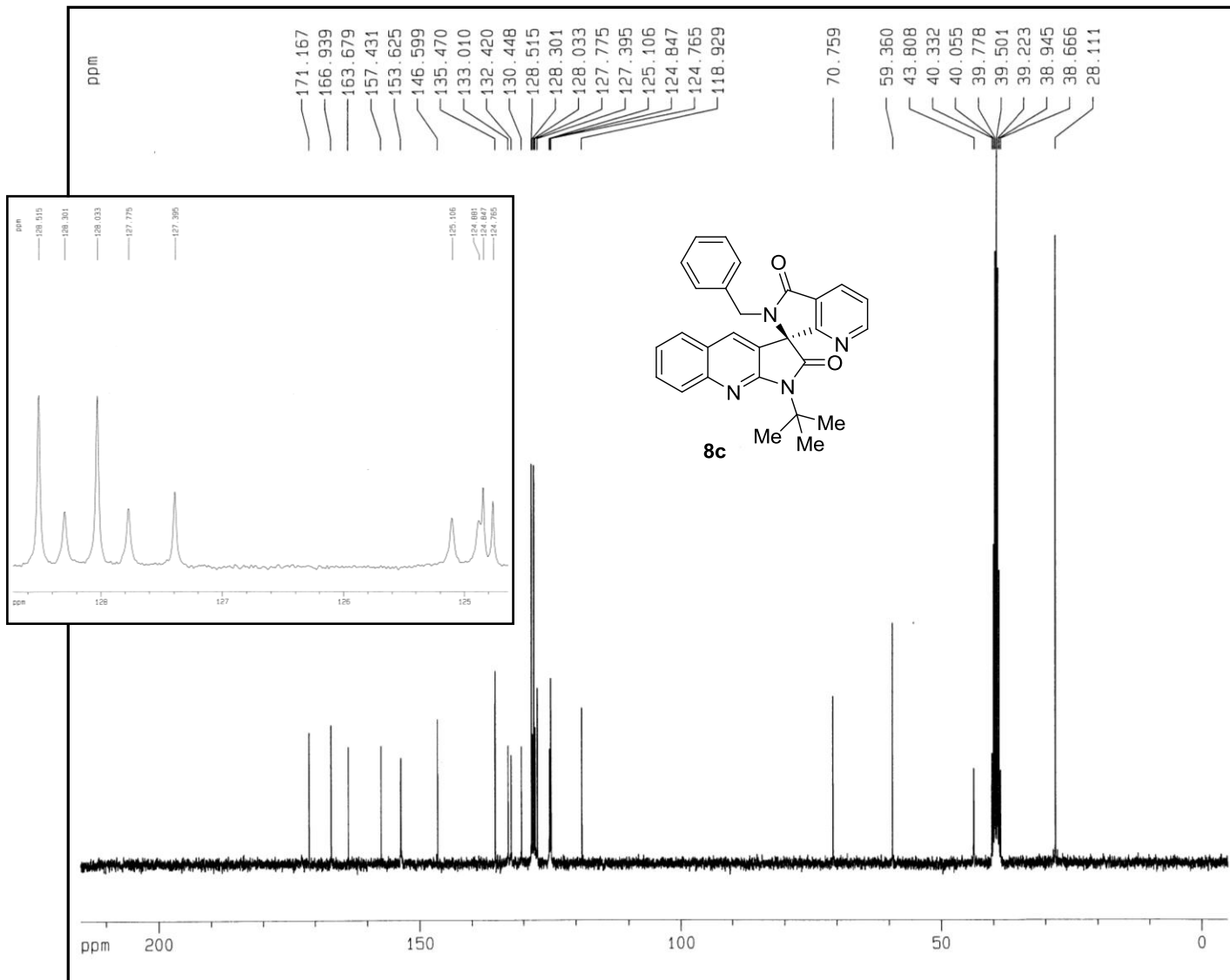


Figure 10. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8c**).

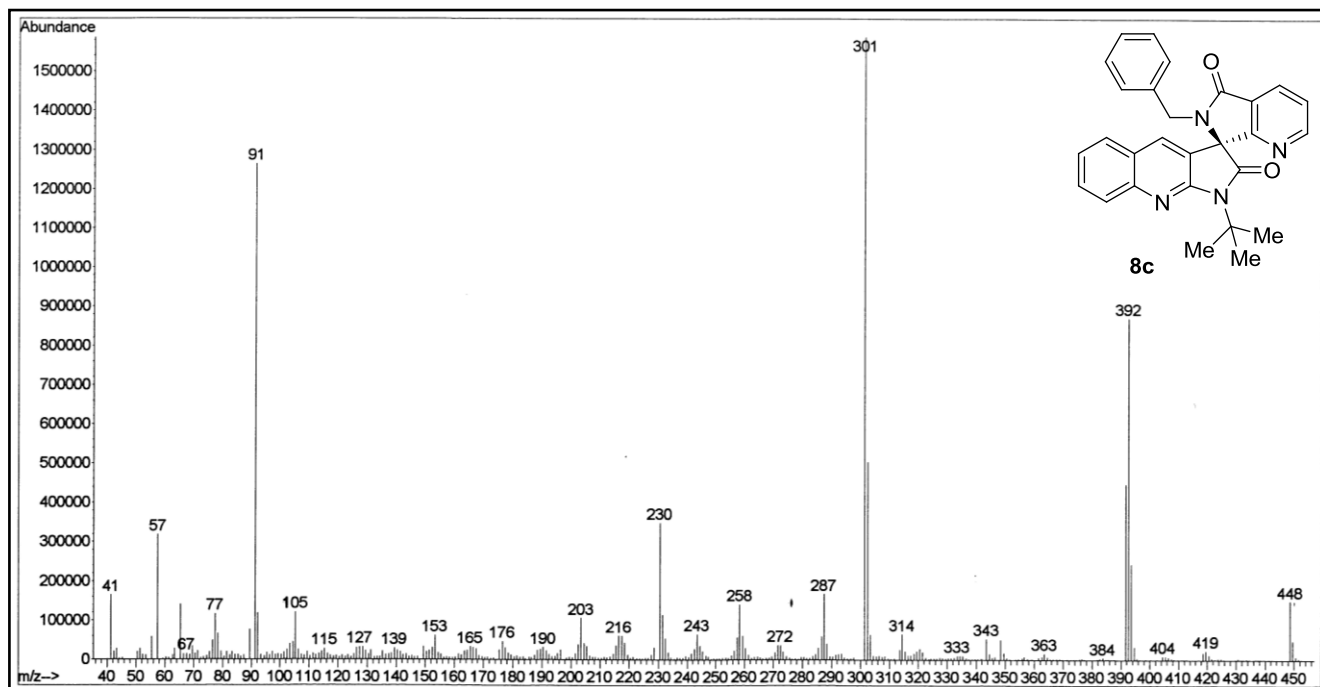


Figure 11. Mass (**8c**).

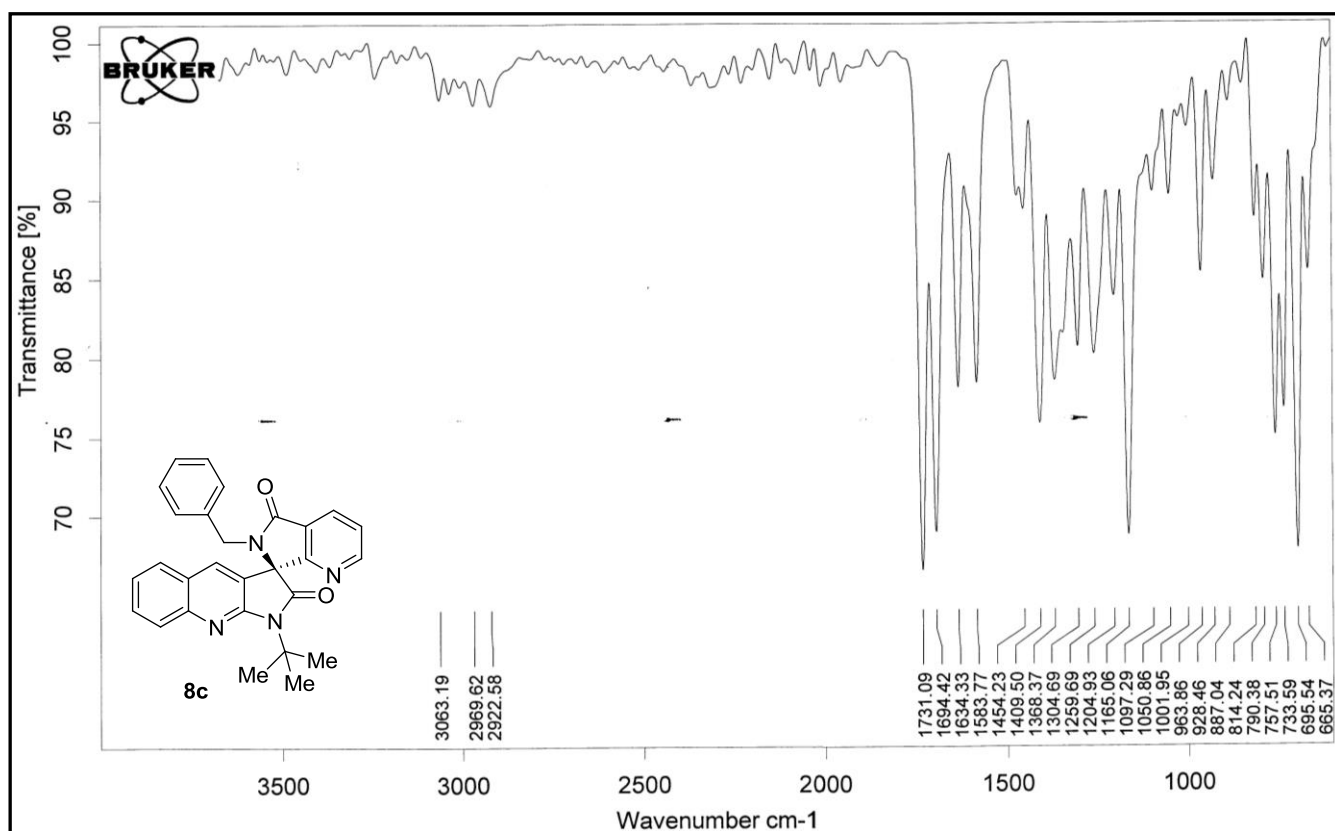


Figure 12. IR (8c).

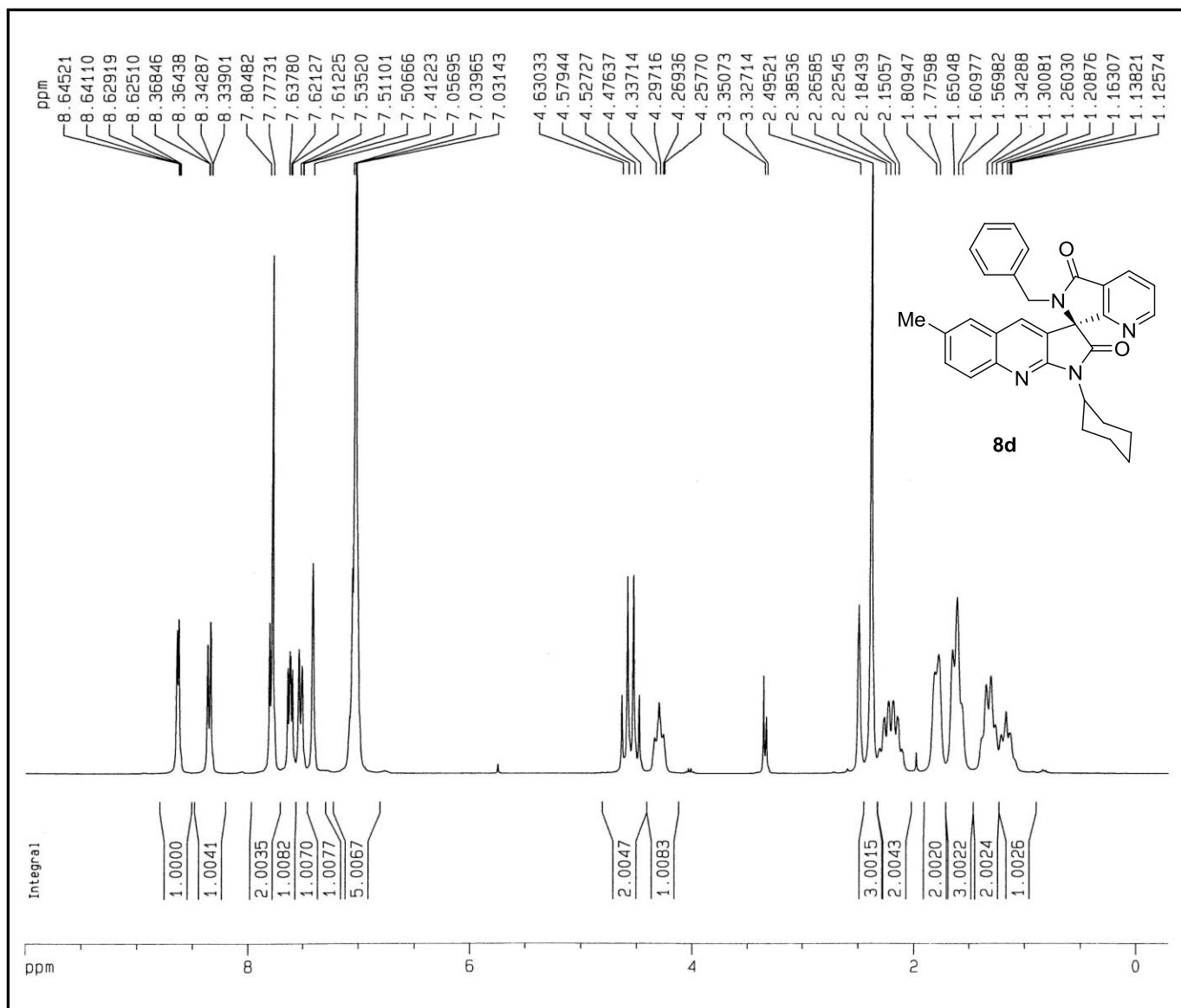
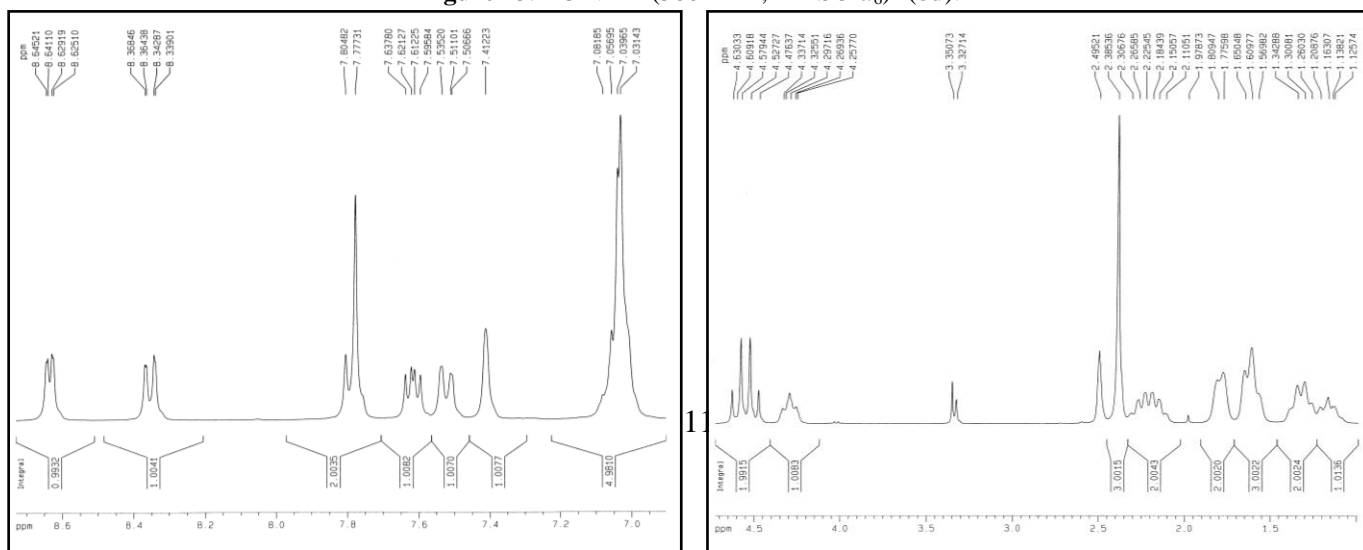


Figure 13. ¹³C NMR (300 MHz, DMSO-*d*₆) (8d).



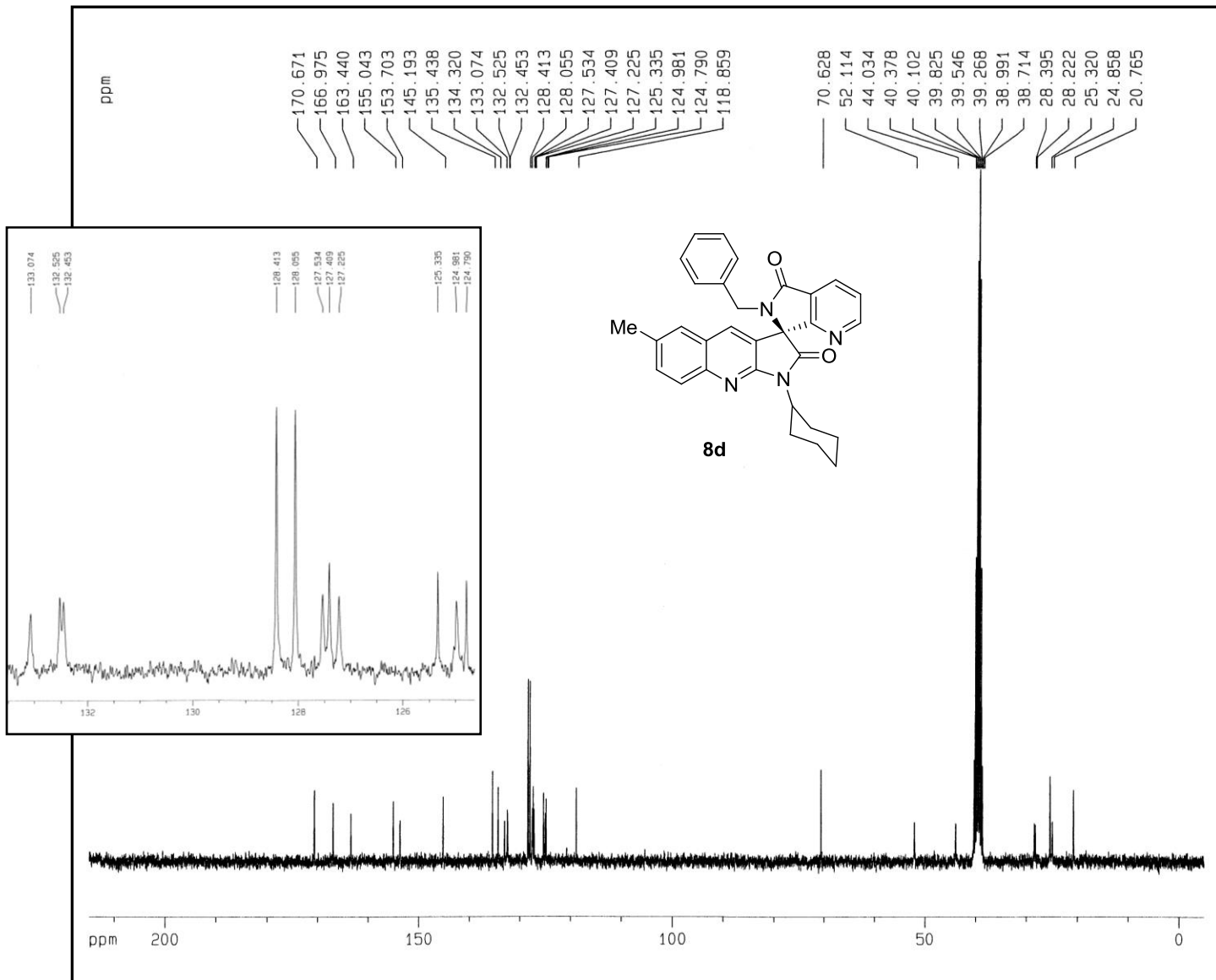
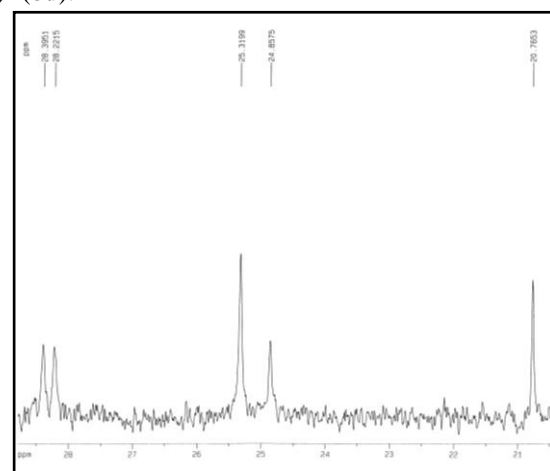


Figure 14. ¹³C NMR (300 MHz, DMSO-d₆) (**8d**).



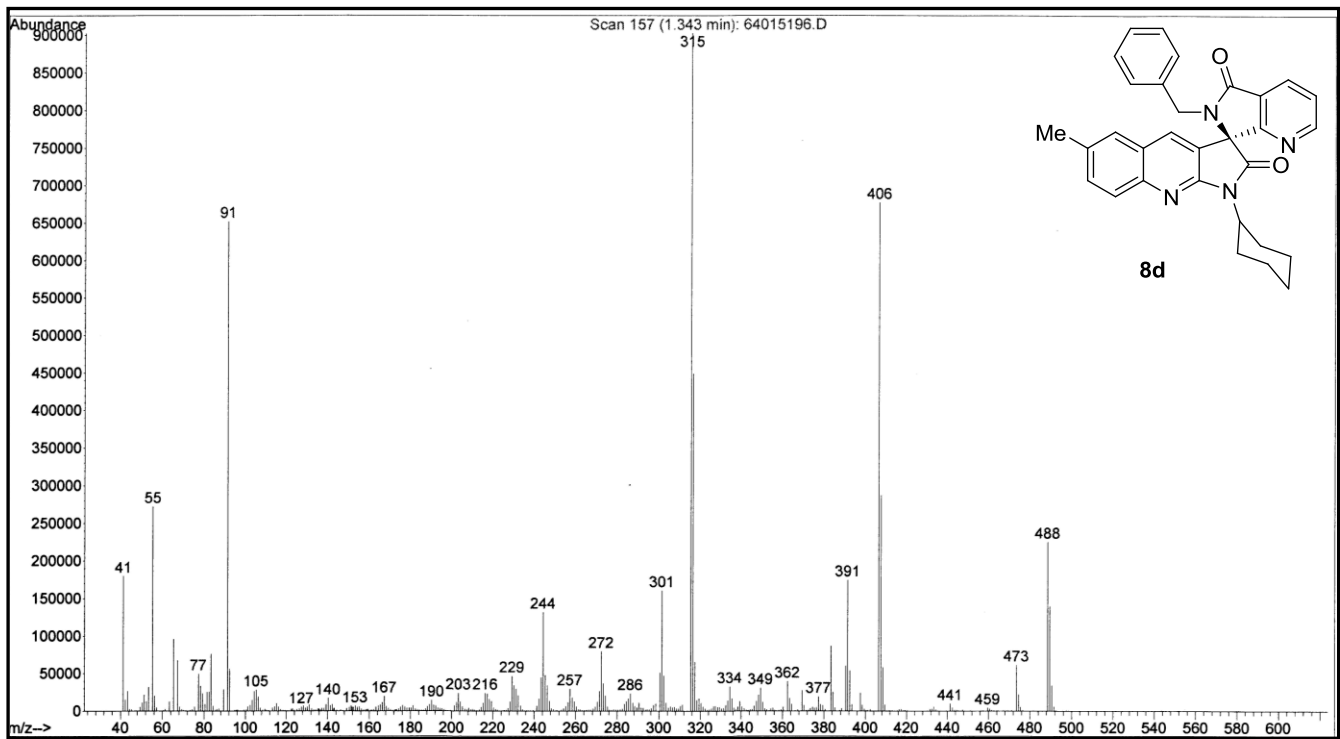


Figure 15. Mass (8d).

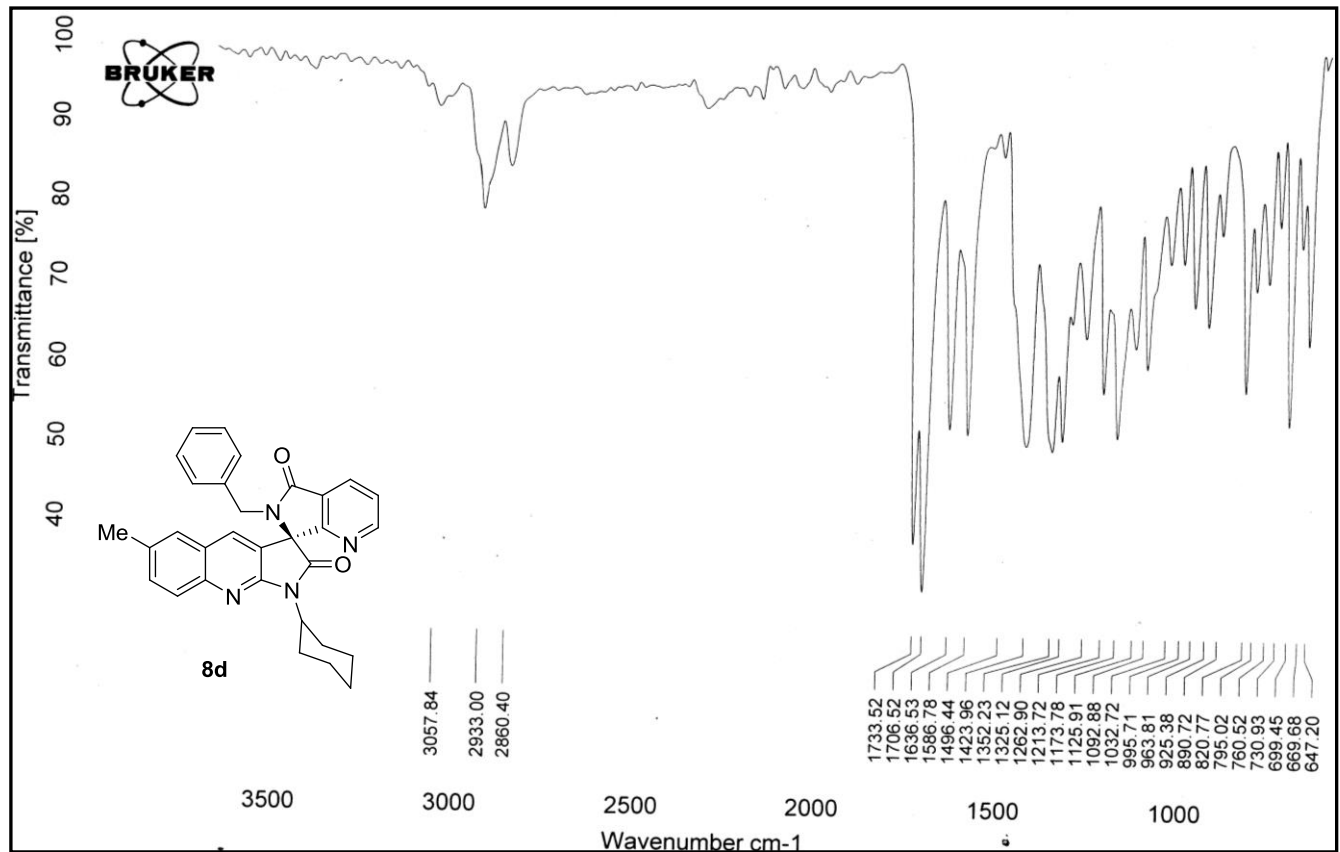


Figure 16. IR (8d).

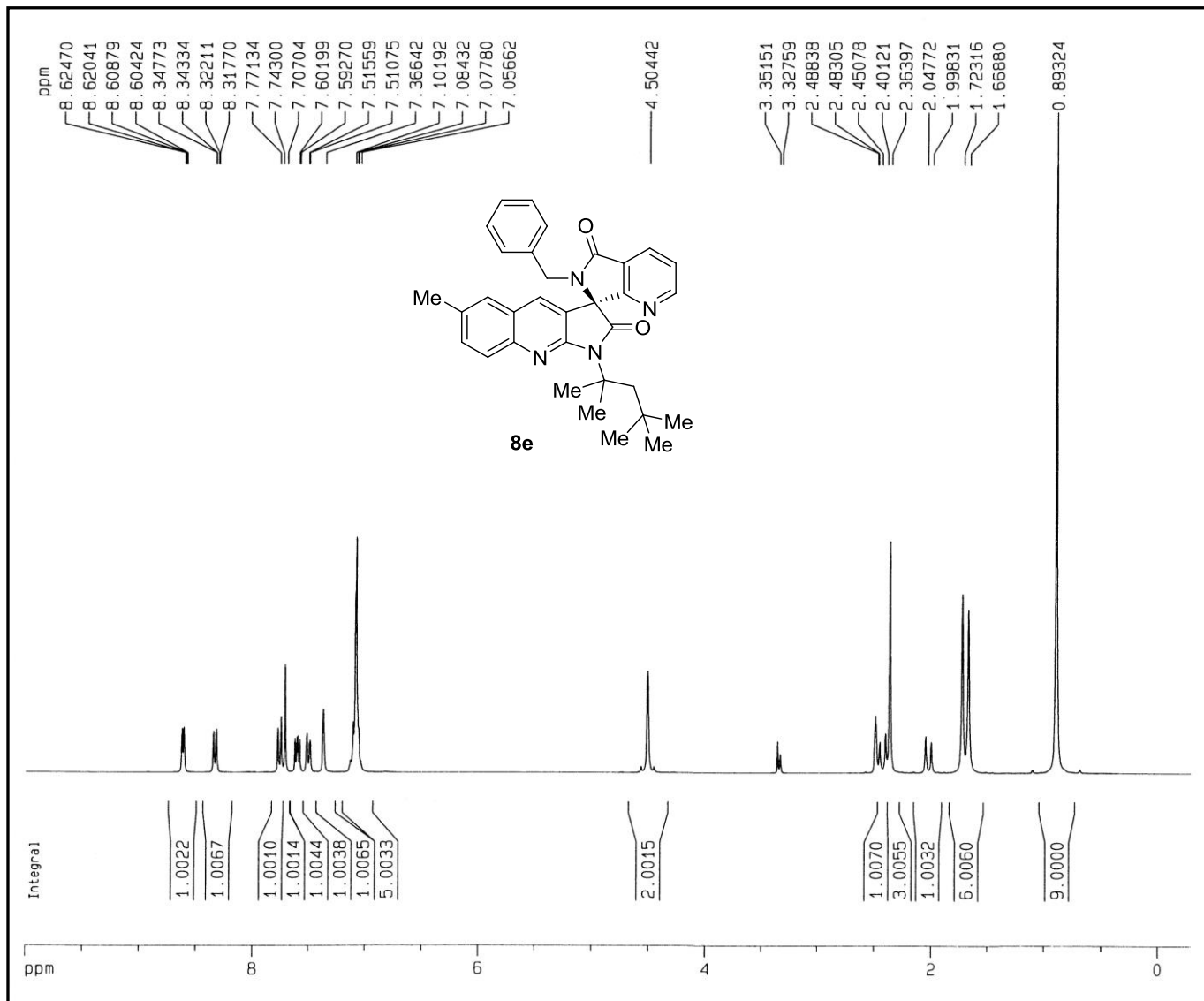
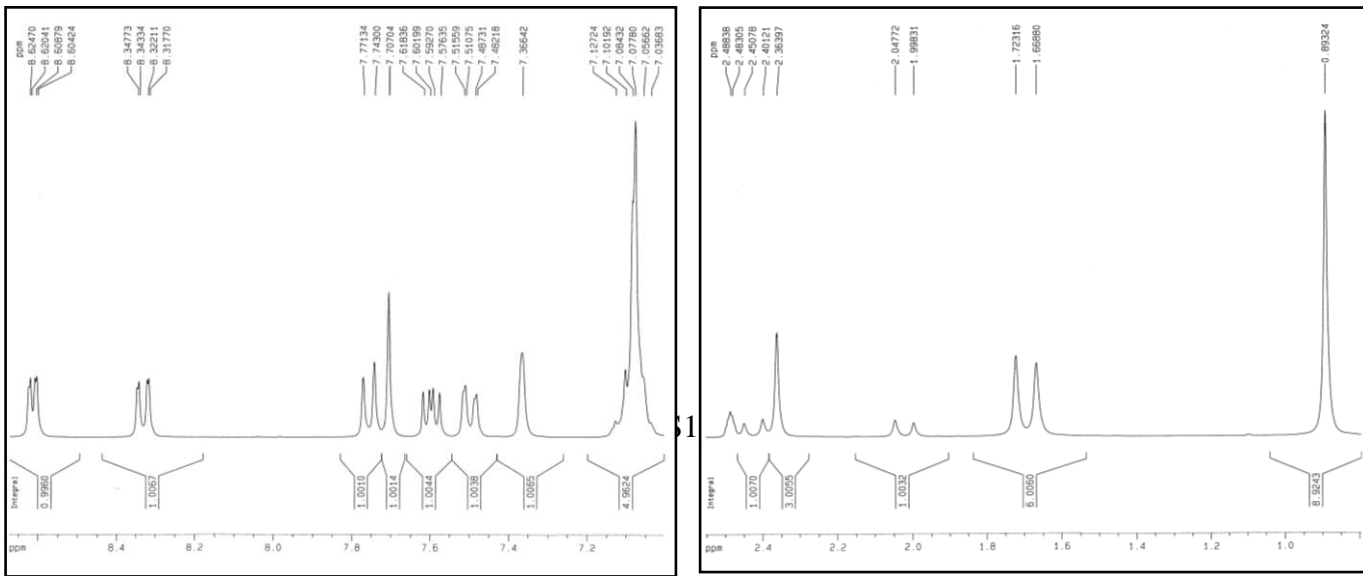


Figure 17. ¹H NMR (300 MHz, DMSO-d₆) (8e).



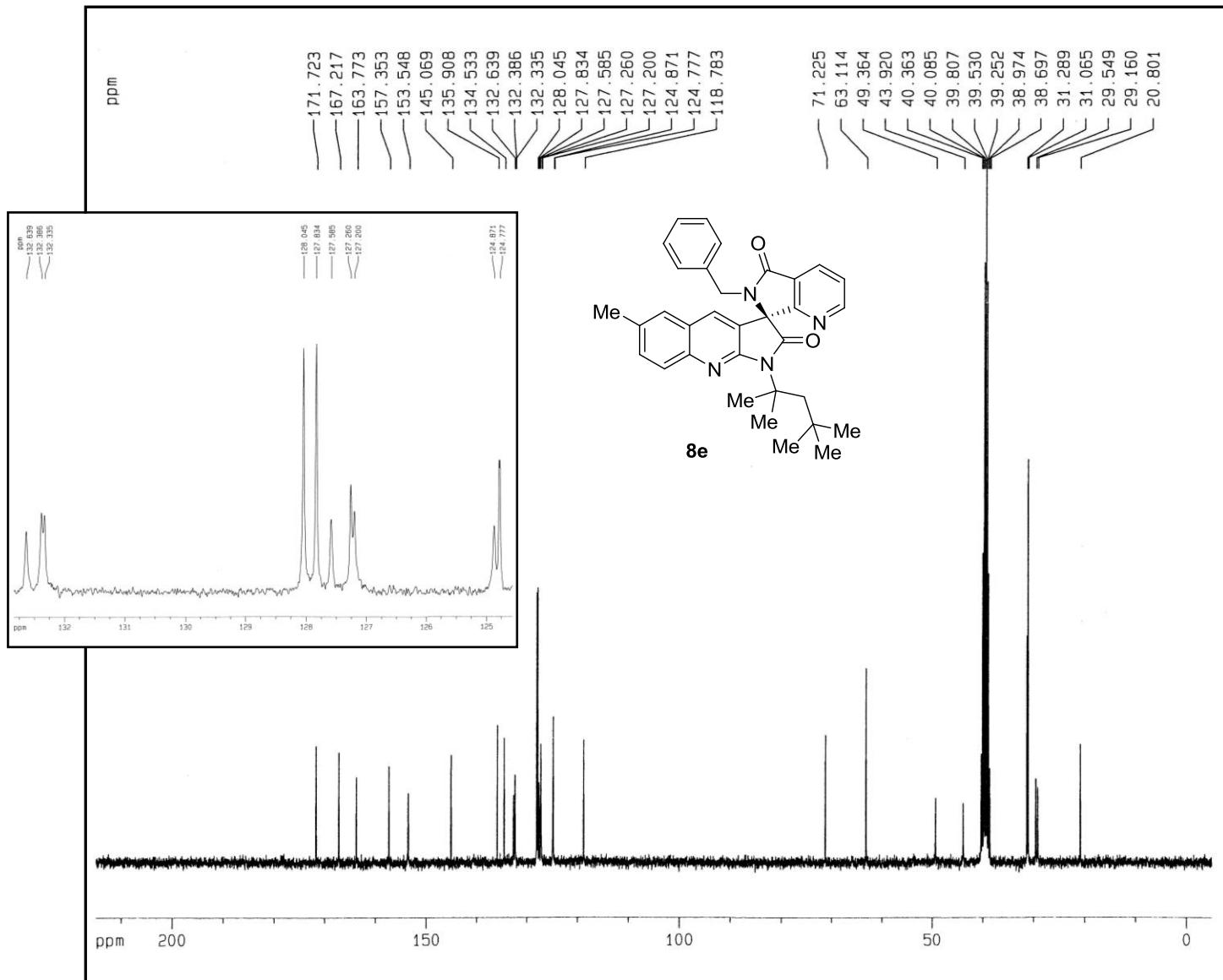


Figure 18. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8e**).

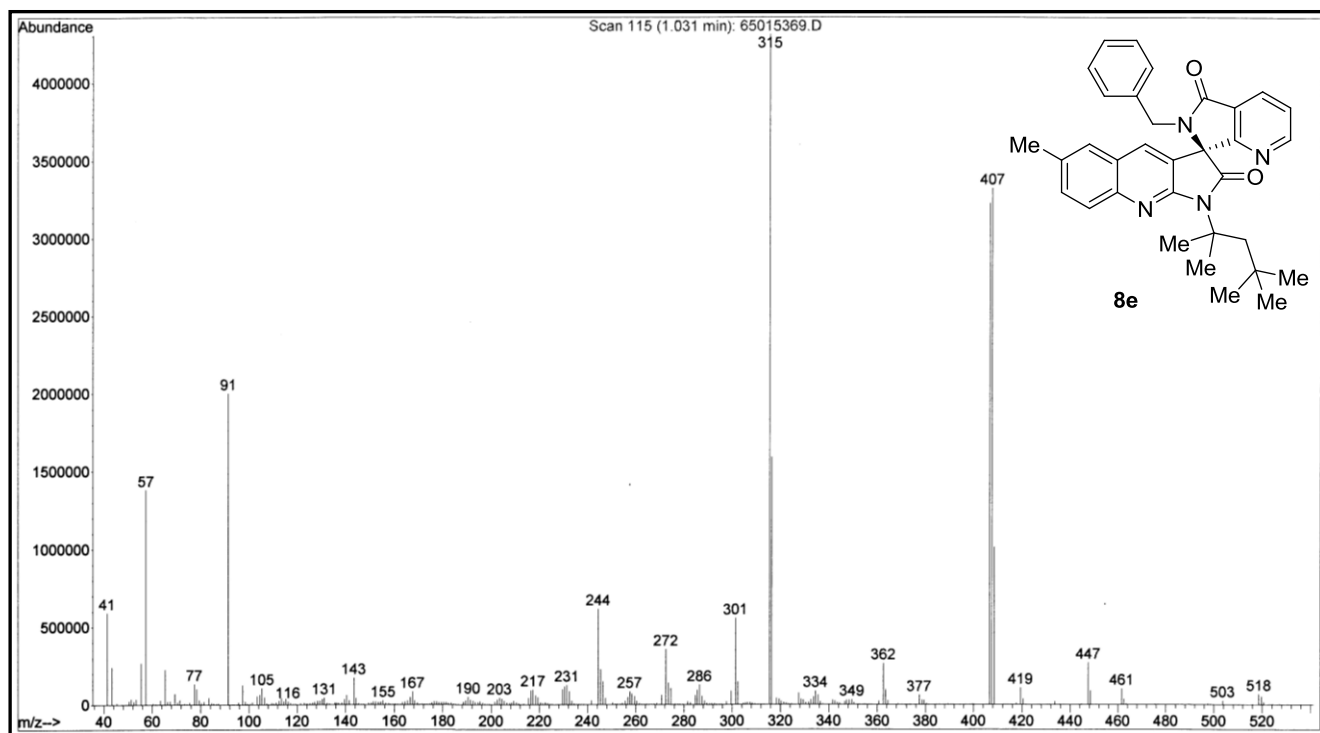


Figure 19. Mass (**8e**).

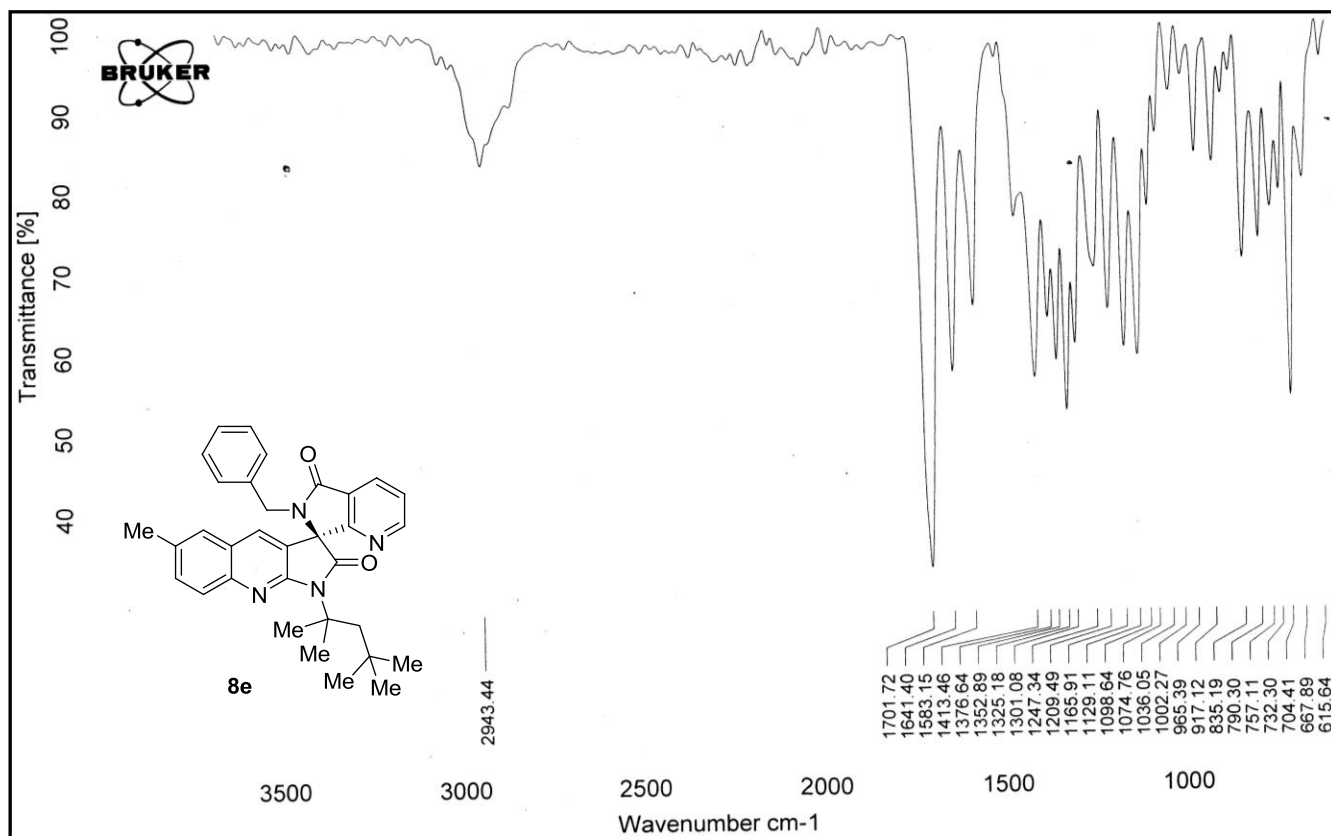


Figure 20. IR (8e).

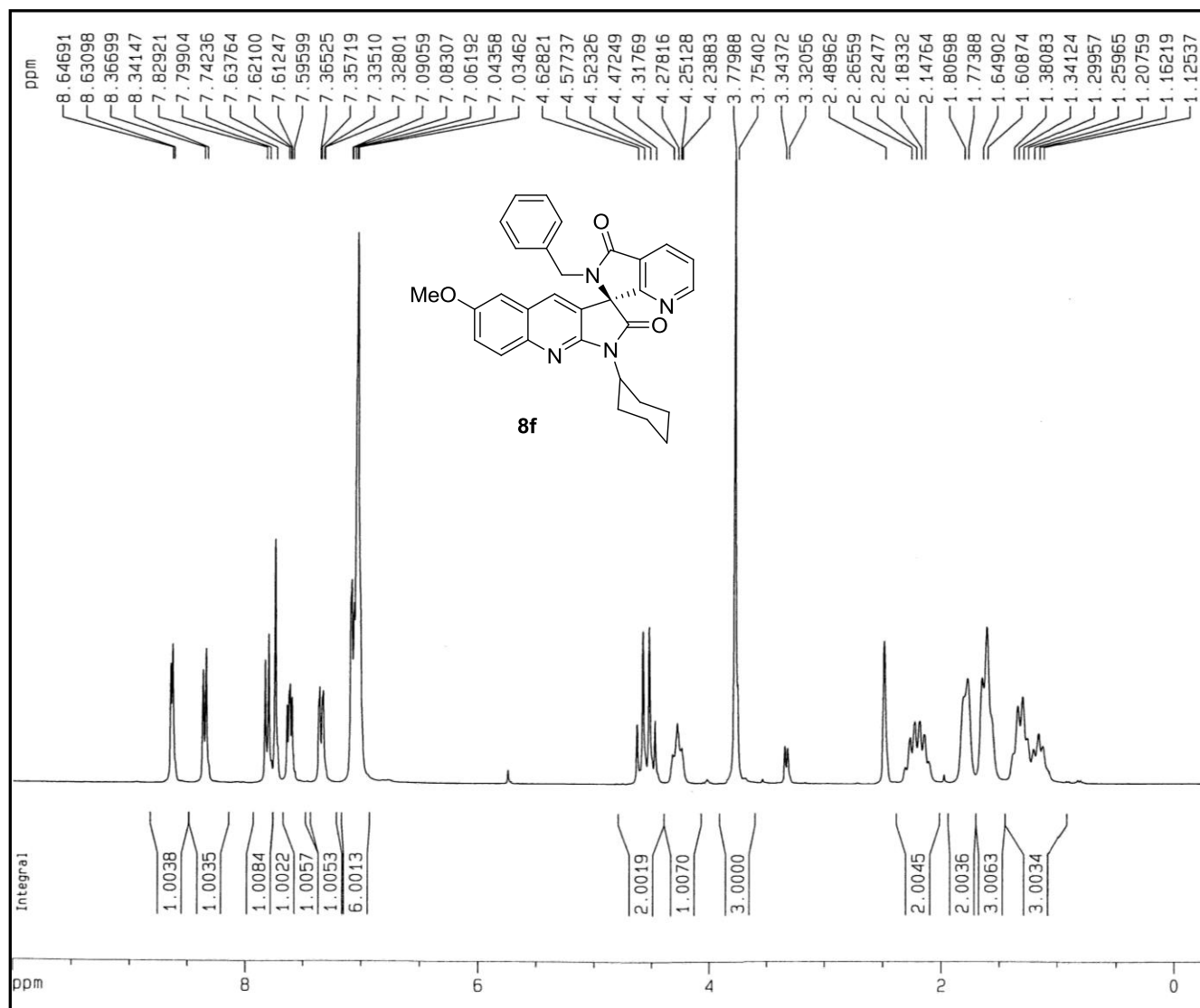
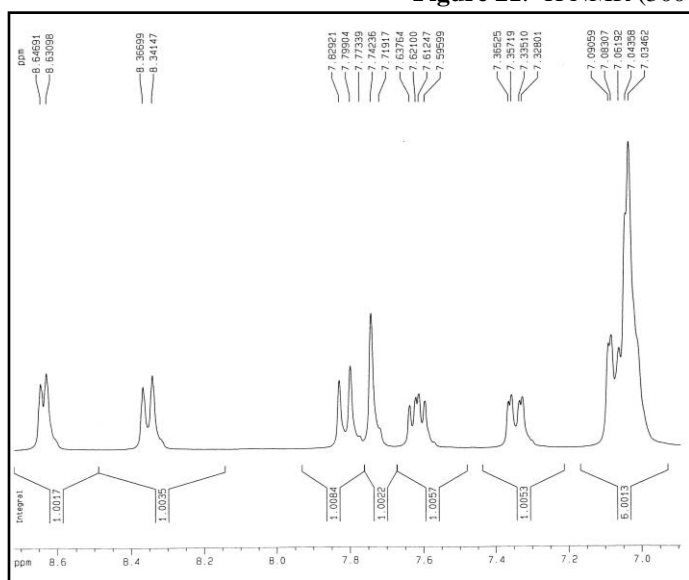


Figure 21. ¹H NMR (300 MHz, DMSO-d₆) (**8f**).



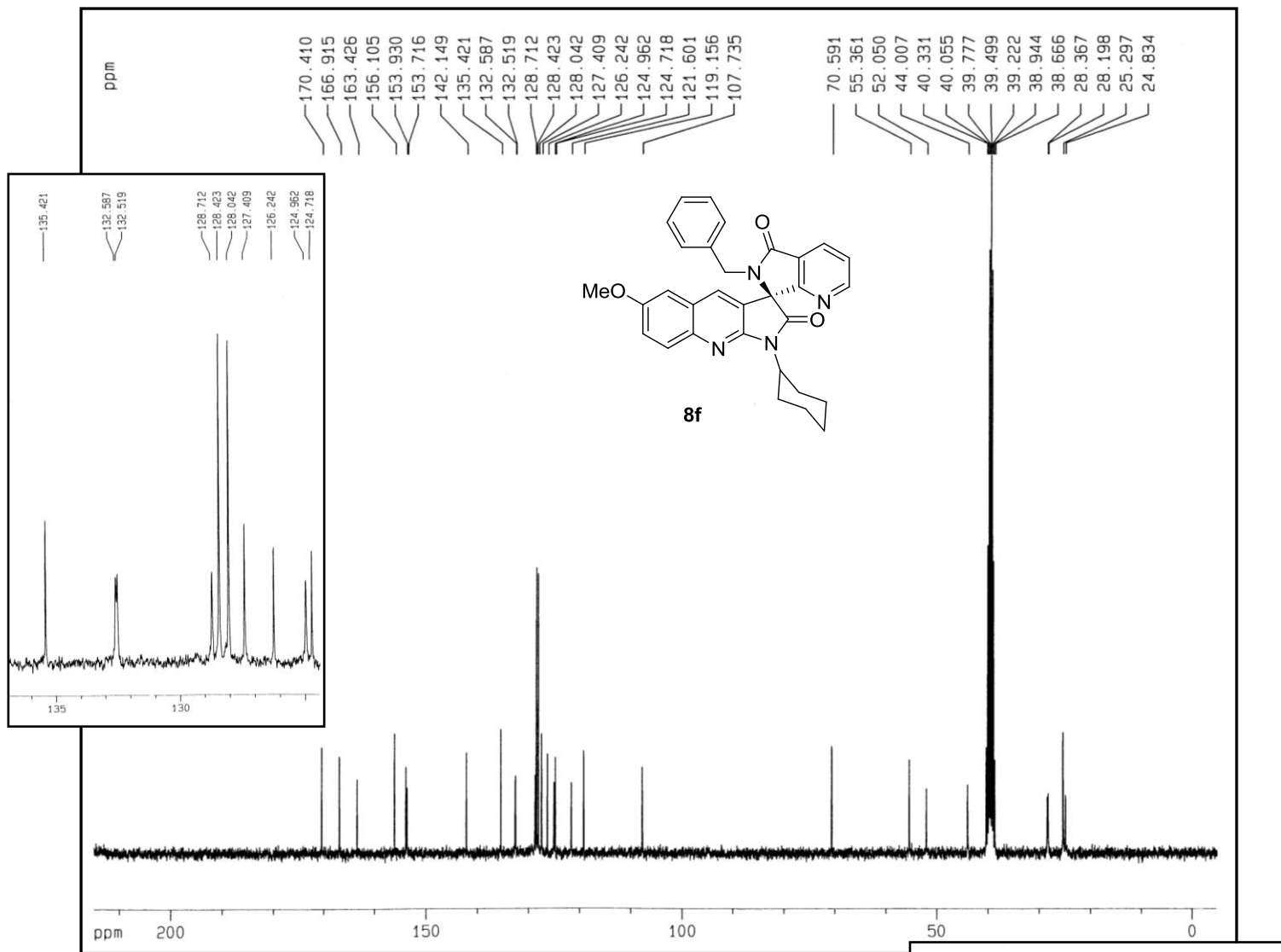
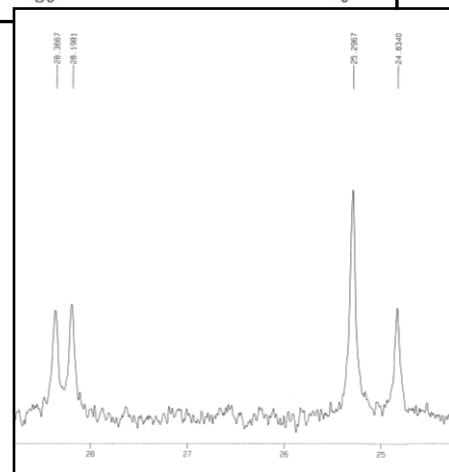


Figure 22. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**8f**).



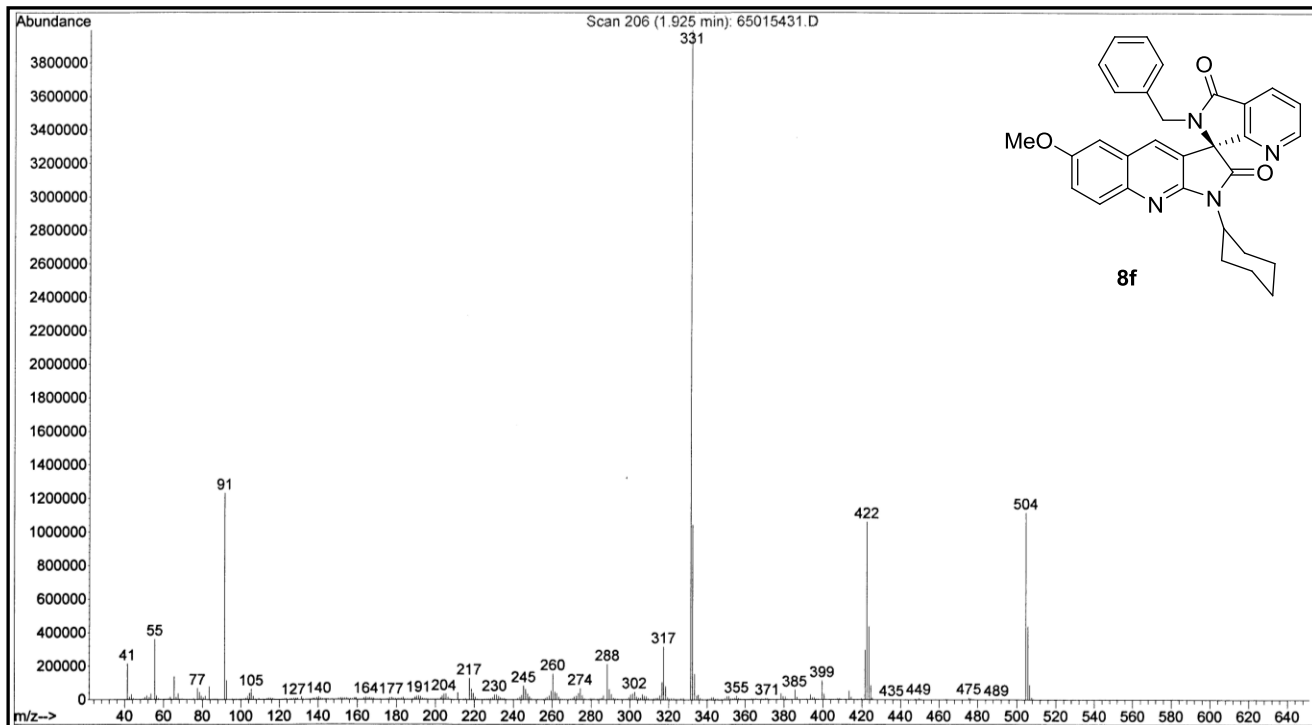


Figure 23. Mass (8f).

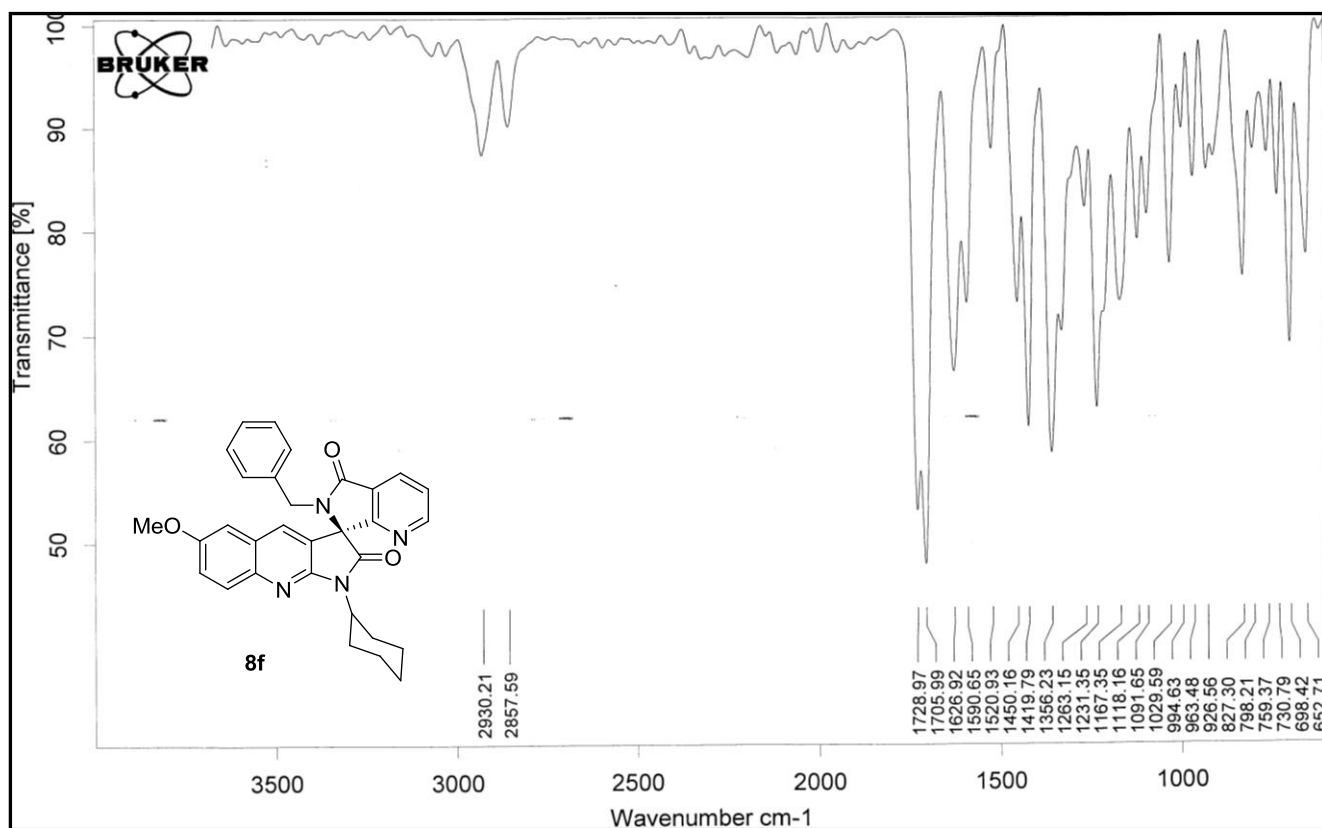


Figure 24. IR (8f).

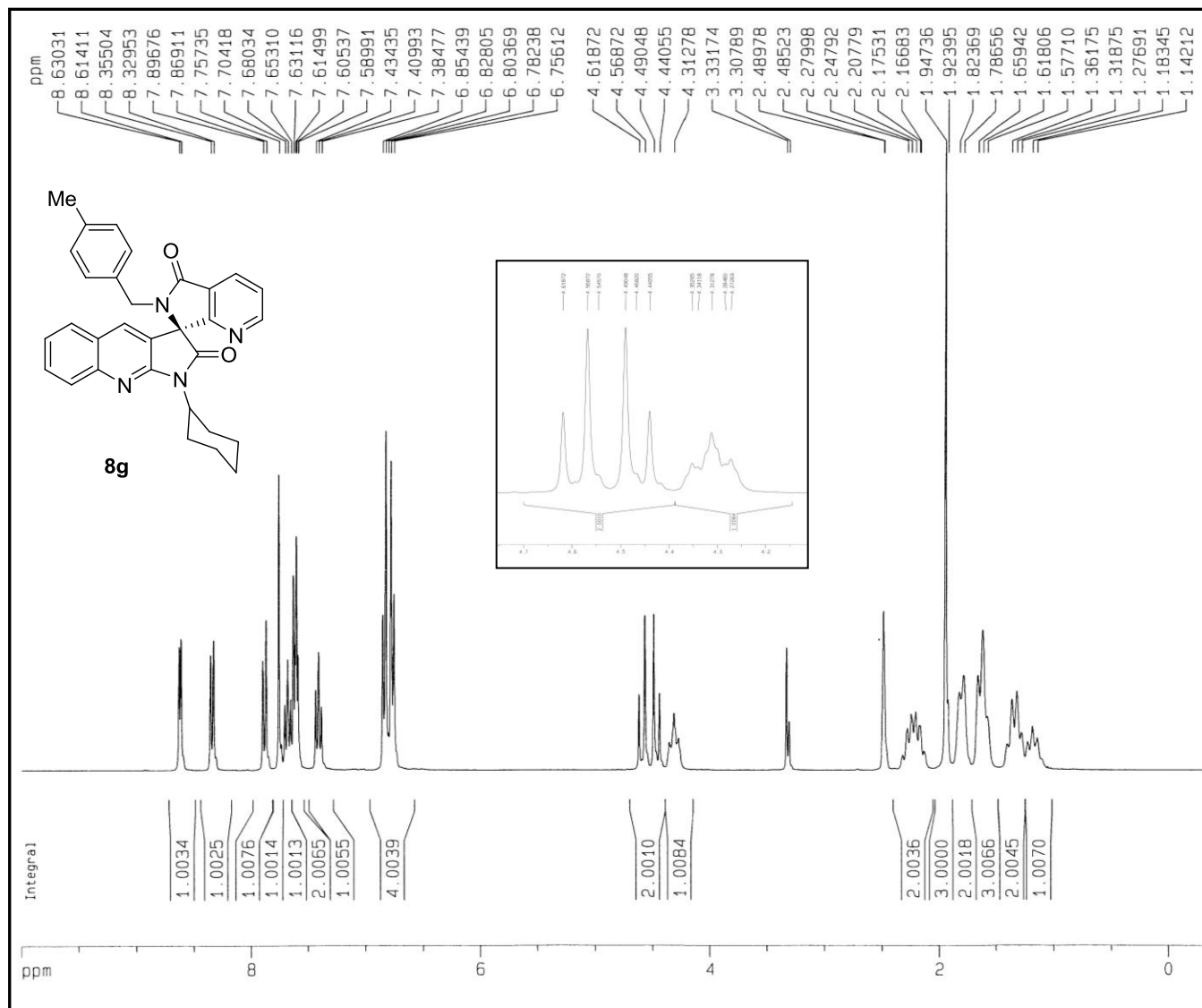
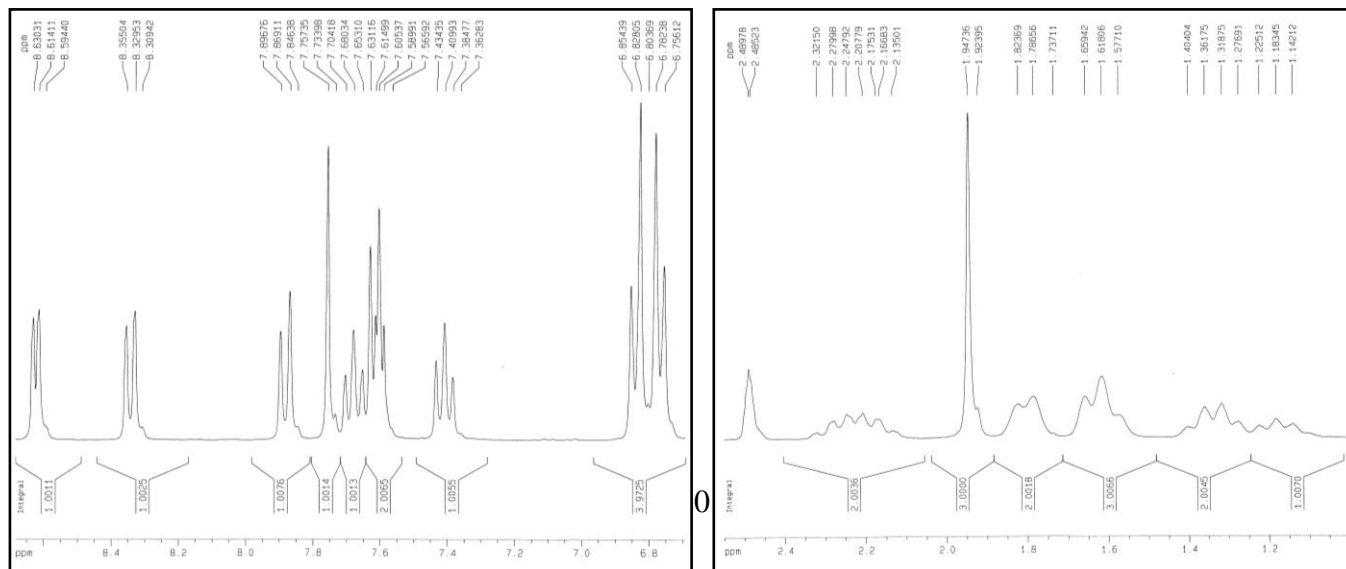


Figure 25. ¹H NMR (300 MHz, DMSO-d₆) (8g).



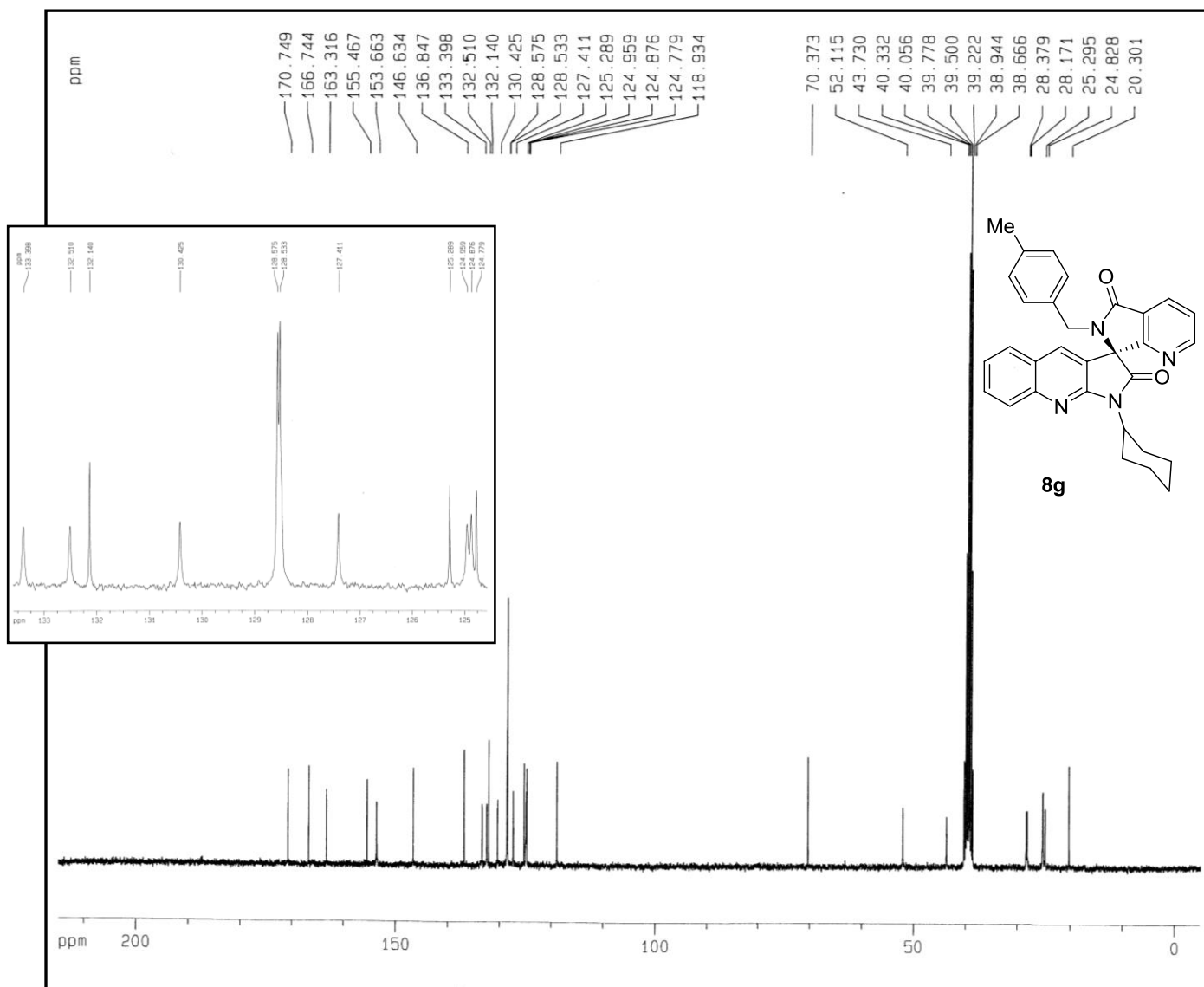


Figure 26. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8g**).

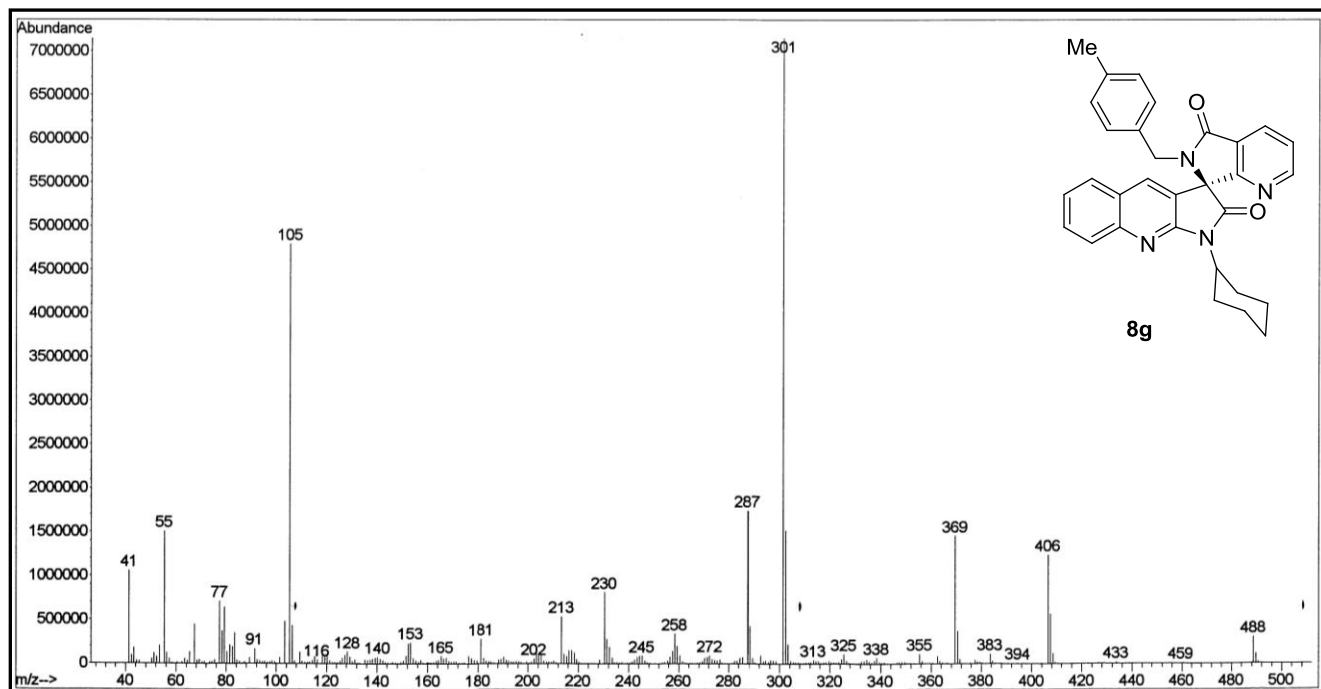


Figure 27. Mass (8g).

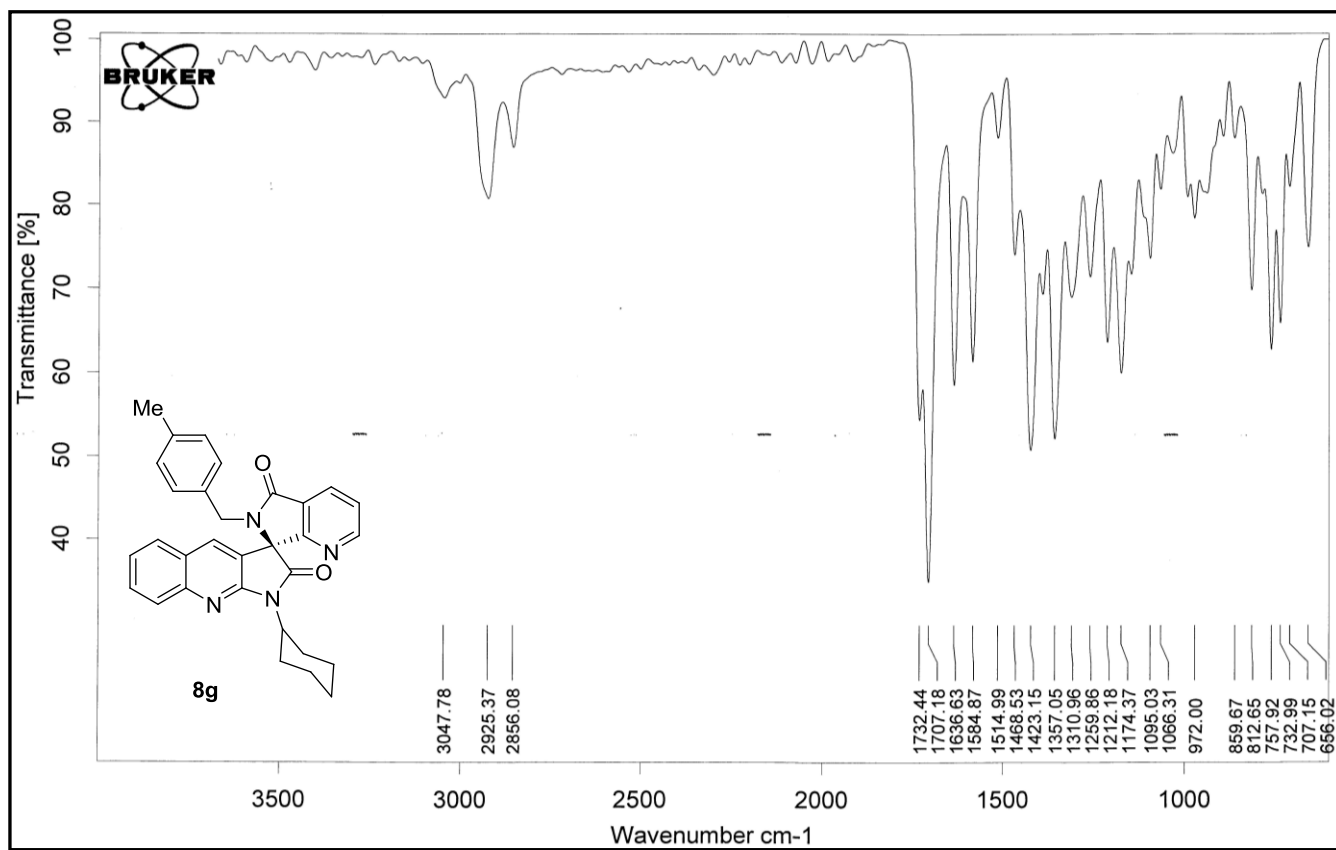


Figure 28. IR (8g).

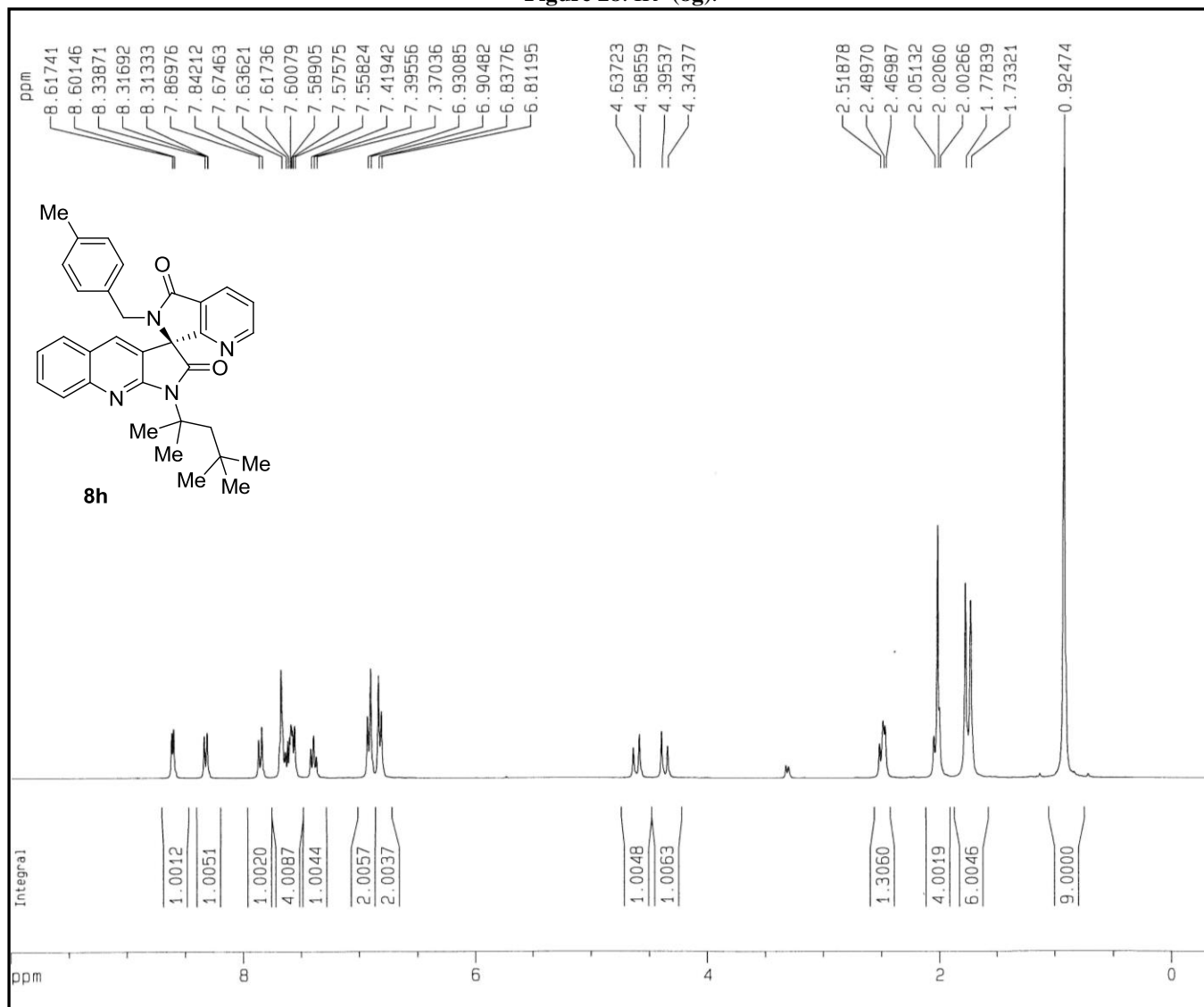
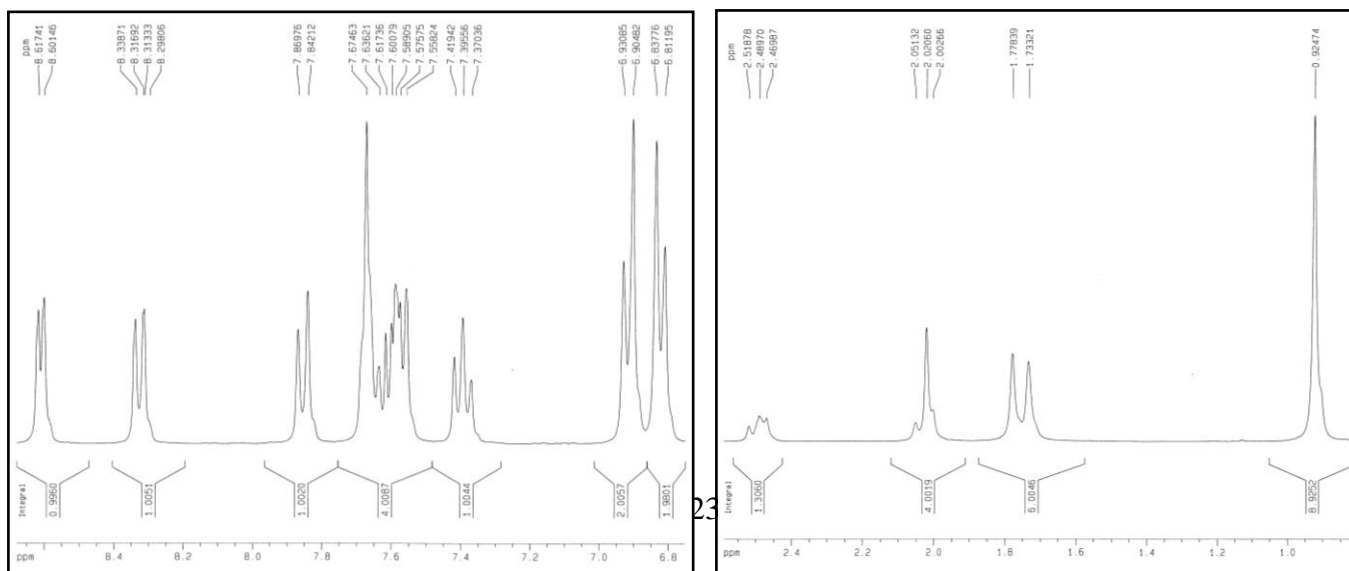
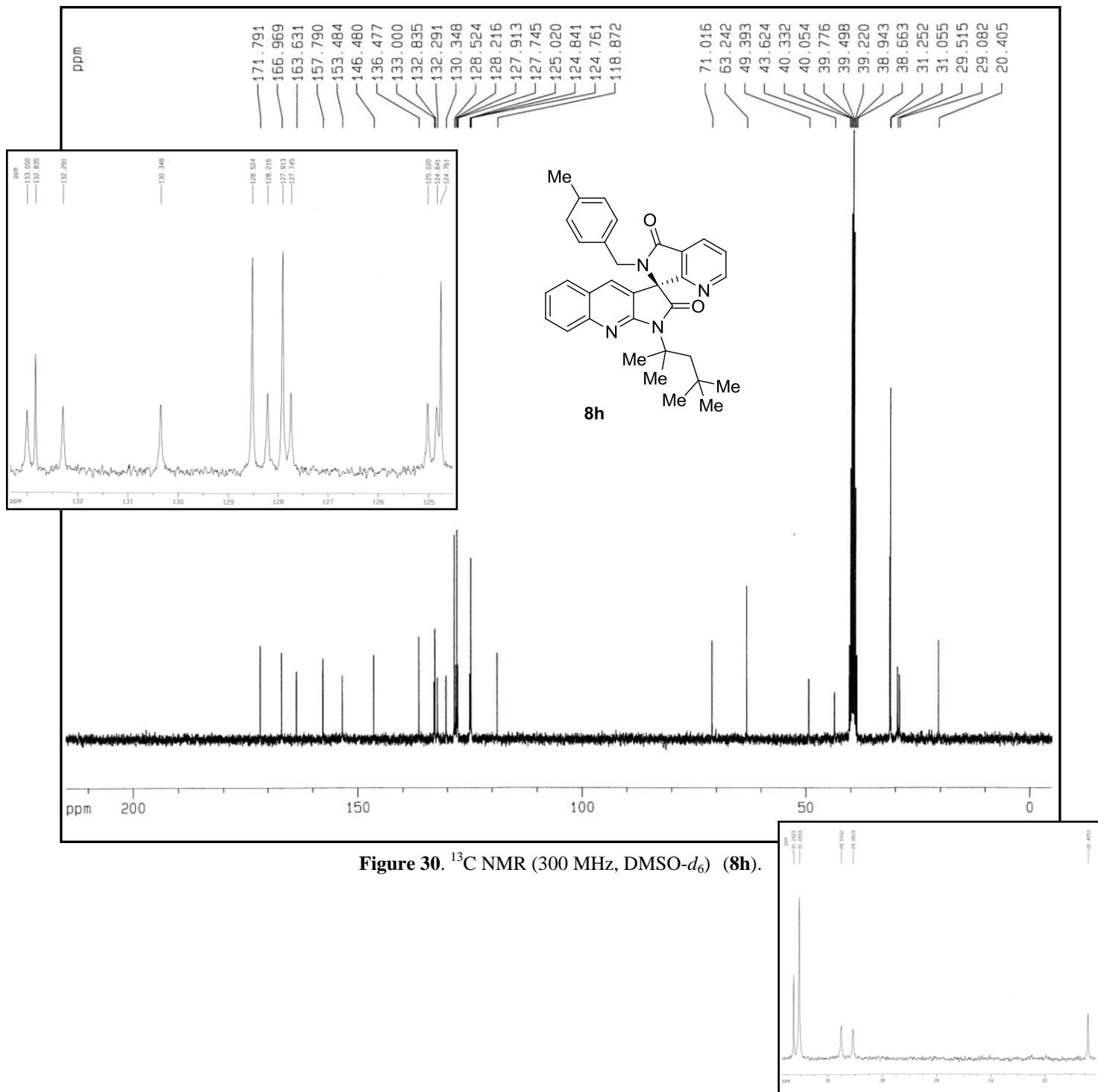


Figure 29. ¹H NMR (300 MHz, DMSO-*d*₆) (**8h**).





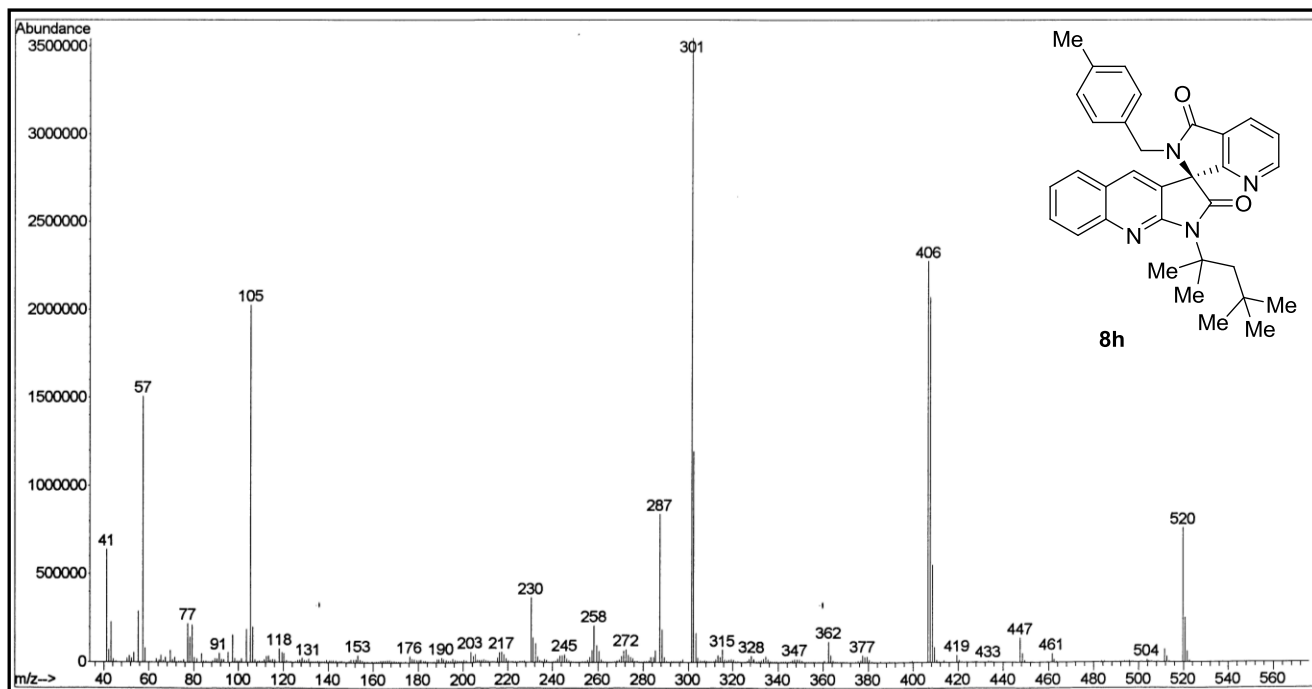


Figure 31. Mass (**8h**).

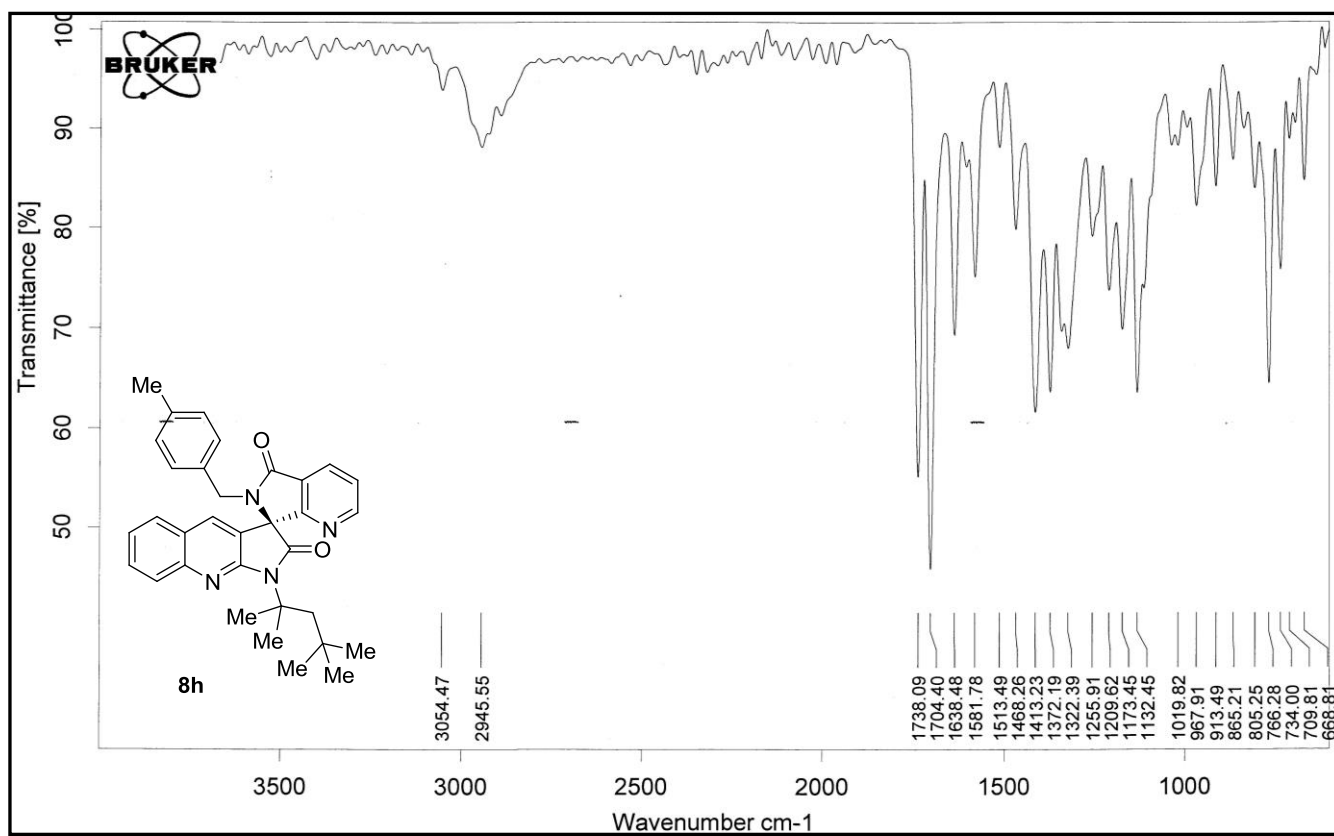


Figure 32. IR (8h).

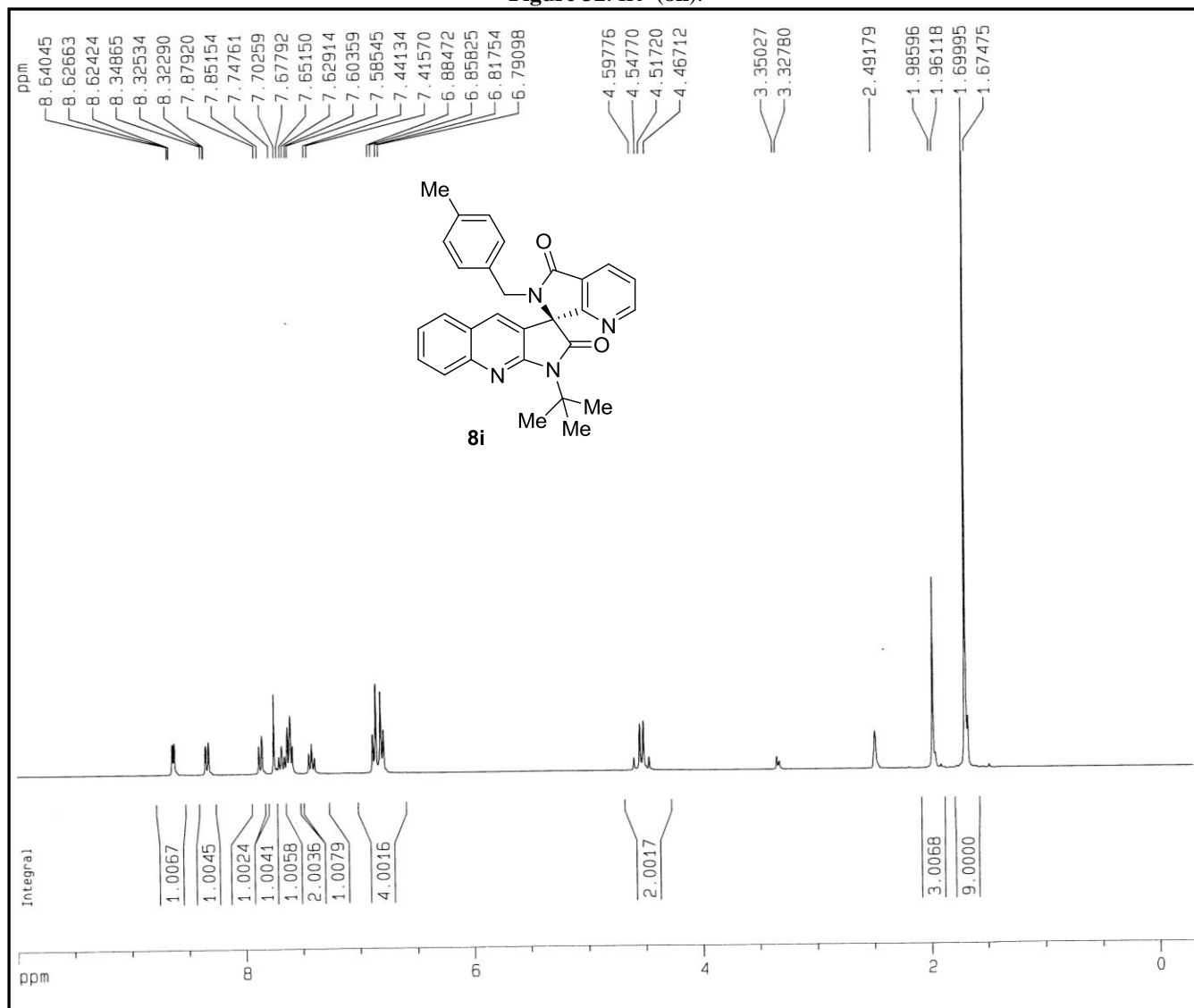
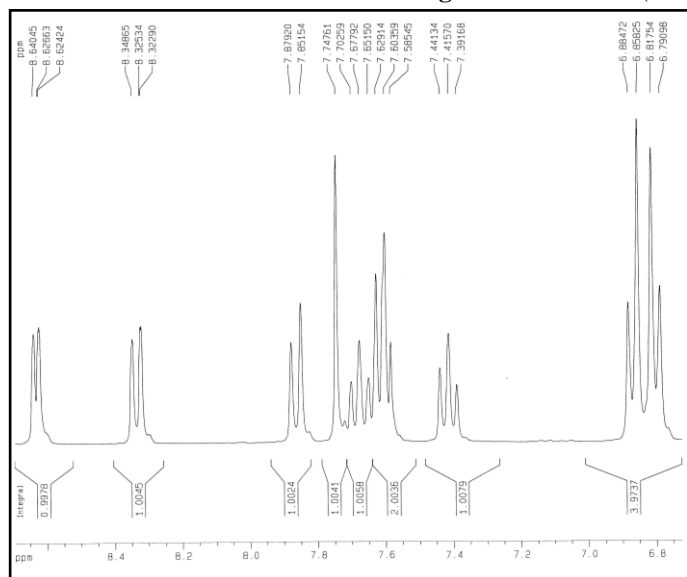


Figure 33. ¹H NMR (300 MHz, DMSO-*d*₆) (**8i**).



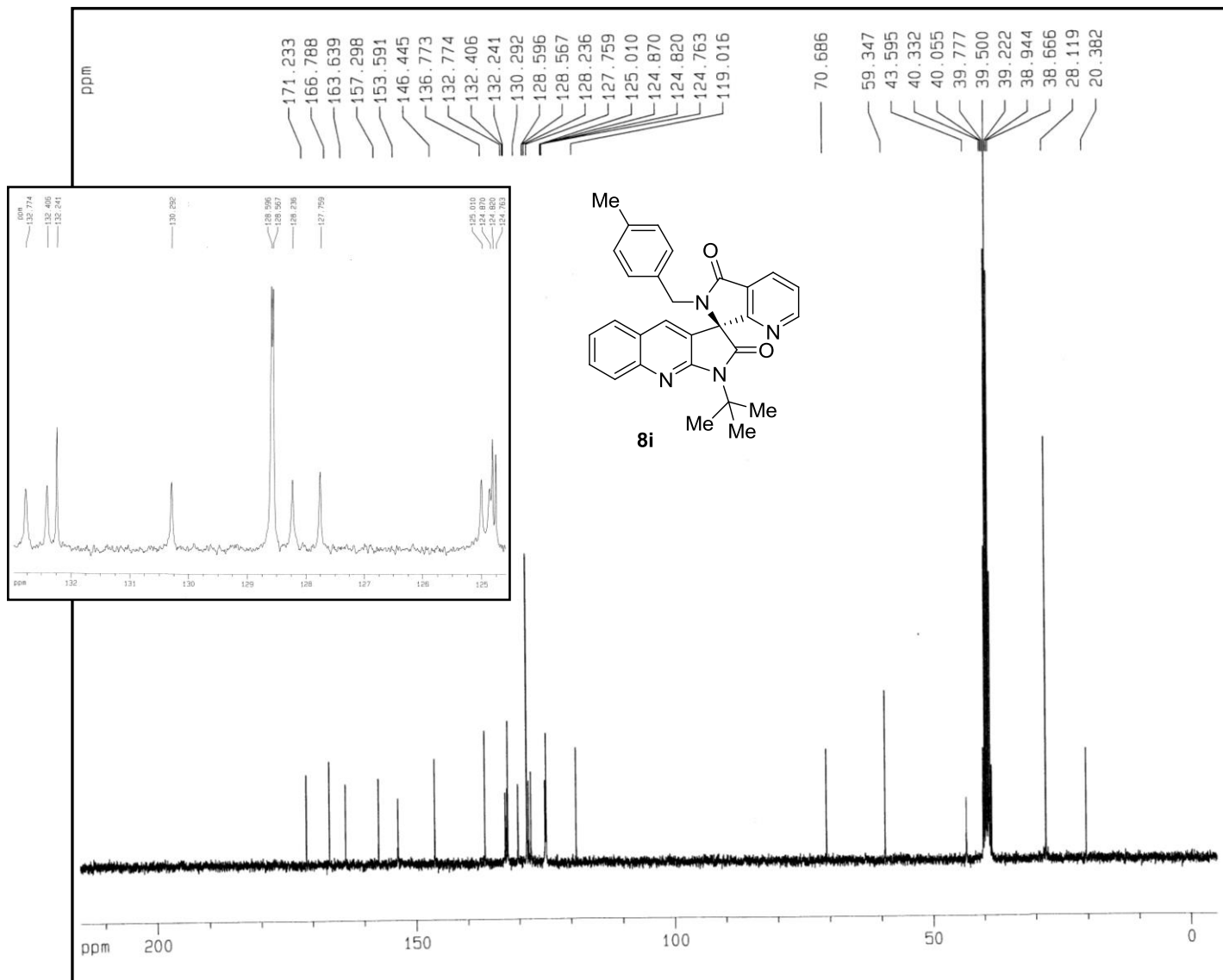


Figure 34. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8i**).

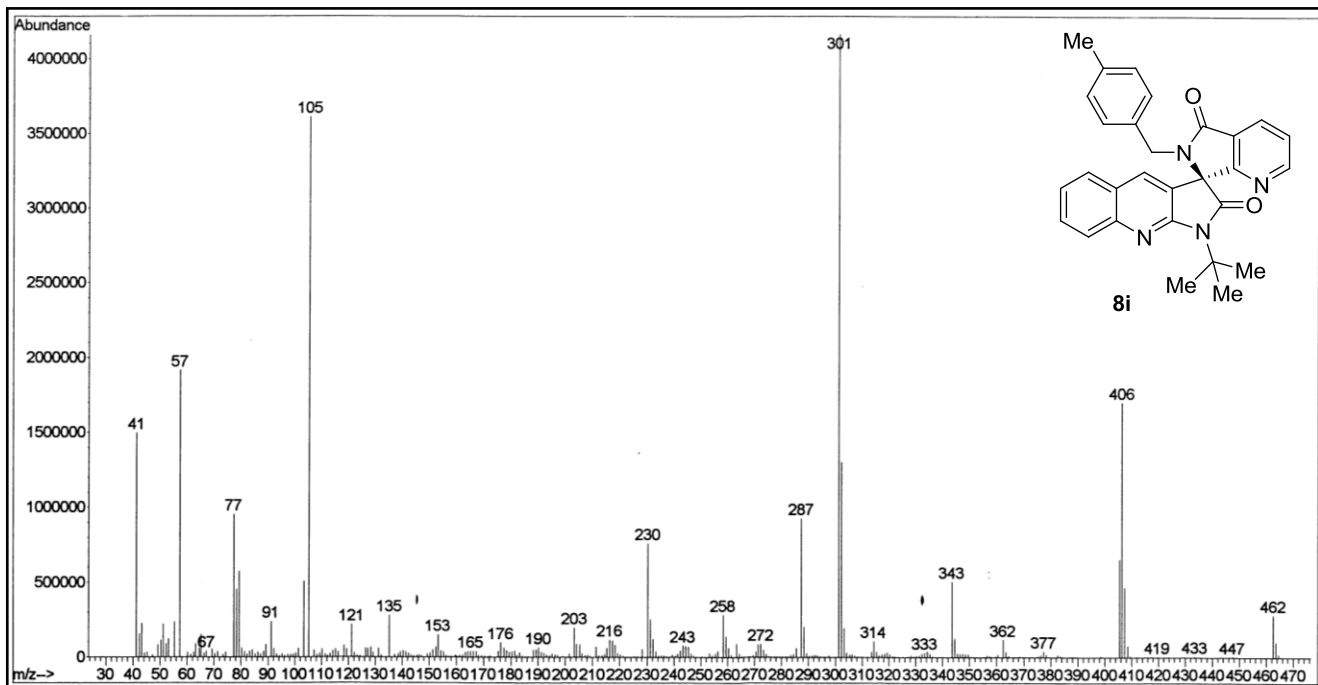


Figure 35. Mass (**8i**).

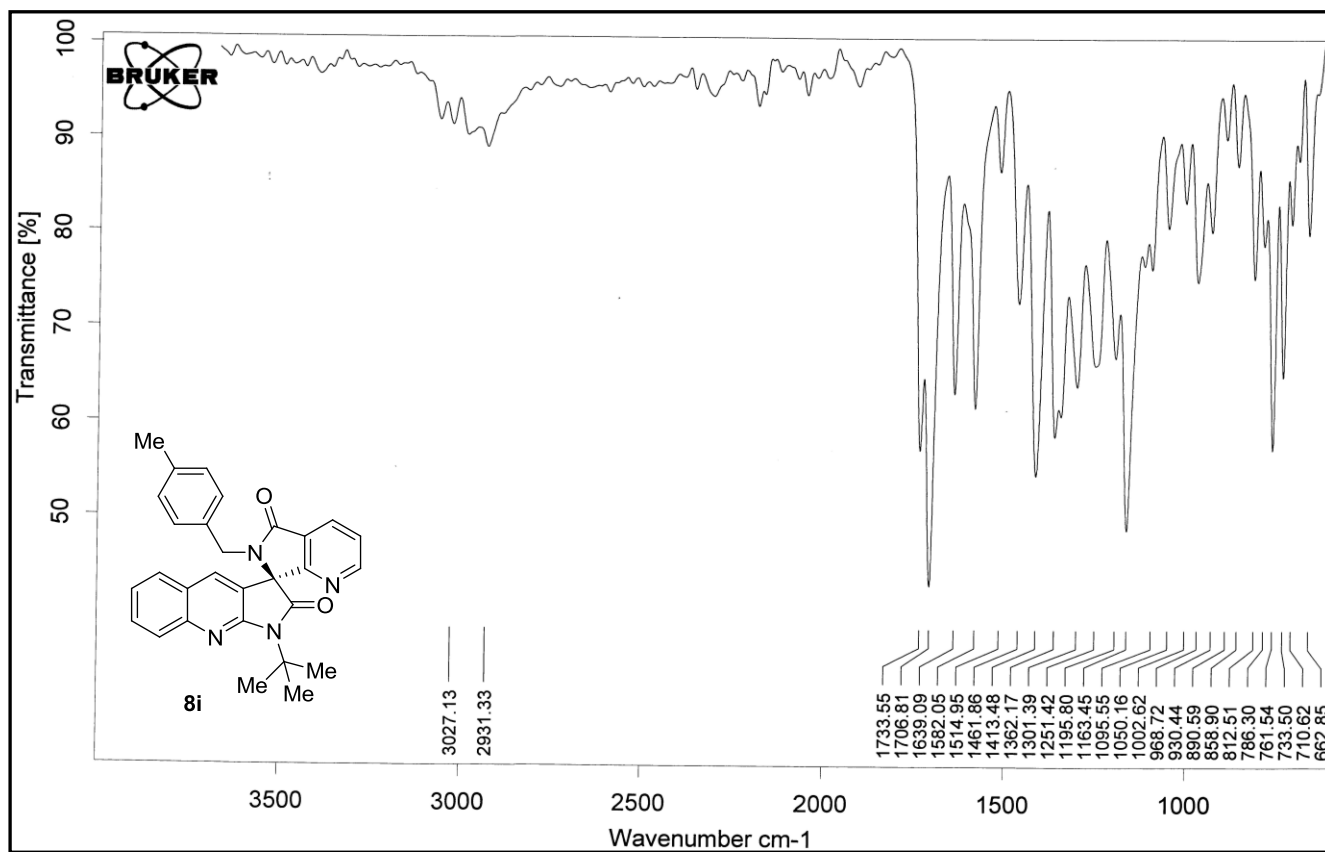


Figure 36. IR (8i).

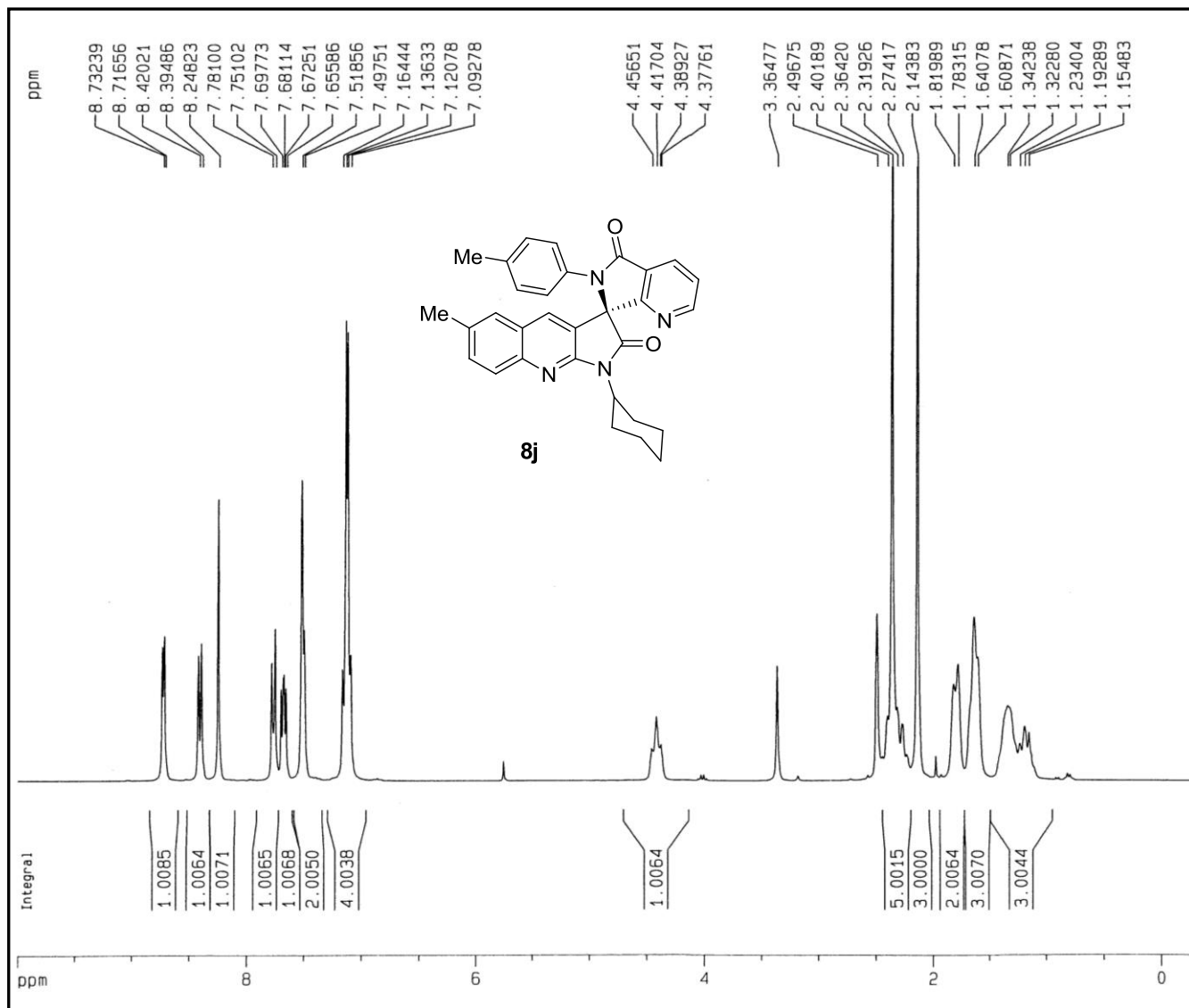
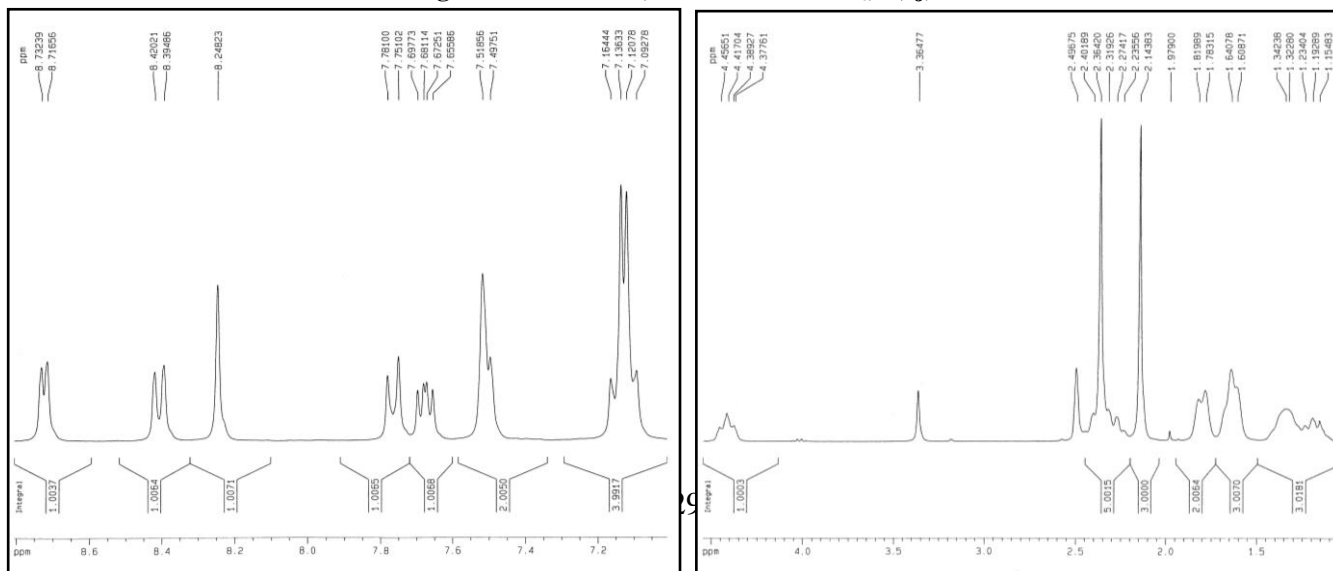


Figure 37. ¹H NMR (300 MHz, DMSO-*d*₆) (**8j**).



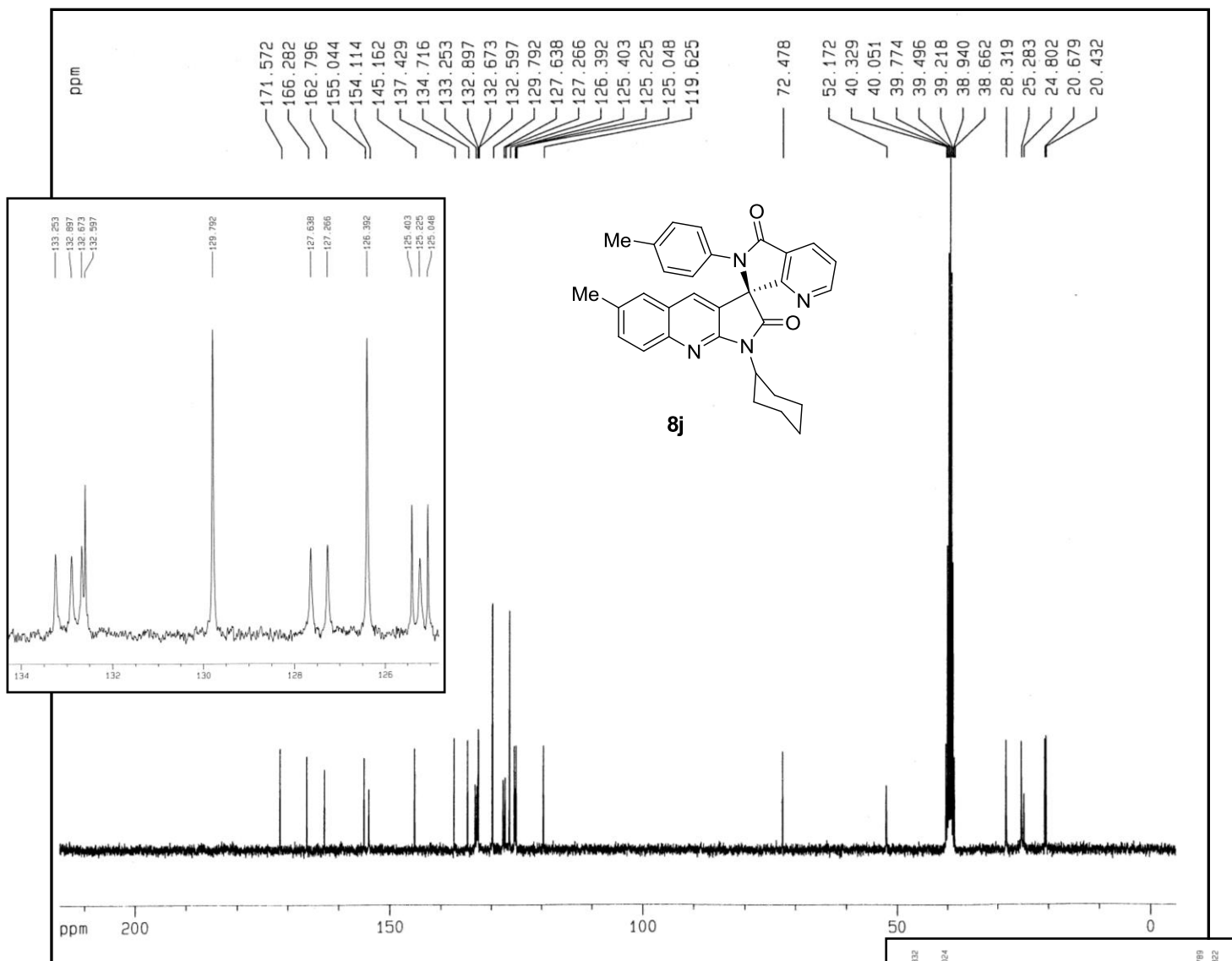
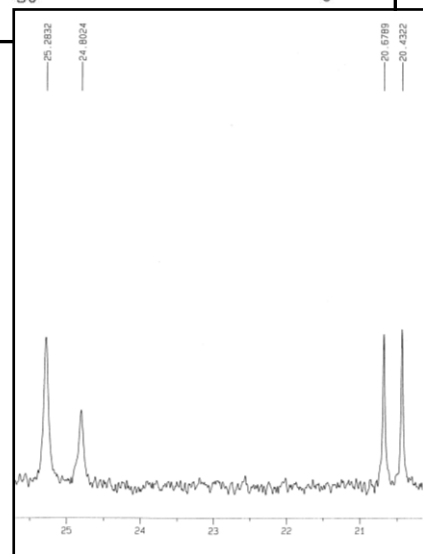


Figure 38. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8j**).



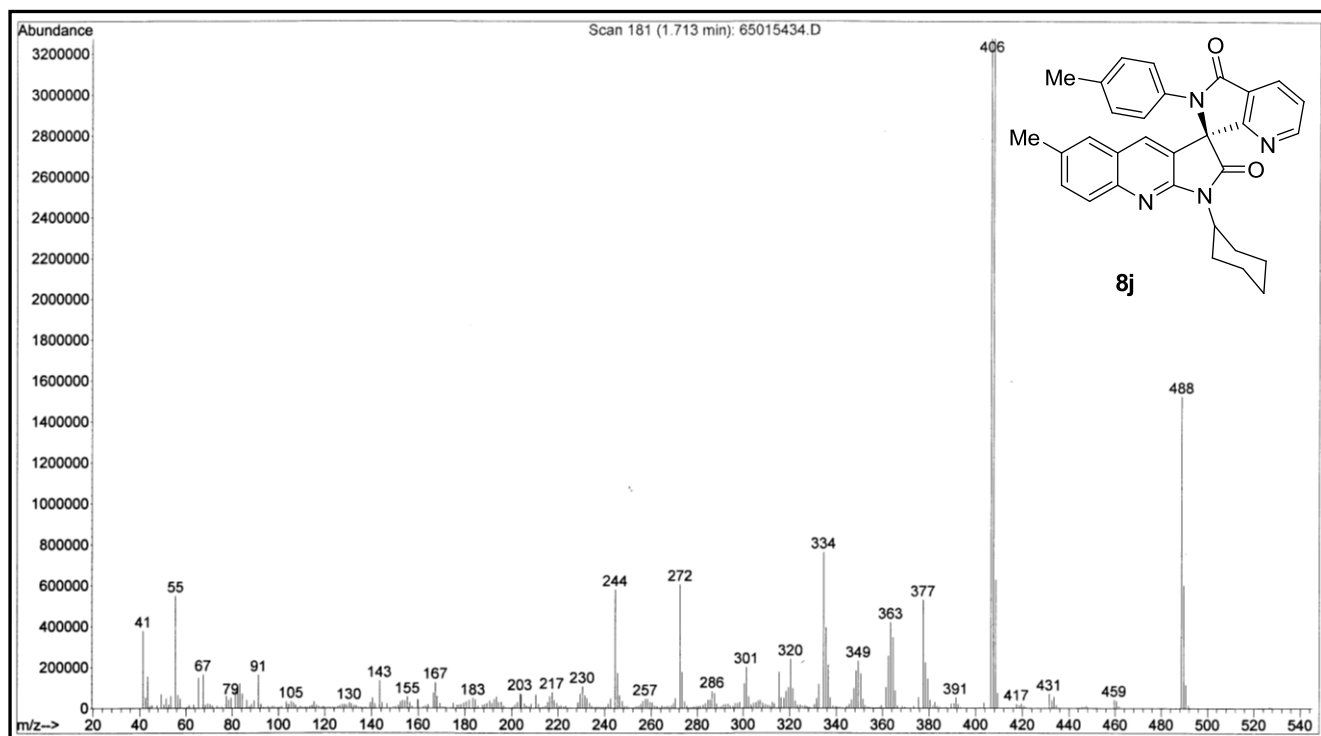


Figure 39. Mass (**8j**).

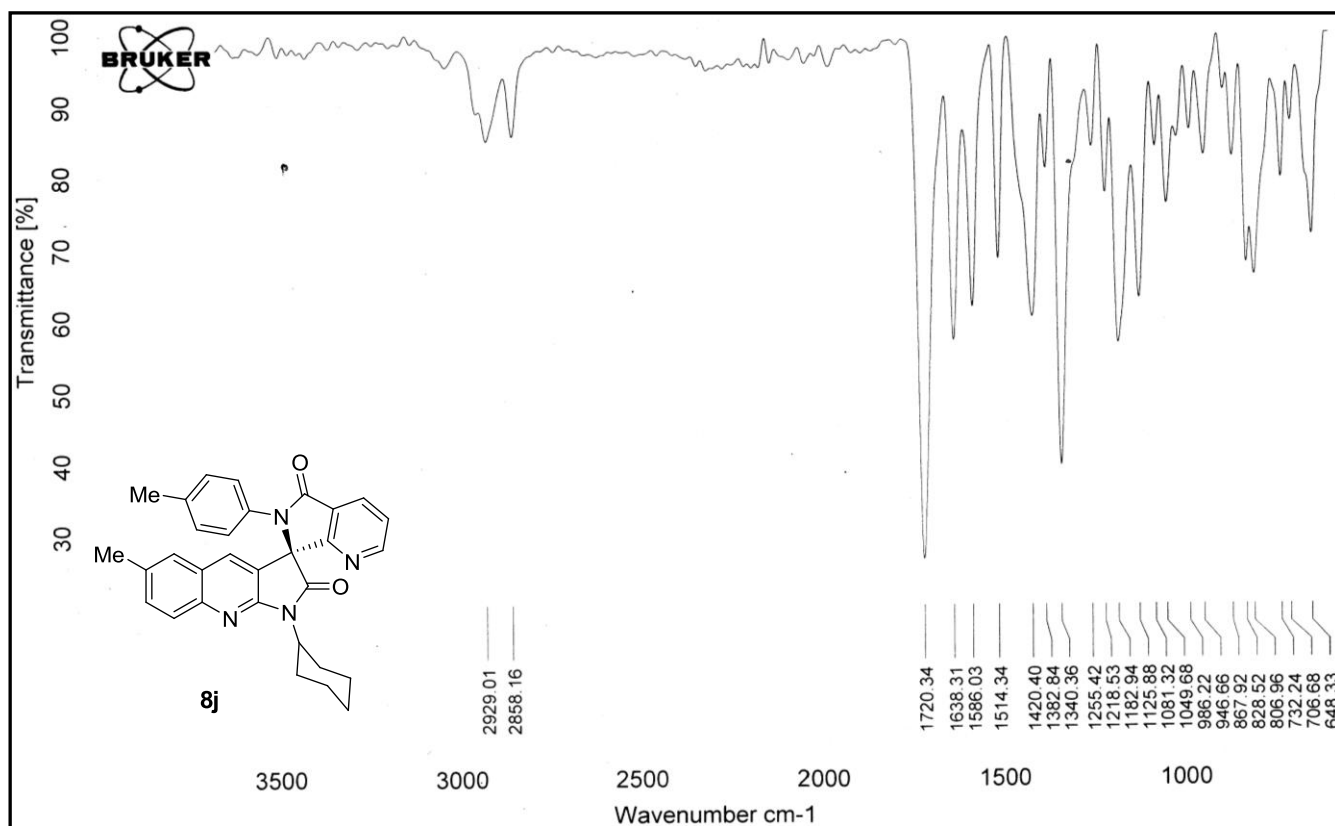


Figure 40. IR (8j).

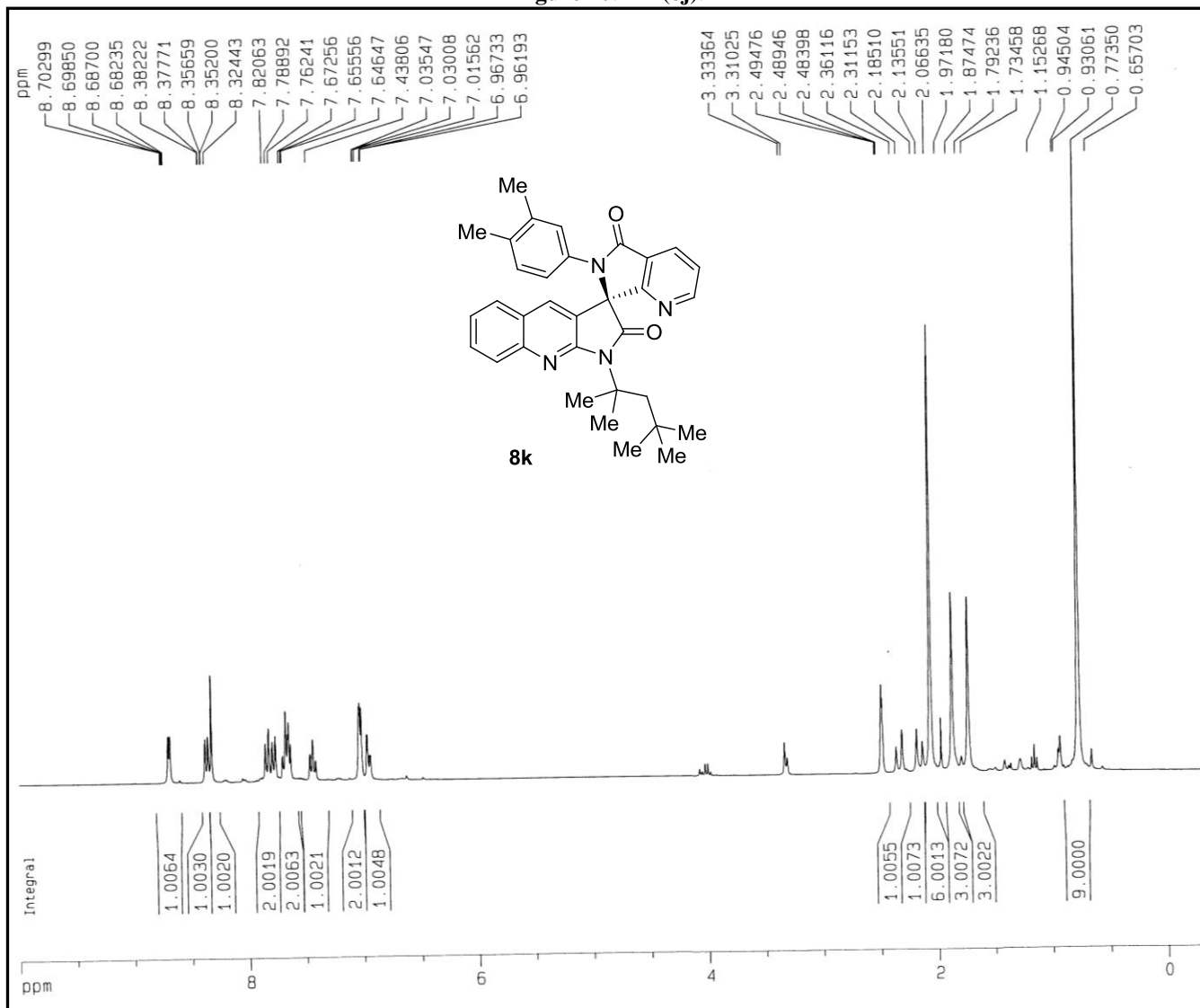
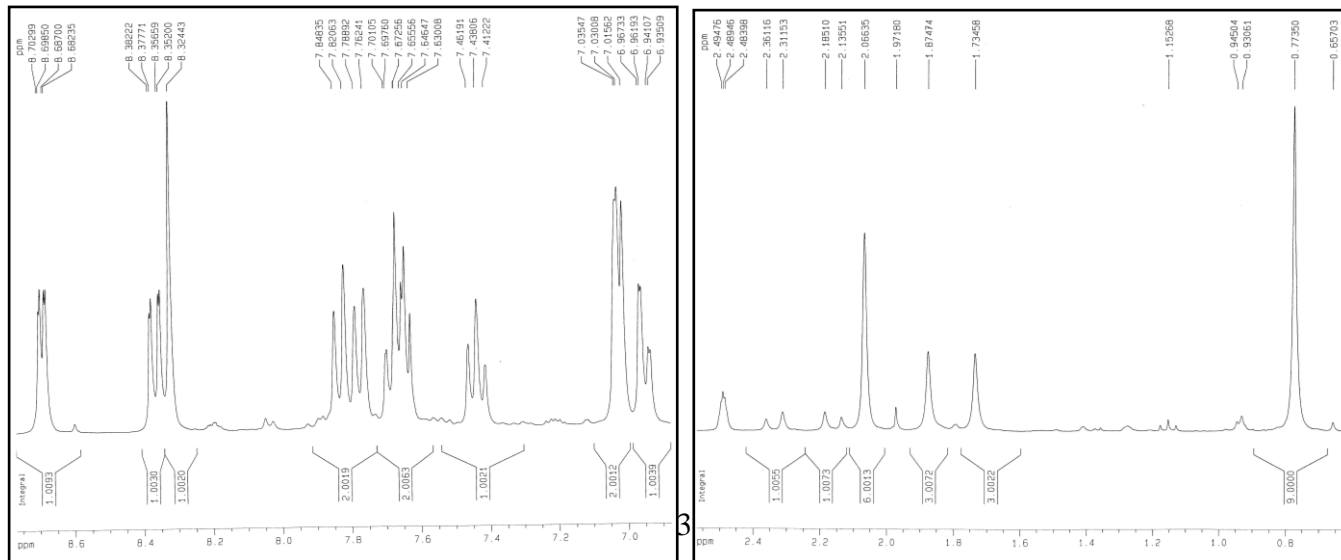


Figure 41. ¹H NMR (300 MHz, DMSO-*d*₆) (**8k**).



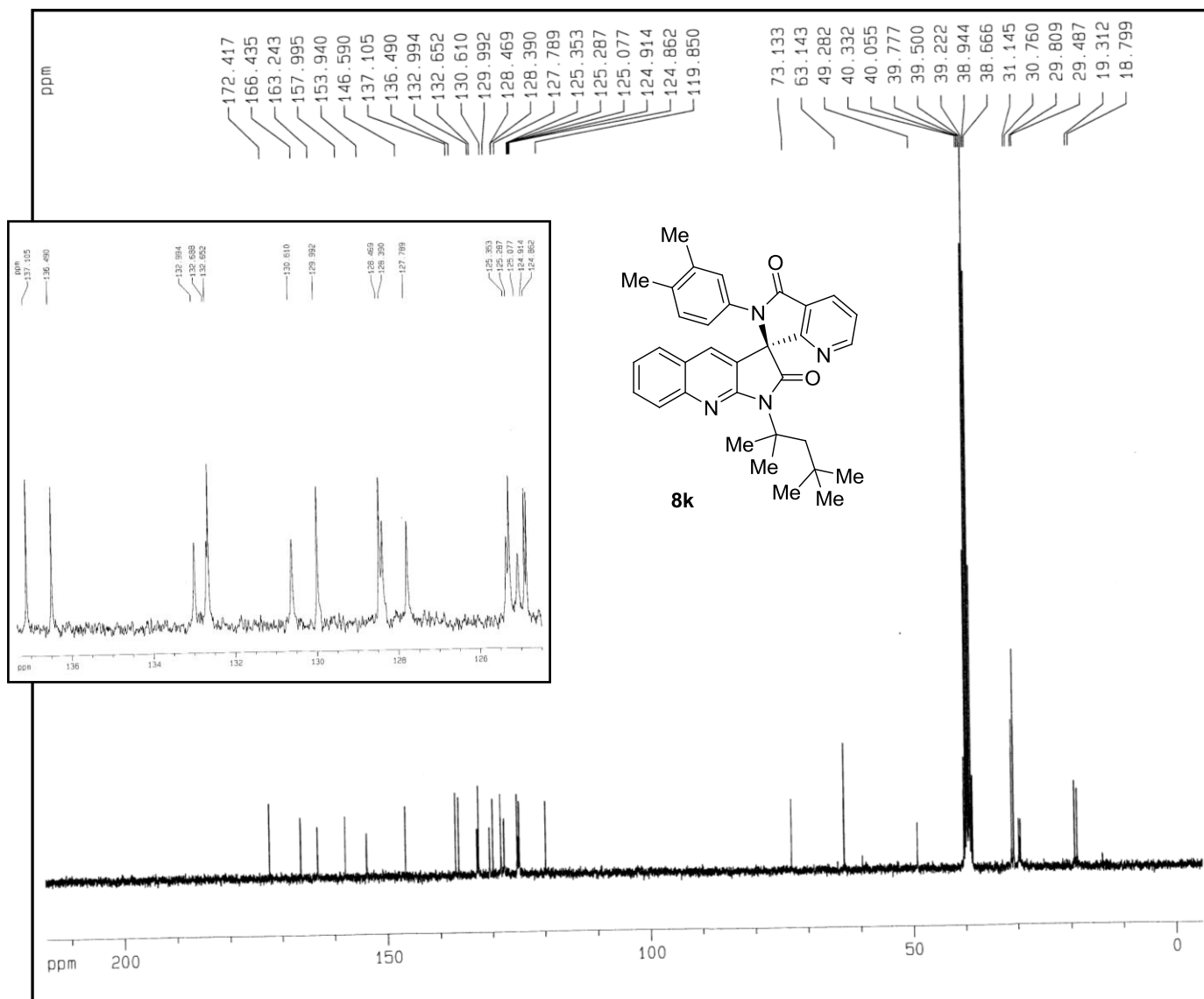
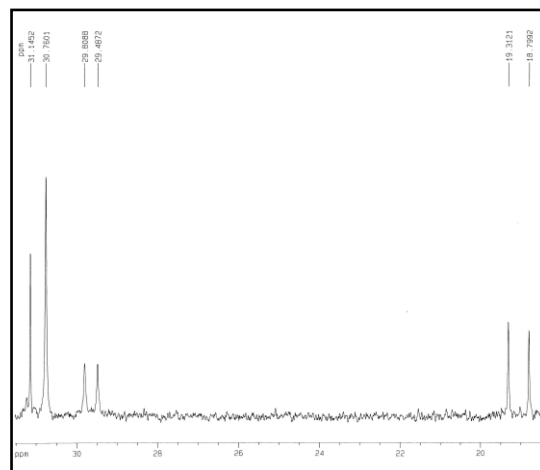


Figure 42. ¹³C NMR (300 MHz, DMSO-d₆) (**8k**).



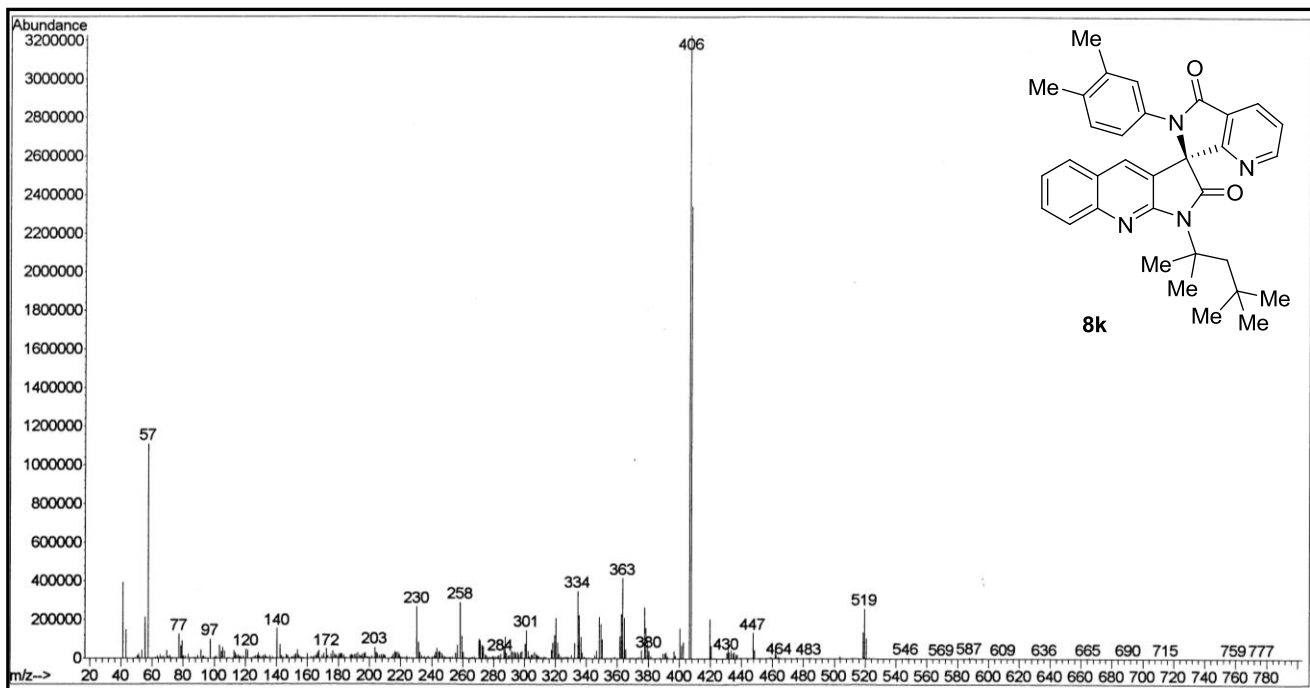


Figure 43. Mass (**8k**).

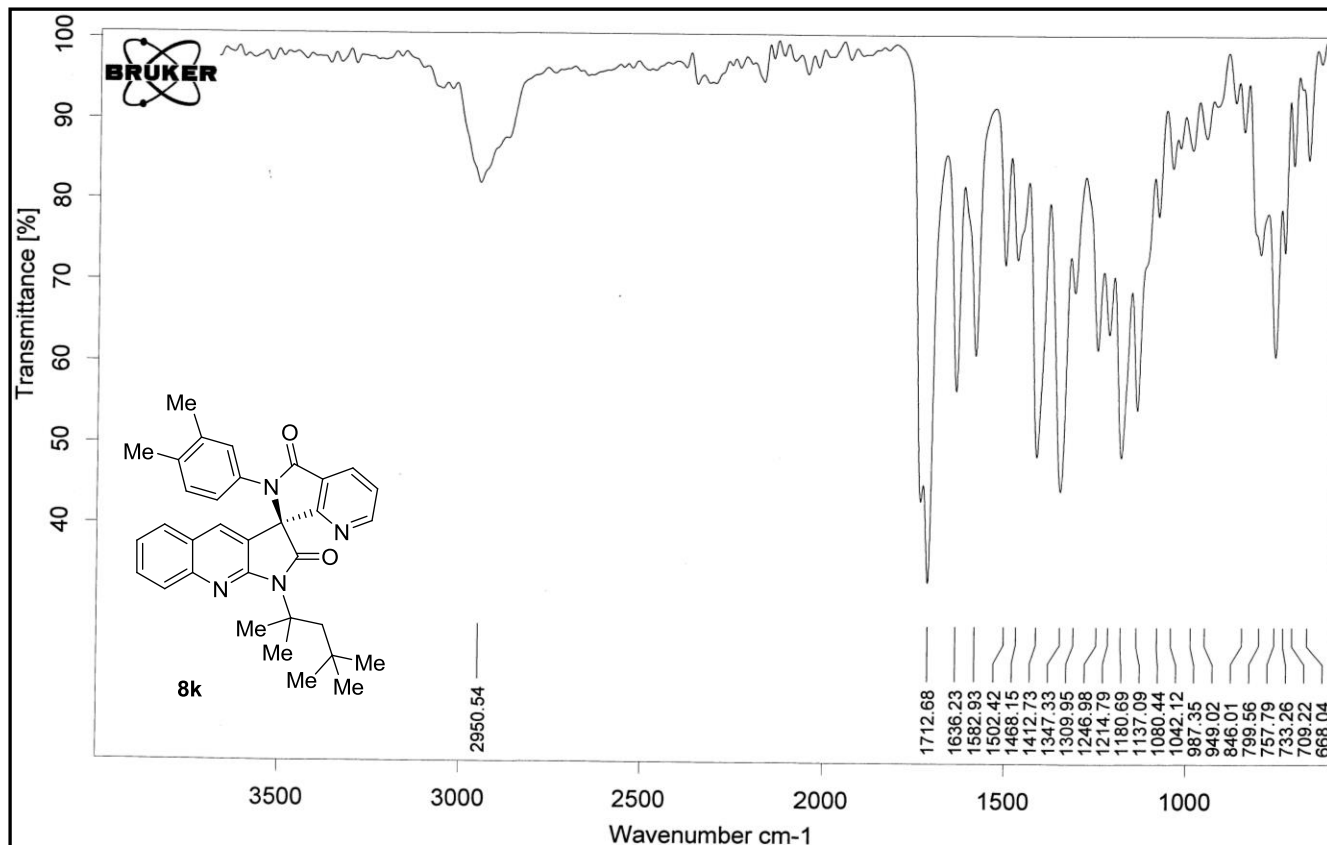


Figure 44. IR (8k).

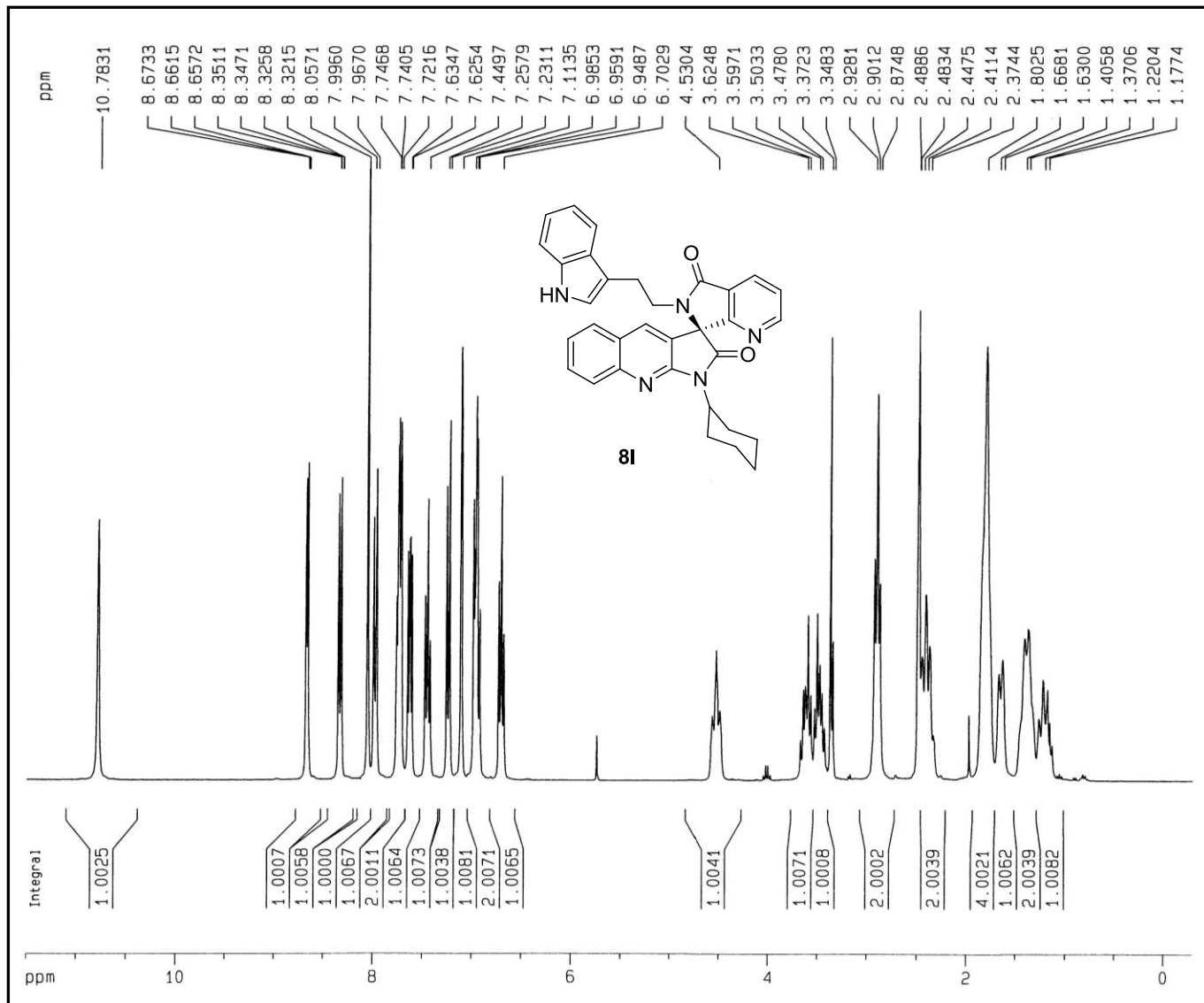
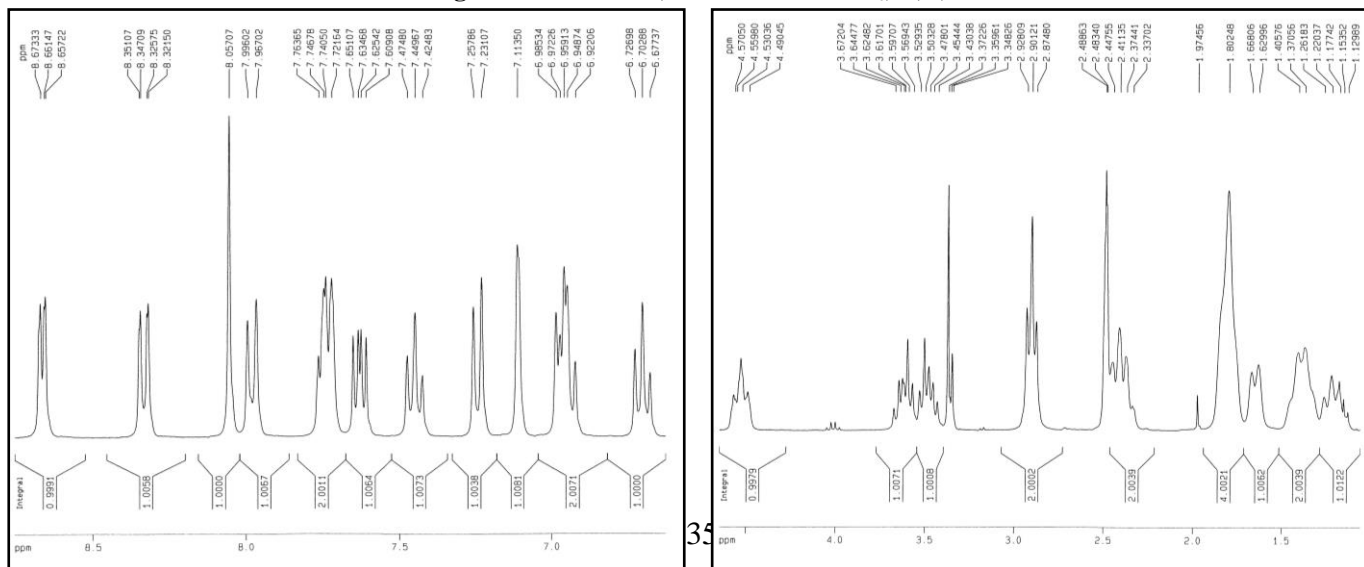


Figure 45. ¹H NMR (300 MHz, DMSO-*d*₆) (**8l**).



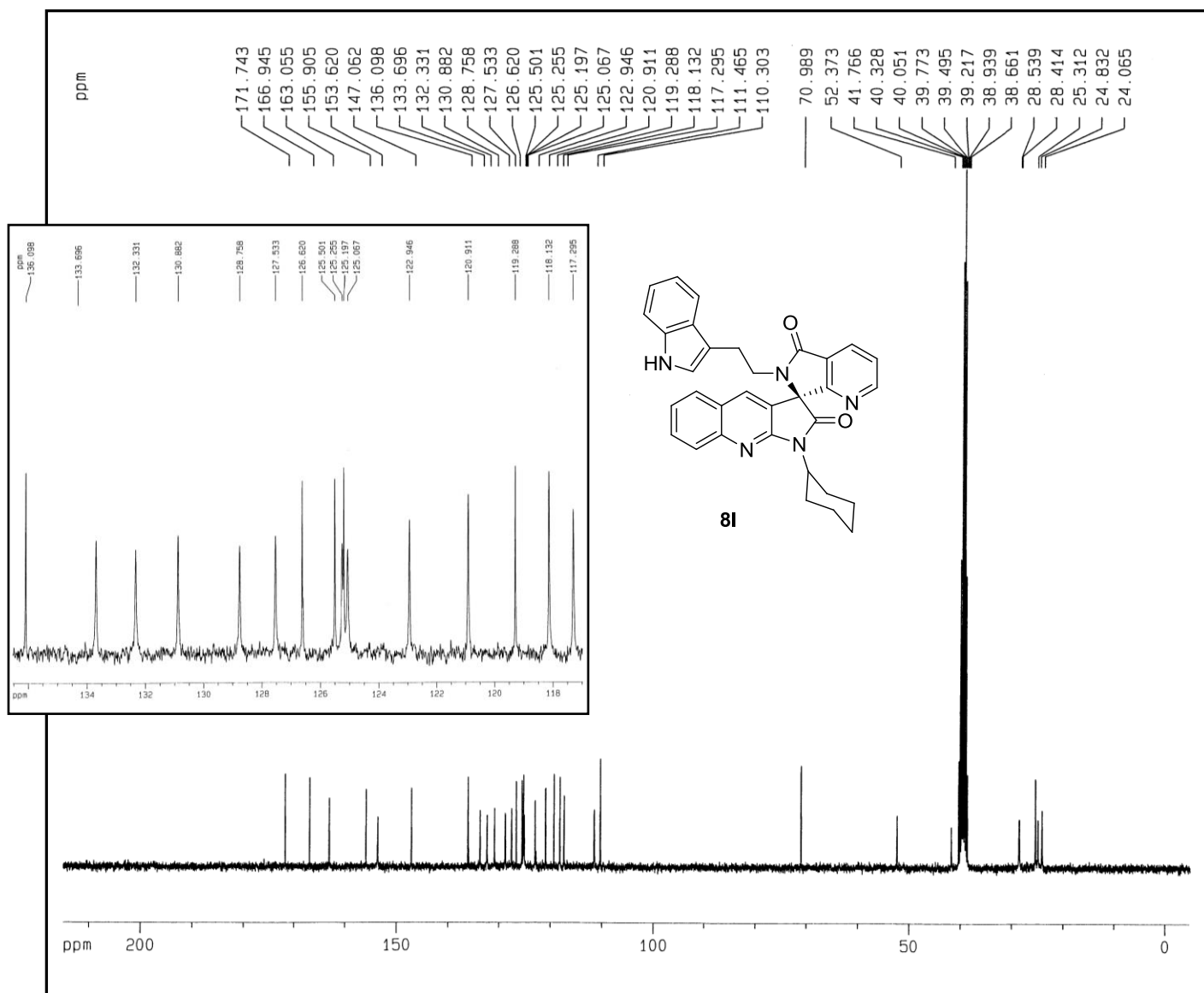


Figure 46. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8I**).

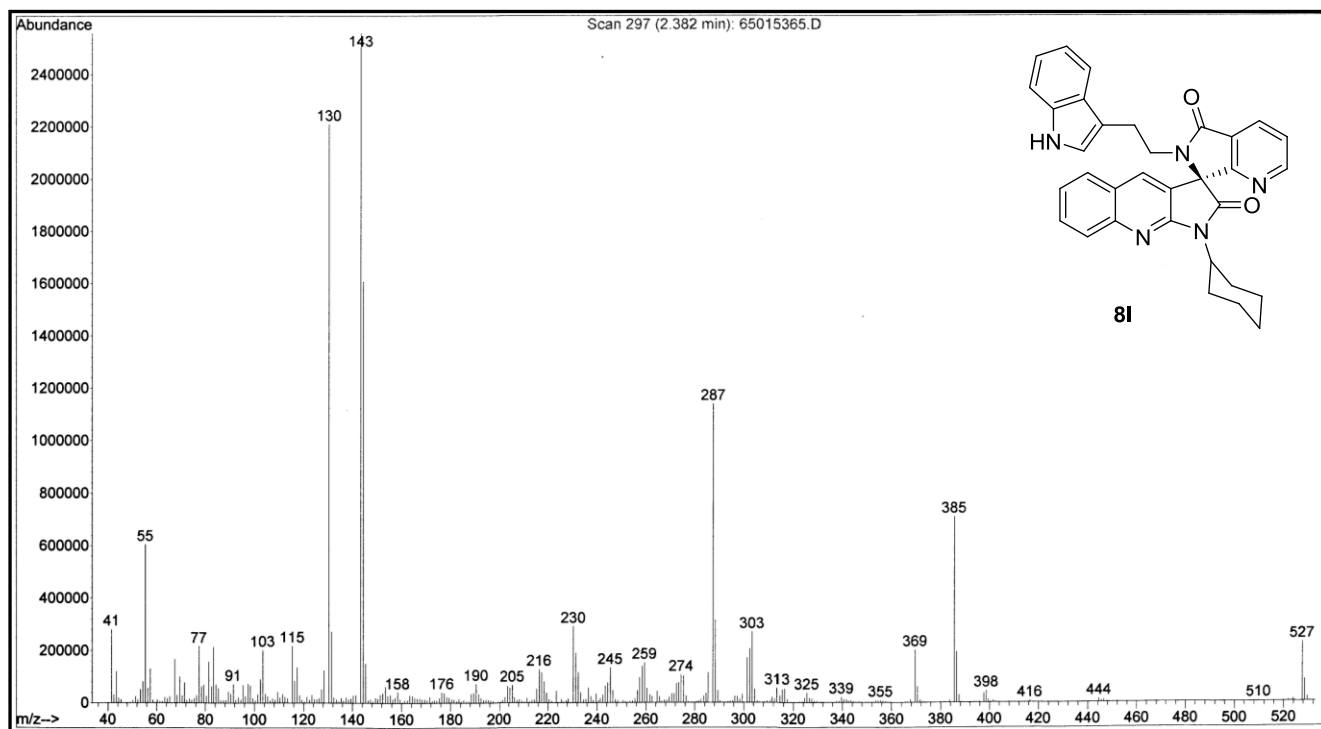


Figure 47. Mass (**81**).

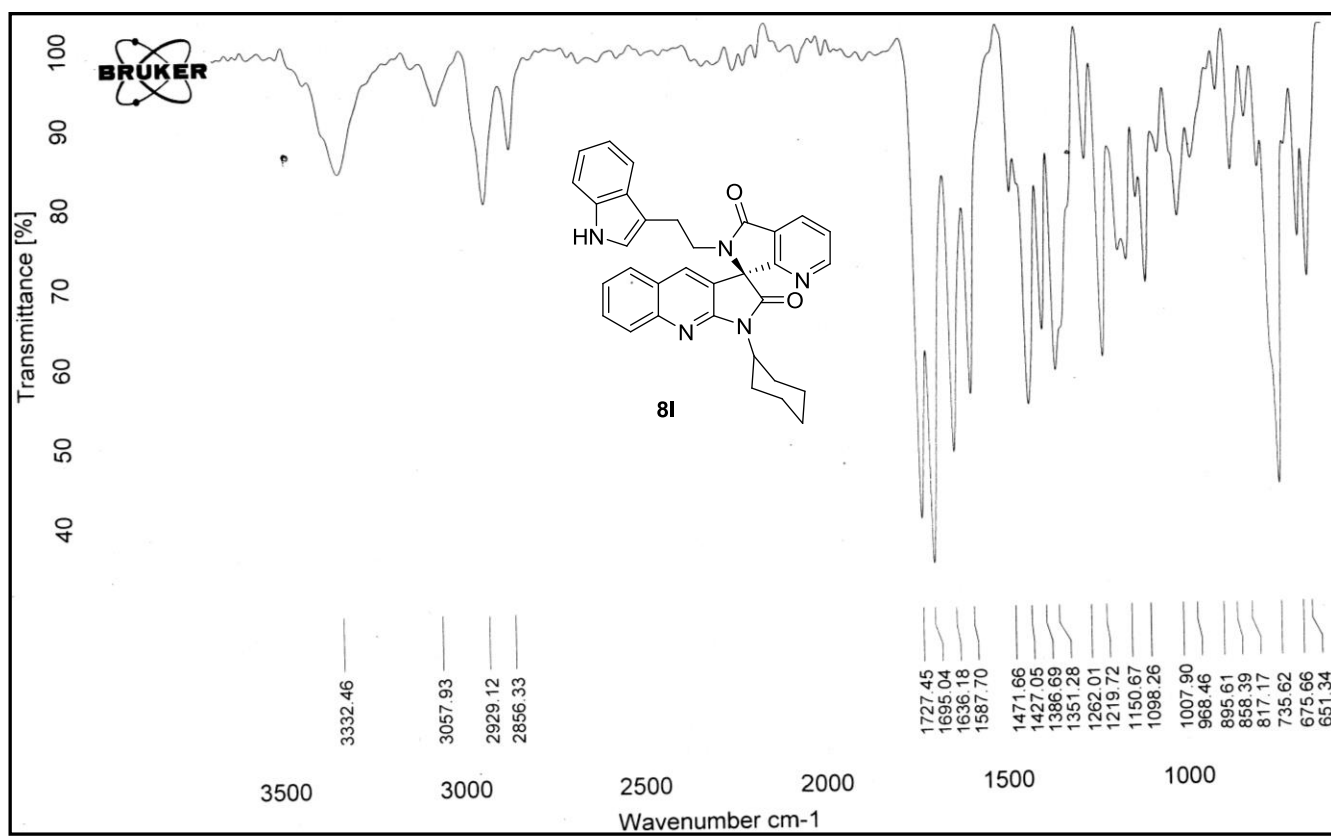


Figure 48. IR (8l).

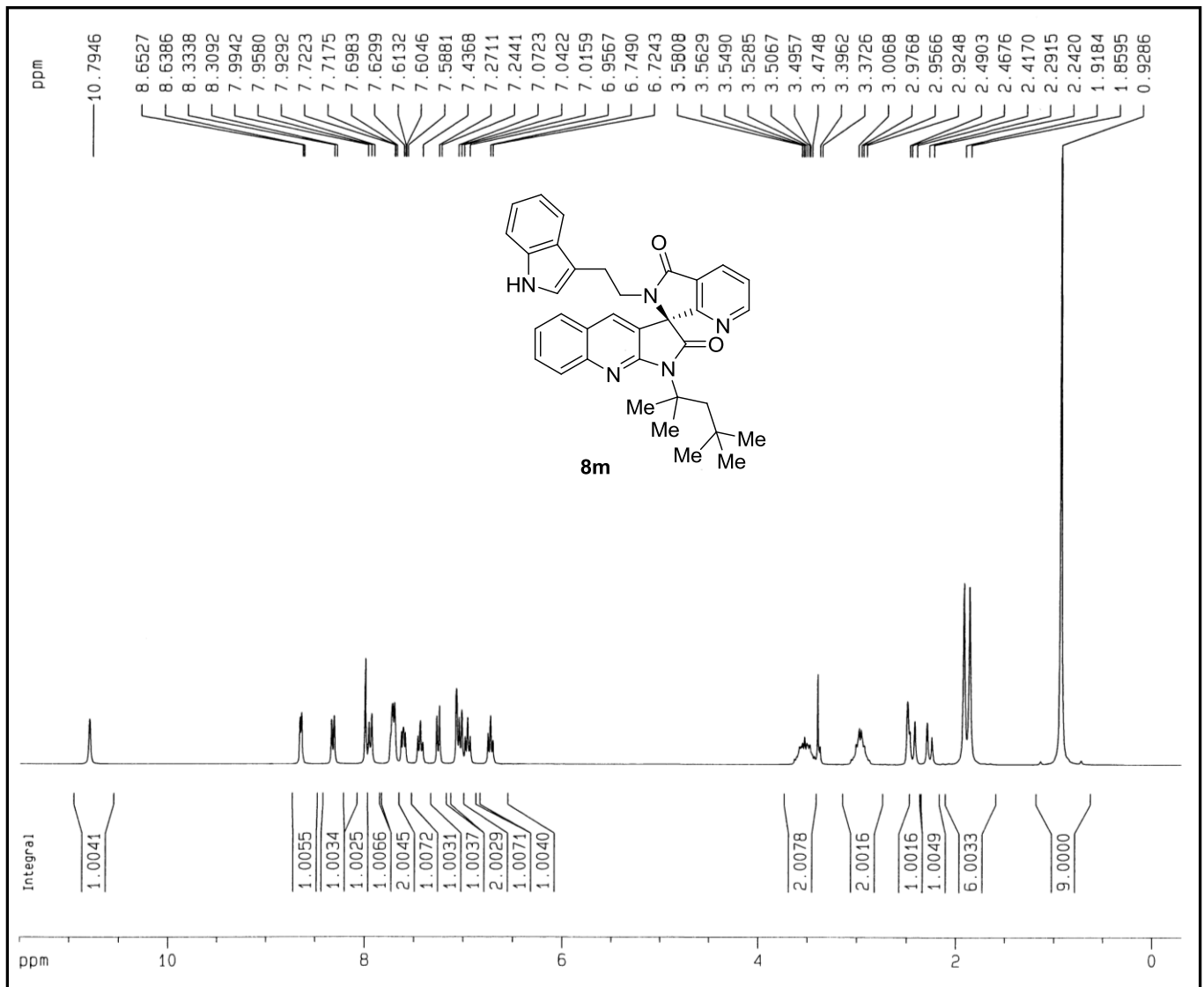
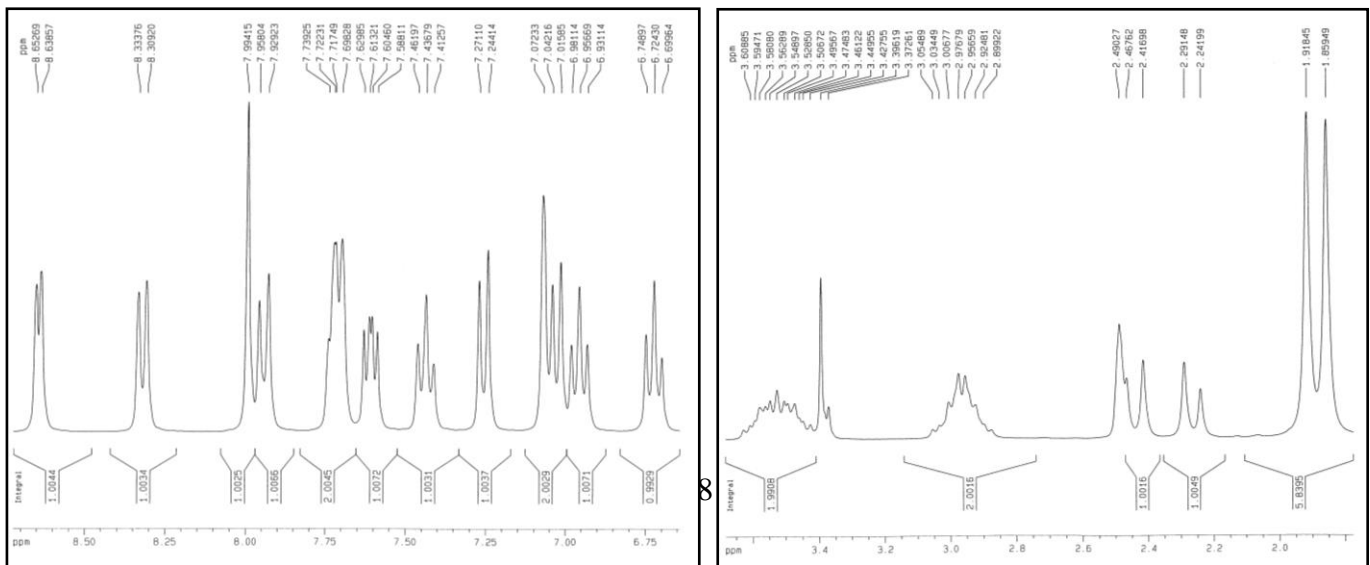


Figure 49. ¹H NMR (300 MHz, DMSO-*d*₆) (**8m**).



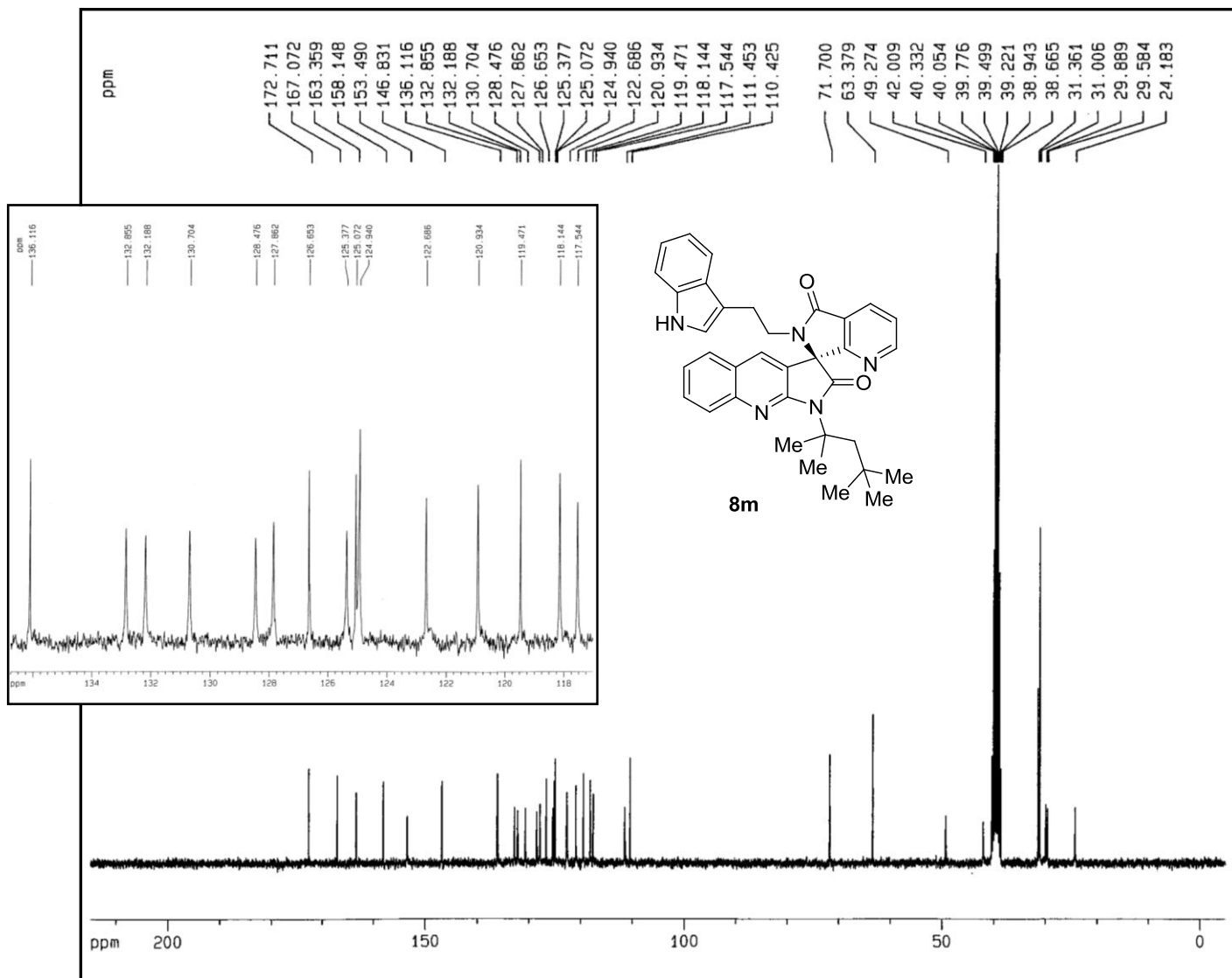
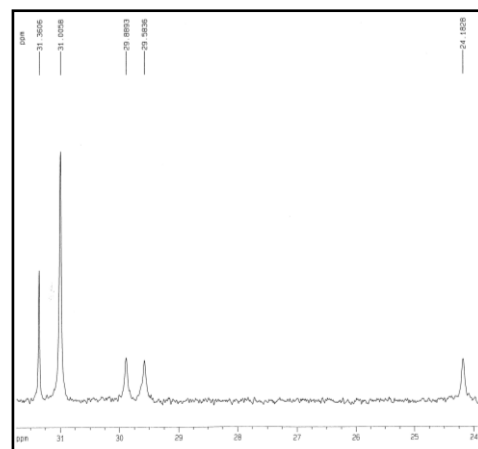


Figure 50. ¹³C NMR (300 MHz, DMSO-*d*₆) (**8m**).



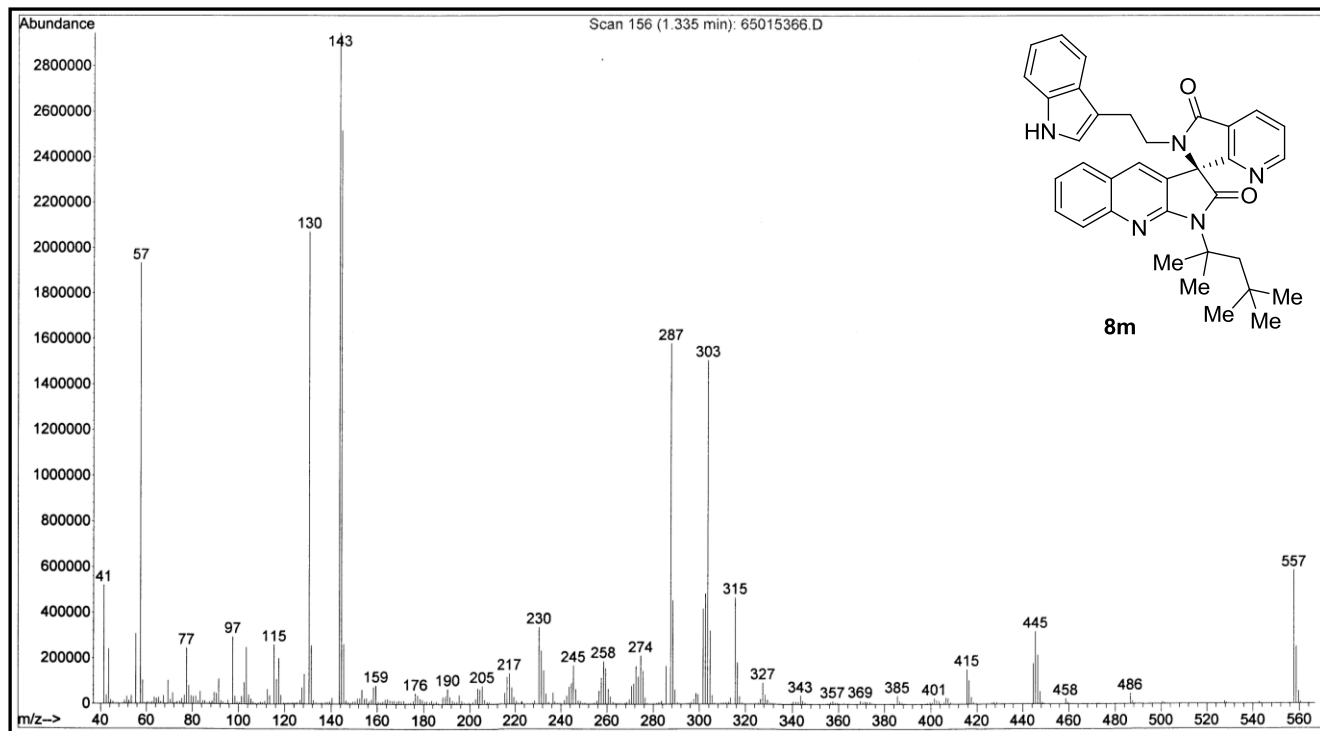


Figure 51. Mass (**8m**).

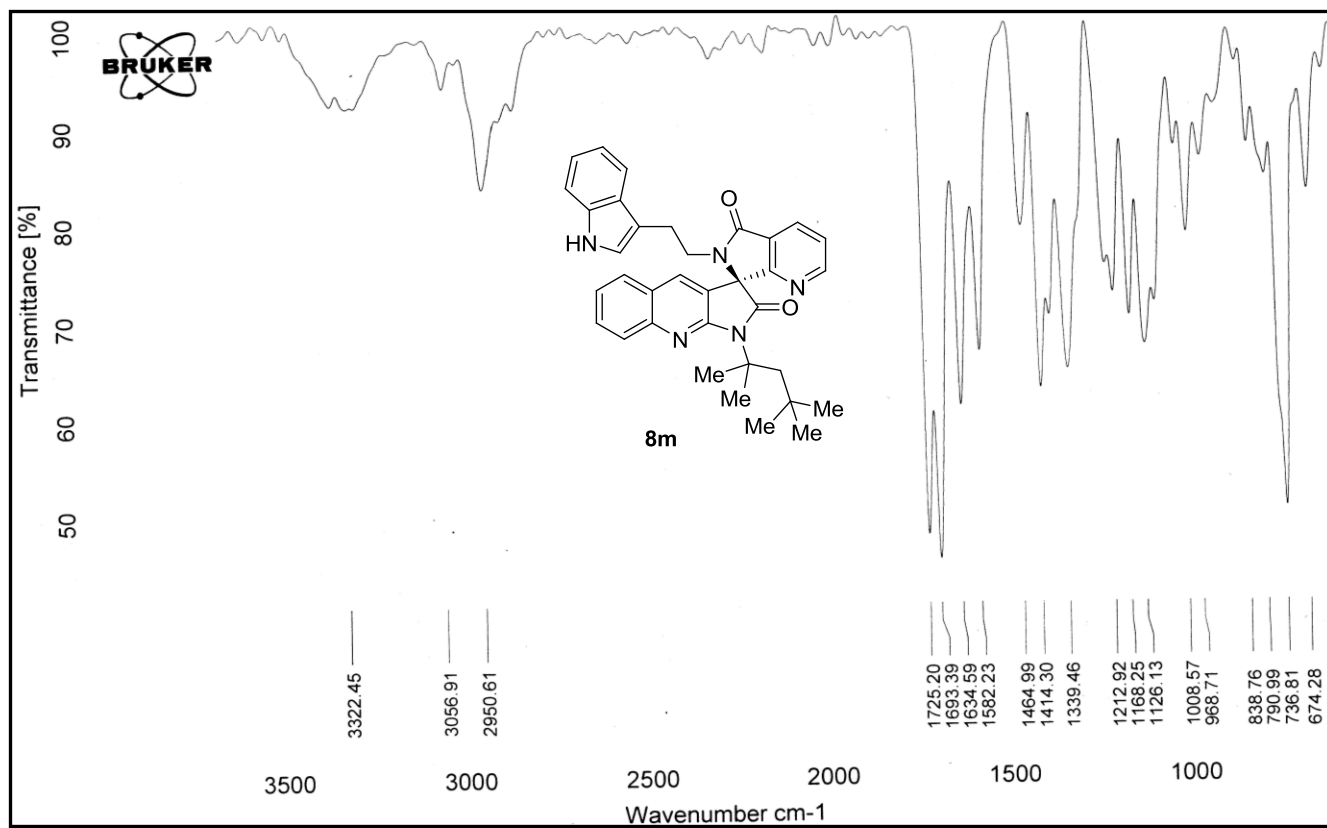


Figure 52. IR (8m).

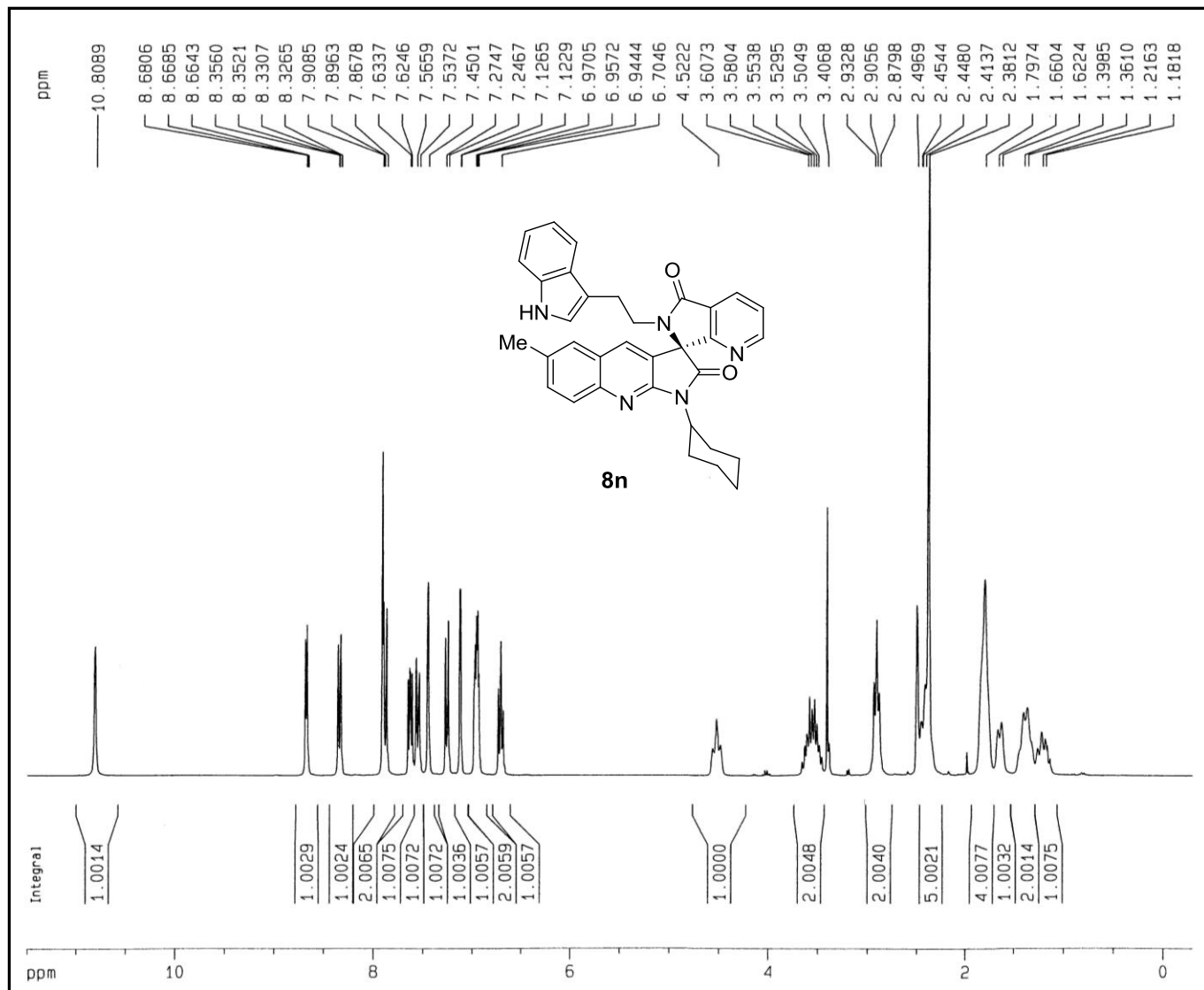
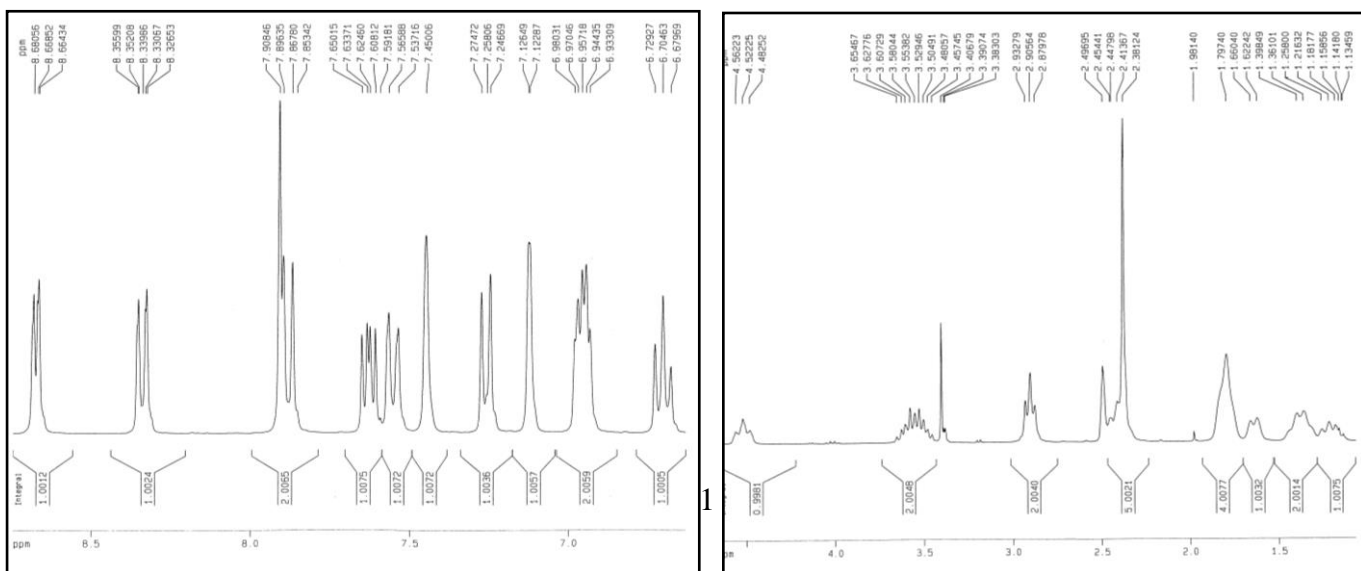
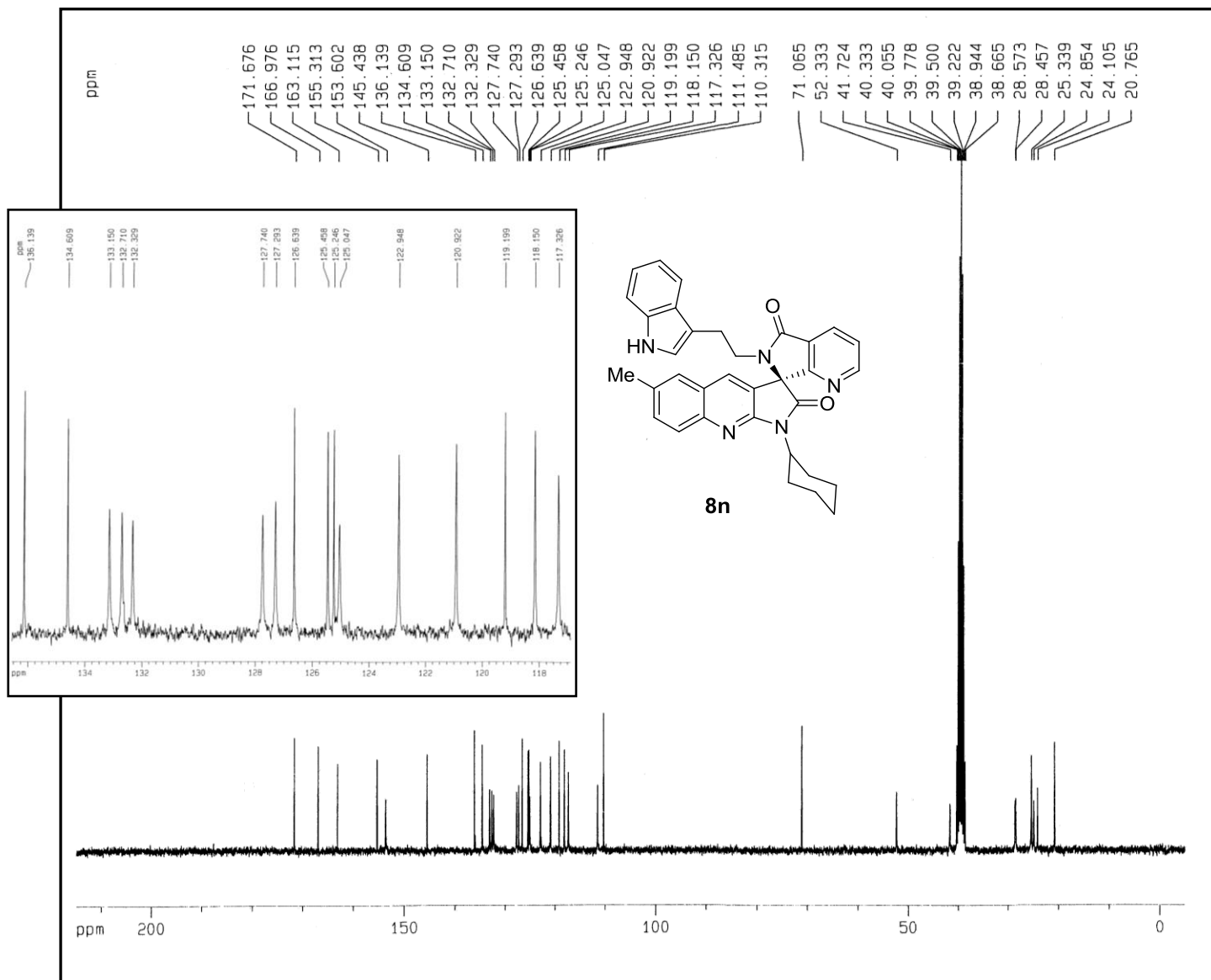


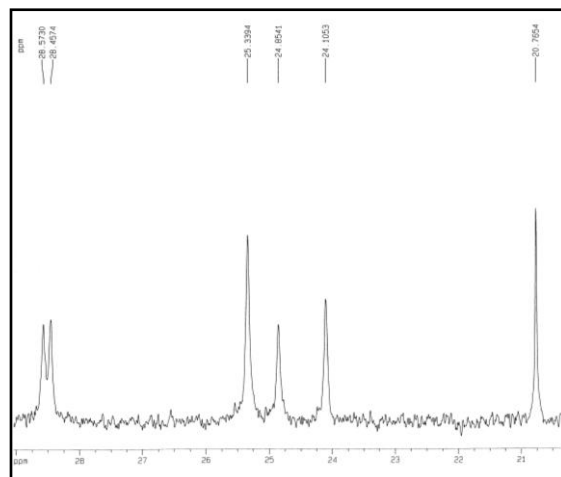
Figure 53. ¹H NMR (300 MHz, DMSO-d₆) (8n).



U. 18



S42



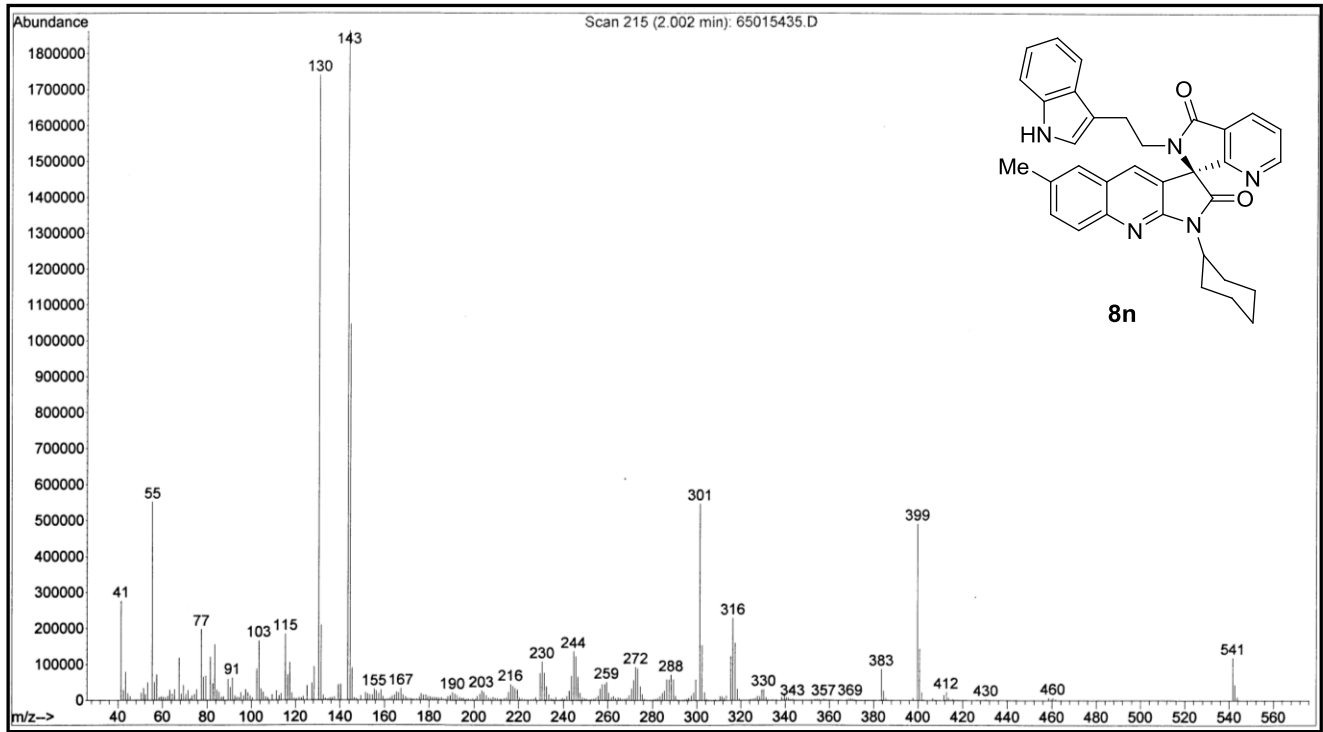


Figure 55. Mass (8n).

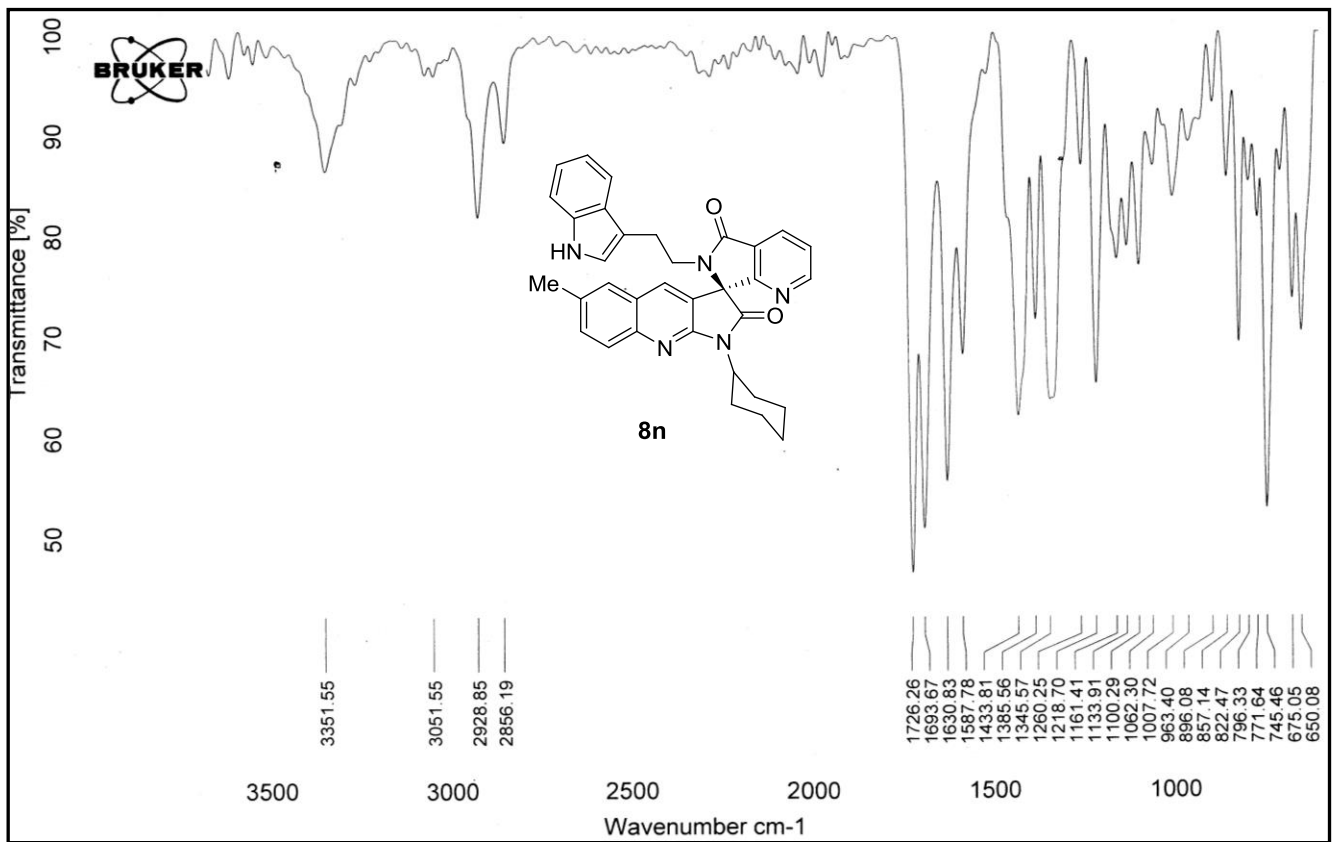


Figure 56. IR (8n).

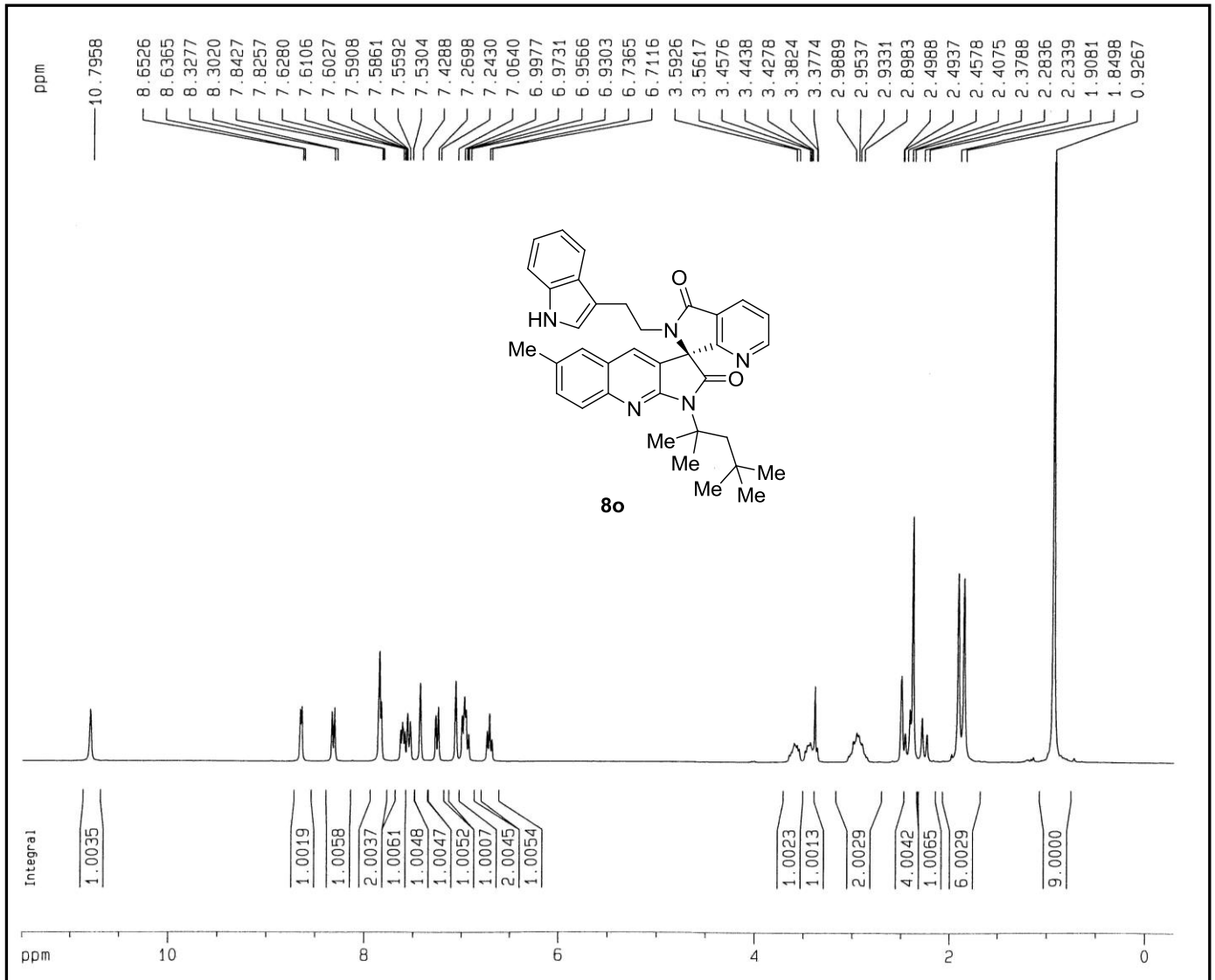
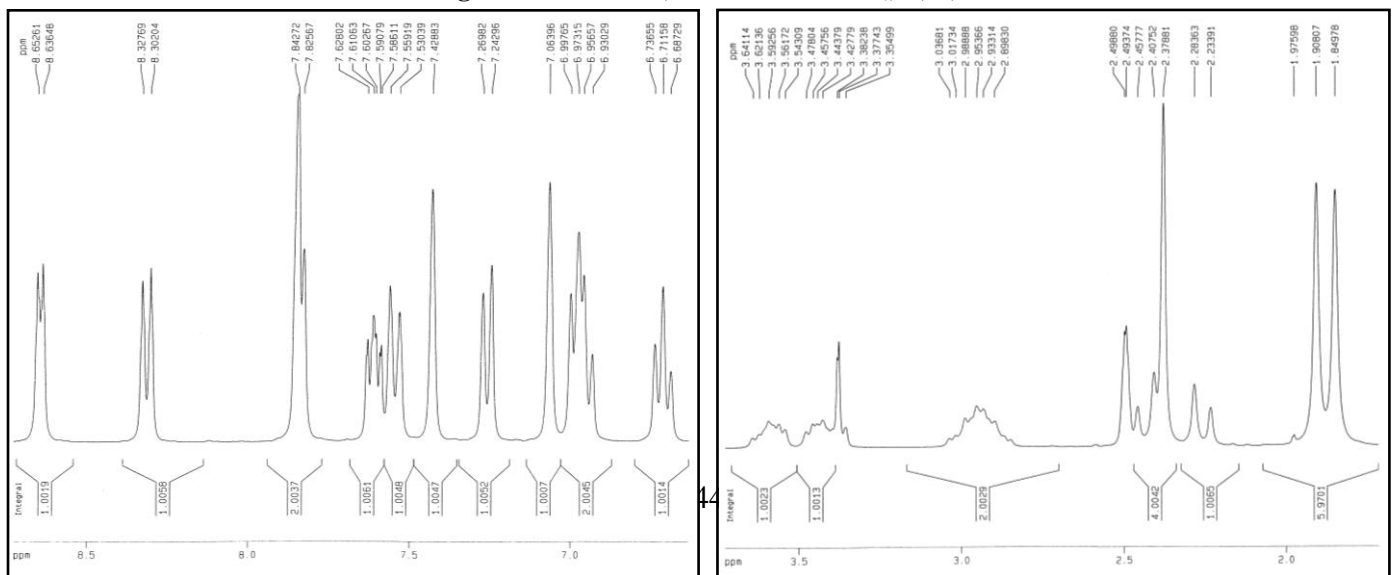


Figure 57. ^1H NMR (300 MHz, $\text{DMSO-}d_6$) (8o).



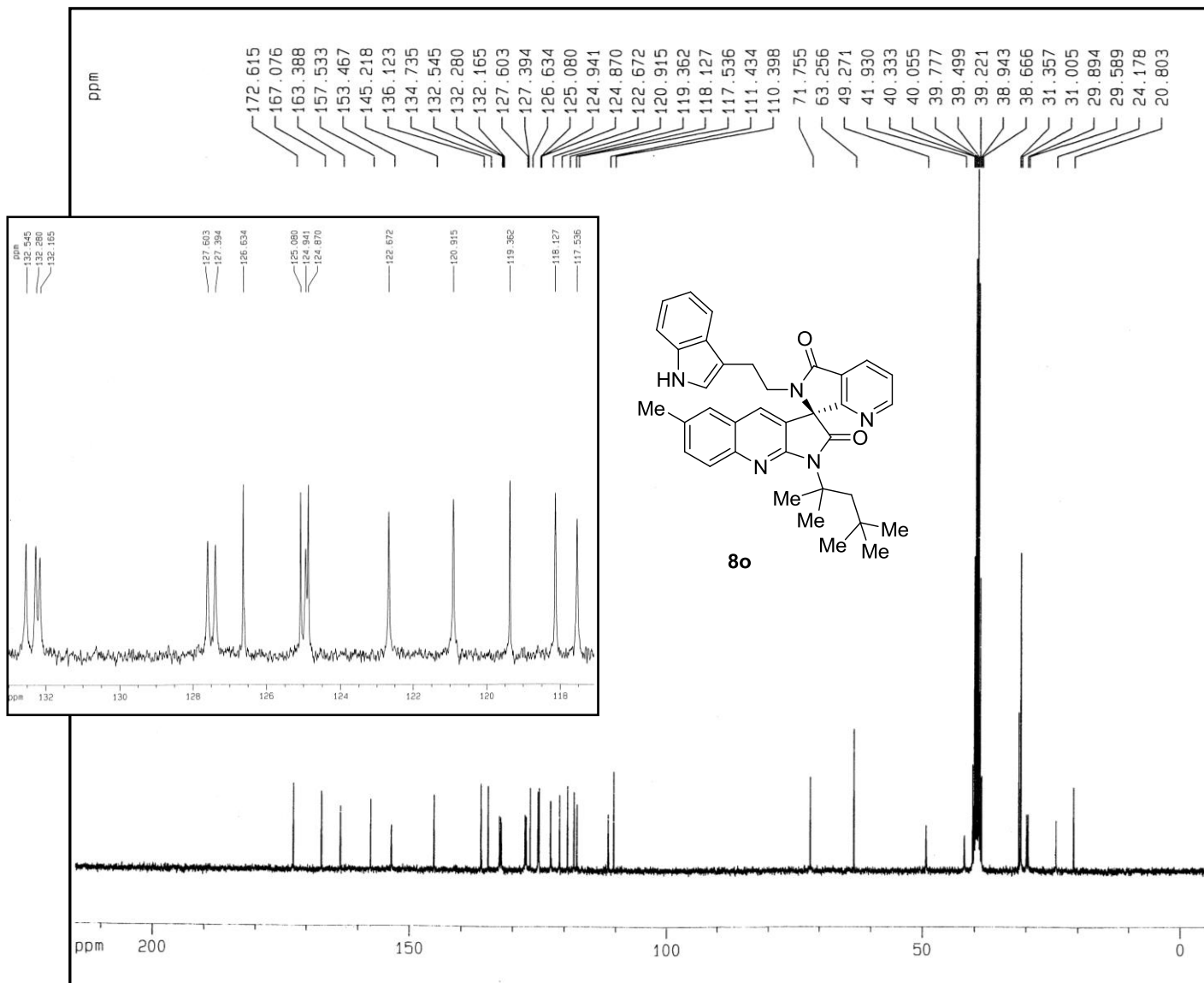


Figure 58. ¹H NMR (300 MHz, DMSO-*d*₆) (**8o**).

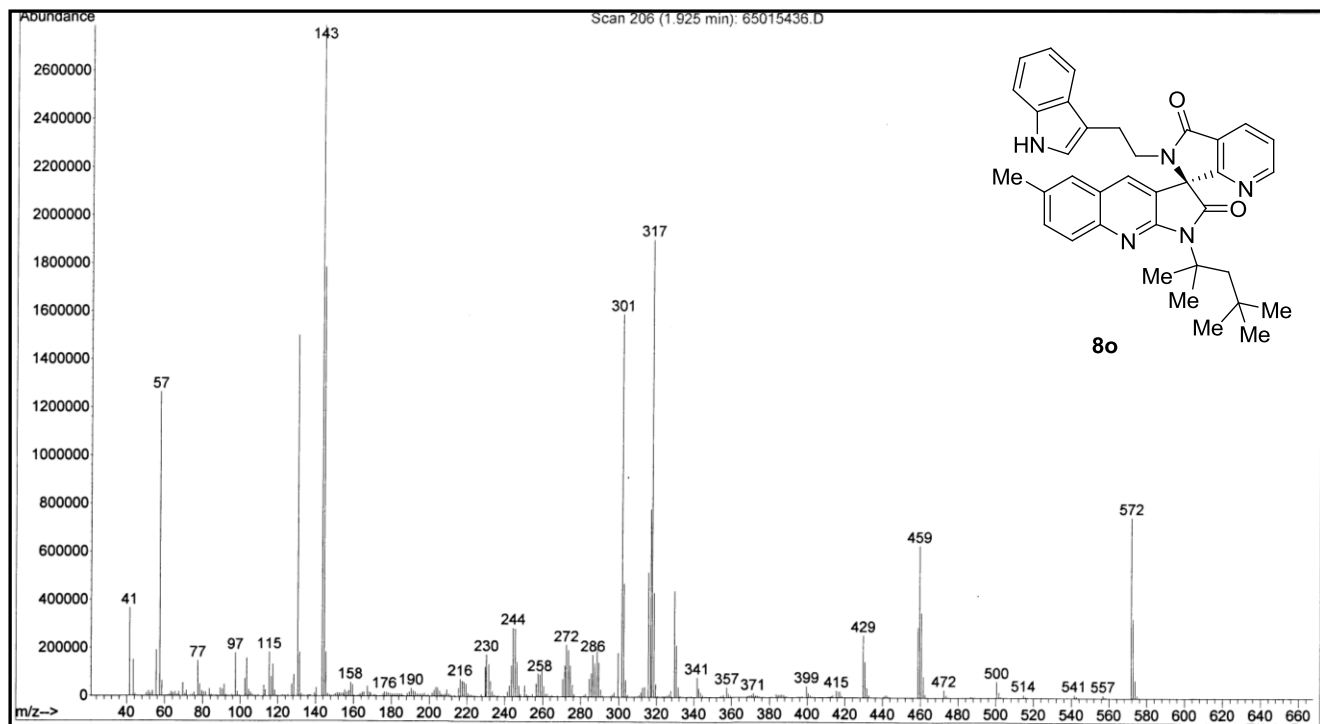


Figure 59. Mass (8o).

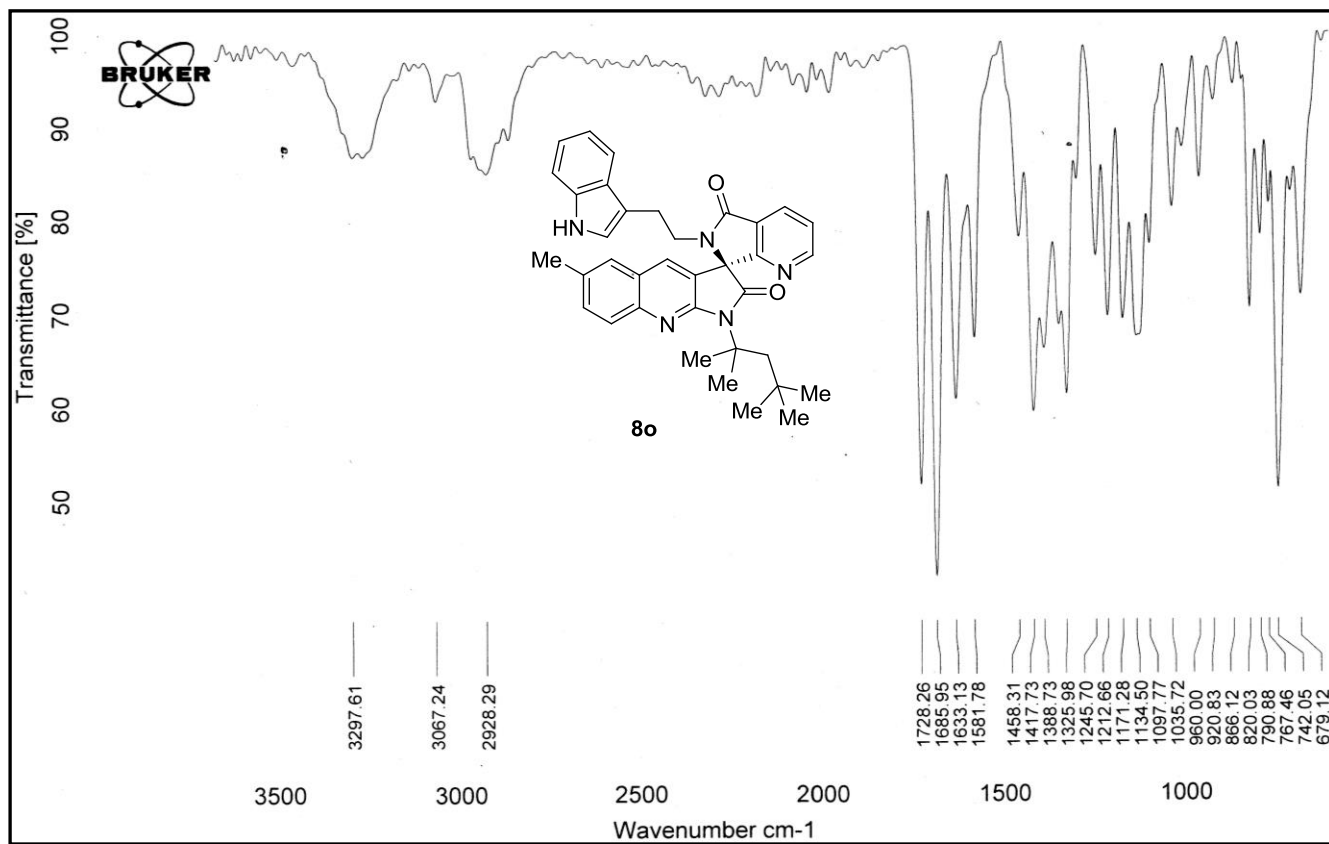


Figure 60. IR (8o).

2. Copies of ^1H and ^{13}C NMR spectra for compounds 10a-l

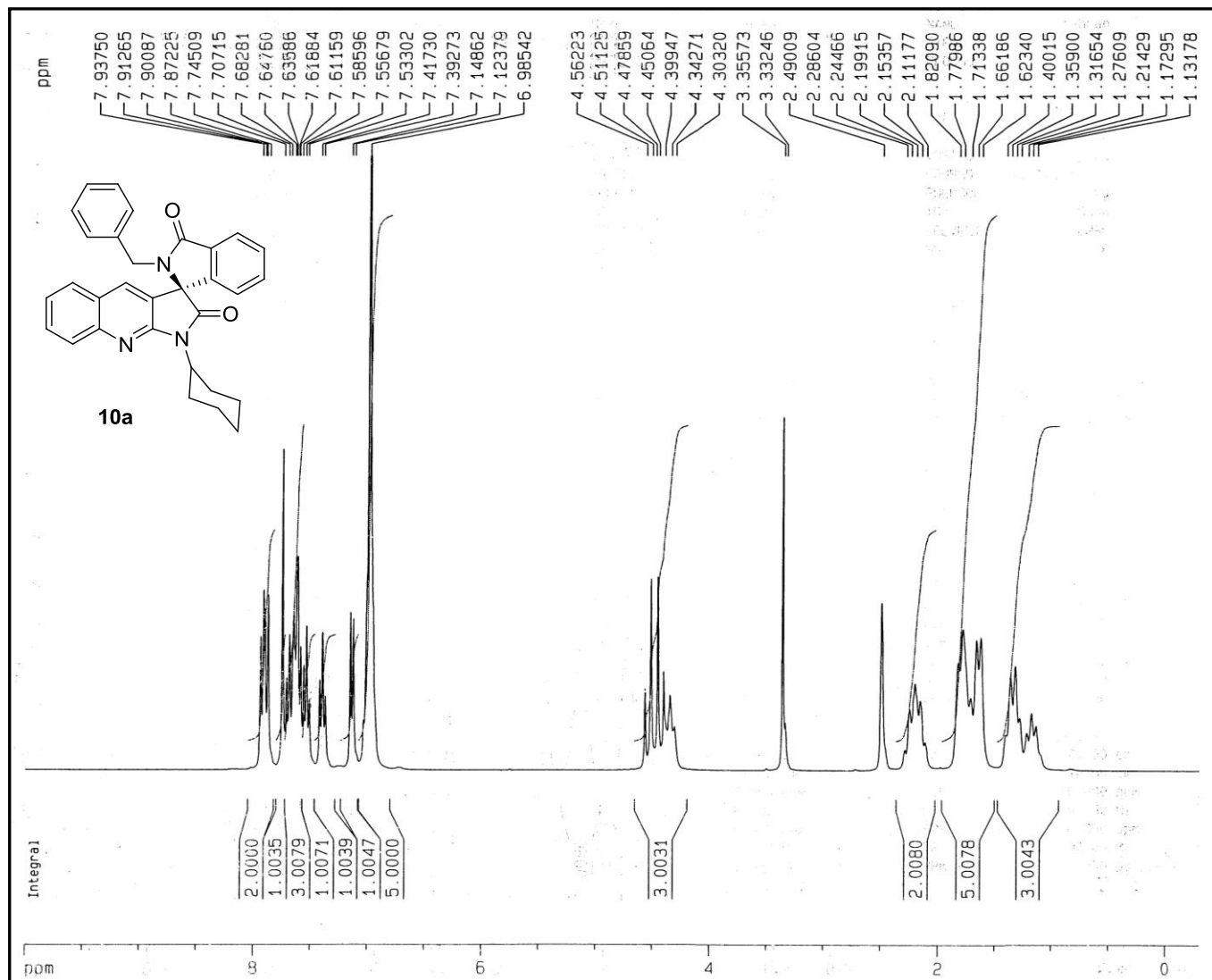
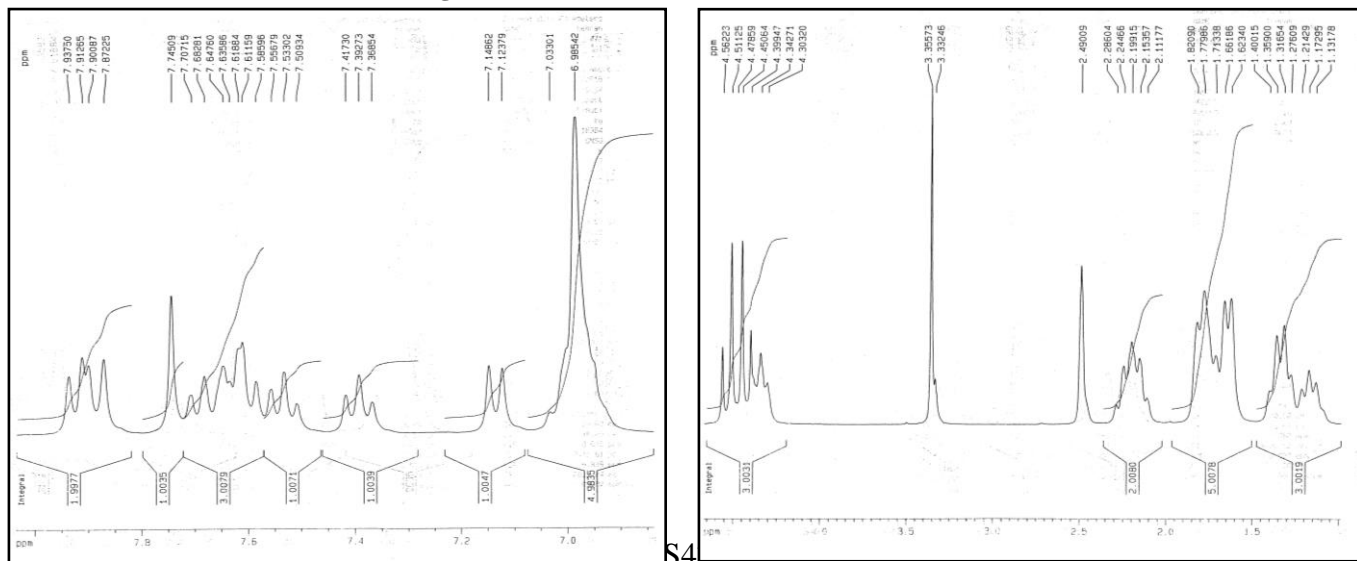


Figure 61. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) (10a).



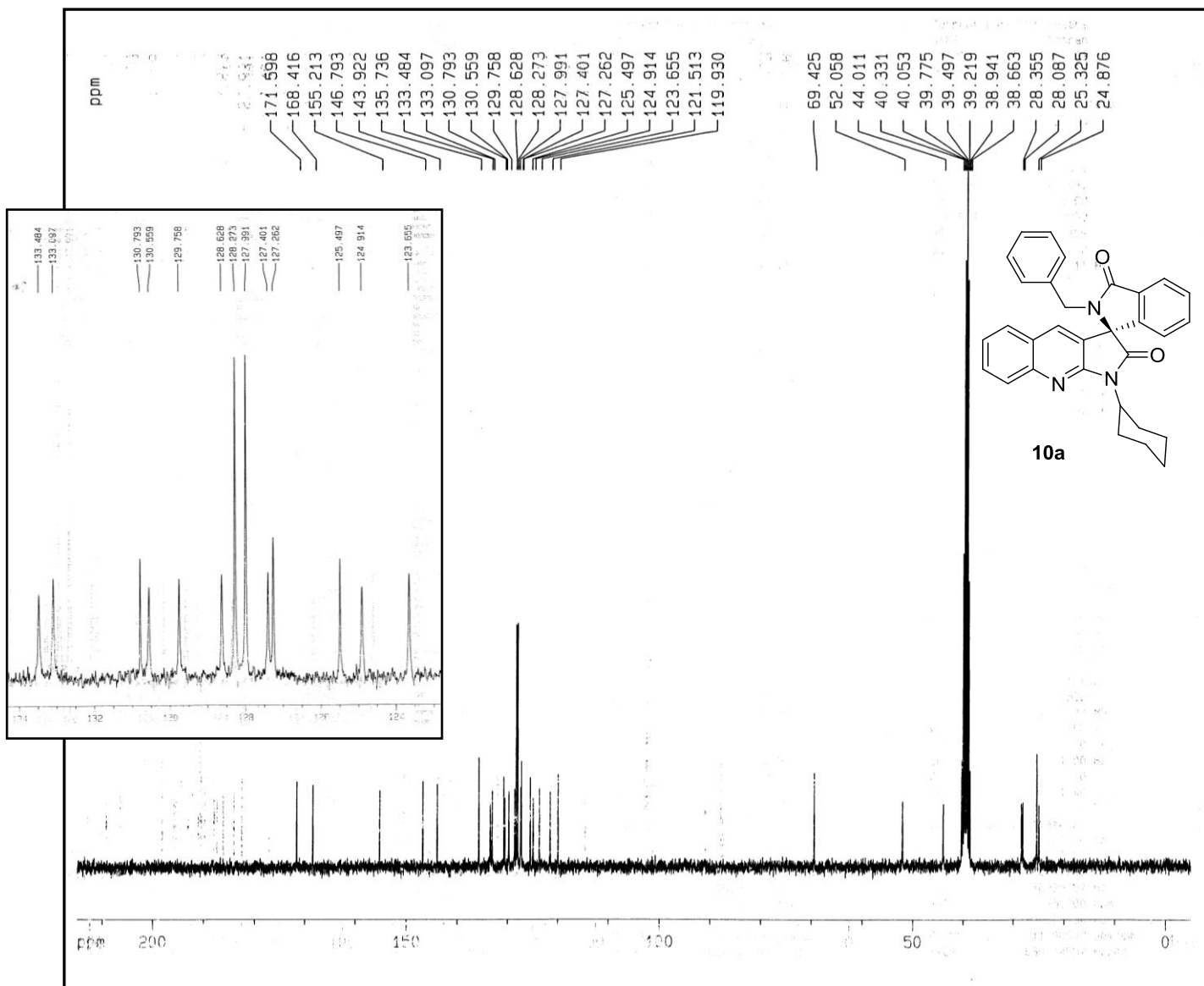


Figure 62. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (10a).

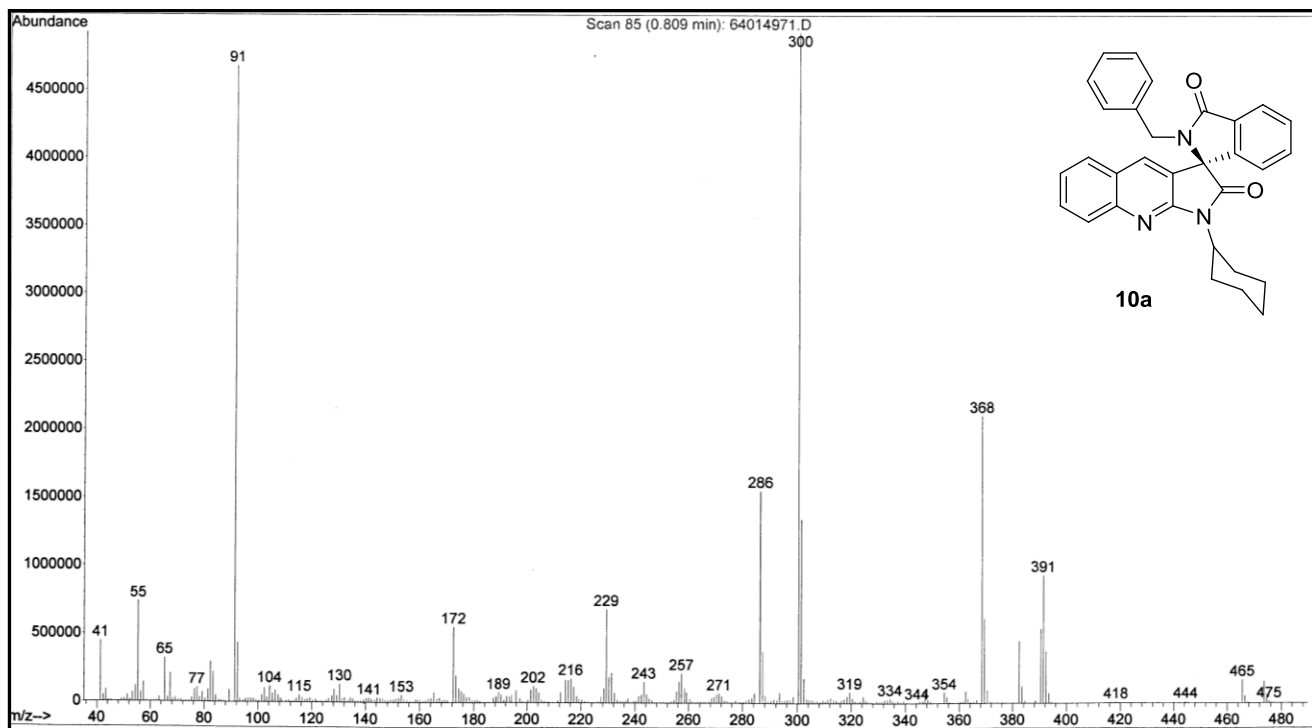


Figure 63. Mass (10a).

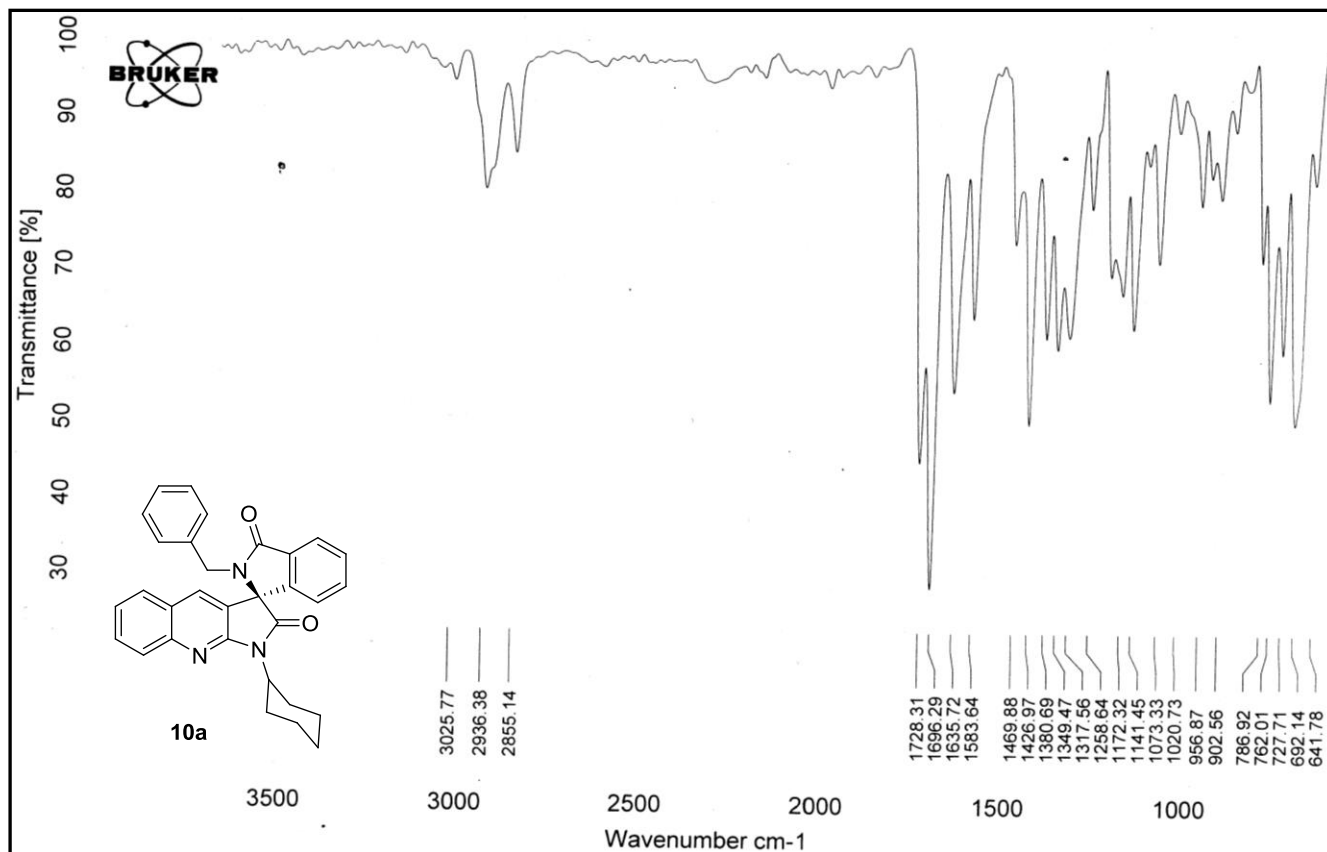


Figure 64. IR (10a).

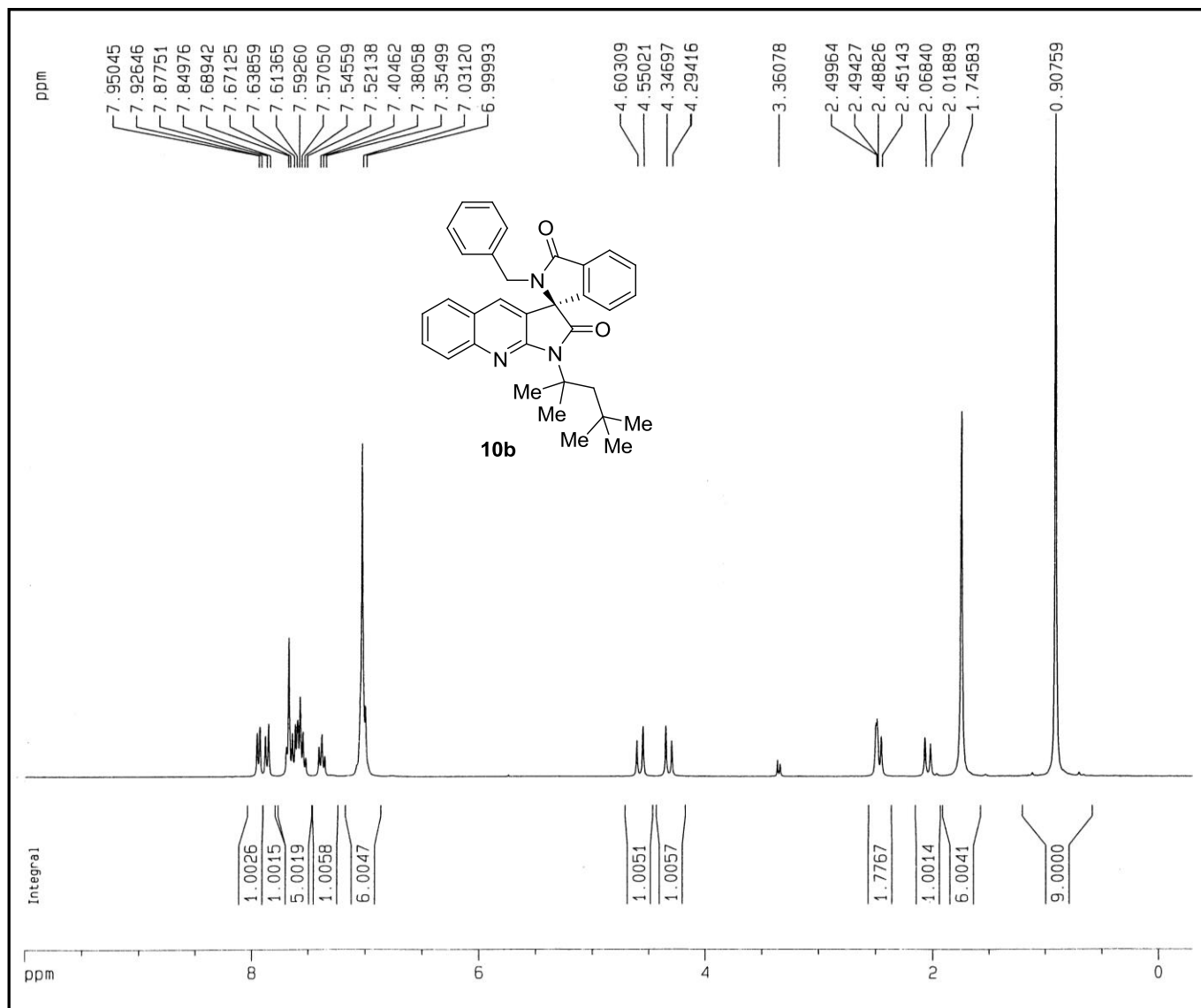
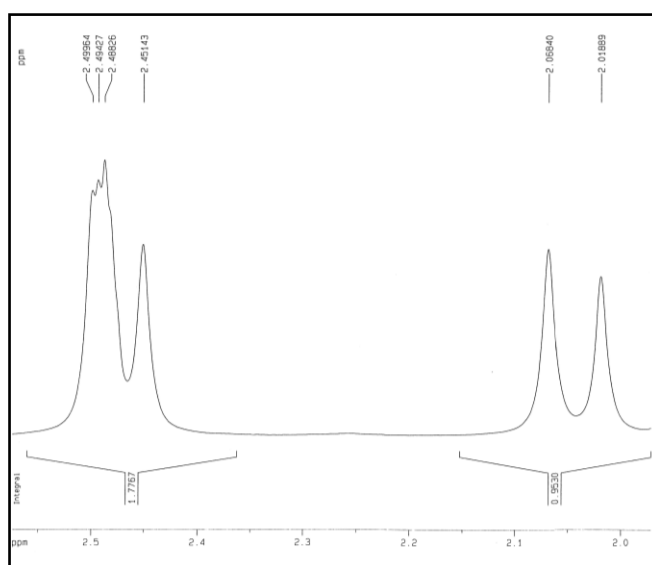
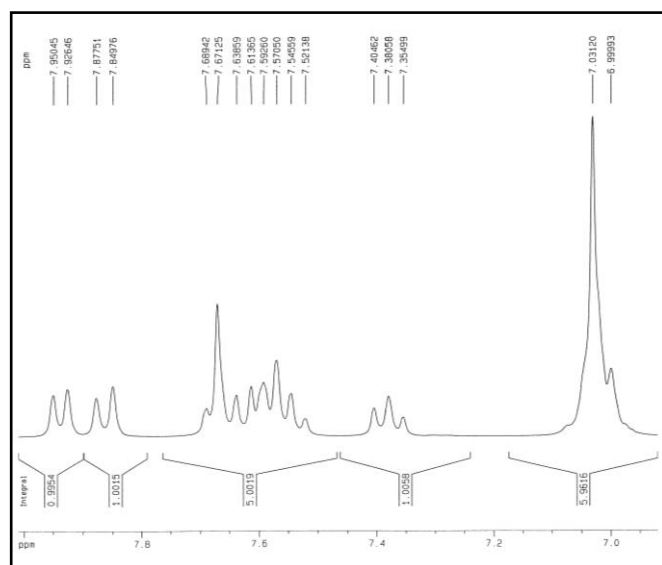


Figure 65. ¹H NMR (300 MHz, DMSO-*d*₆) (**10b**).



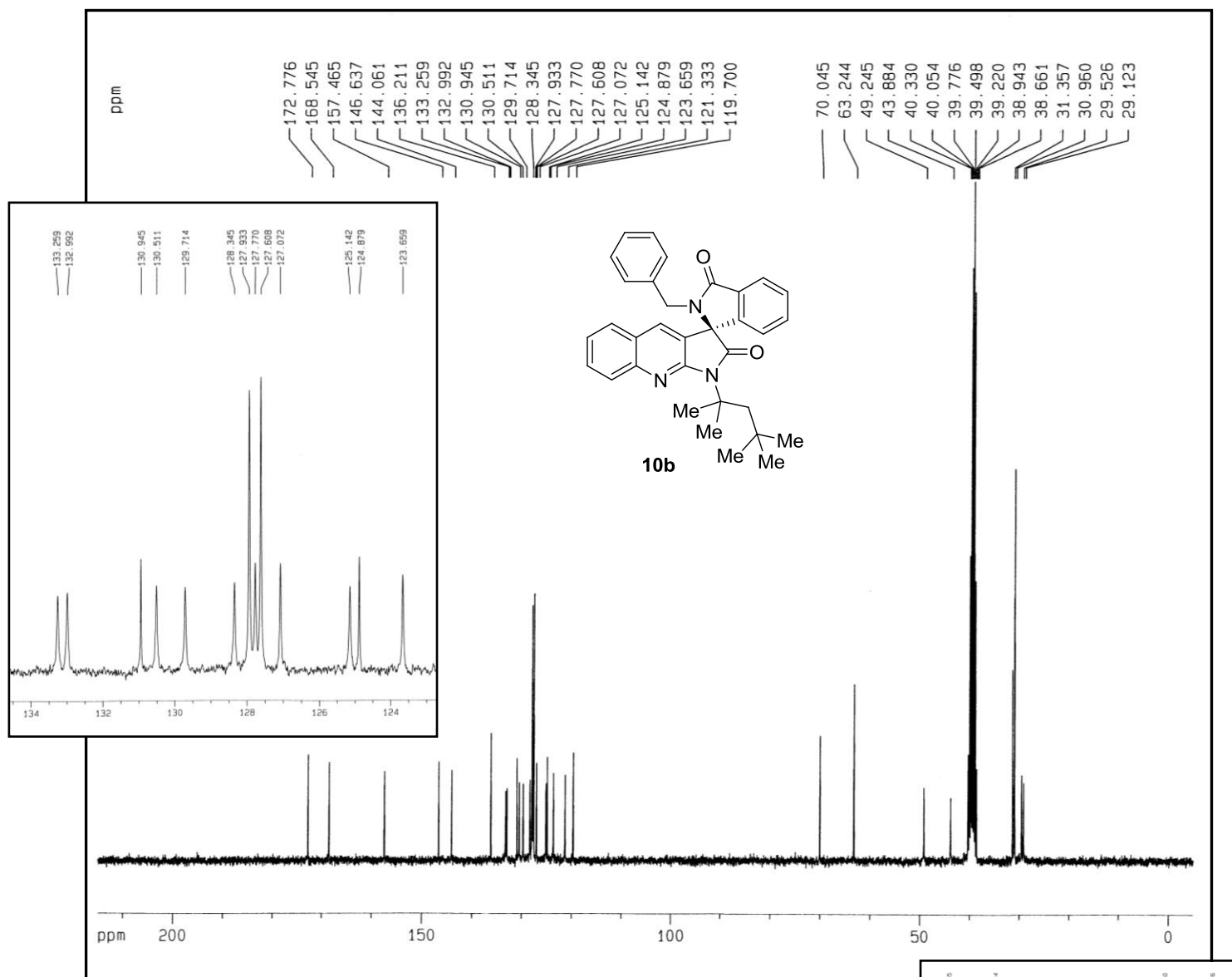
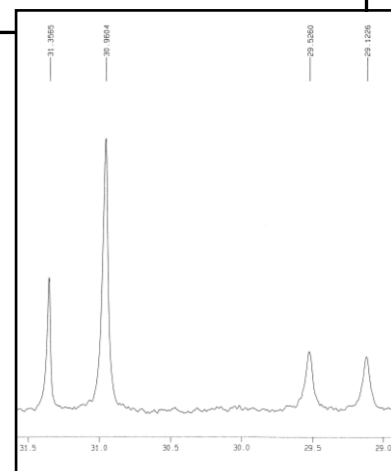


Figure 66. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10b**).



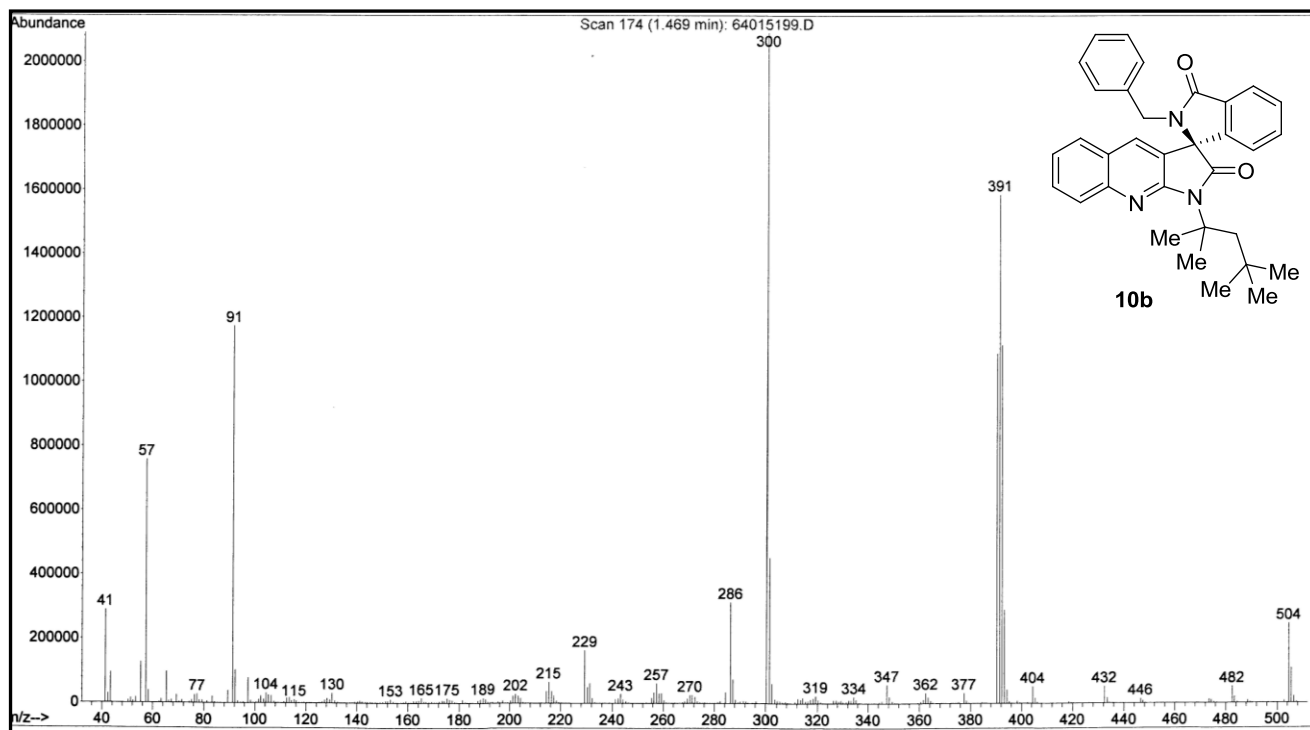


Figure 67. Mass (10b).

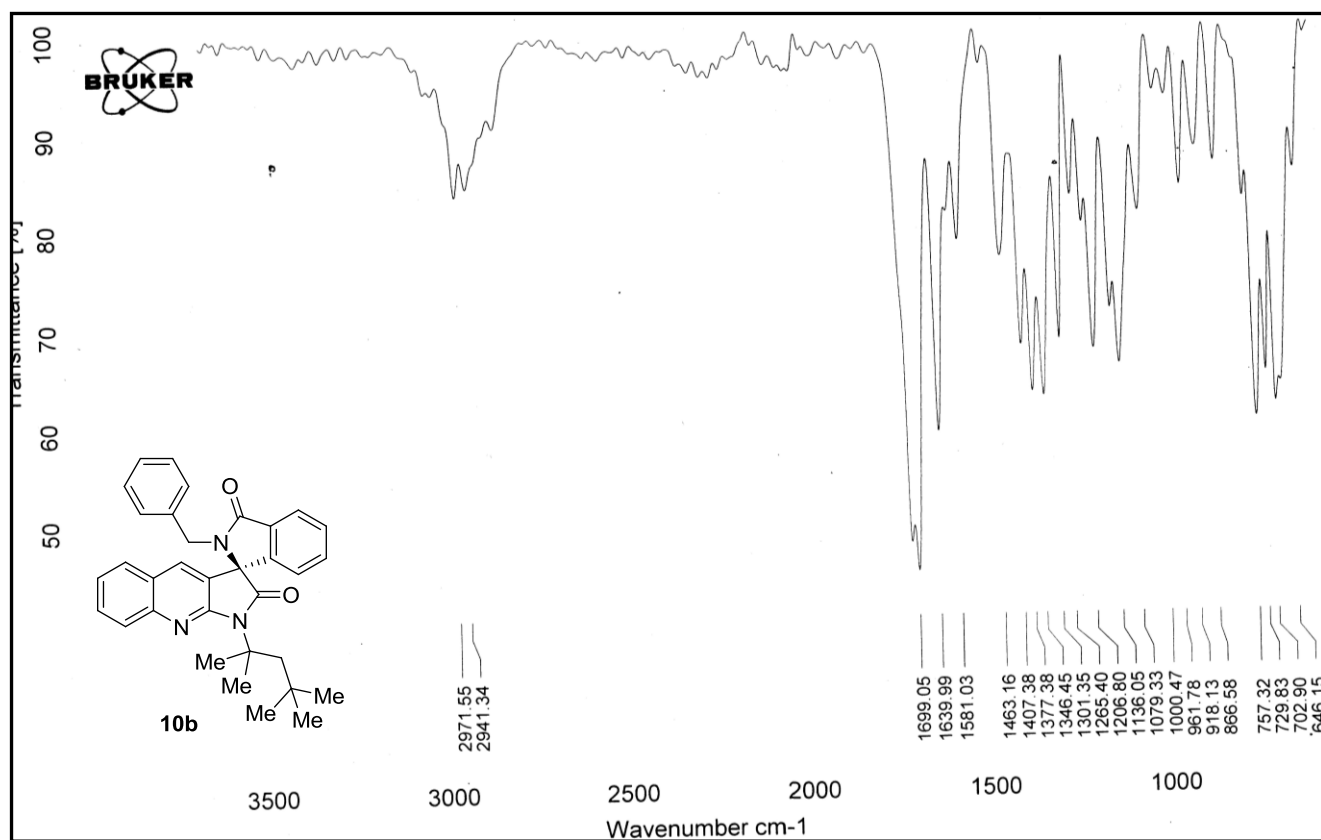


Figure 68. IR (10b).

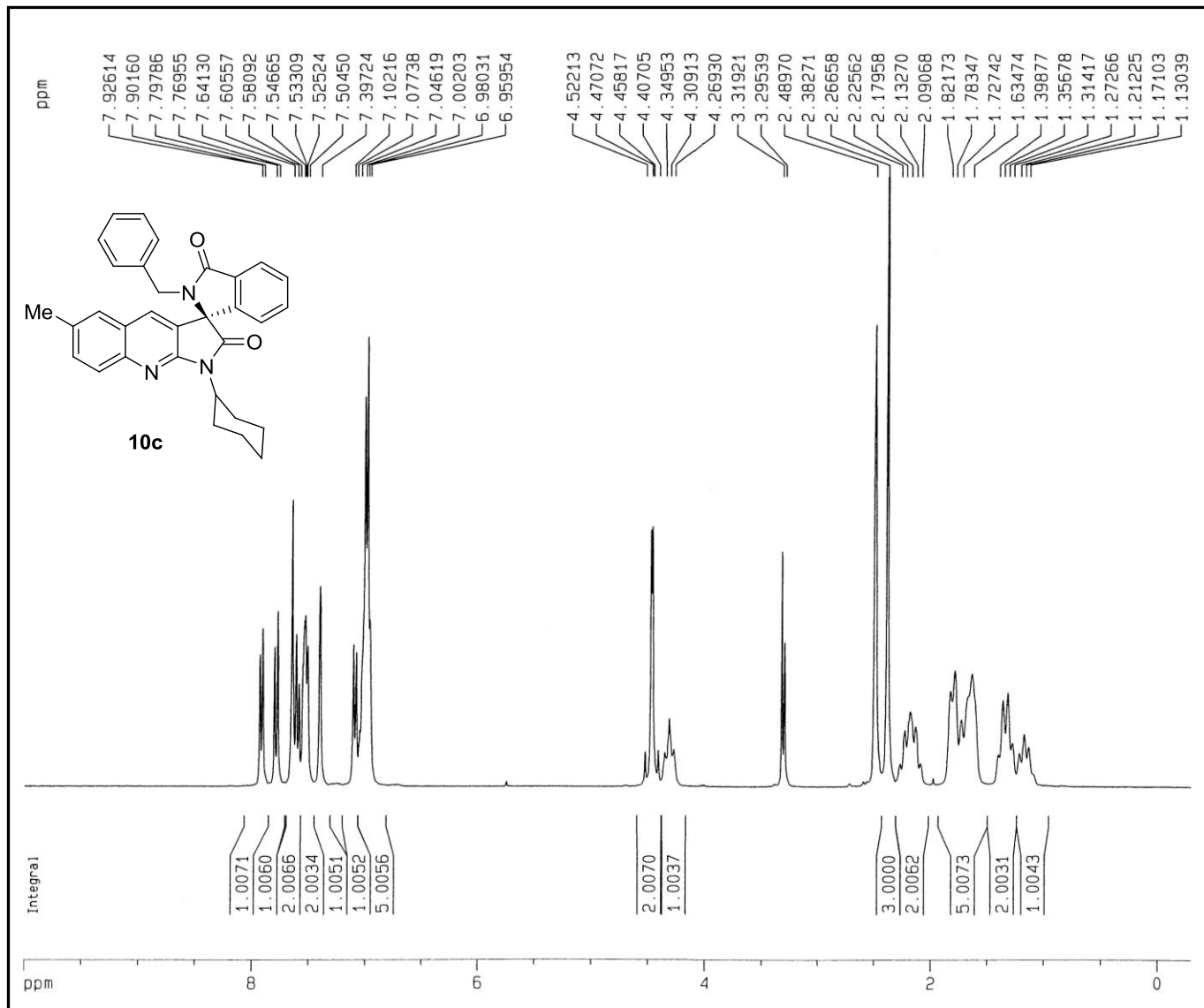
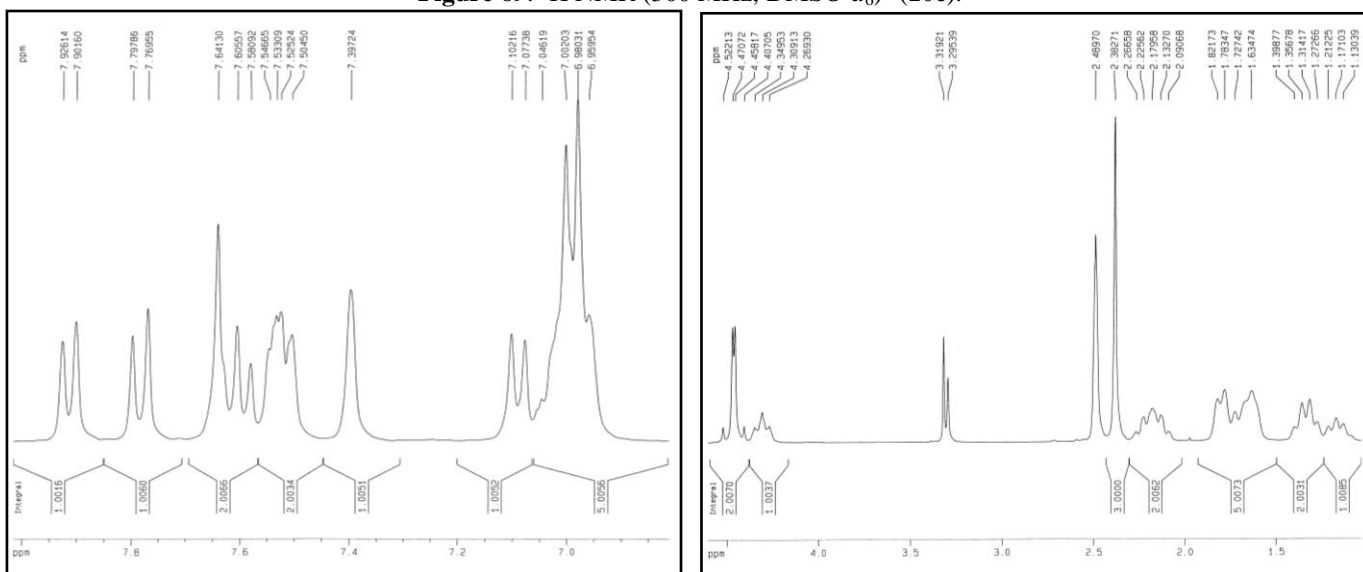


Figure 69. ¹H NMR (300 MHz, DMSO-*d*₆) (**10c**).



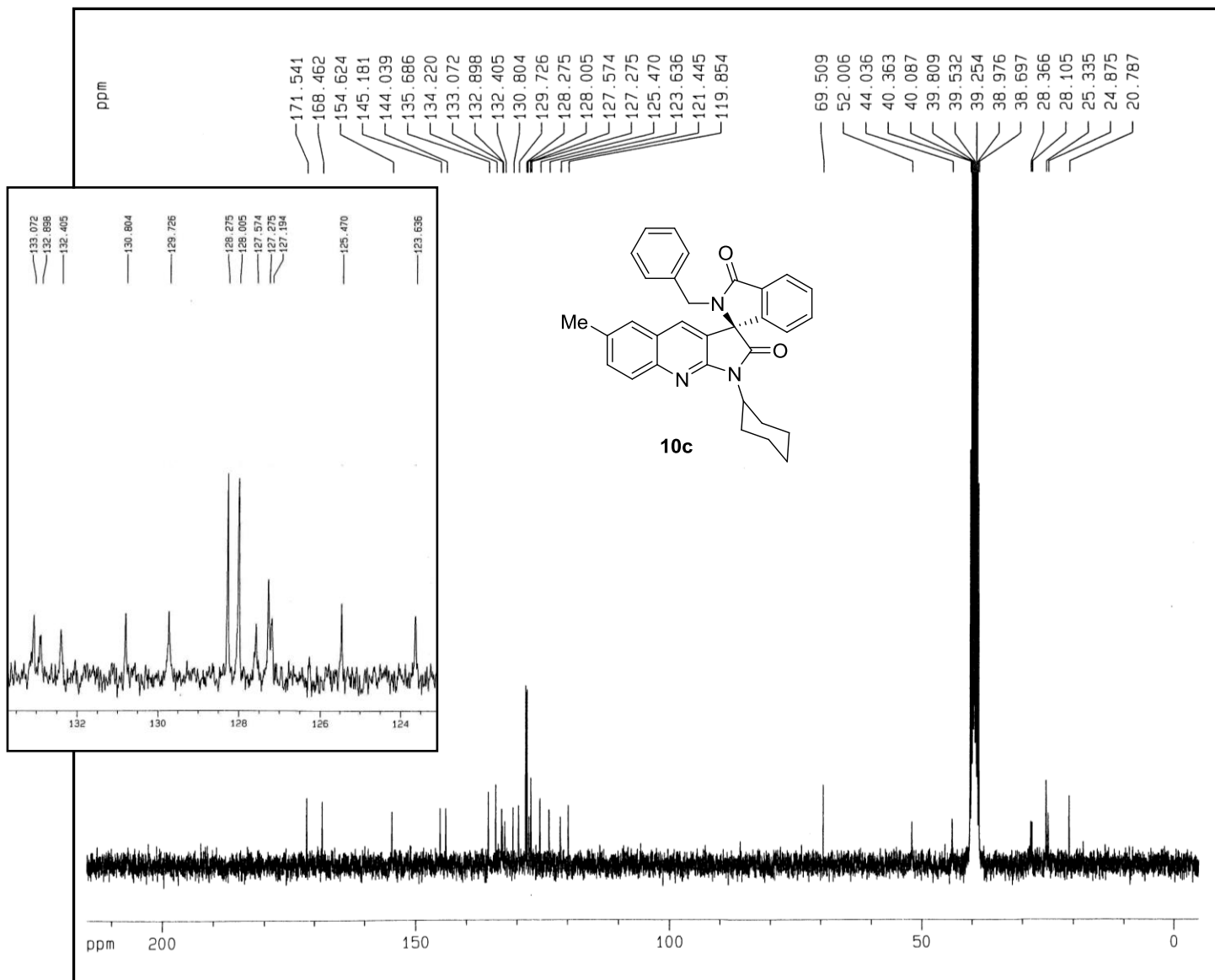


Figure 70. ¹³C NMR (300 MHz, DMSO-*d*₆) (**10c**).

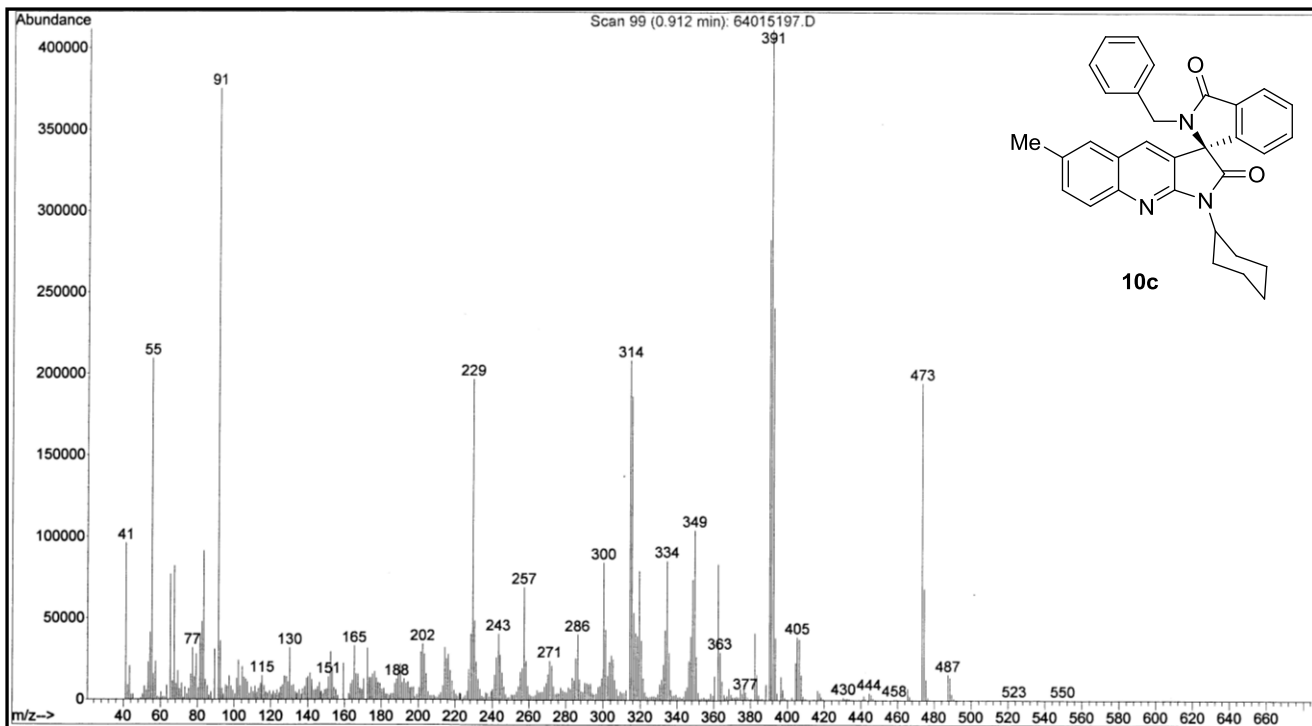


Figure 71. Mass (**10c**).

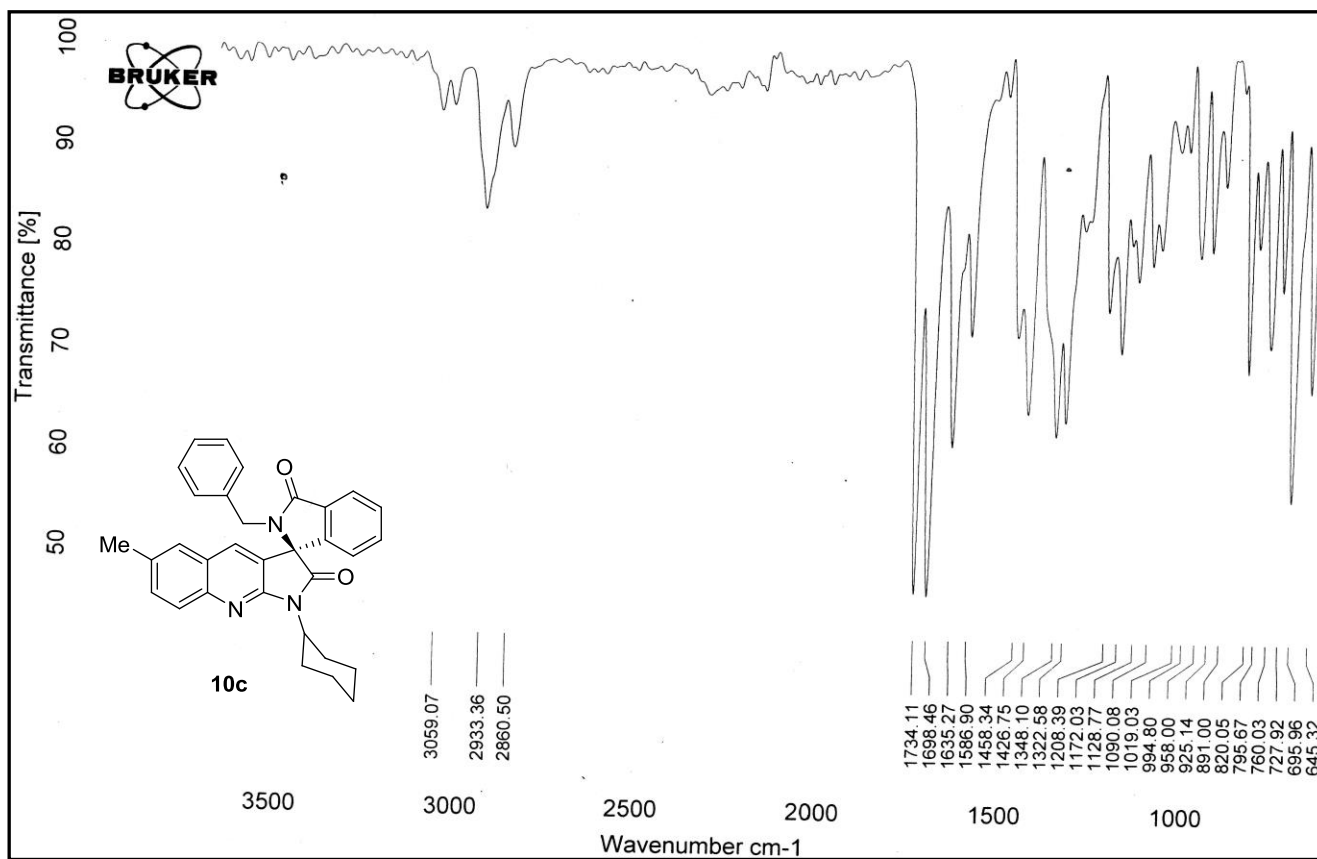


Figure 72. IR (**10c**).

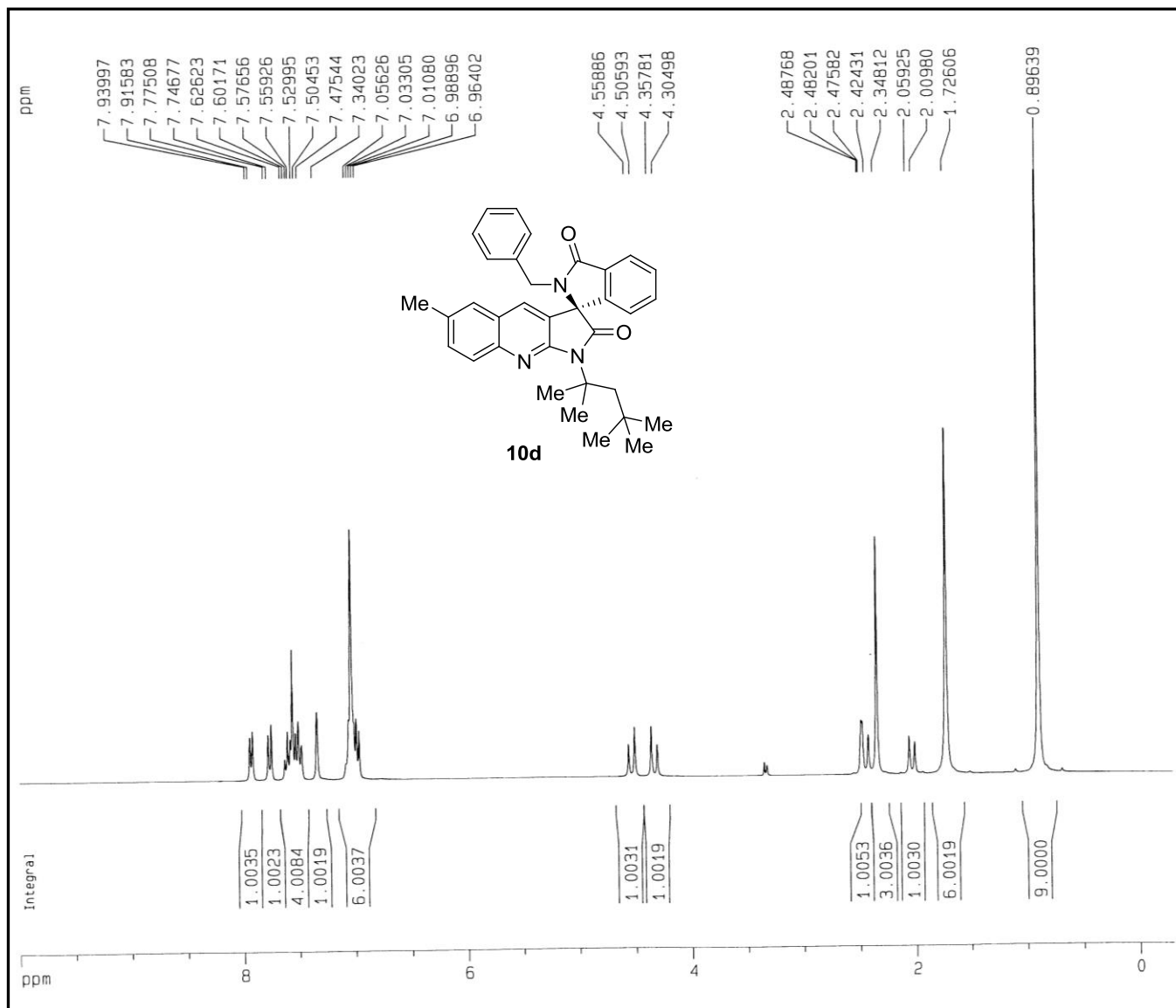
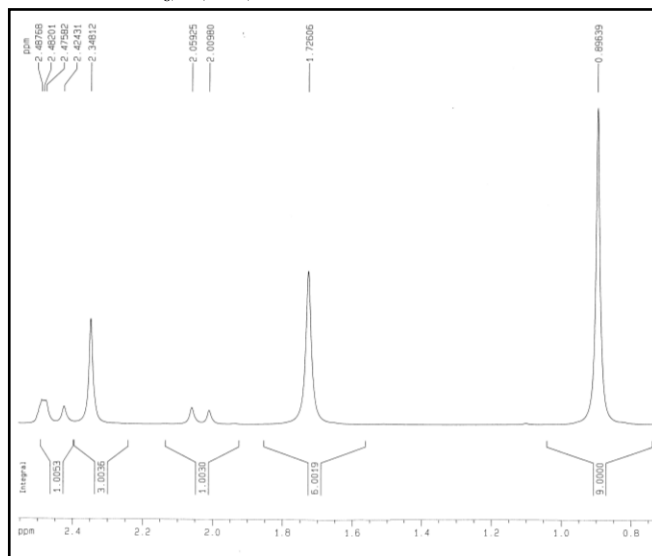
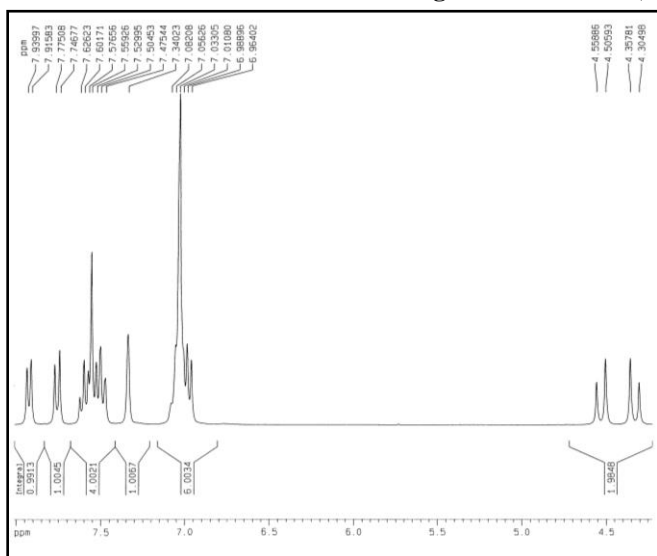


Figure 73. ^1H NMR (300 MHz, $\text{DMSO-}d_6$) (**10d**).



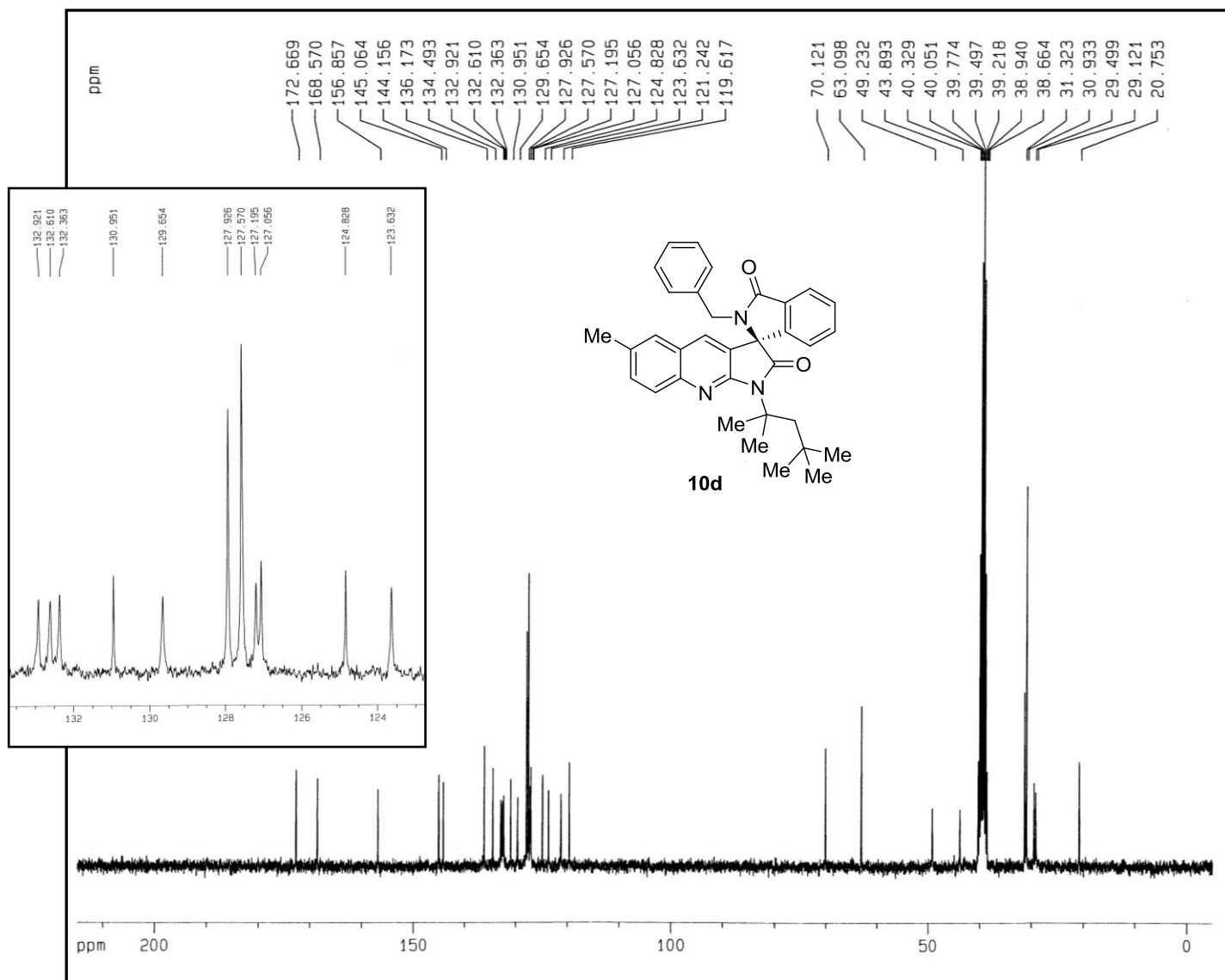


Figure 74. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10d**).

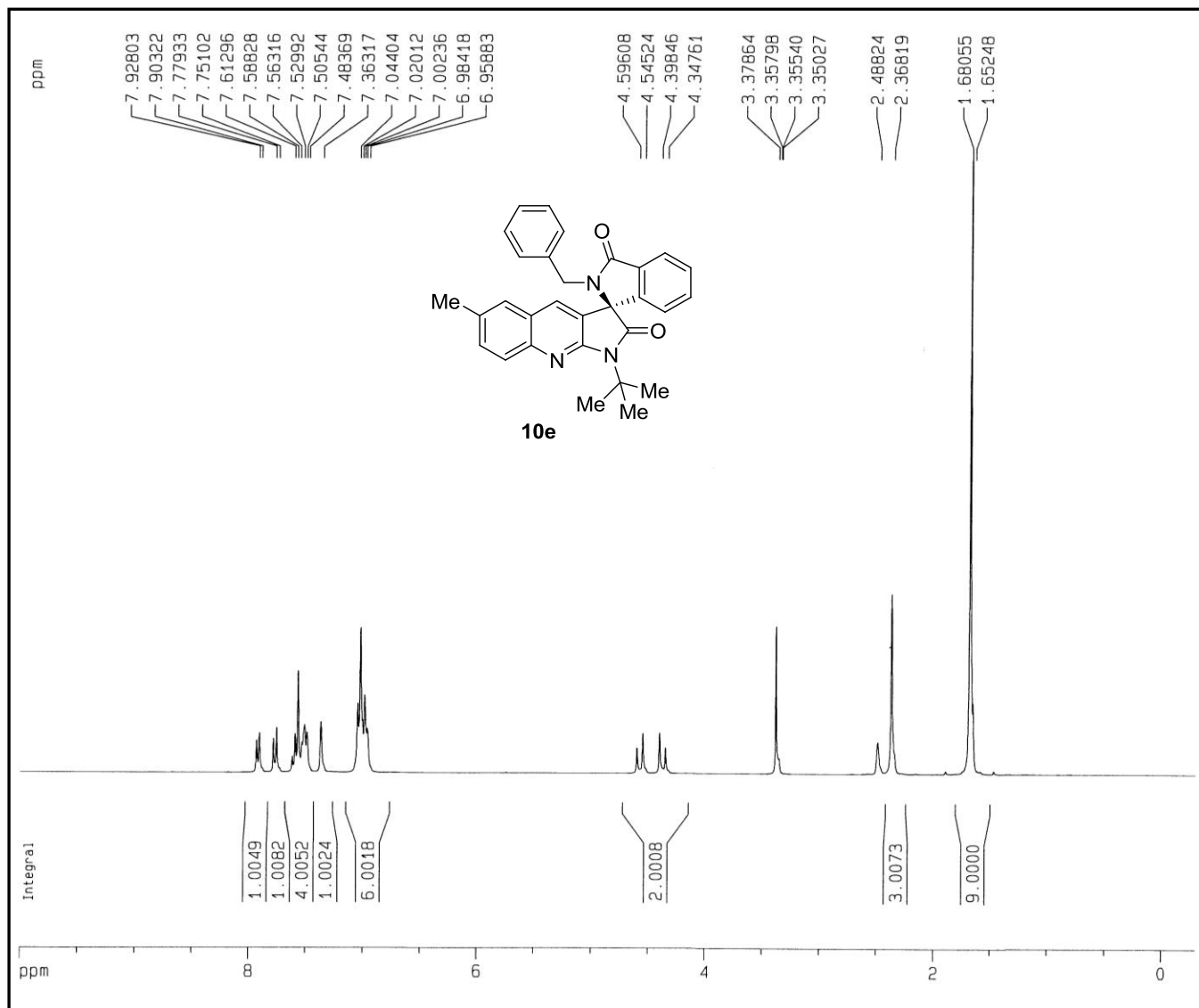
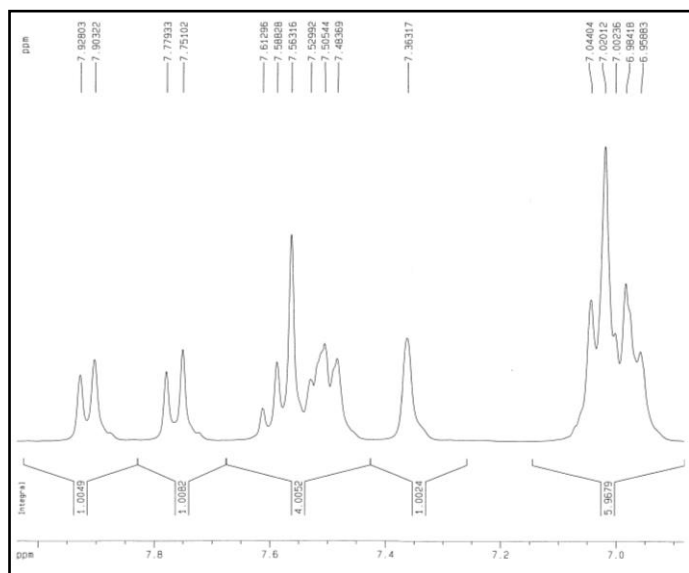


Figure 77. ¹H NMR (300 MHz, DMSO-*d*₆) (**10e**).



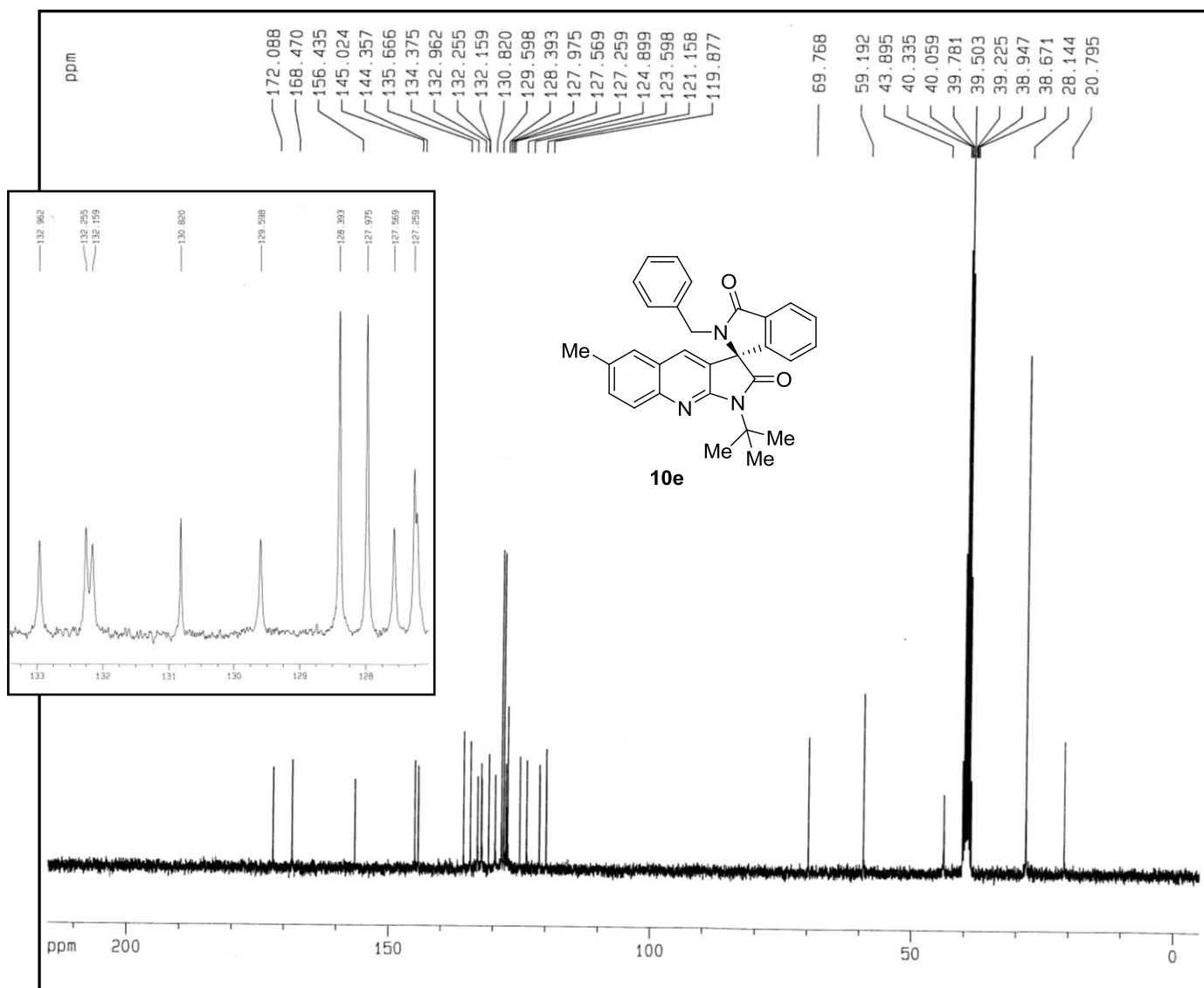


Figure 78. ¹³C NMR (300 MHz, DMSO-*d*₆) (**10e**).

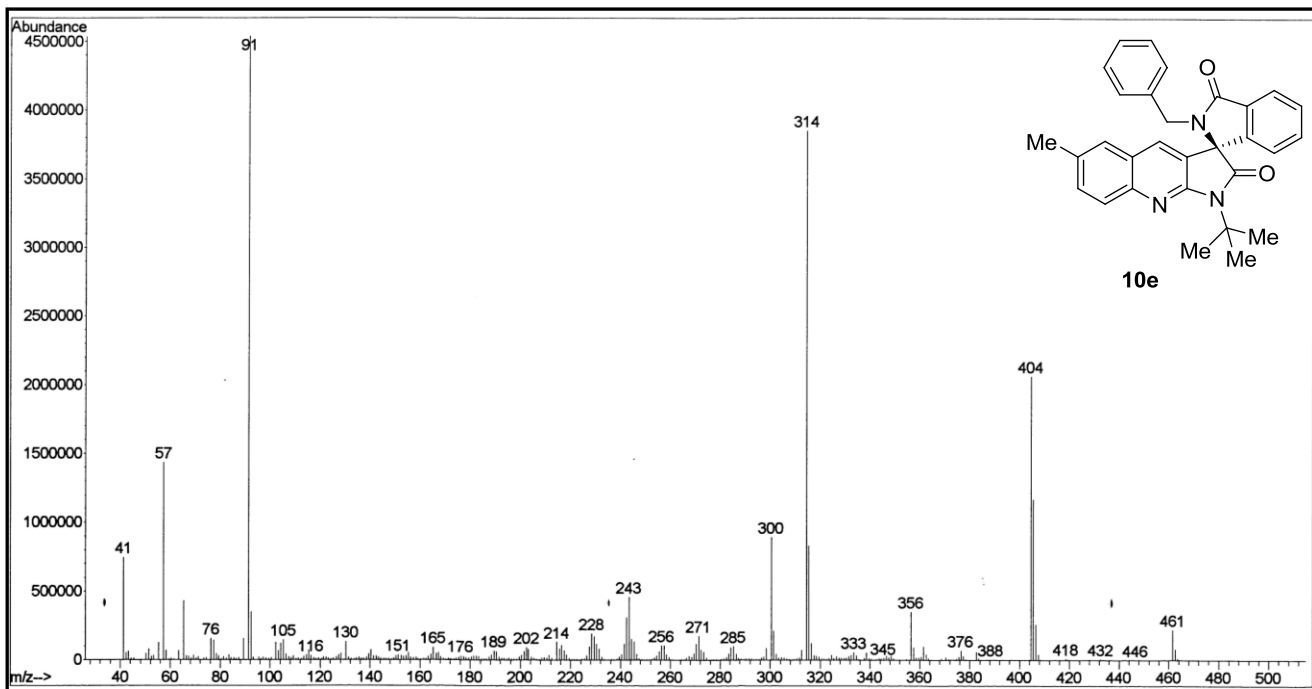


Figure 79. Mass (10e).

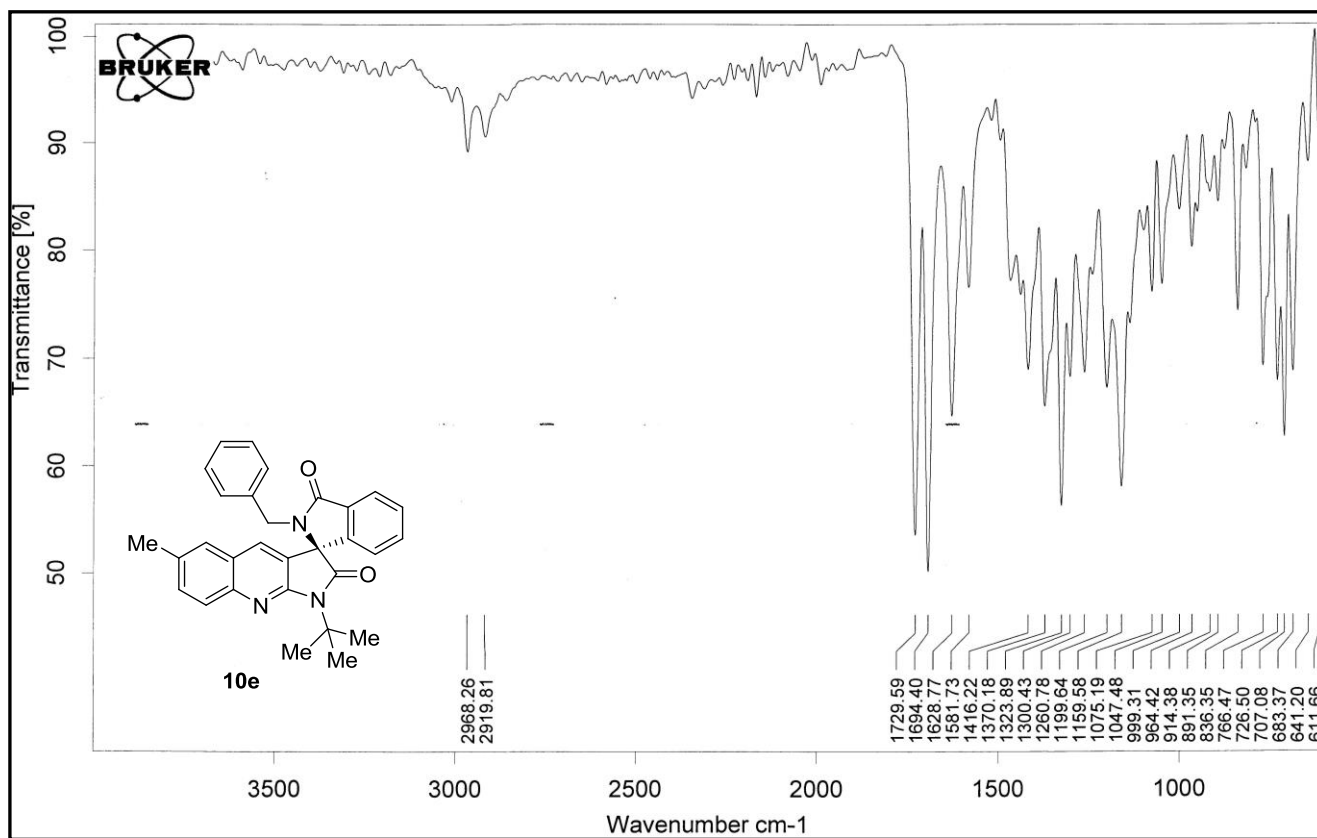


Figure 80. IR (10e).

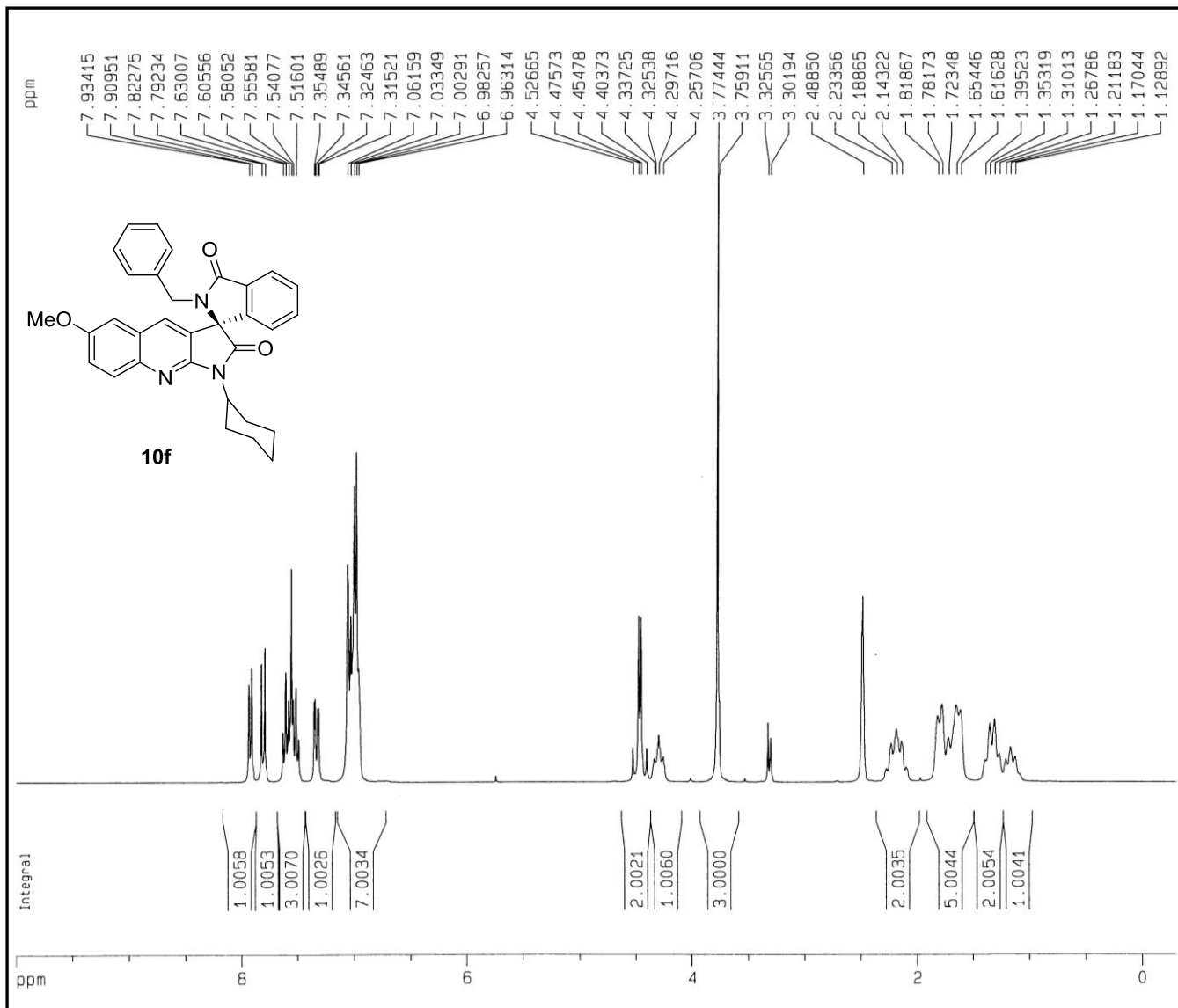
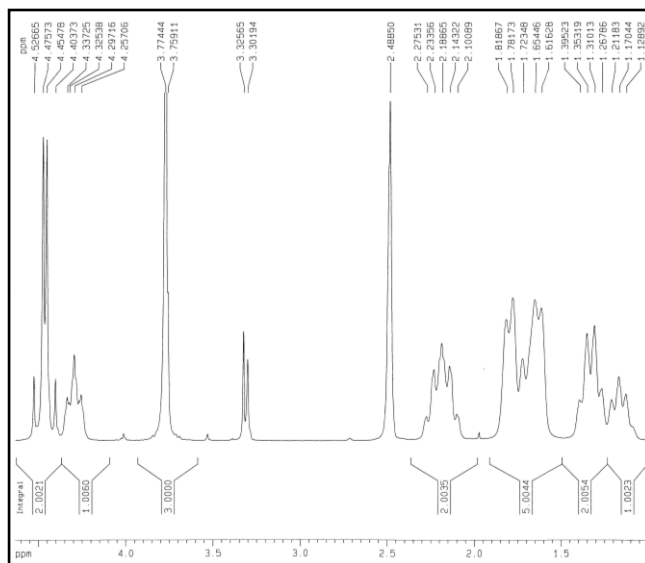
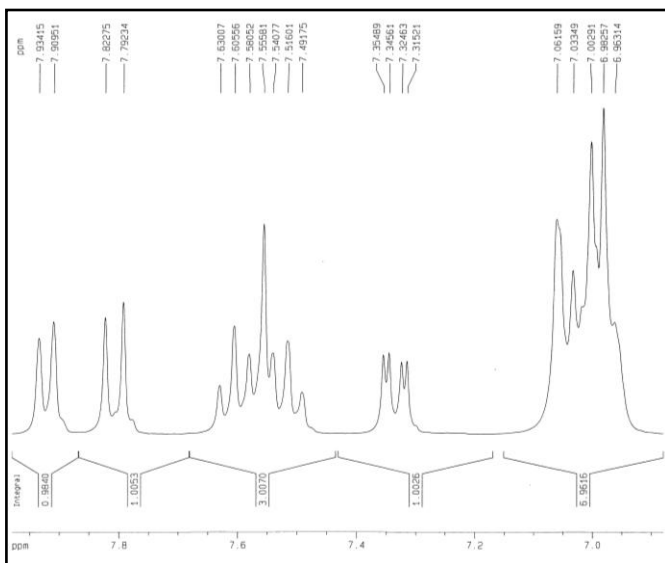


Figure 81. ^1H NMR (300 MHz, $\text{DMSO-}d_6$) (**10f**).



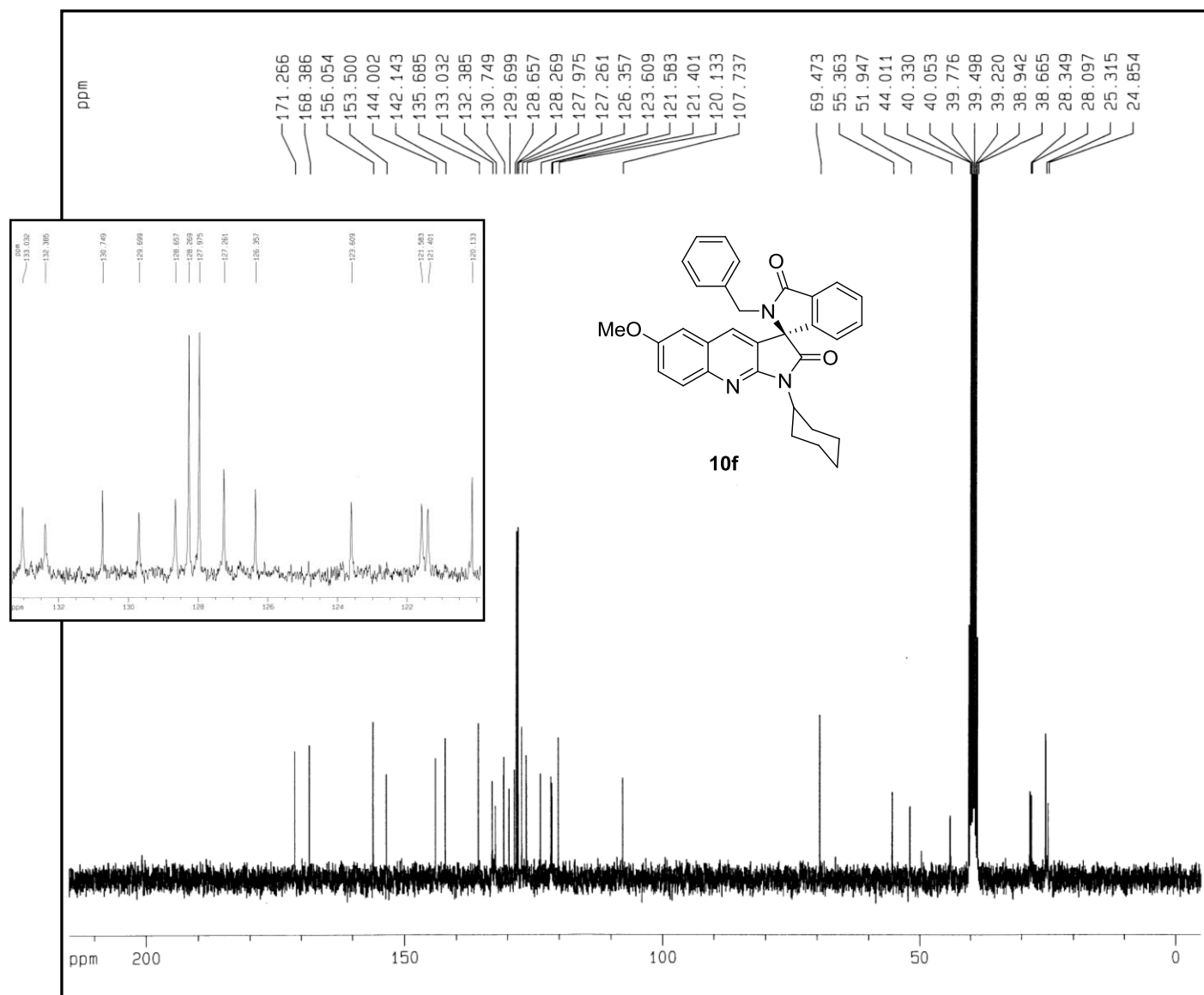


Figure 82. ¹³C NMR (75 MHz, DMSO-*d*₆) (**10f**).

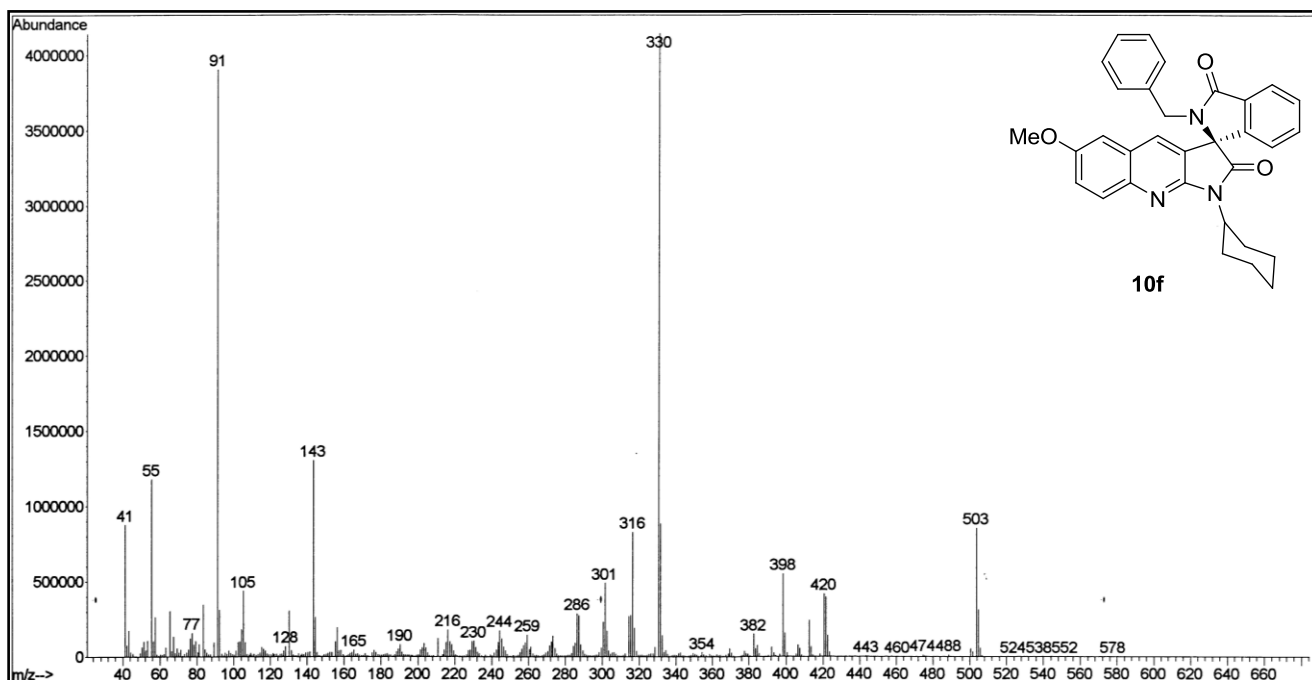


Figure 83. Mass (10f).

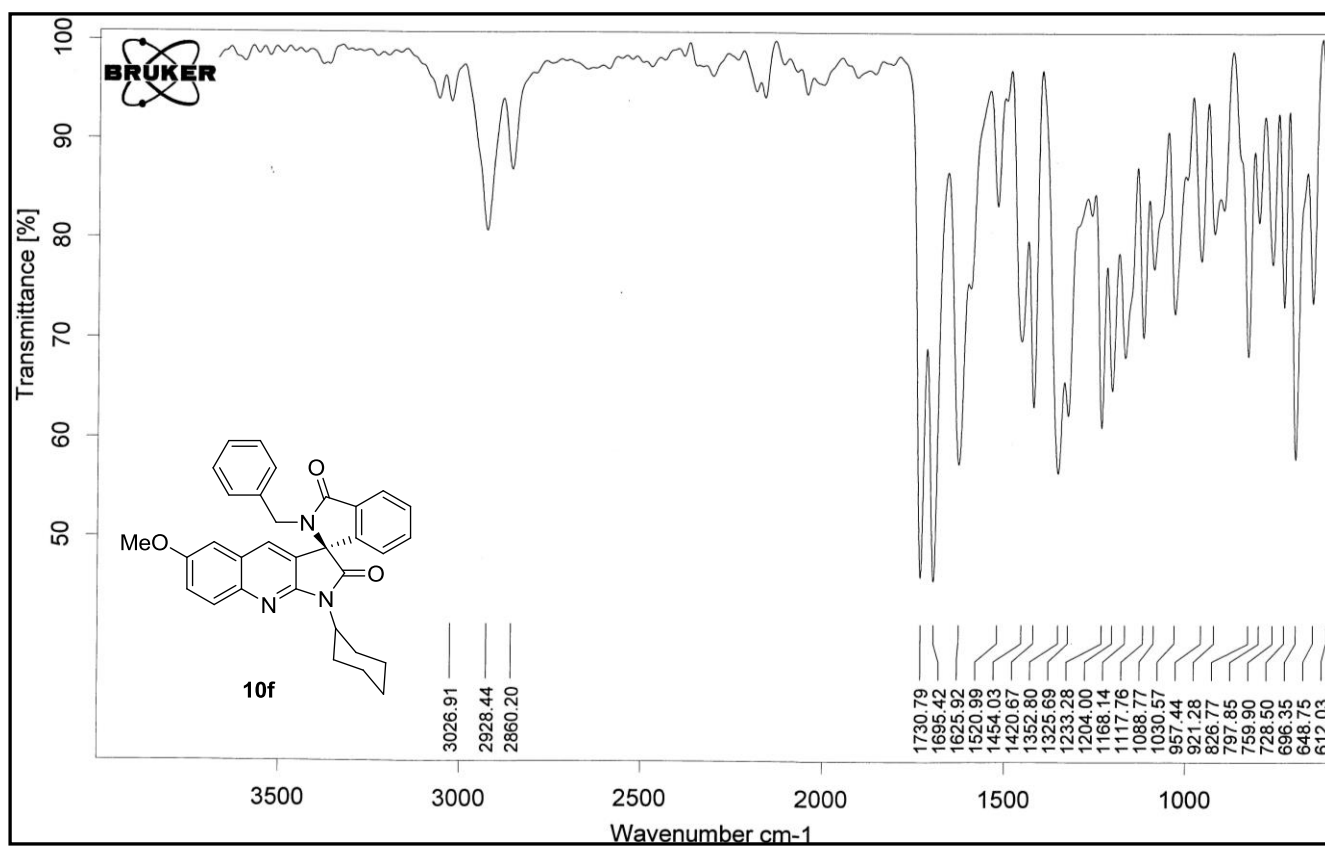


Figure 84. IR (10f).

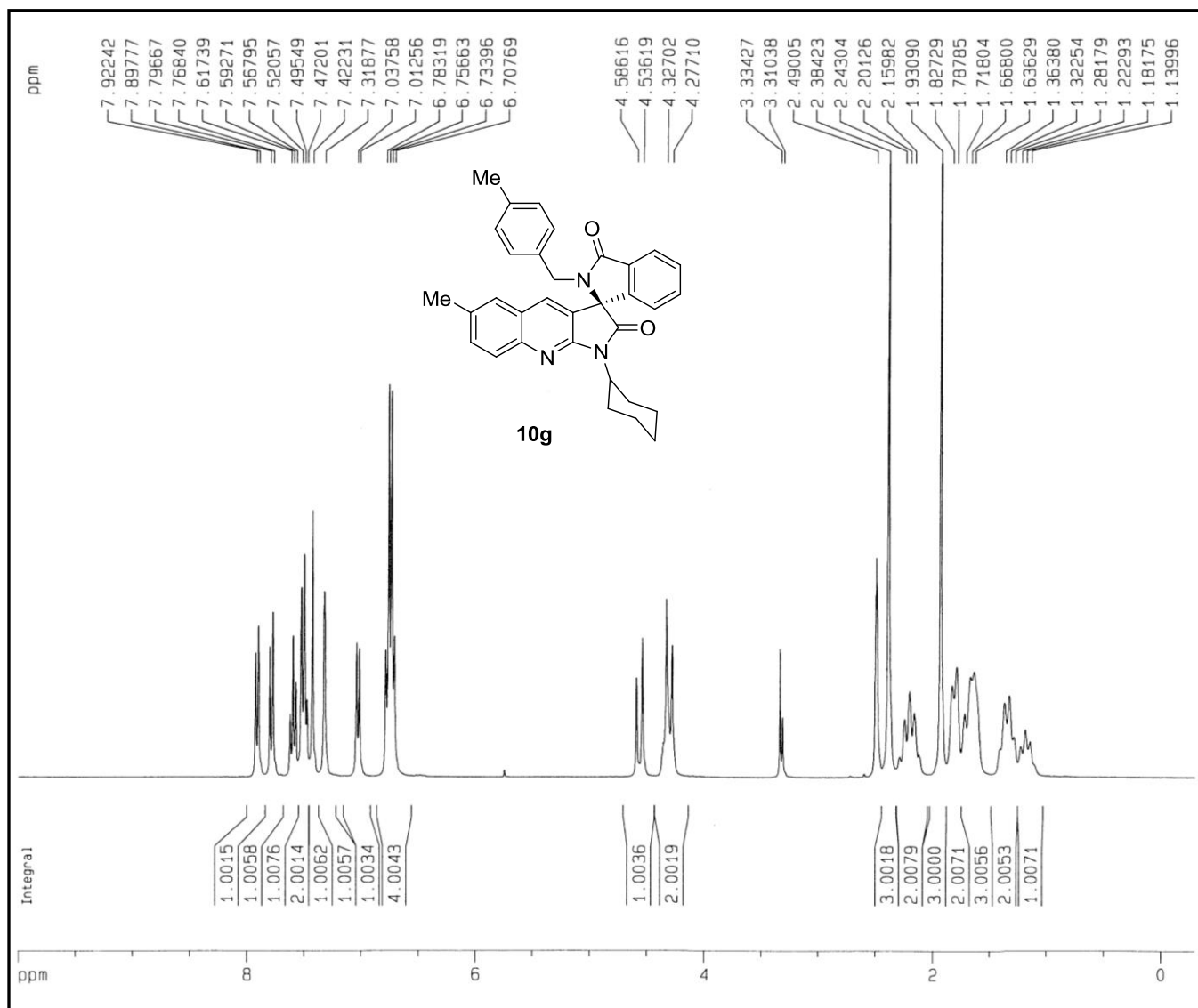
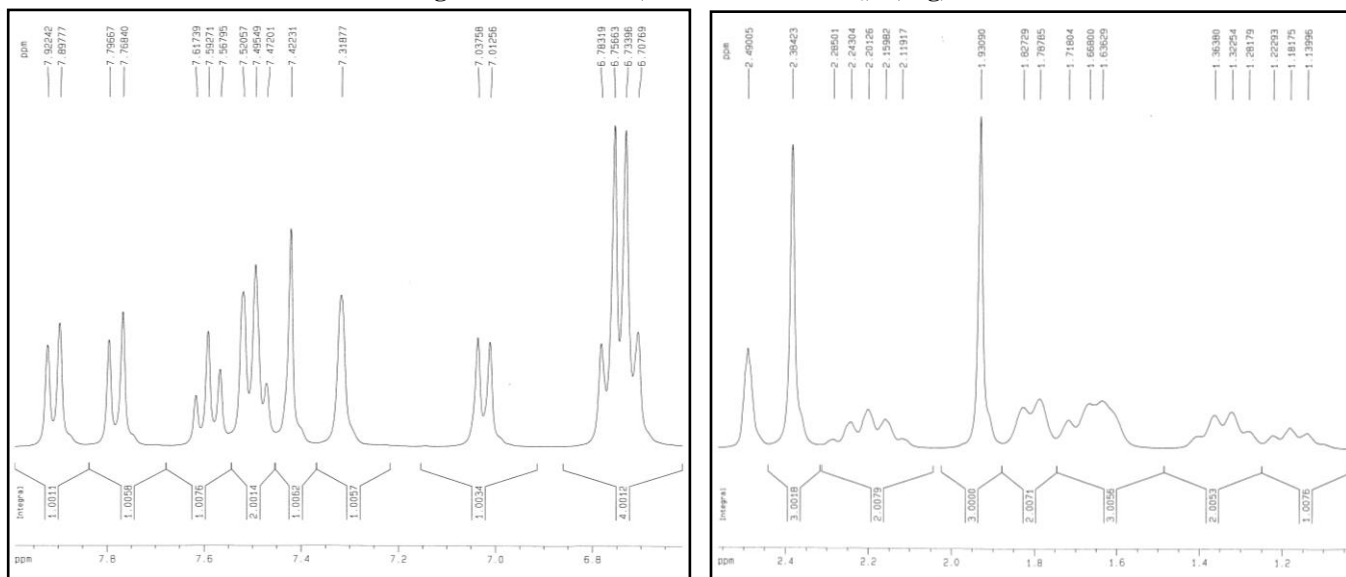


Figure 85. ¹H NMR (300 MHz, DMSO-*d*₆) (**10g**).



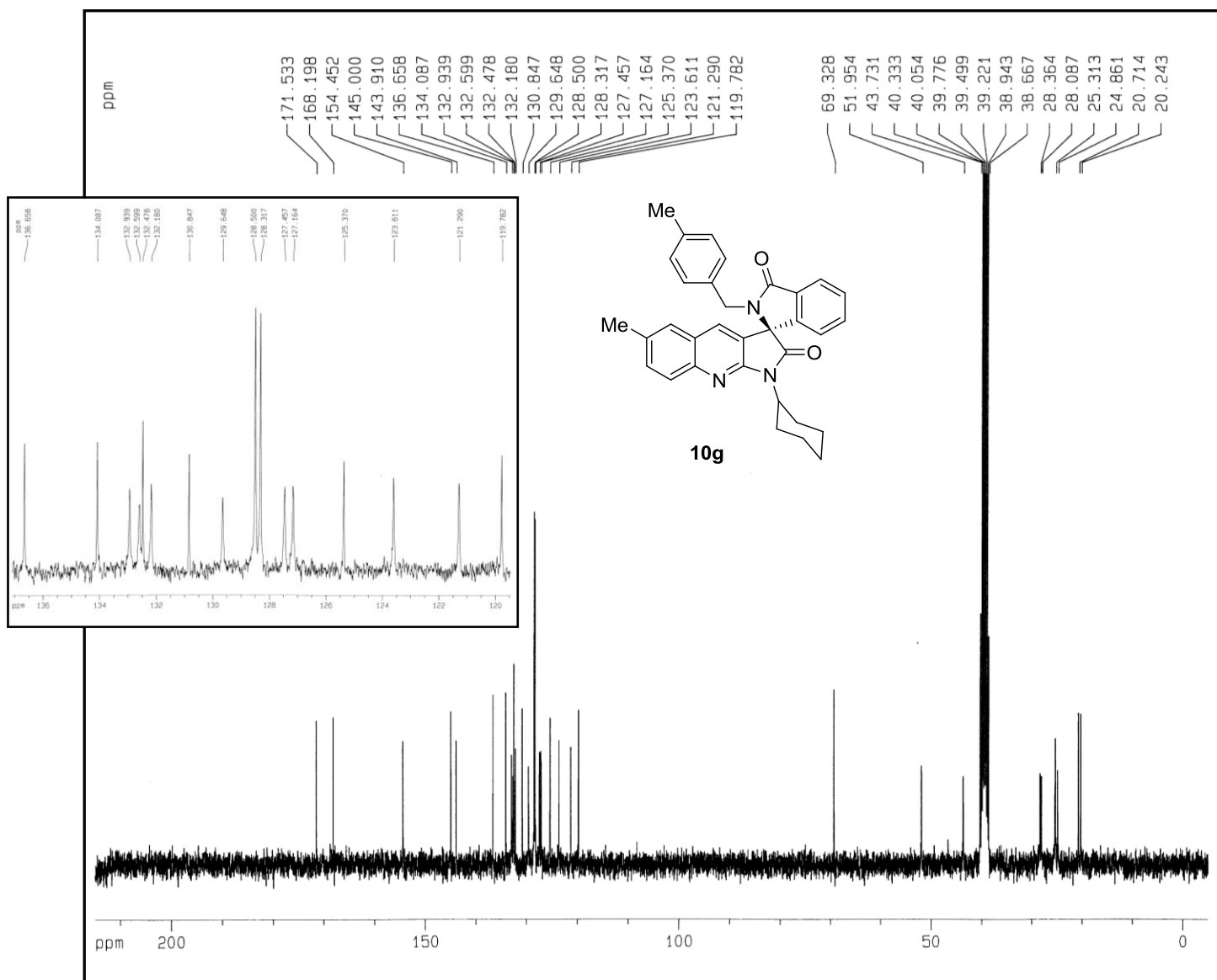


Figure 86. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10g**).

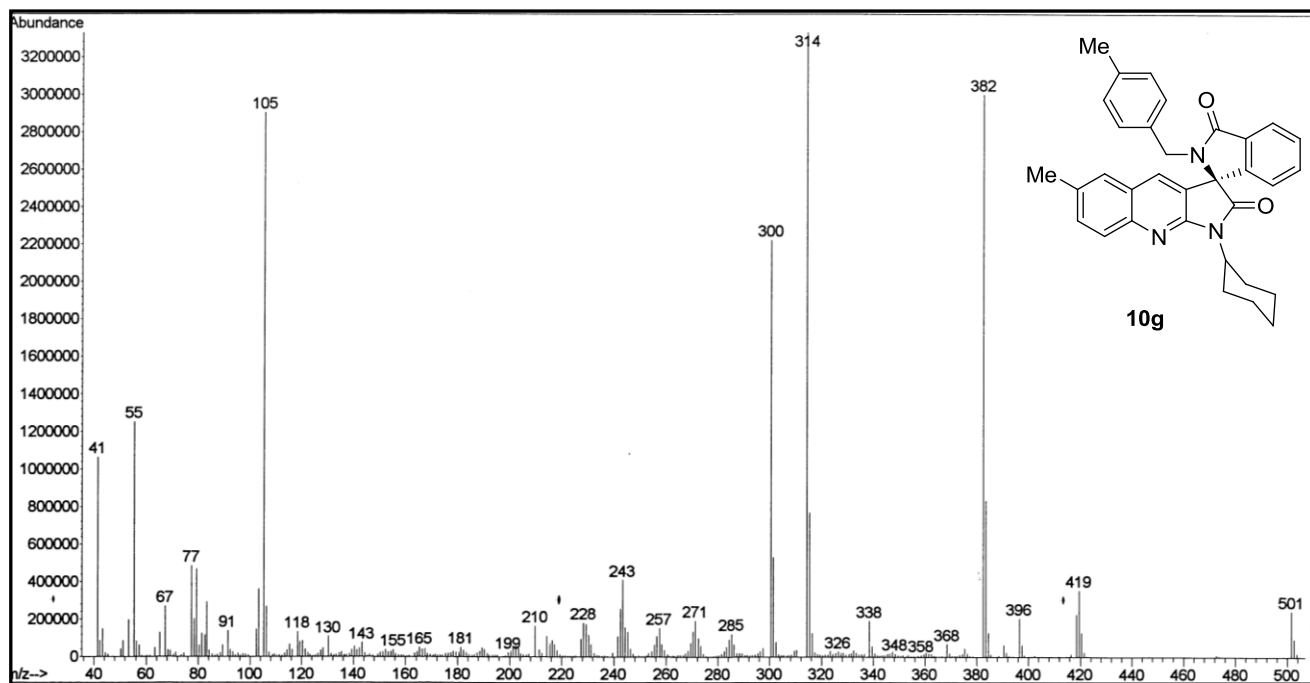


Figure 87. Mass (10g).

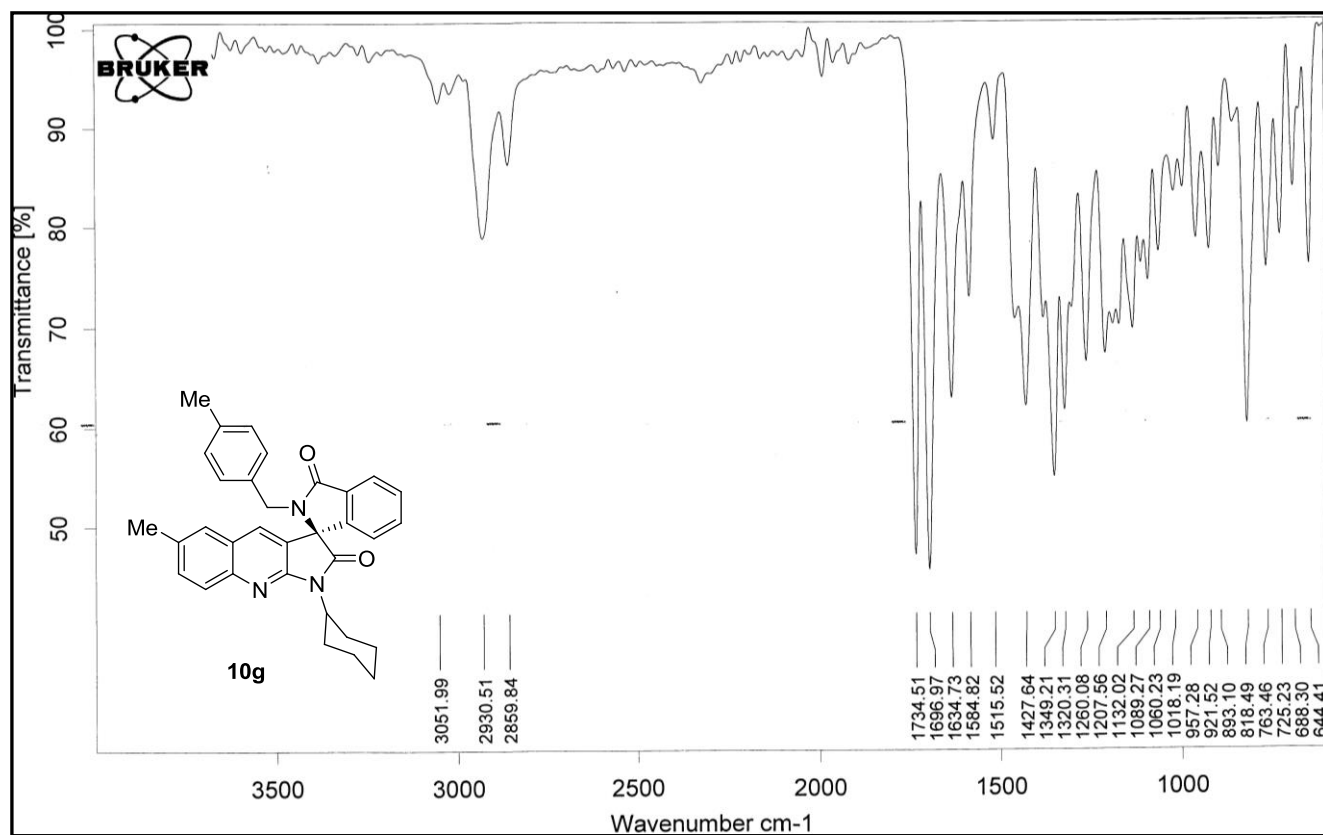


Figure 88. IR (10g).

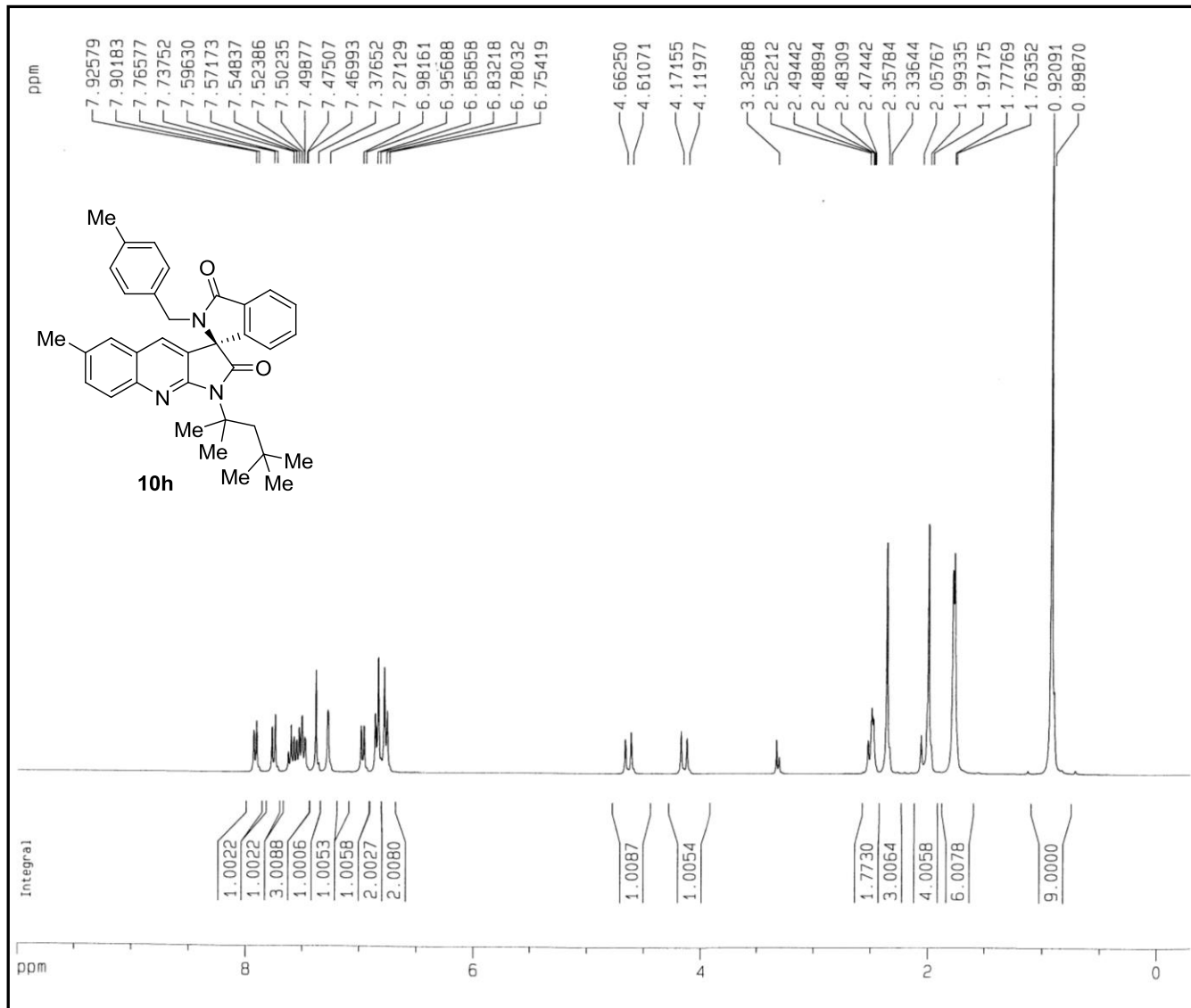
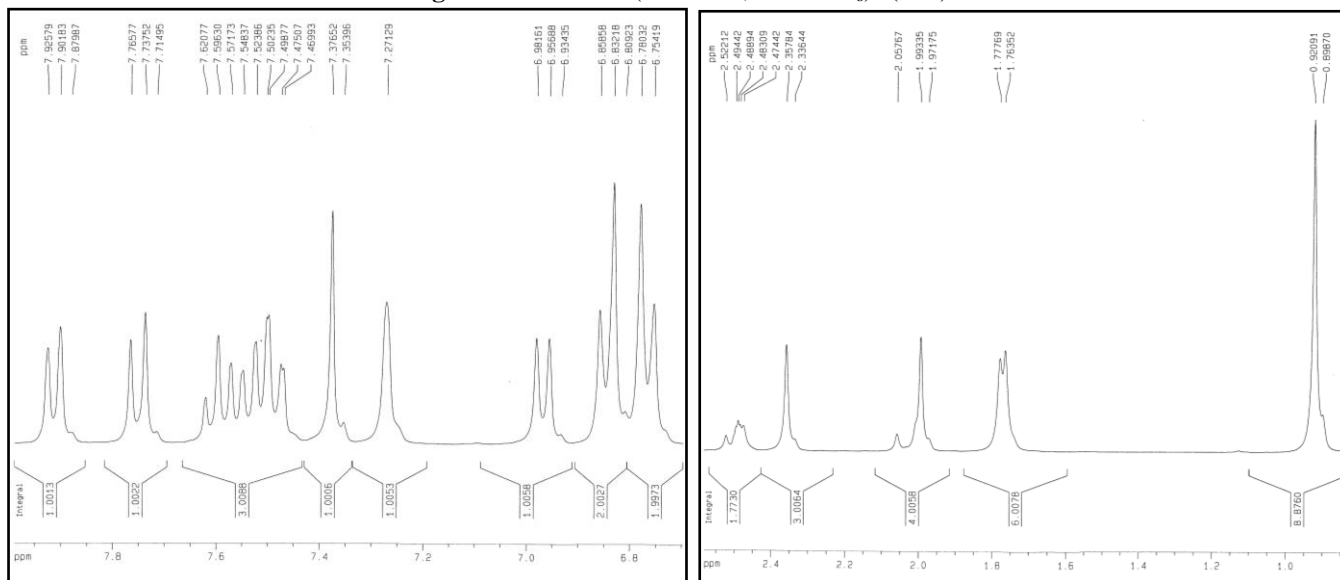


Figure 89. ¹H NMR (300 MHz, DMSO-*d*₆) (**10h**).



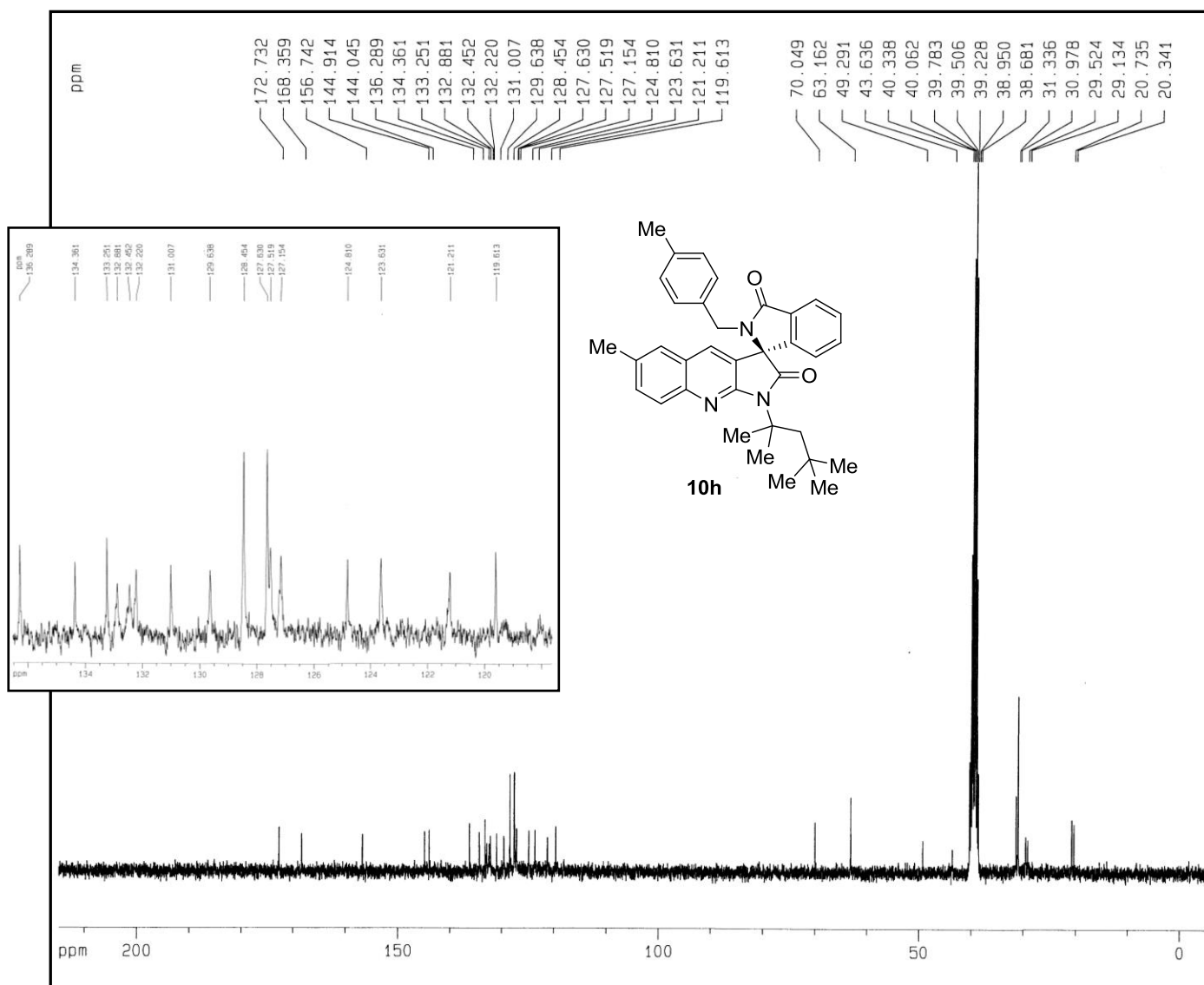


Figure 90. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10h**).

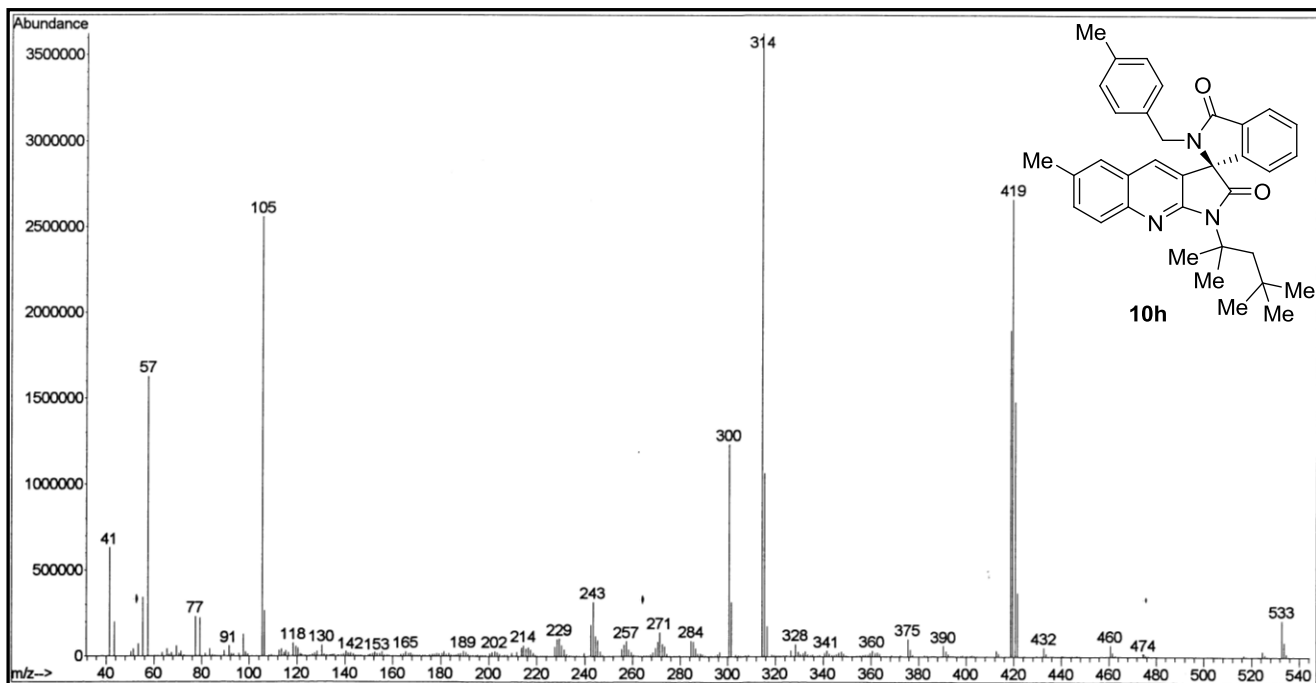


Figure 91. Mass (10h).

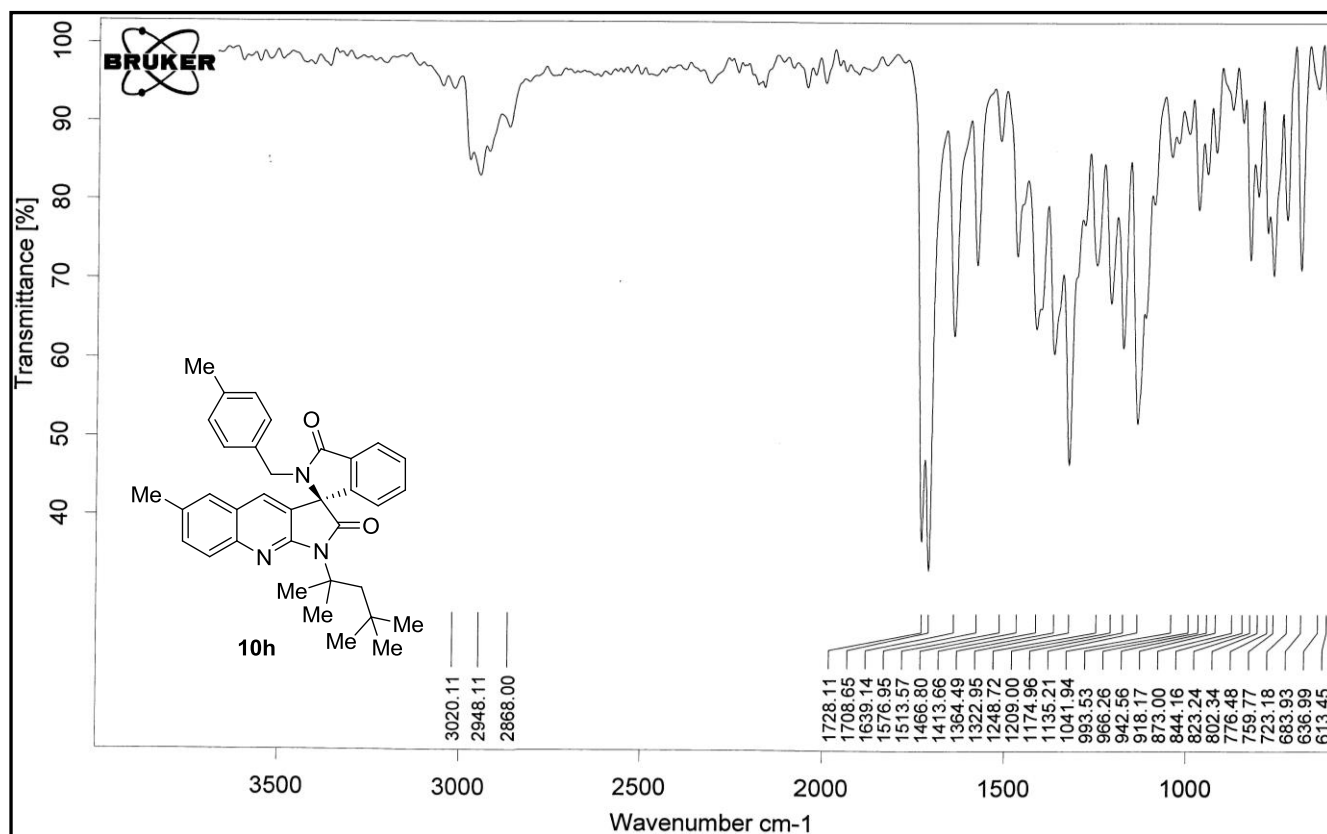


Figure 92. IR (10h).

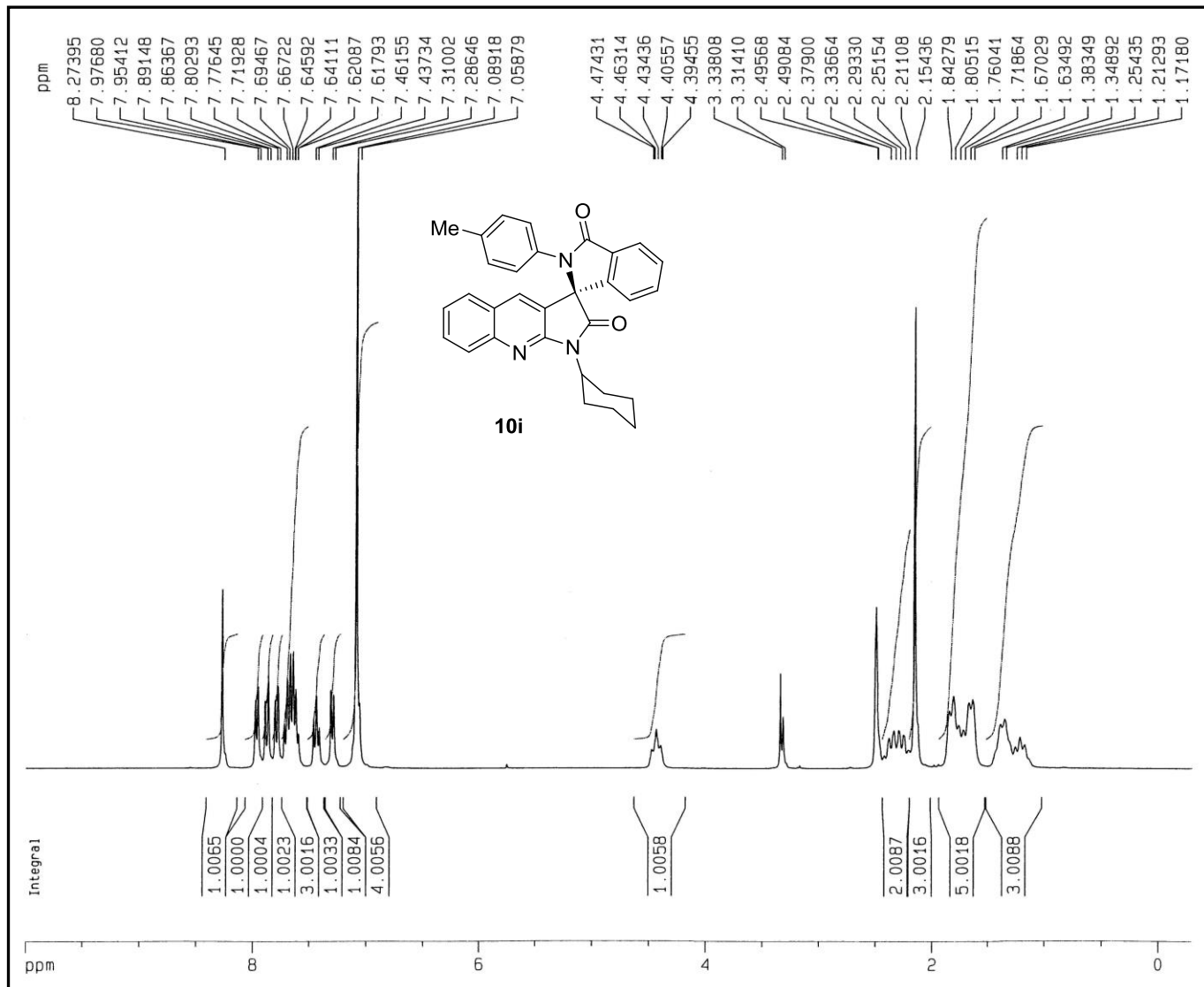
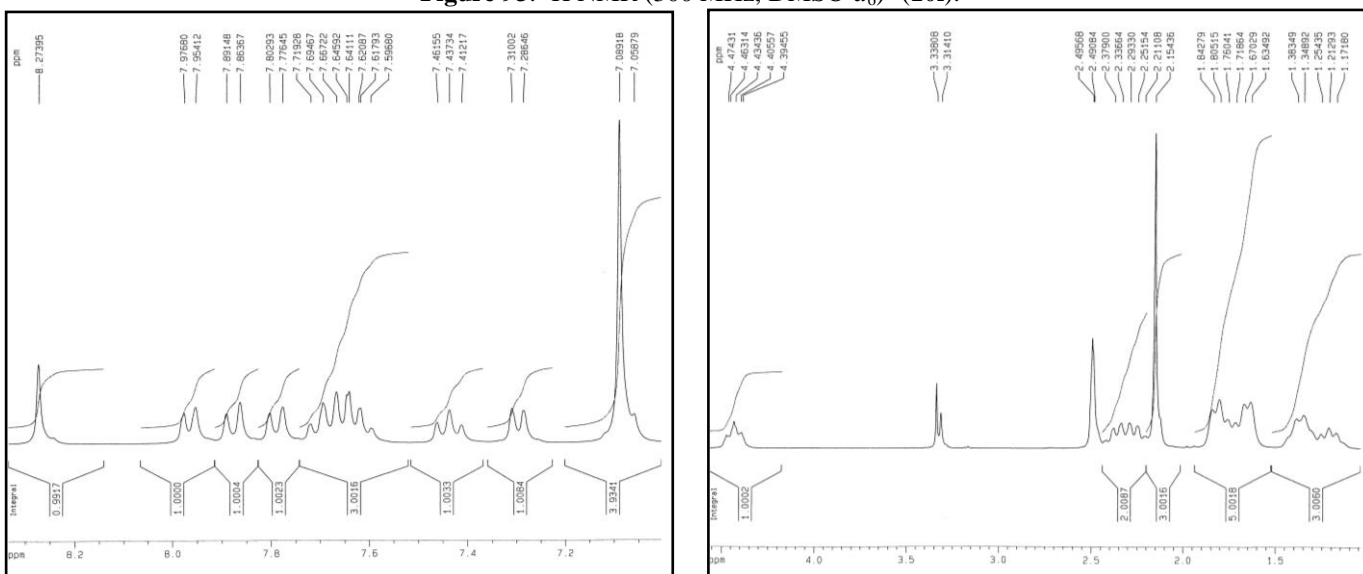
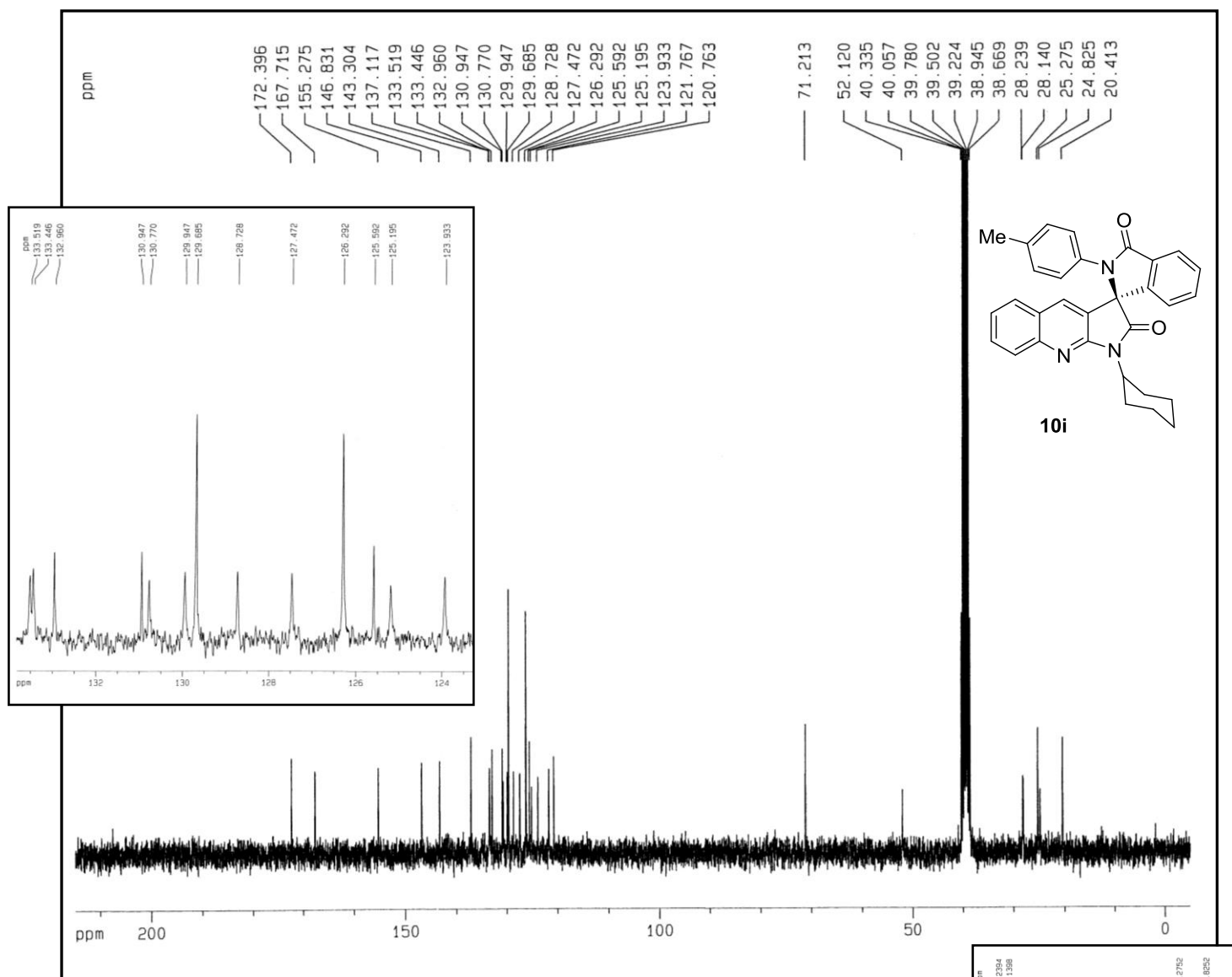


Figure 93. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) (**10i**).





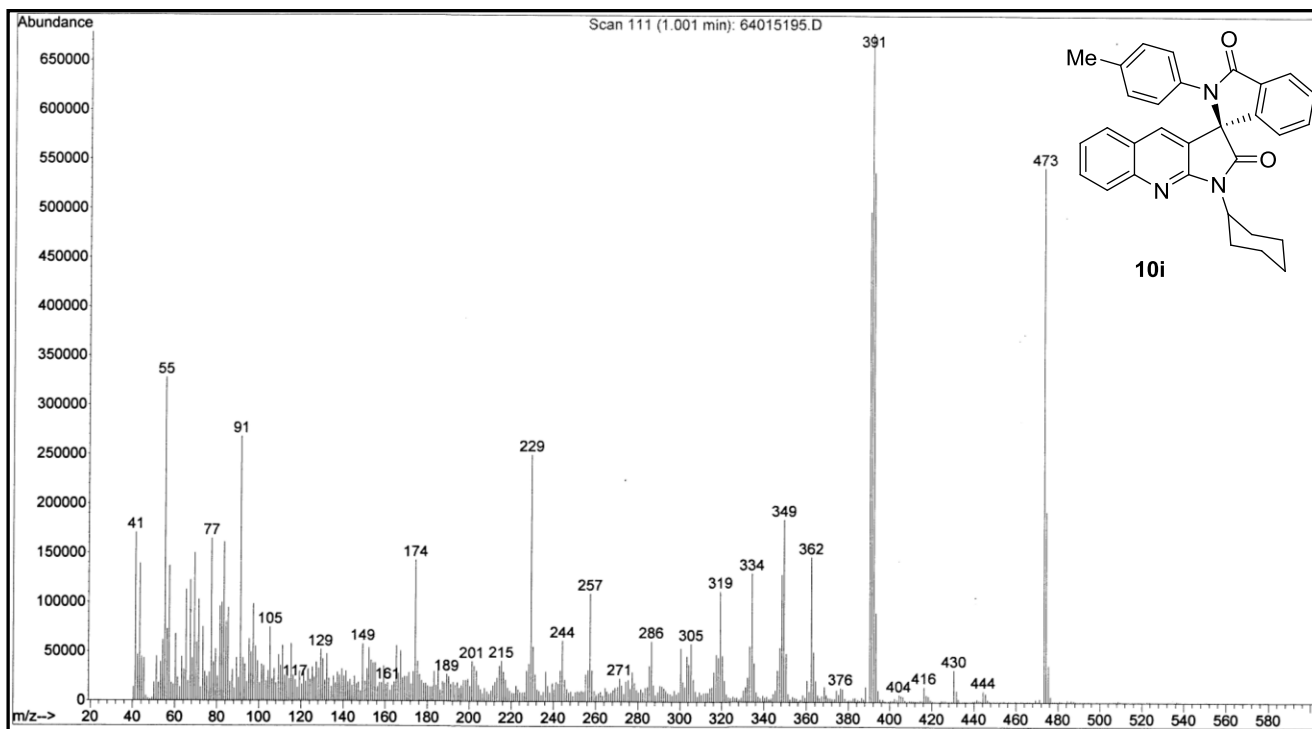


Figure 95. Mass (10i).

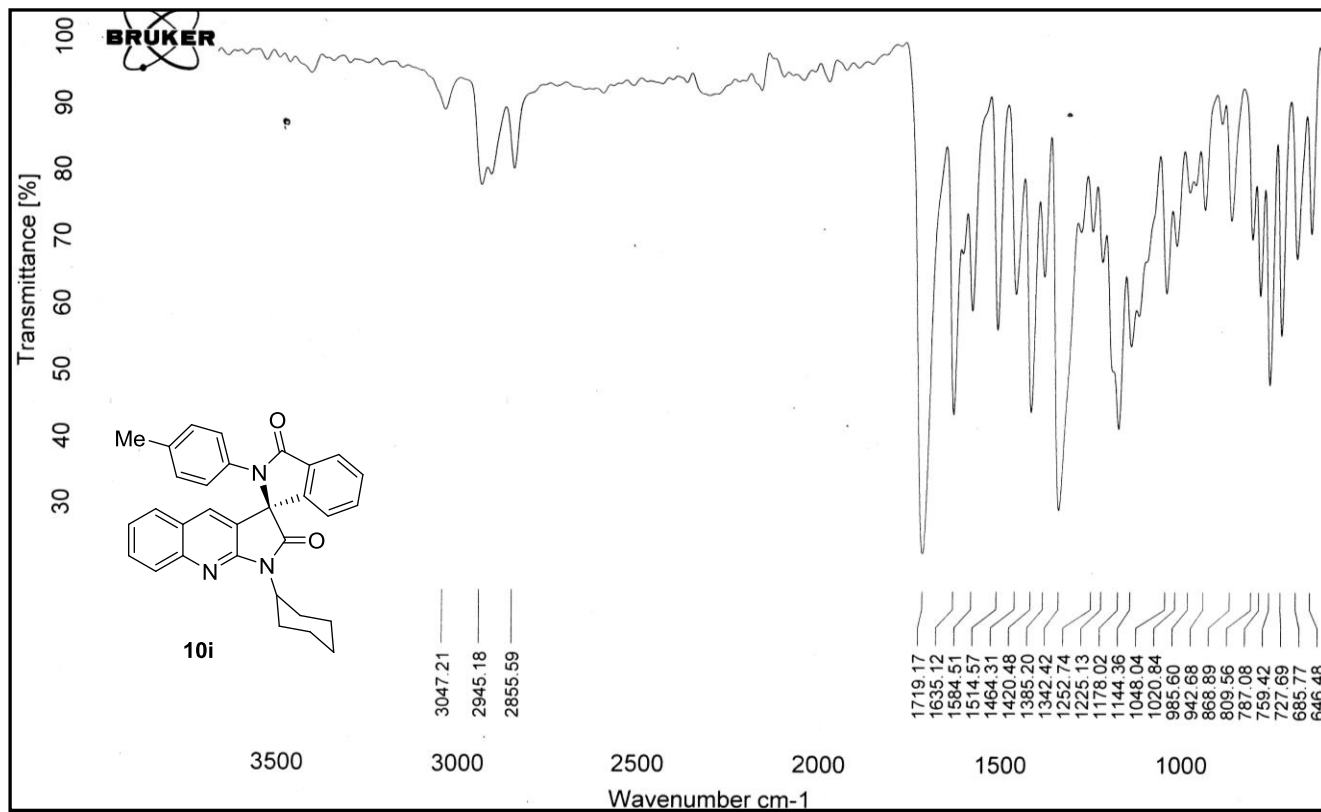


Figure 96. IR (10i).

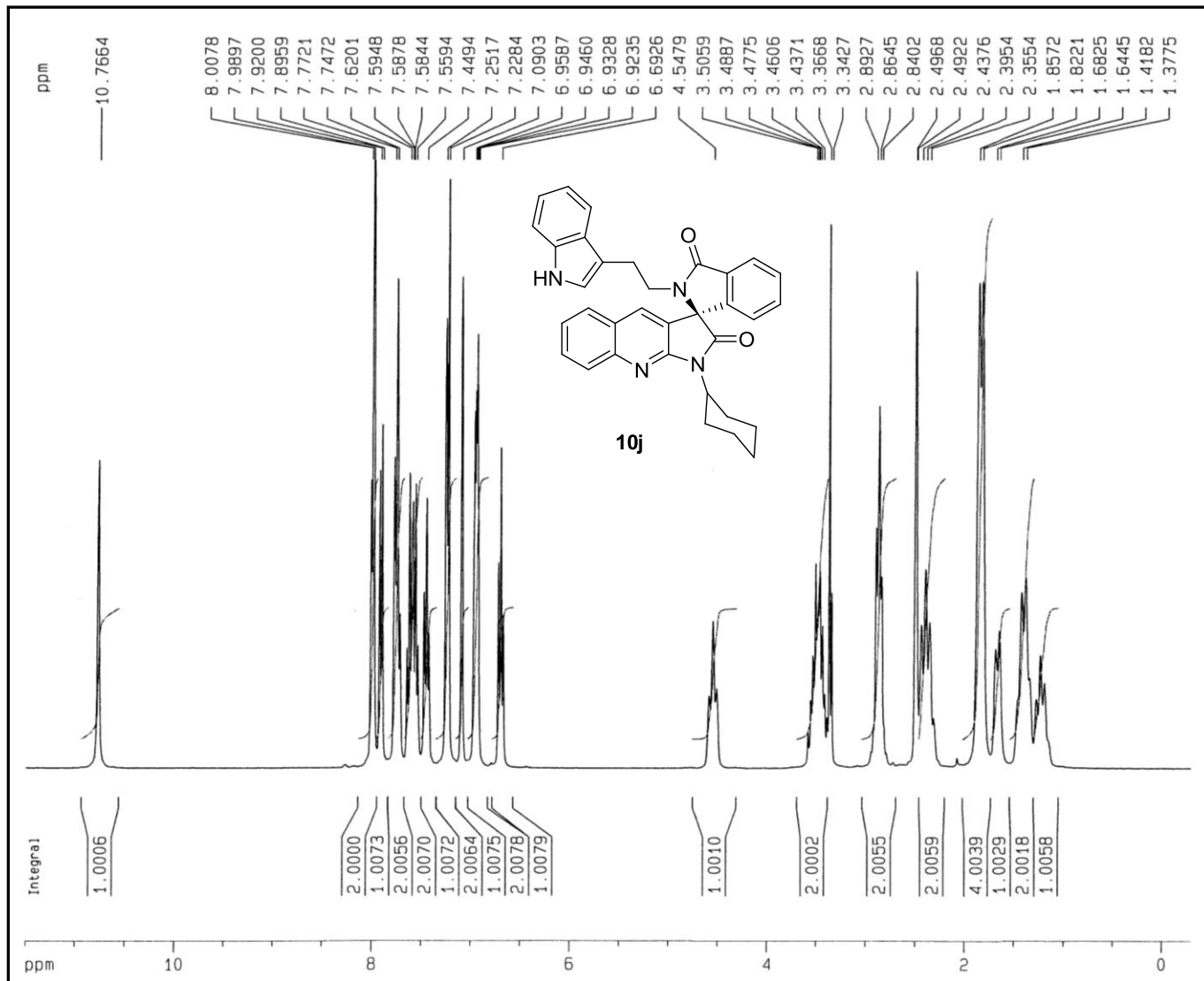
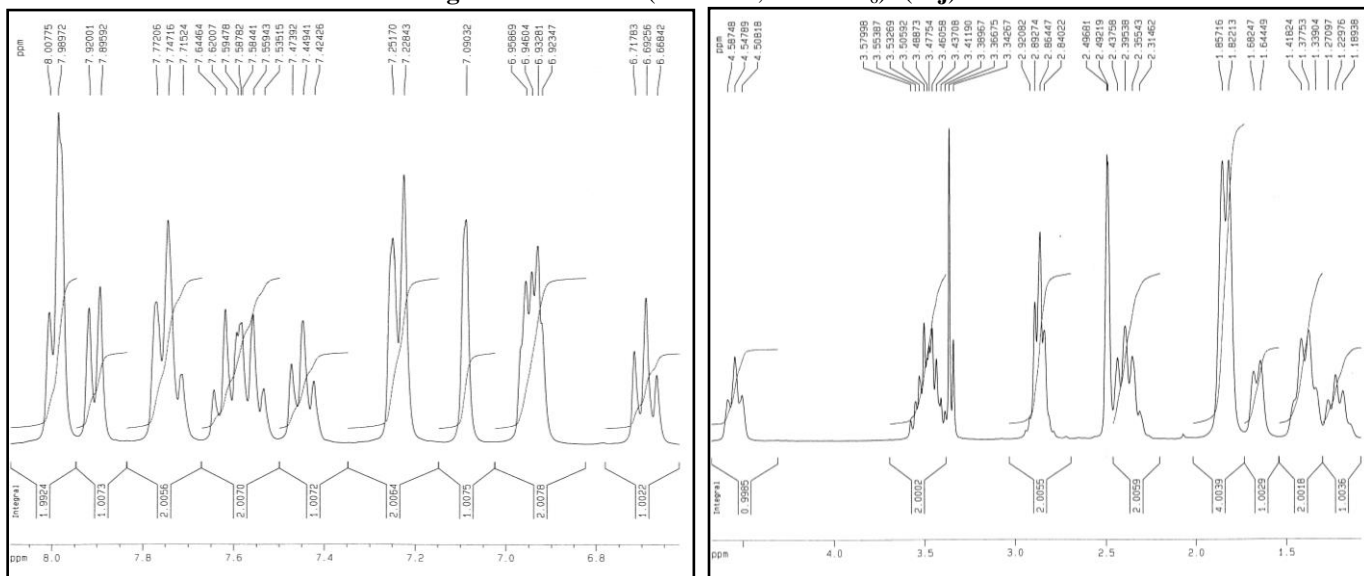


Figure 97. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) (**10j**).



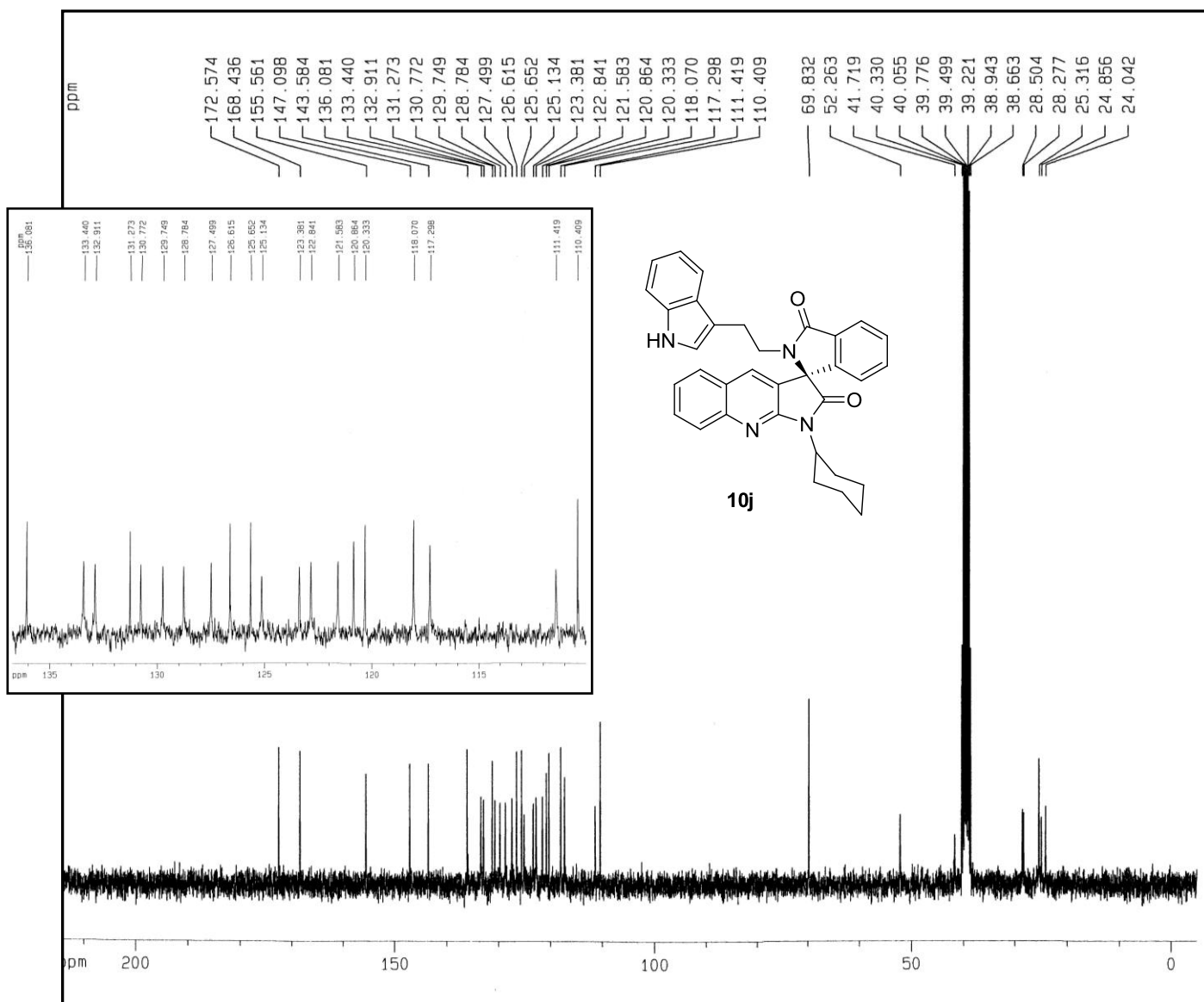


Figure 98. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10j**).

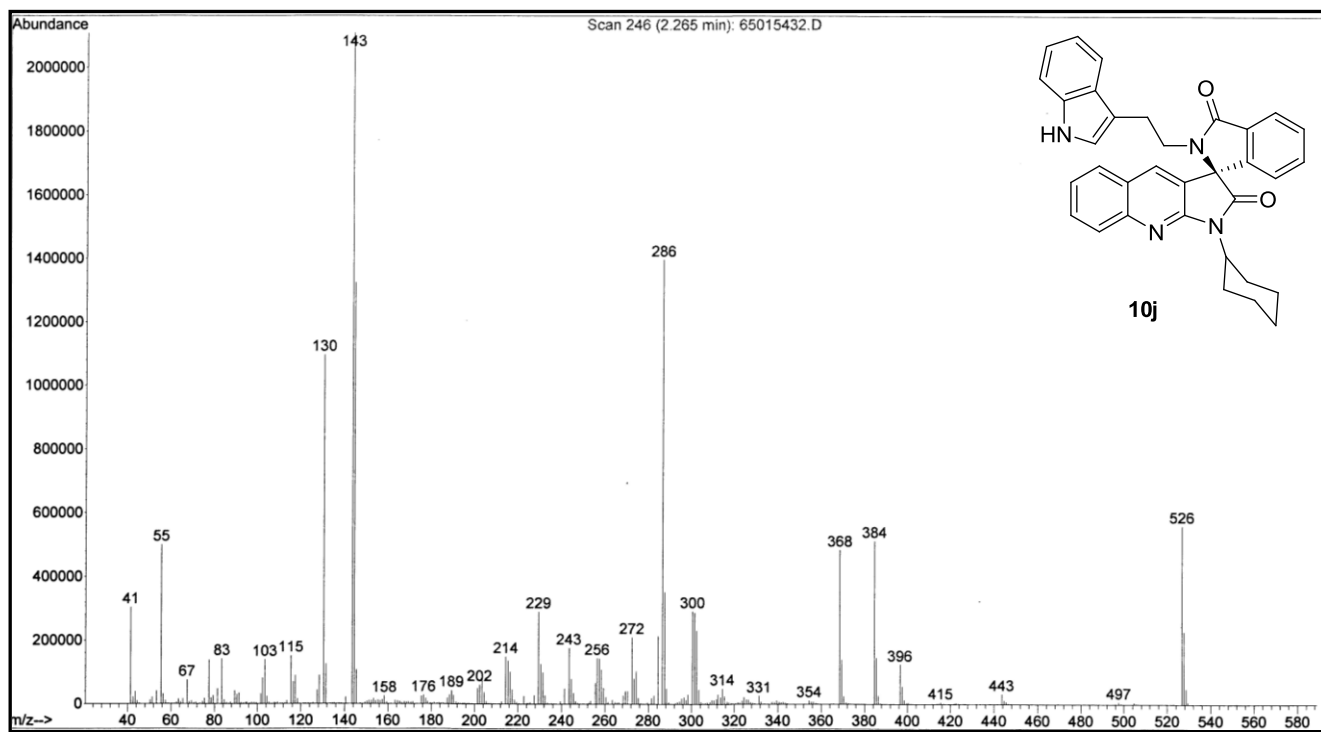


Figure 99. Mass (10j).

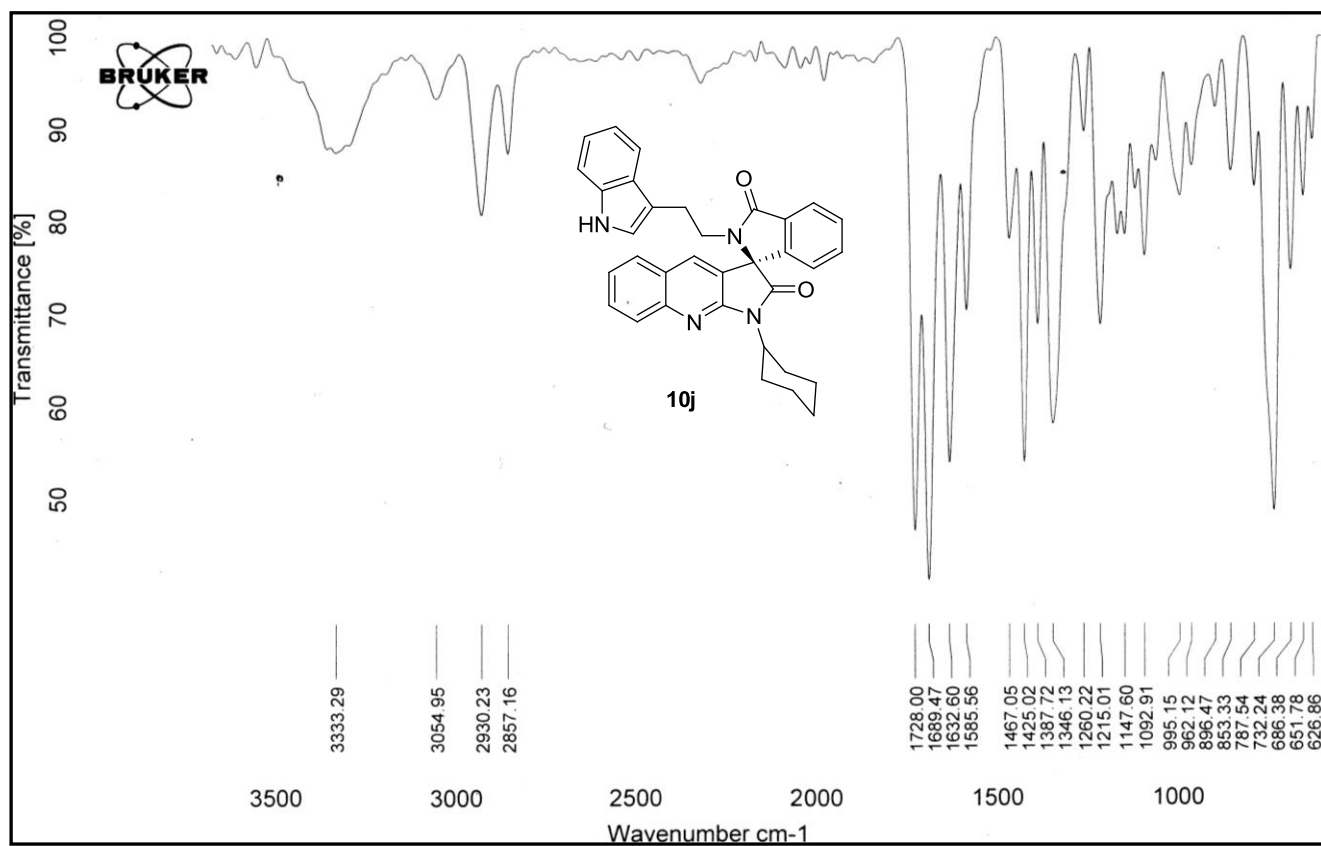


Figure 100. IR (10j).

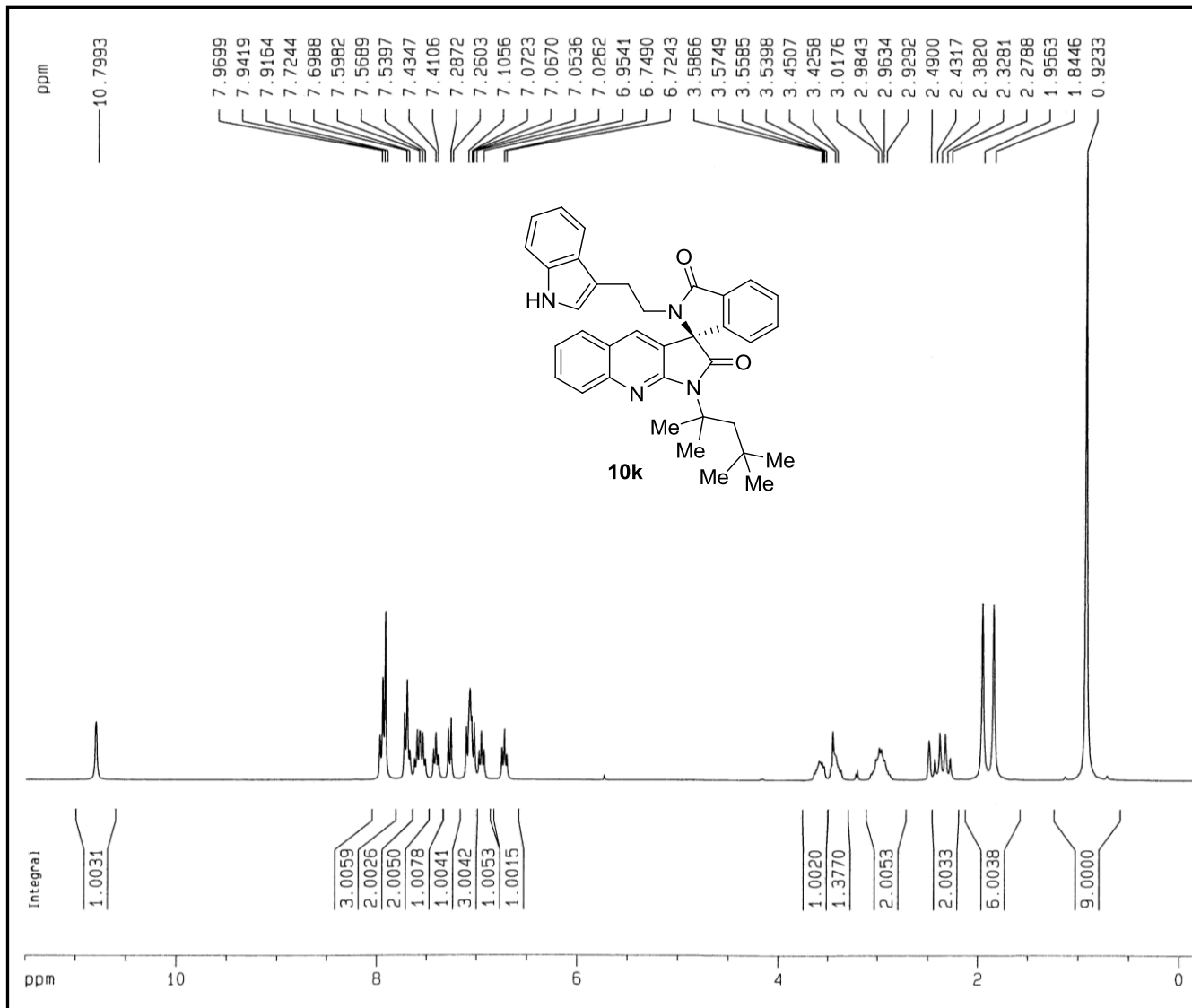
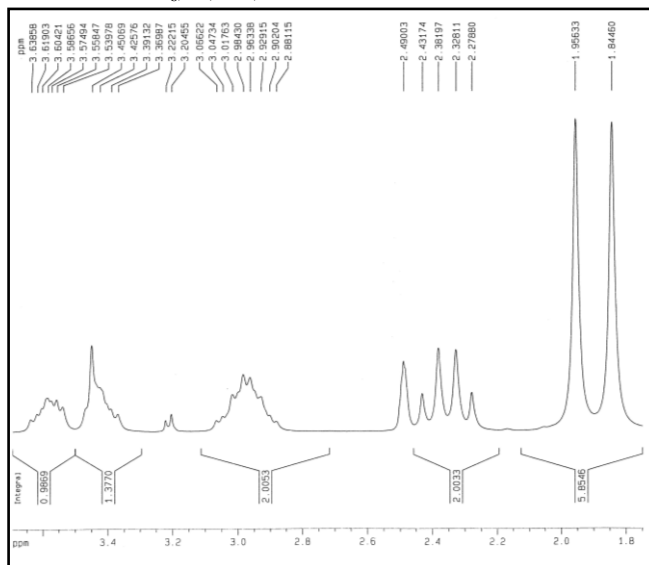
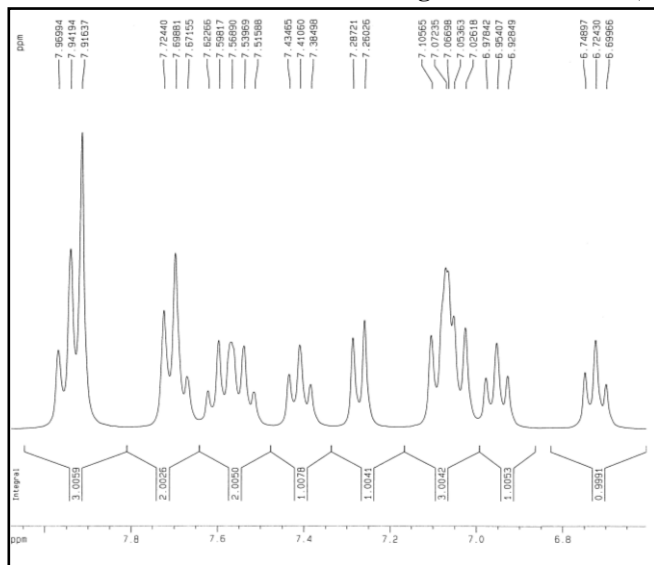


Figure 101. ¹H NMR (300 MHz, DMSO-*d*₆) (**10k**).



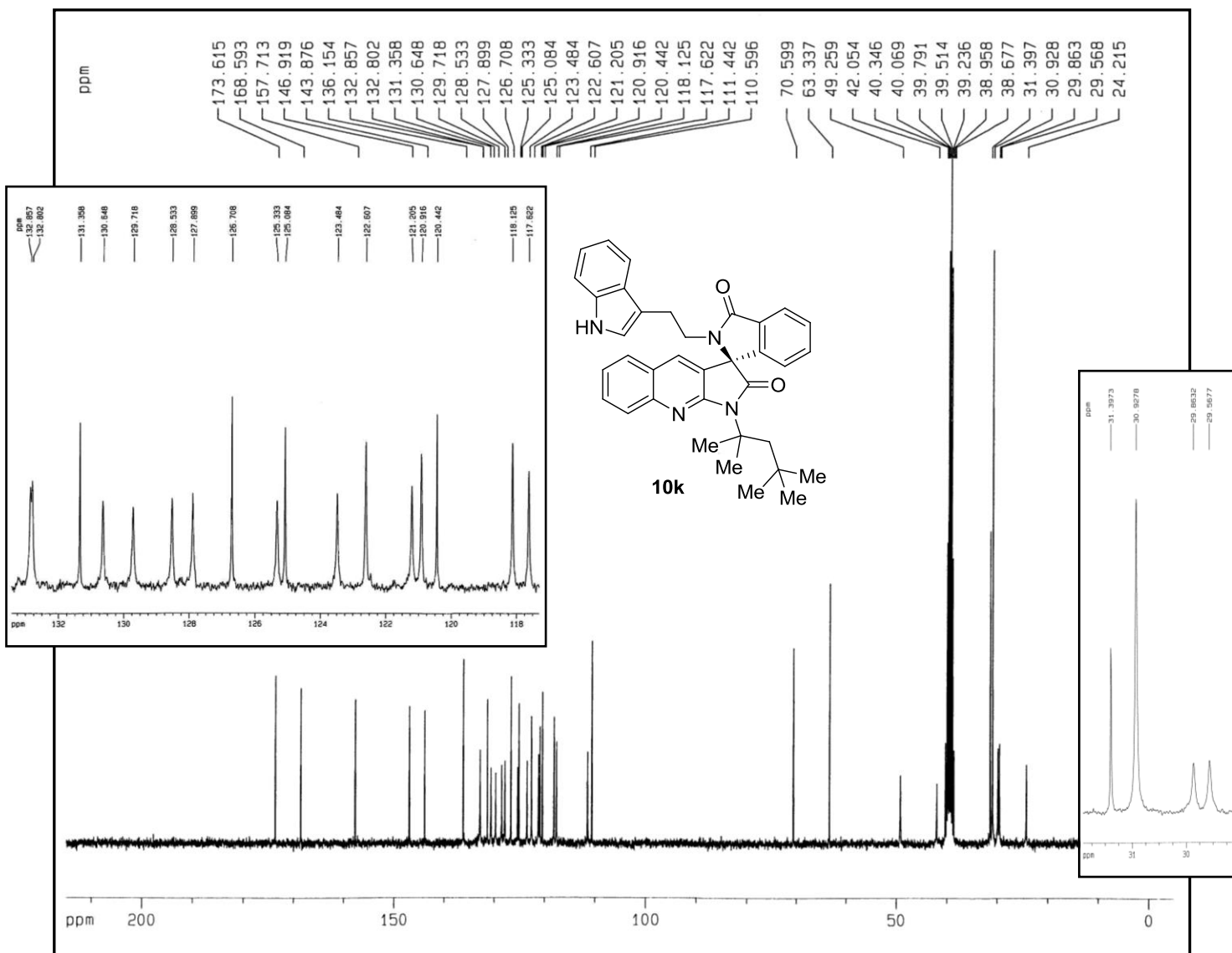


Figure 102. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10k**).

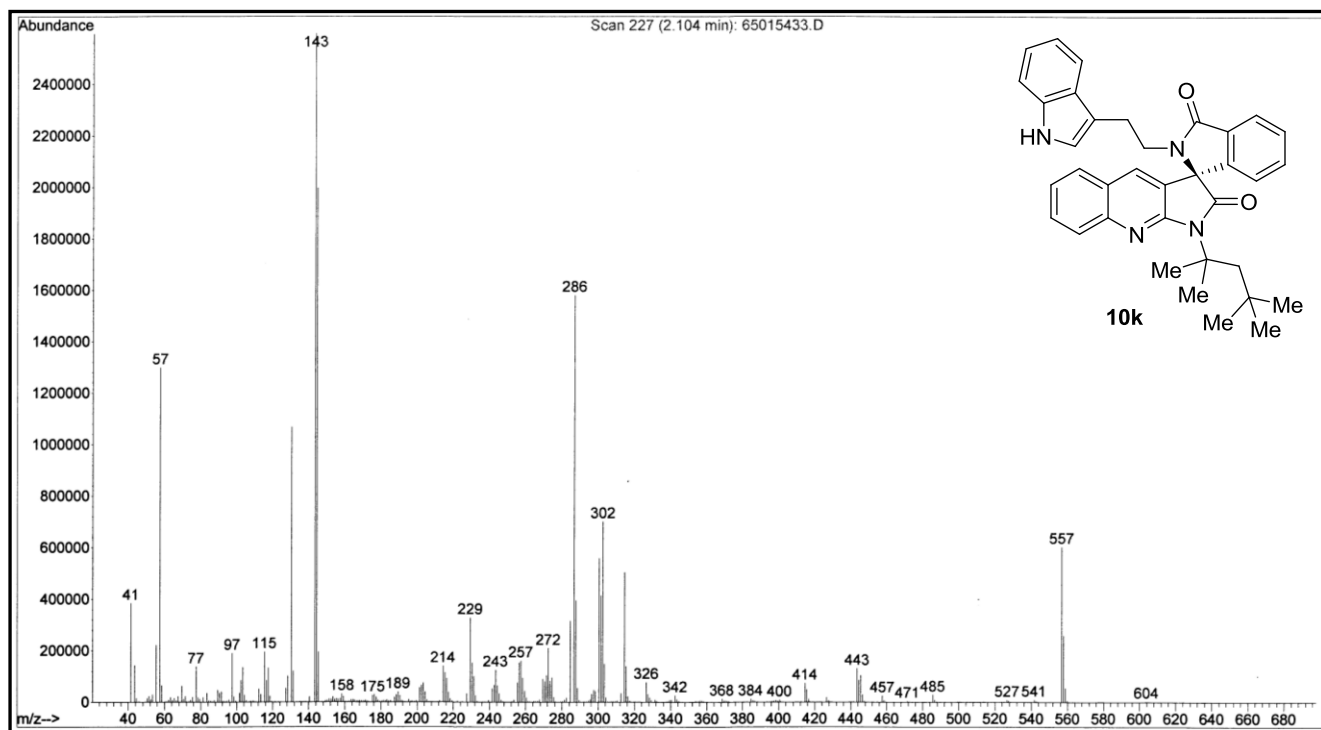


Figure 103. Mass (10k).

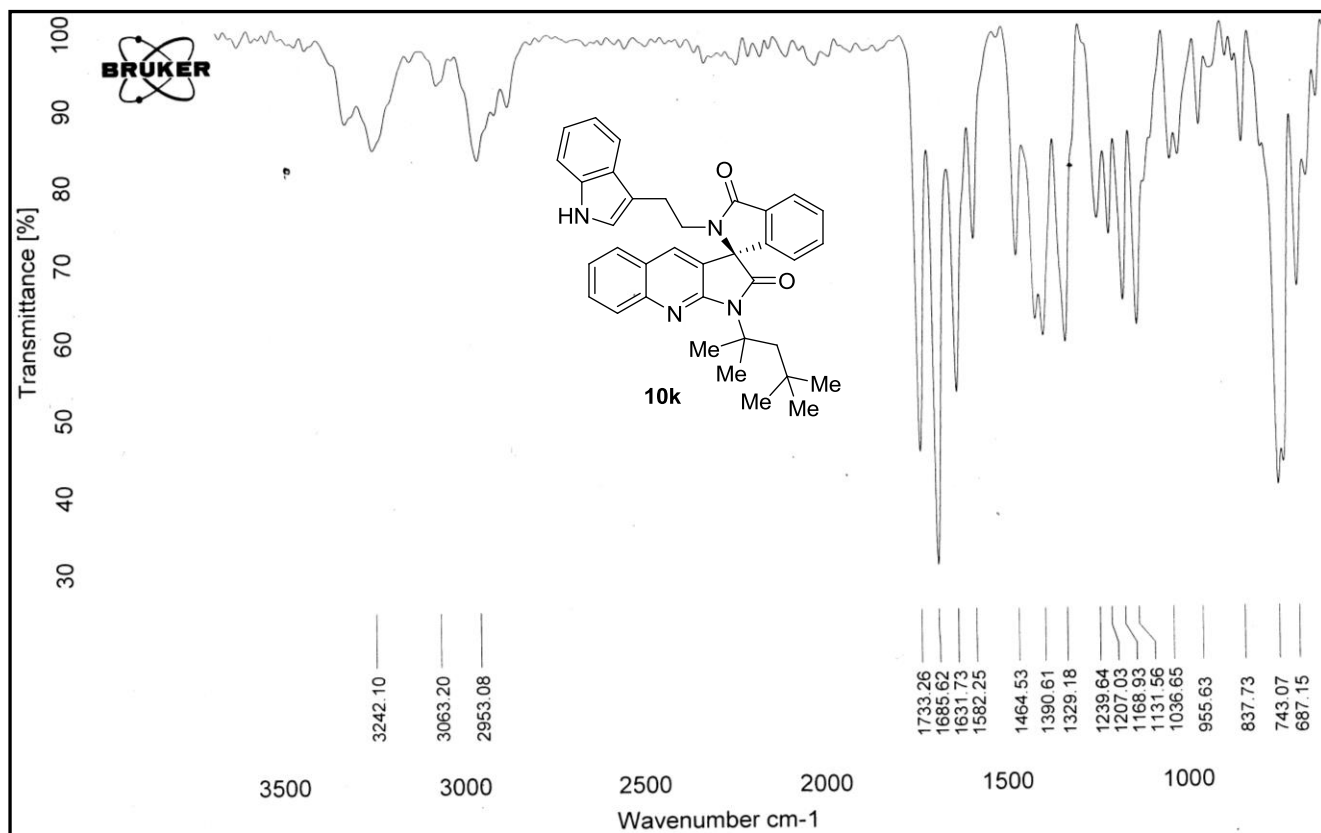


Figure 104. IR (10k).

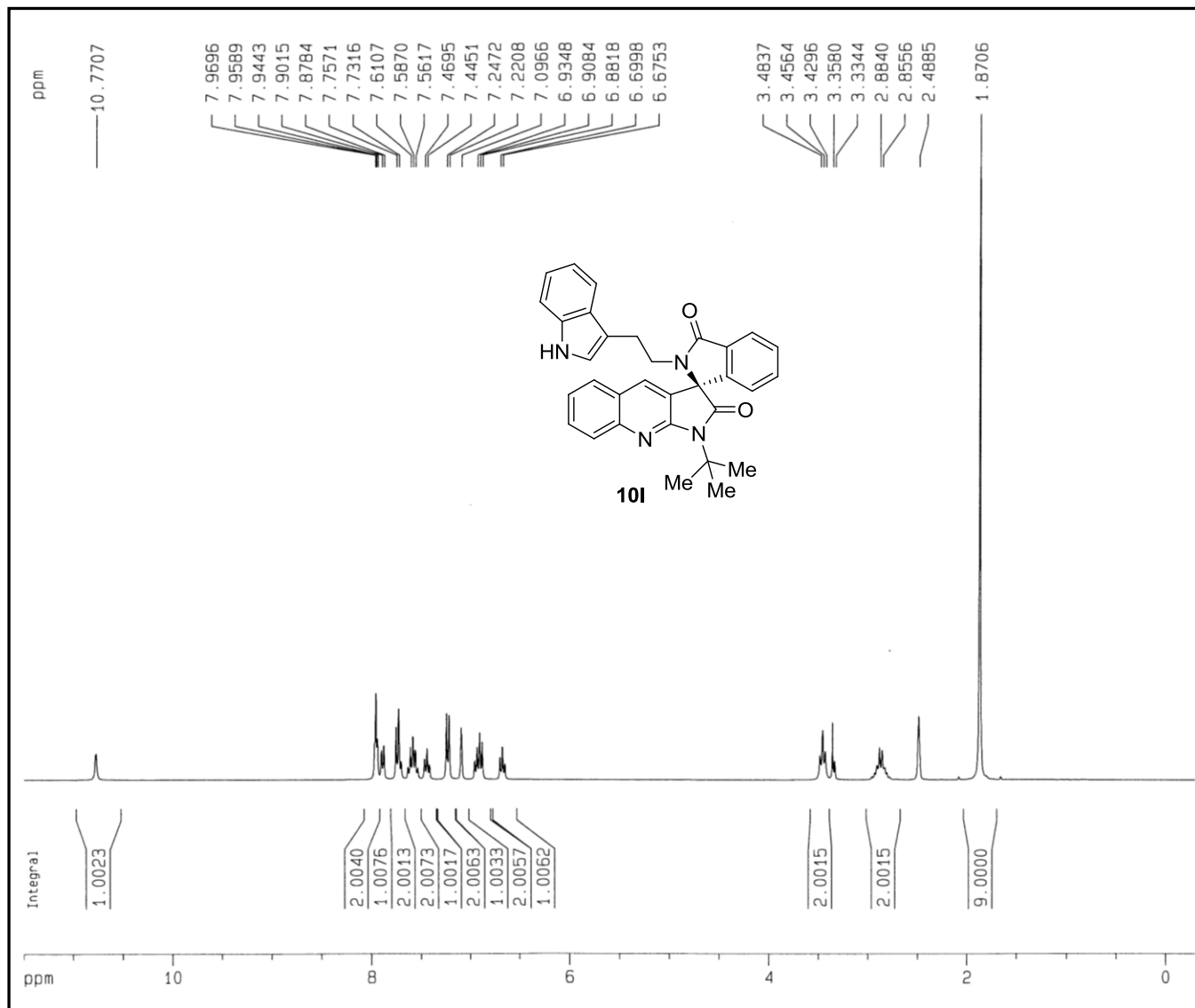
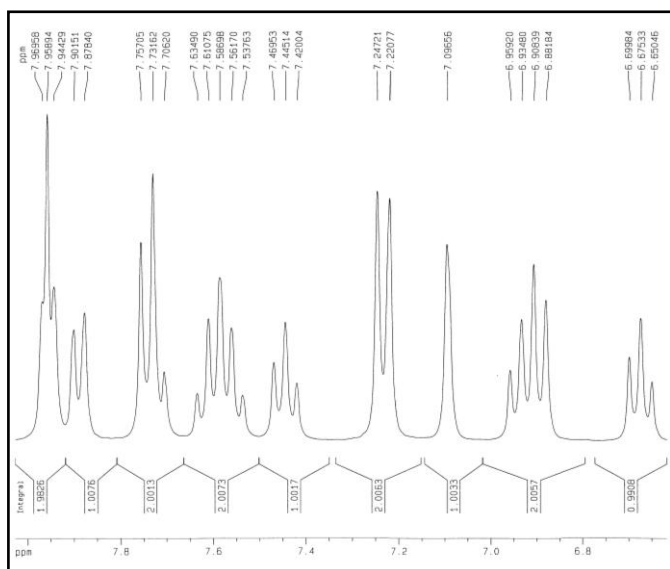


Figure 105. ¹H NMR (300 MHz, DMSO-*d*₆) (**101**).



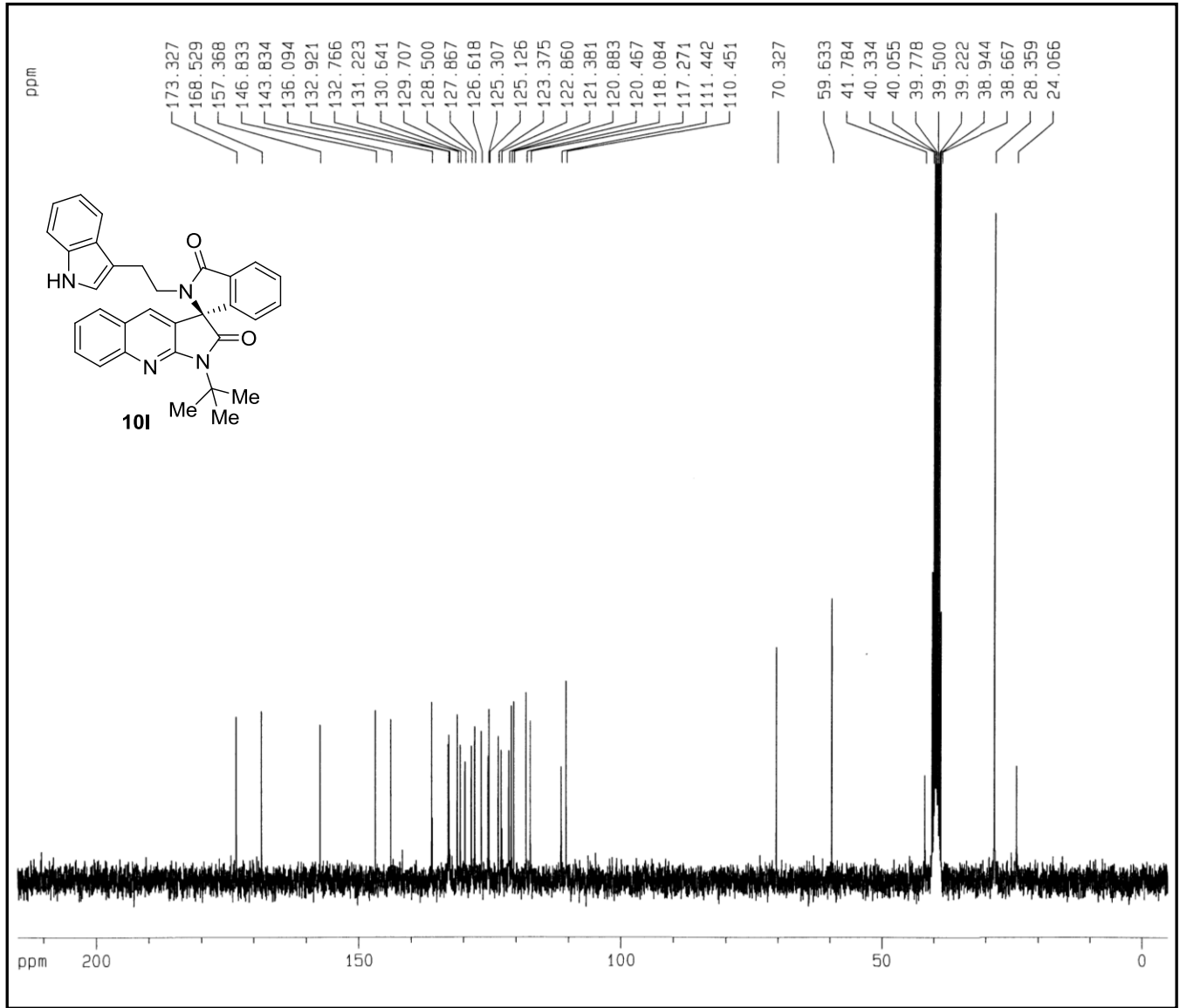


Figure 106. ^{13}C NMR (300 MHz, $\text{DMSO-}d_6$) (**10l**).

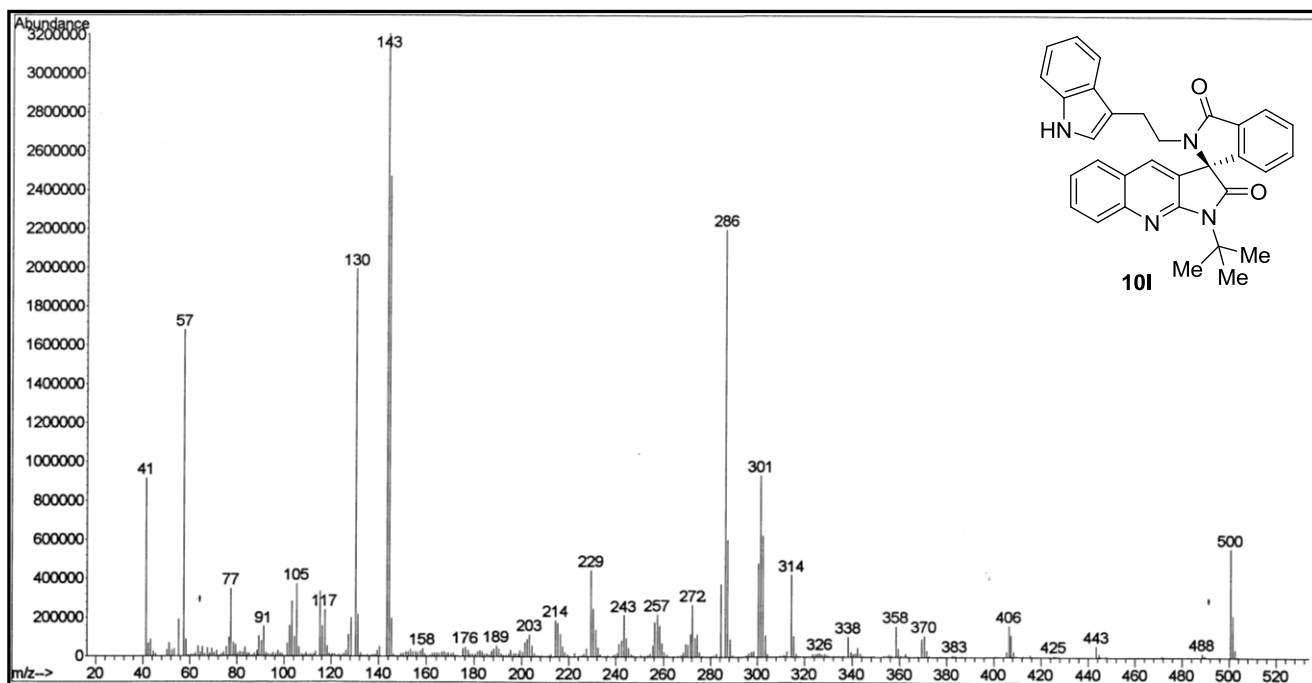


Figure 107. Mass (10I).

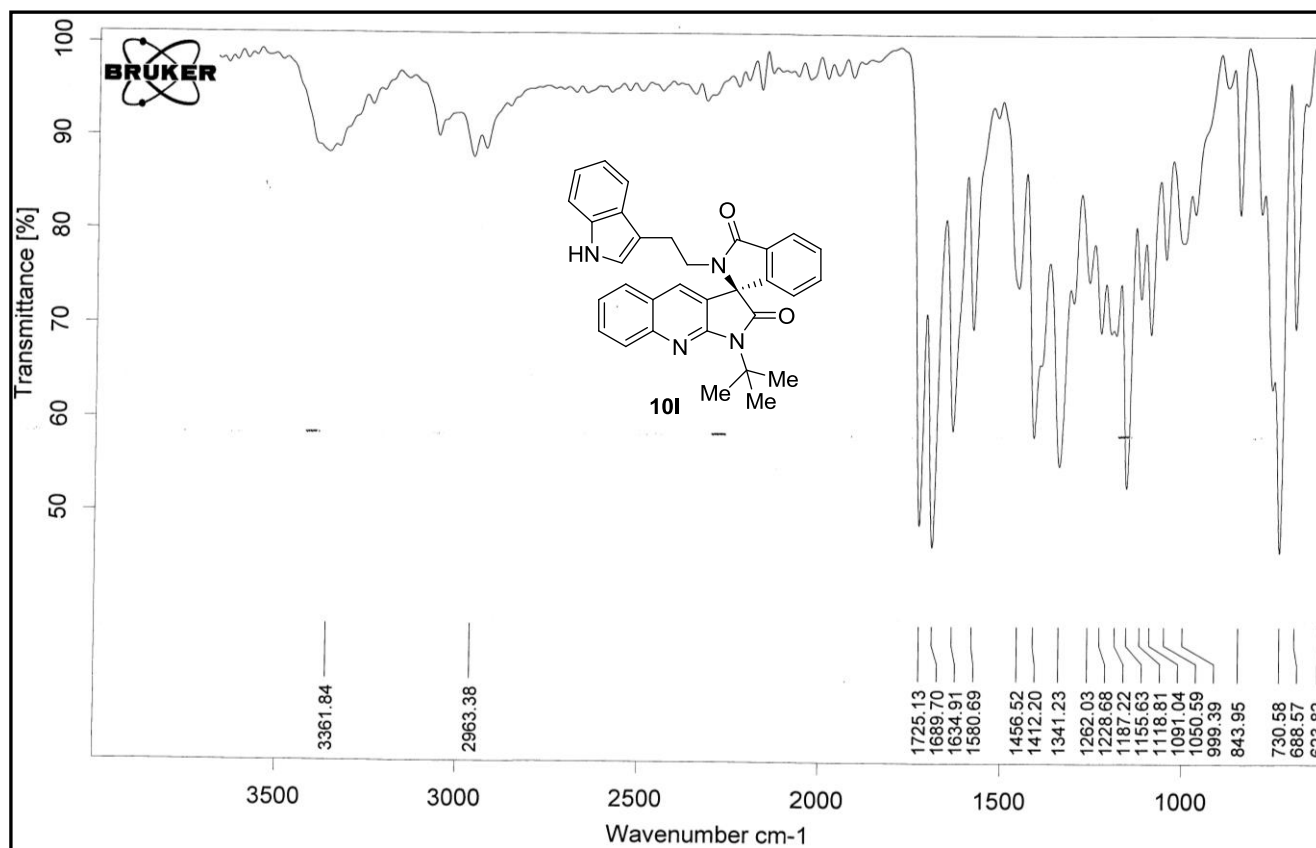


Figure 108. IR (10I).

3. X-ray Crystallography: CIF in separate file.

Crystallographic data **8a** (CCDC 1010288) and **10j** (CCDC 1053522)

The CCDC deposition number for compound **8a** is 1010288. Formula: C₃₀H₂₆N₄O₂. Unit Cell

Parameters: $a = 8.1907(16)$, $b = 9.4346(19)$, $c = 32.024(6)$, space group P21/c.

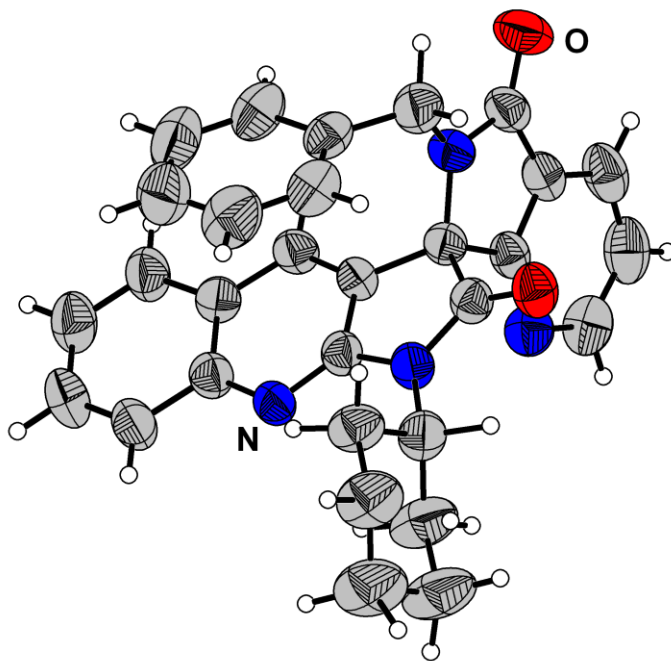


Figure 109. ORTEP diagram of spiro compound **8a**.

The CCDC deposition number for compound **10j** is 1053522 Formula: C₃₄H₃₀N₄O₂. Unit Cell Parameters: $a = 11.299(2)$, $b = 11.724(2)$, $c = 14.051(3)$, space group P-1.

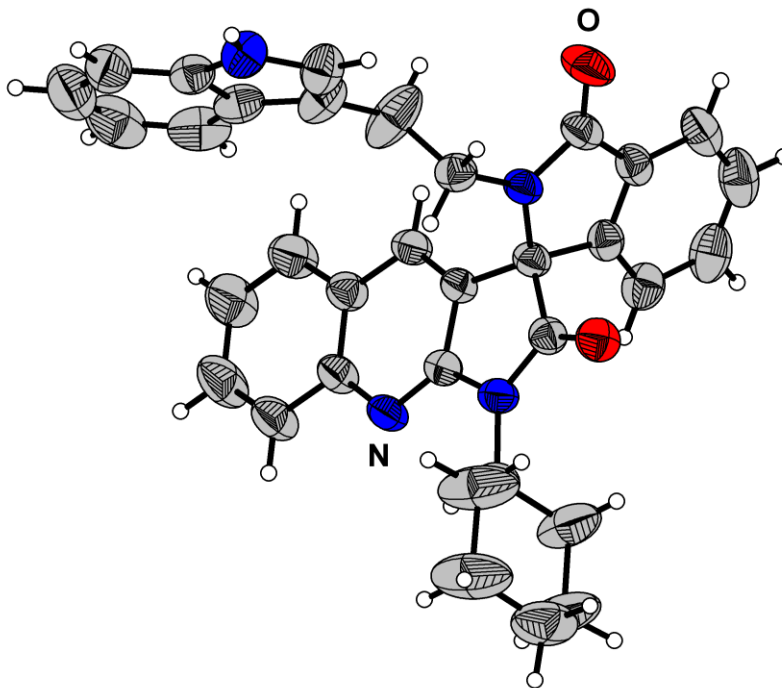


Figure 110. ORTEP diagram of spiro compound **10j**.