

Supplementary Information

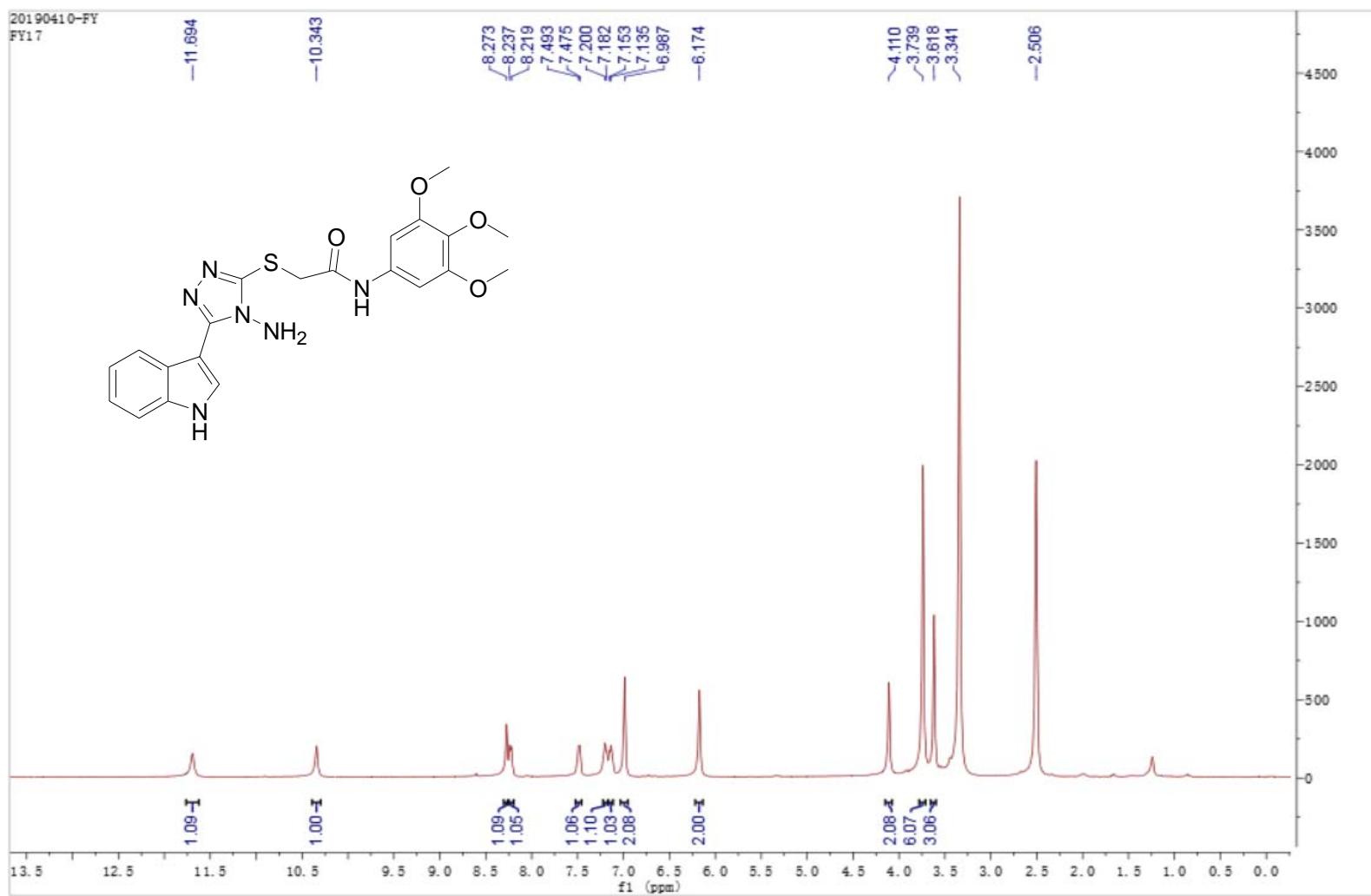
Discovery of new indole-based 1,2,4-triazole derivatives as potent tubulin polymerization inhibitors with anticancer activity

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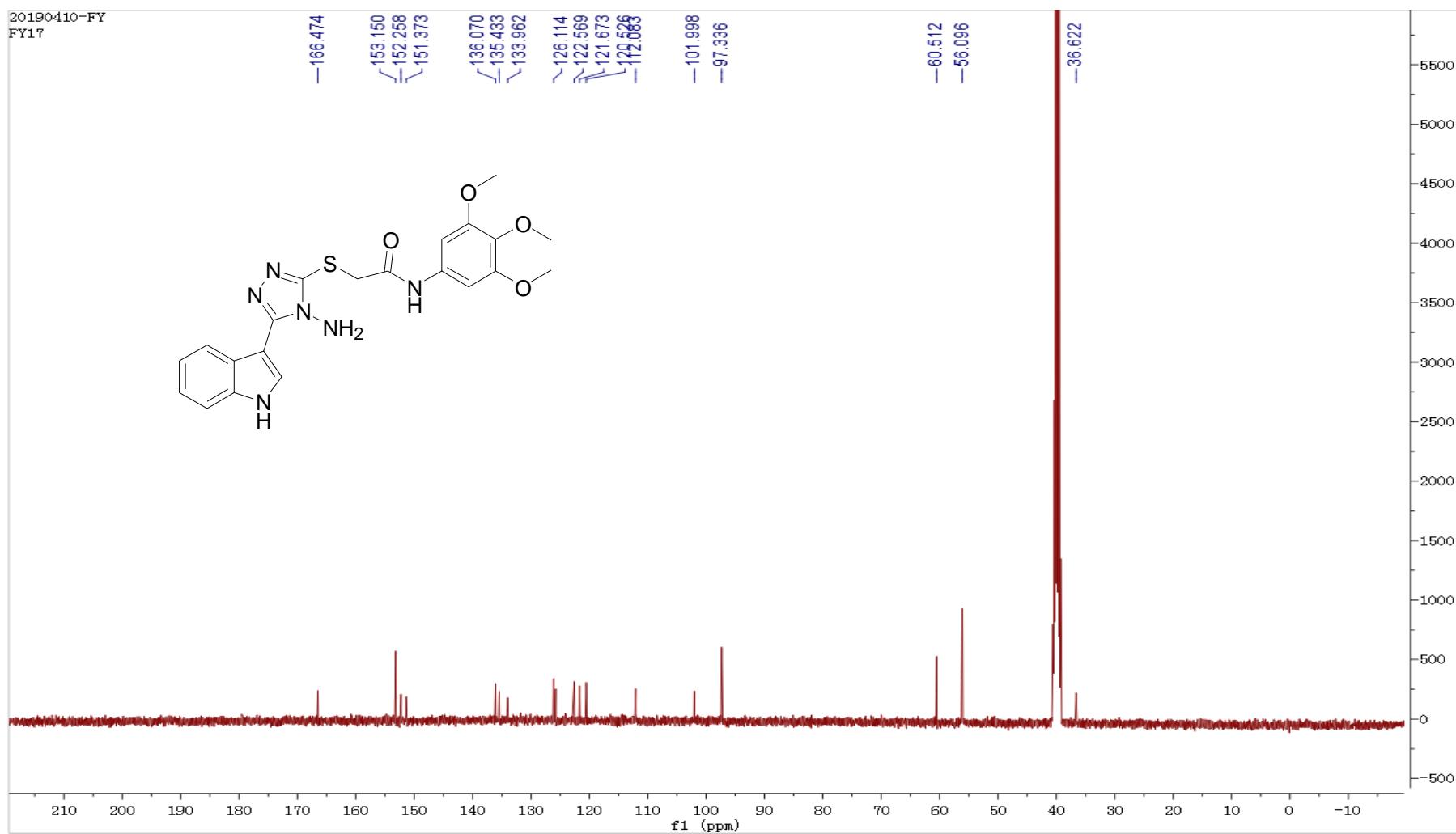


Figure 2. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound 9a.

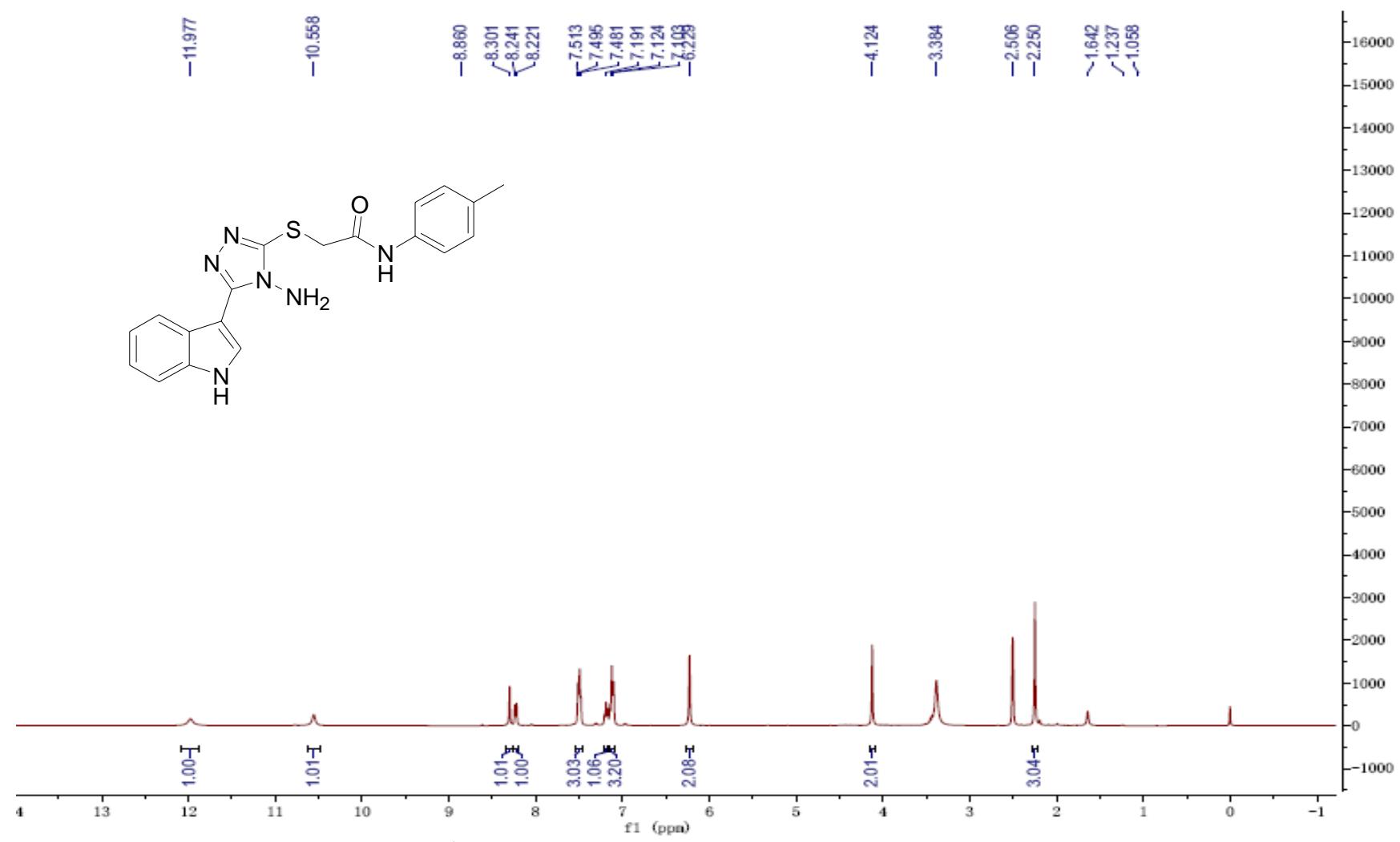


Figure 3. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **9b**.

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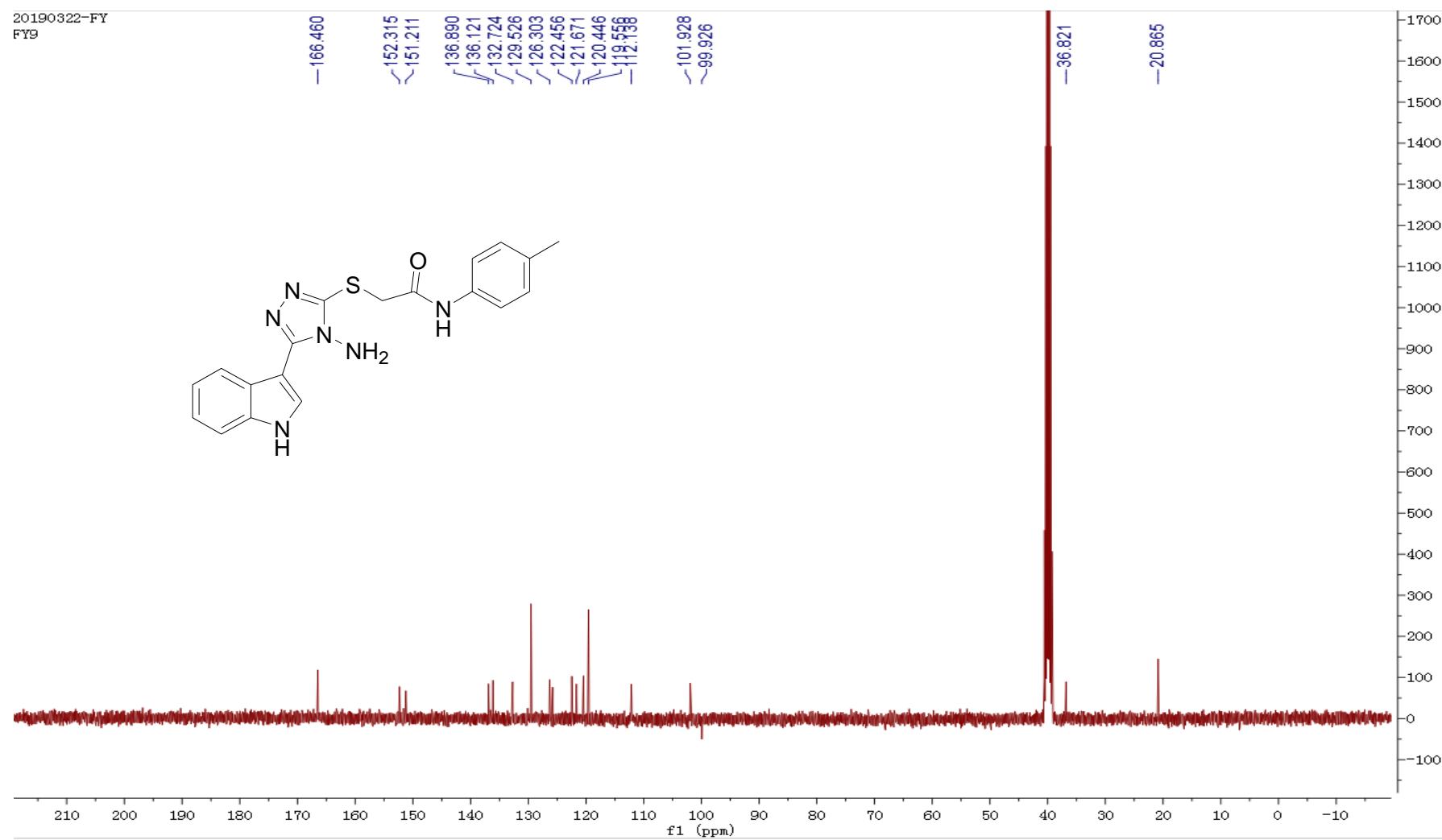


Figure 4. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of compound **9b**.

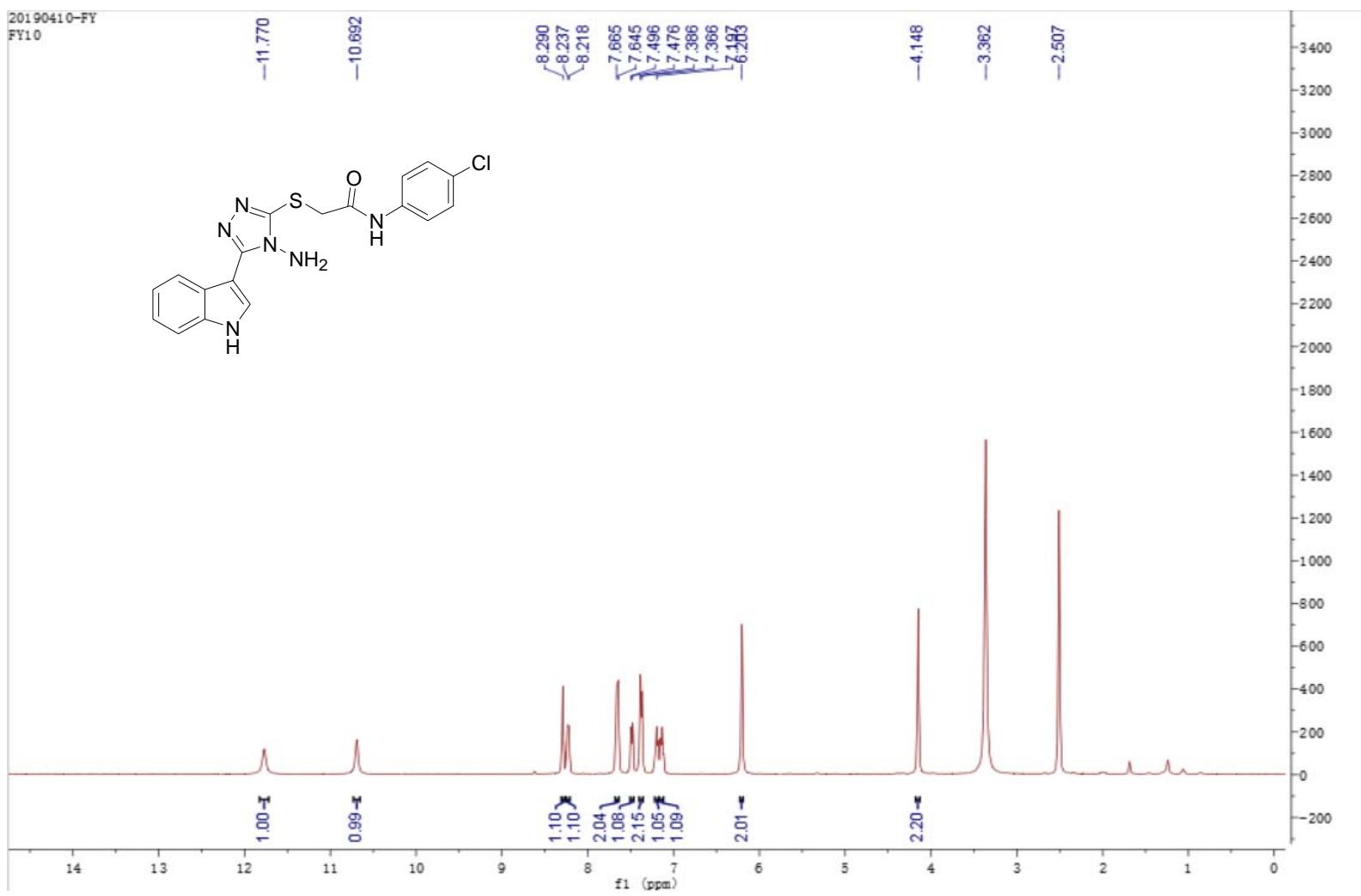


Figure 5. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound 9c.

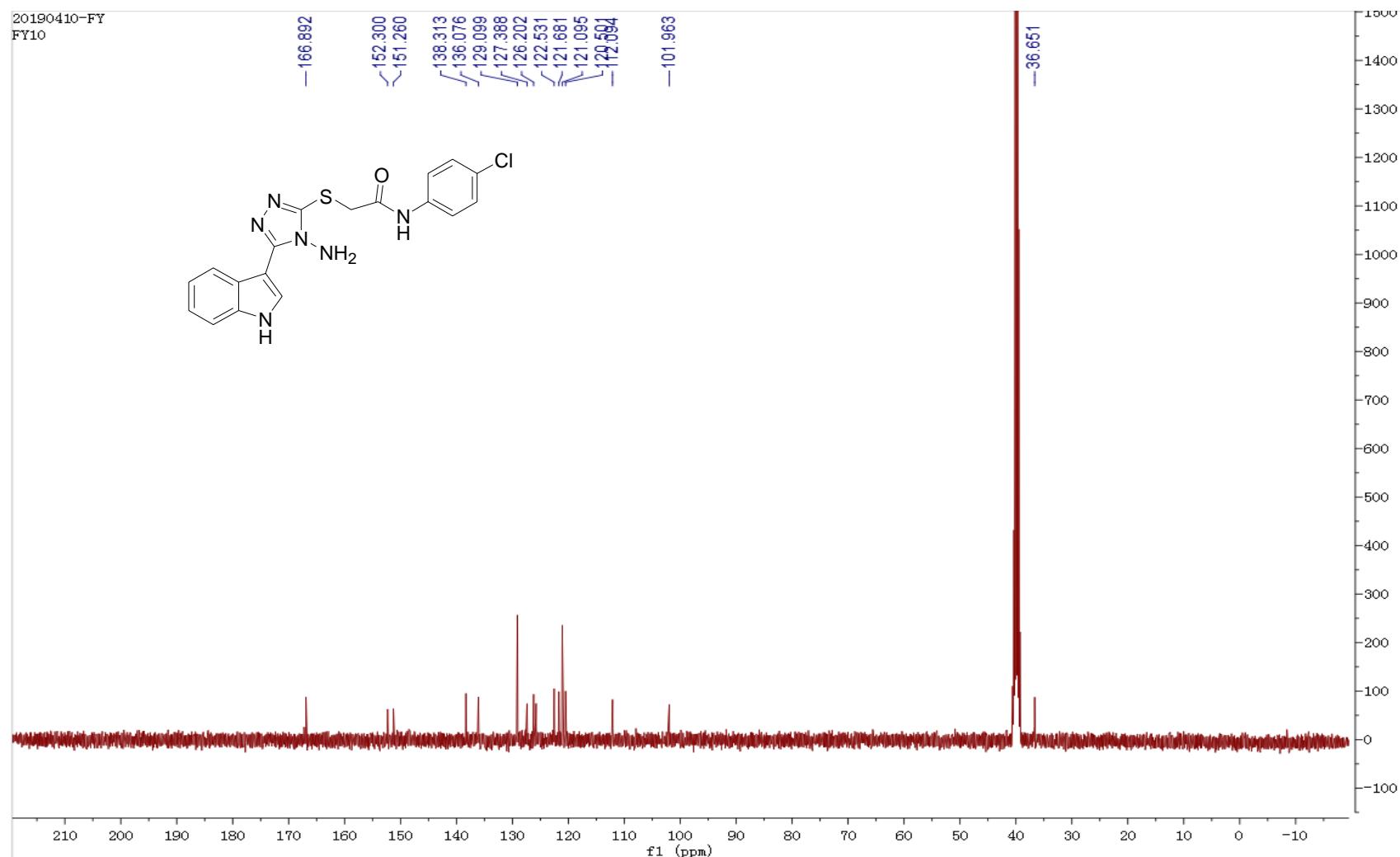


Figure 6. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9c**.

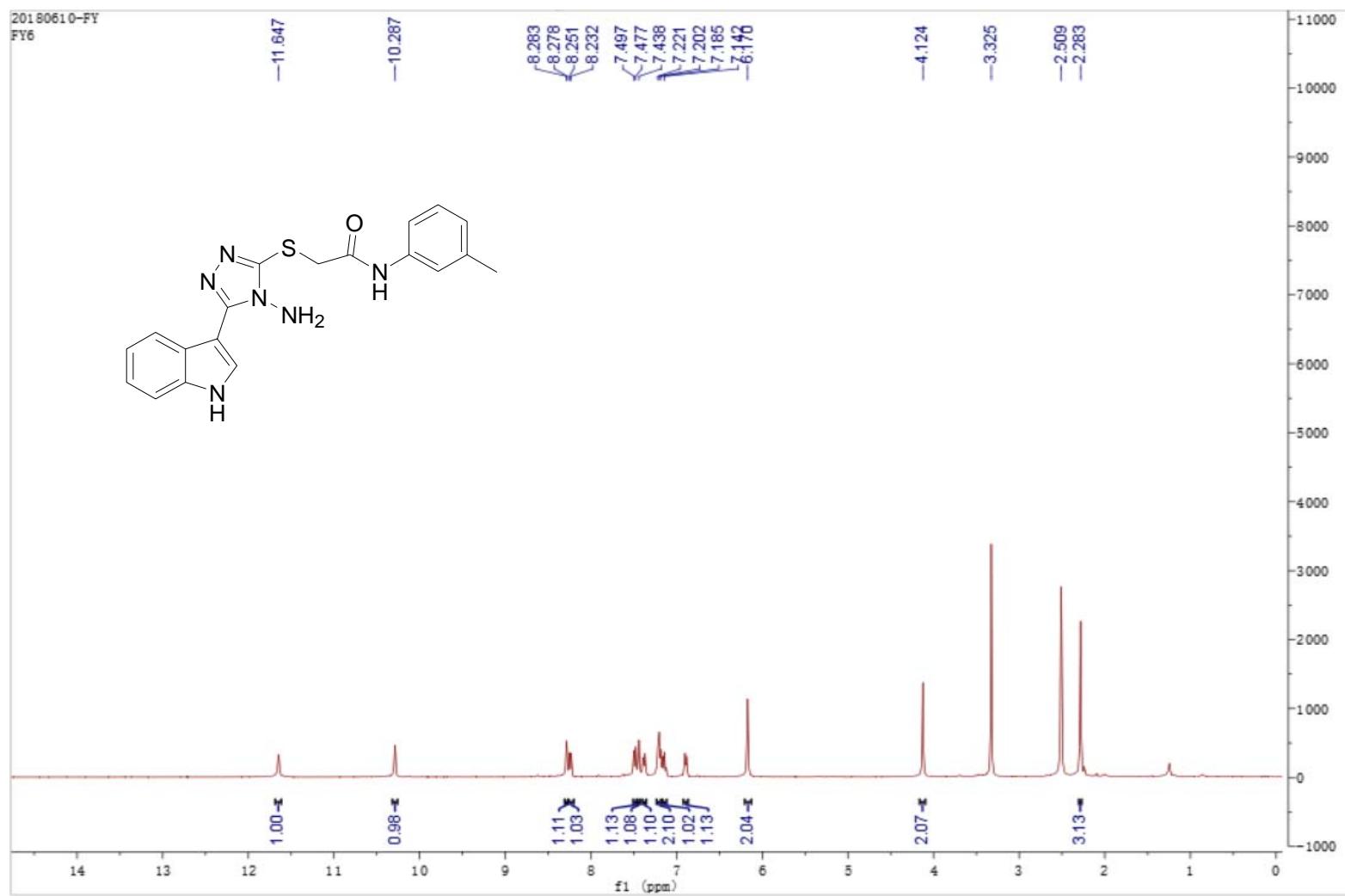


Figure 7. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound 9d.

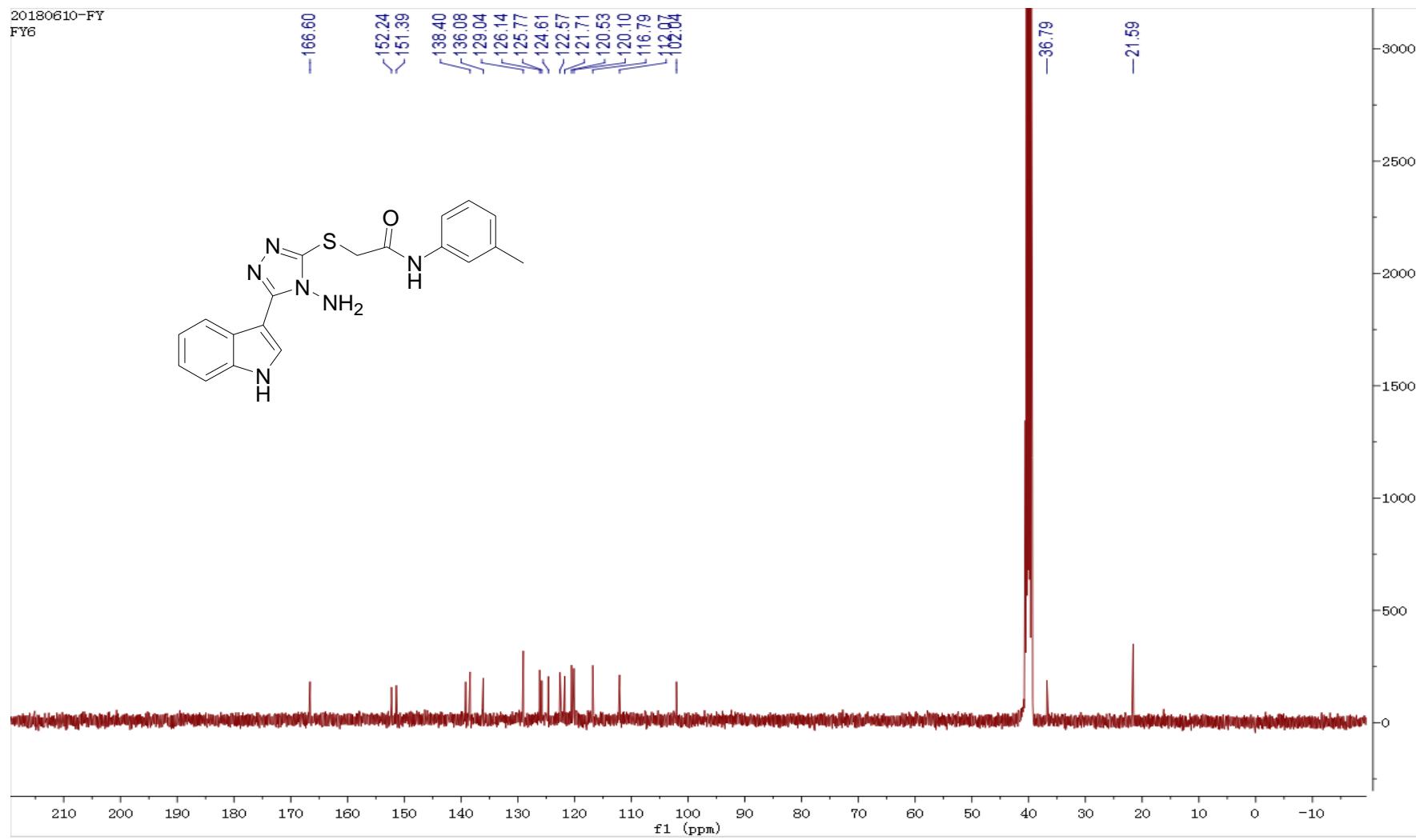


Figure 8. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9d**.

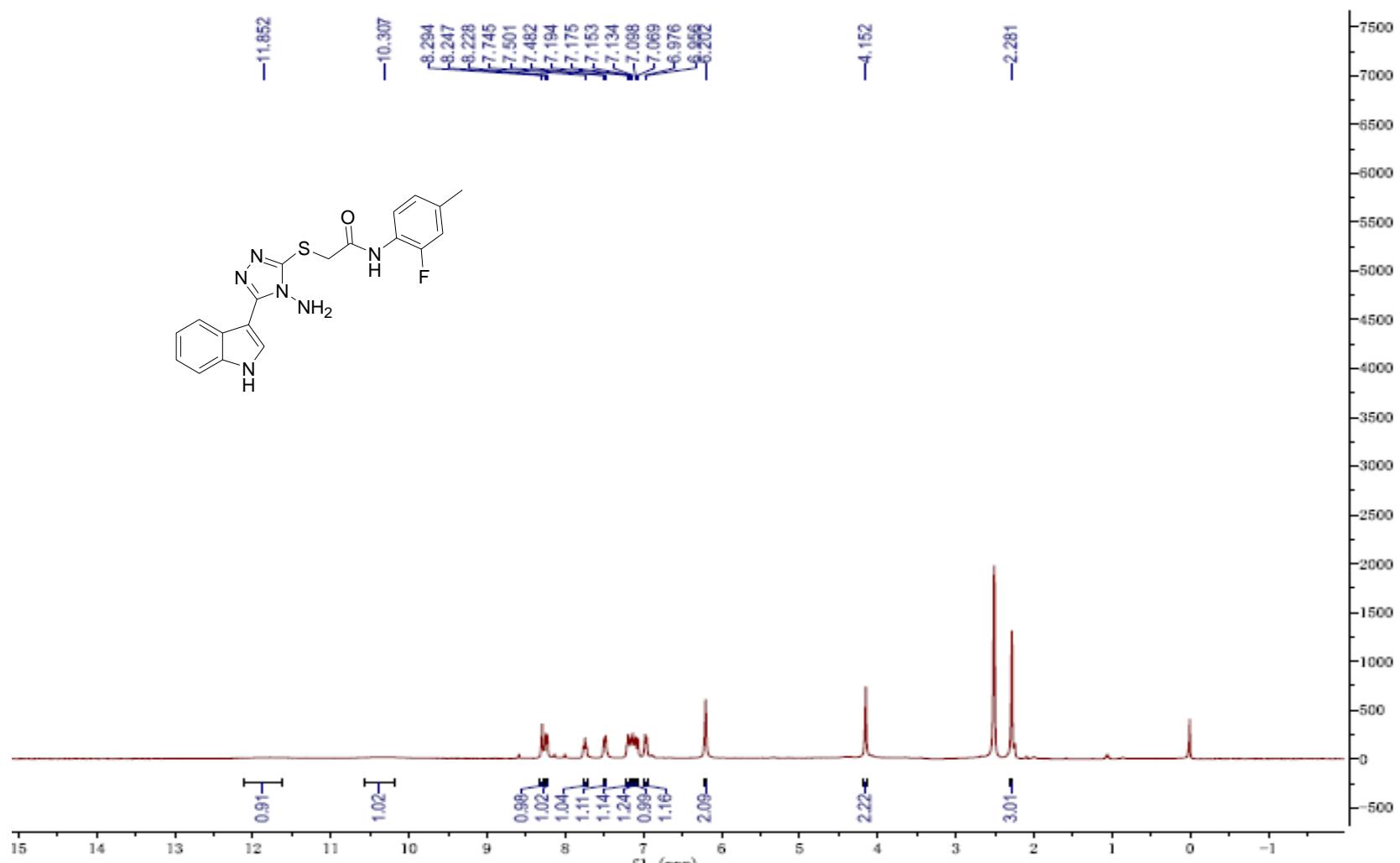


Figure 9. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 9e.

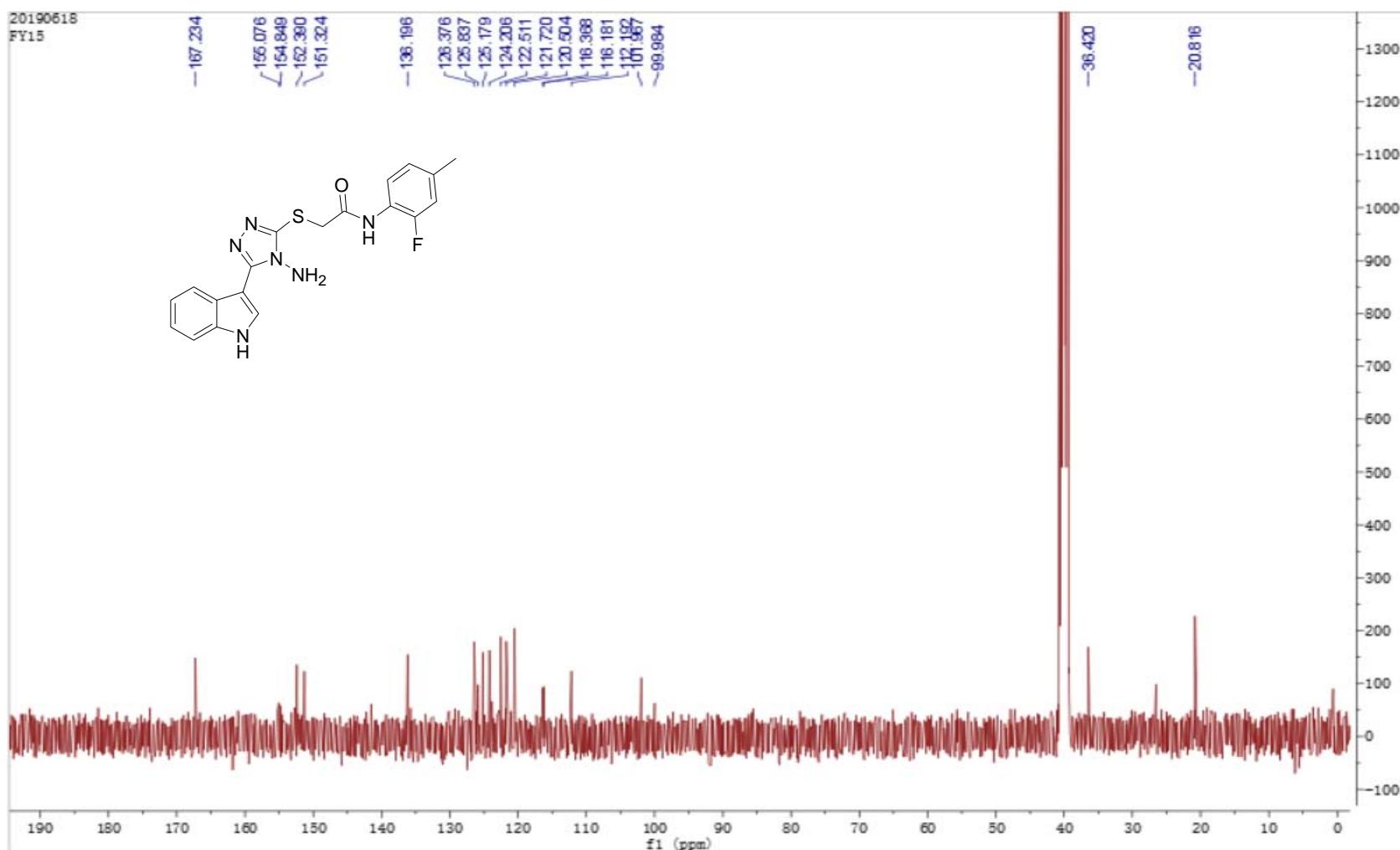


Figure 10. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound 9e.

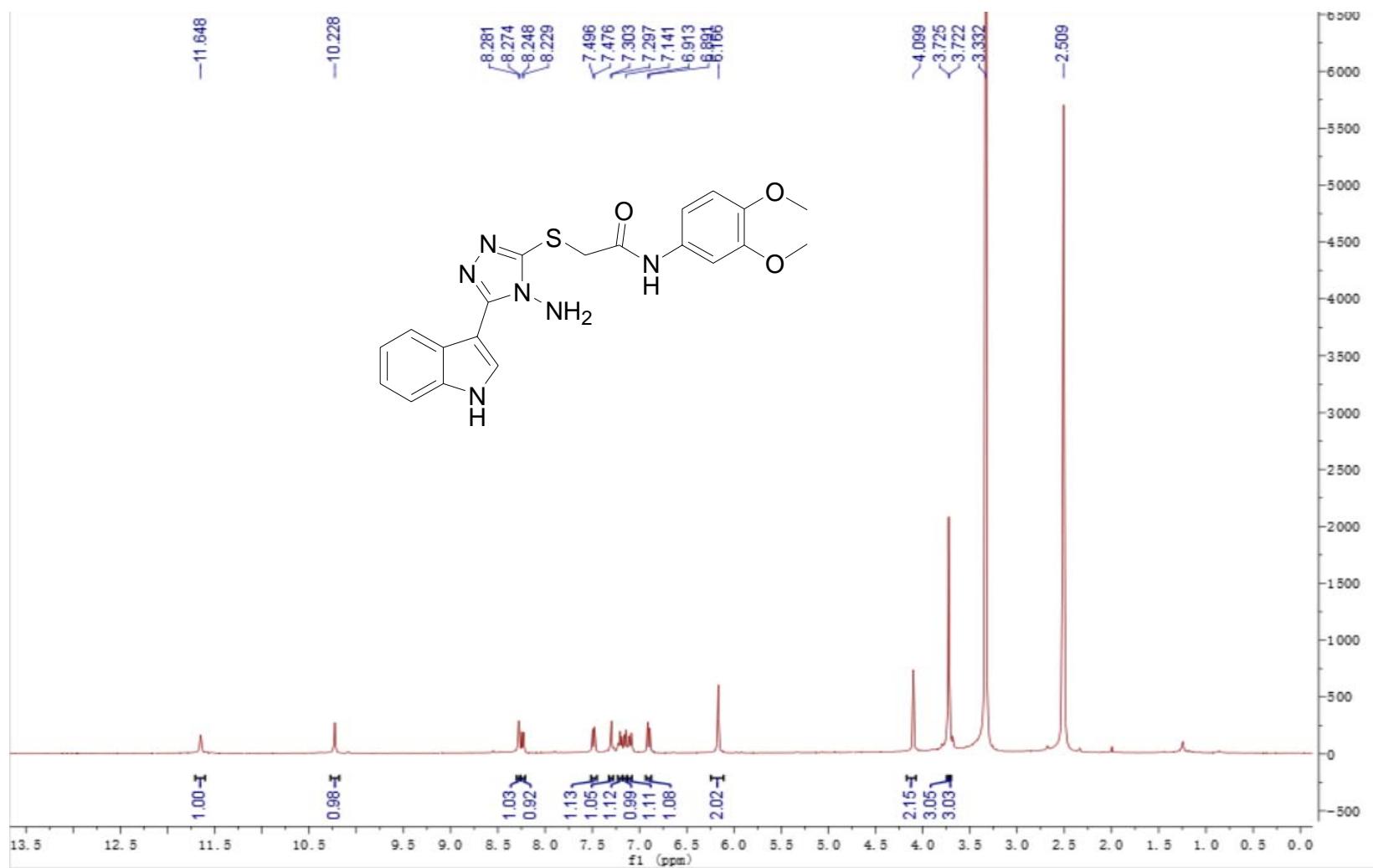


Figure 11. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **9f**.

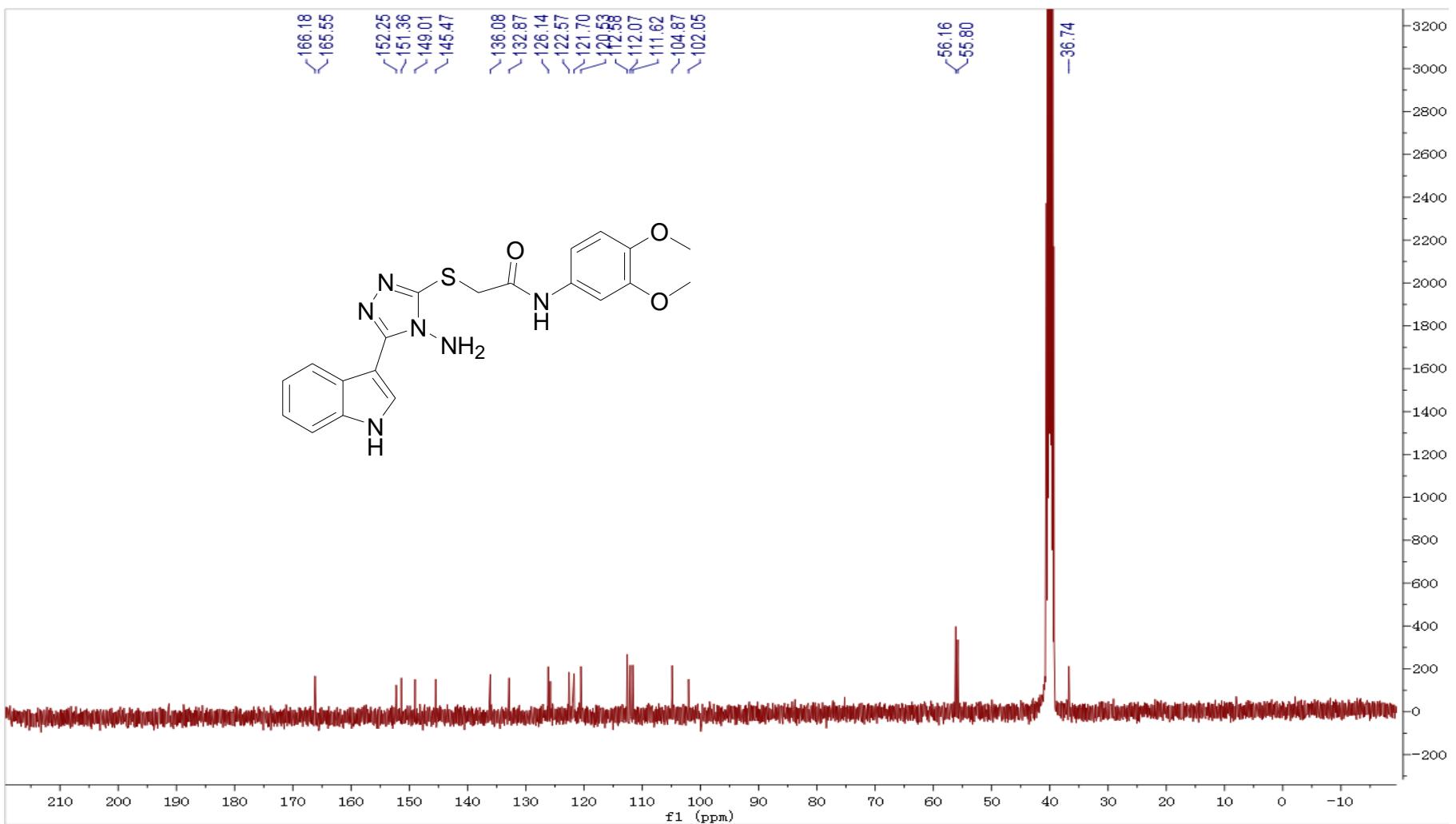


Figure 12. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9f**.

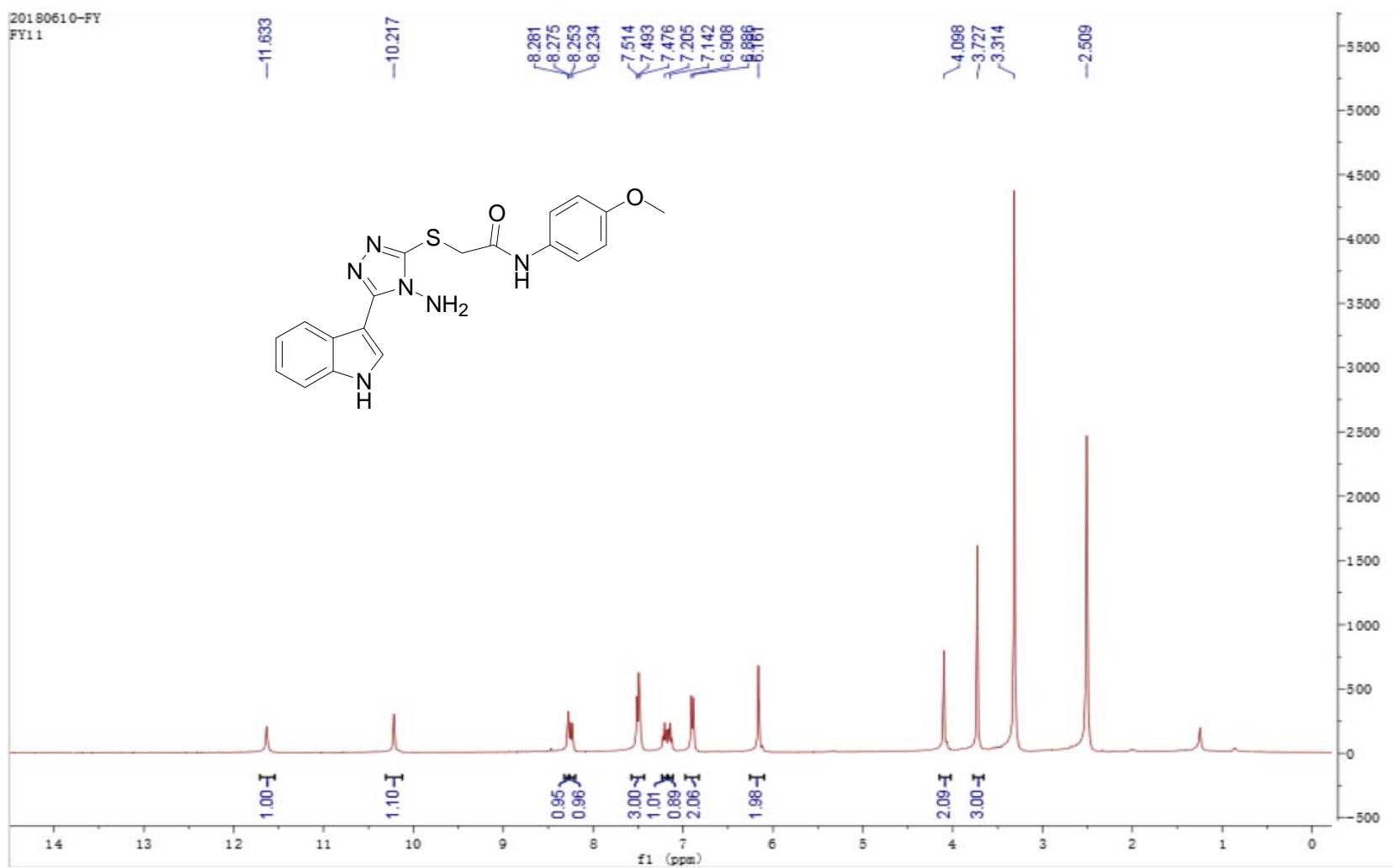


Figure 13. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 9g.

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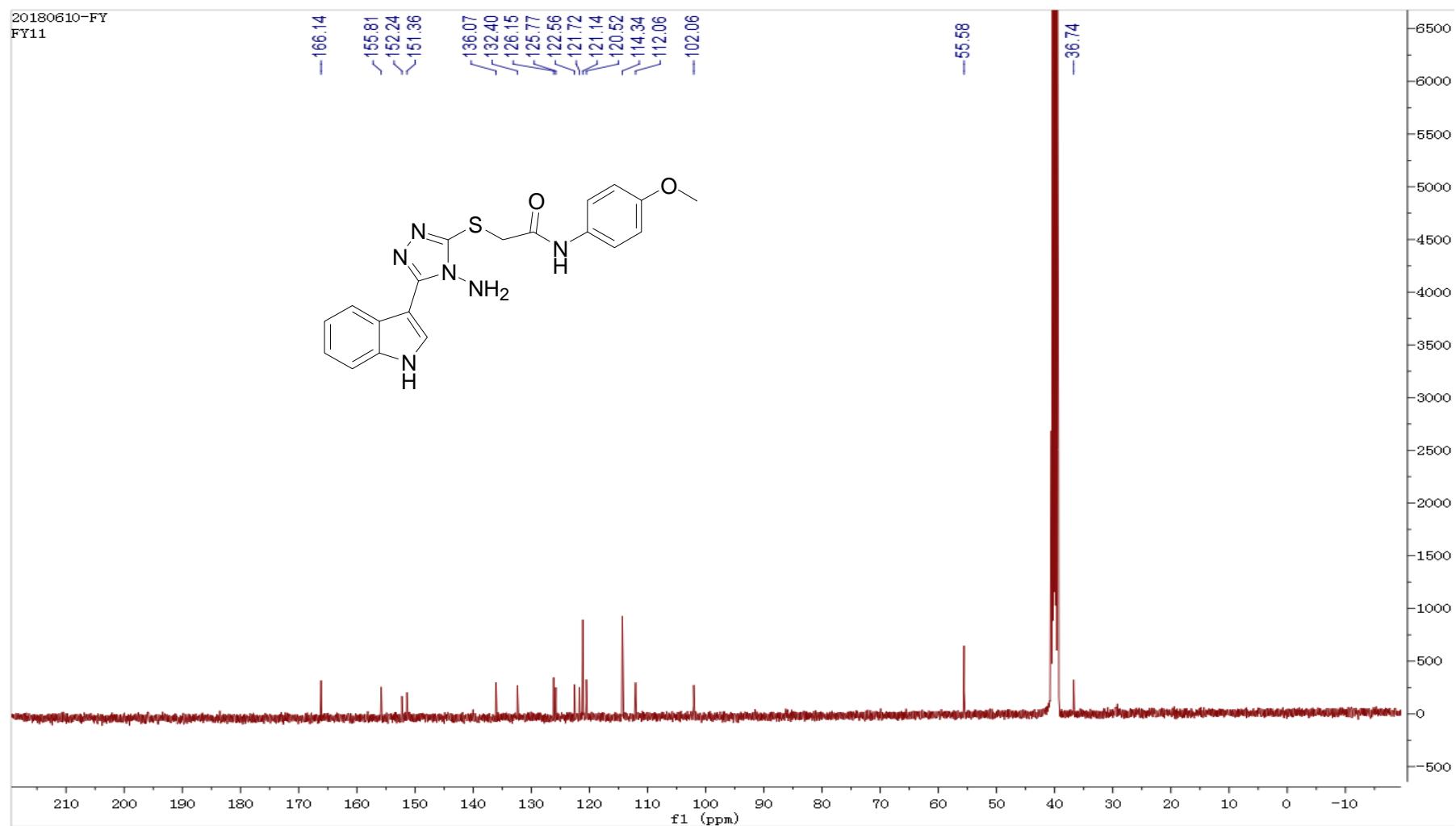


Figure 14. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of compound **9g**.

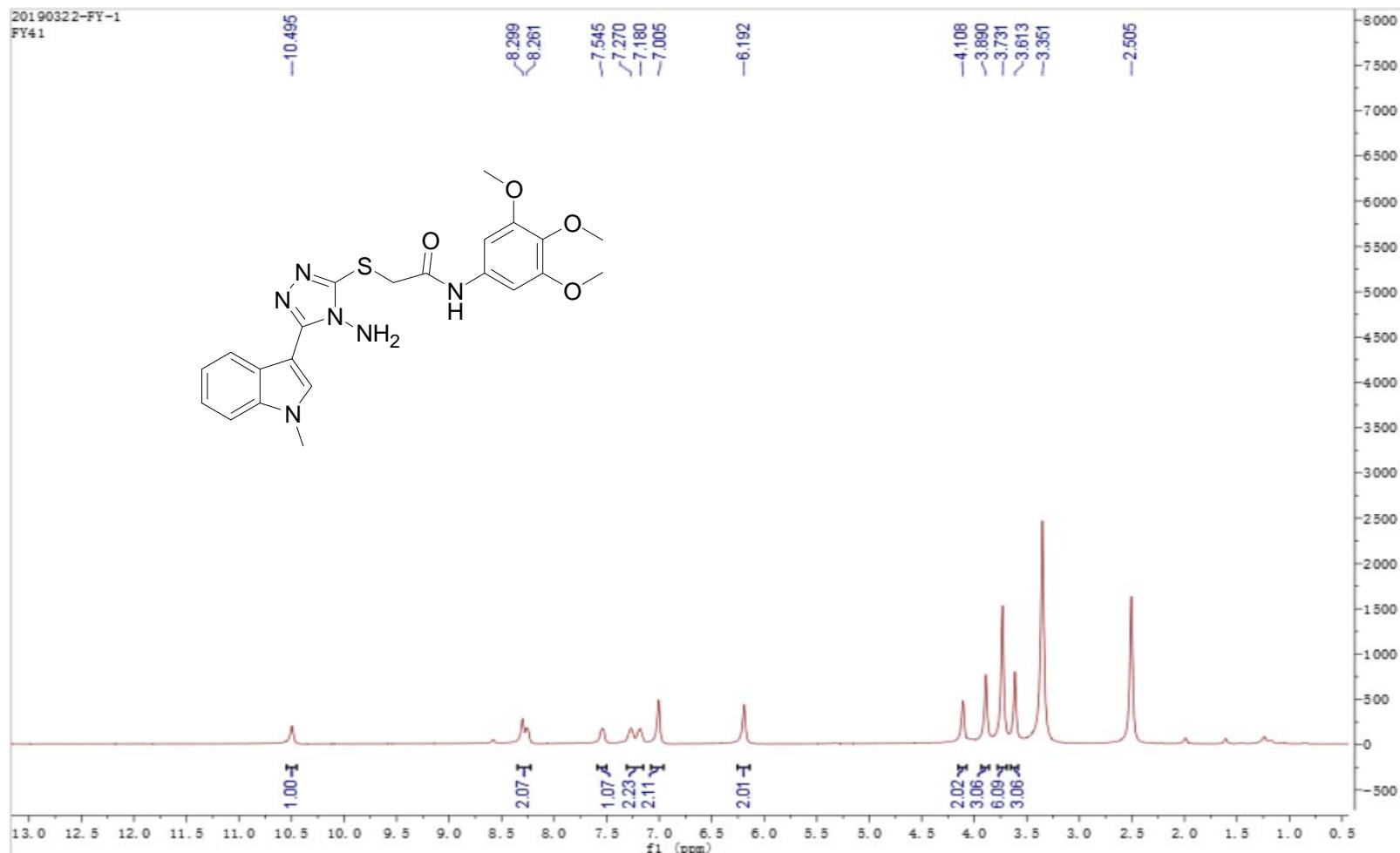


Figure 15. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 9h.

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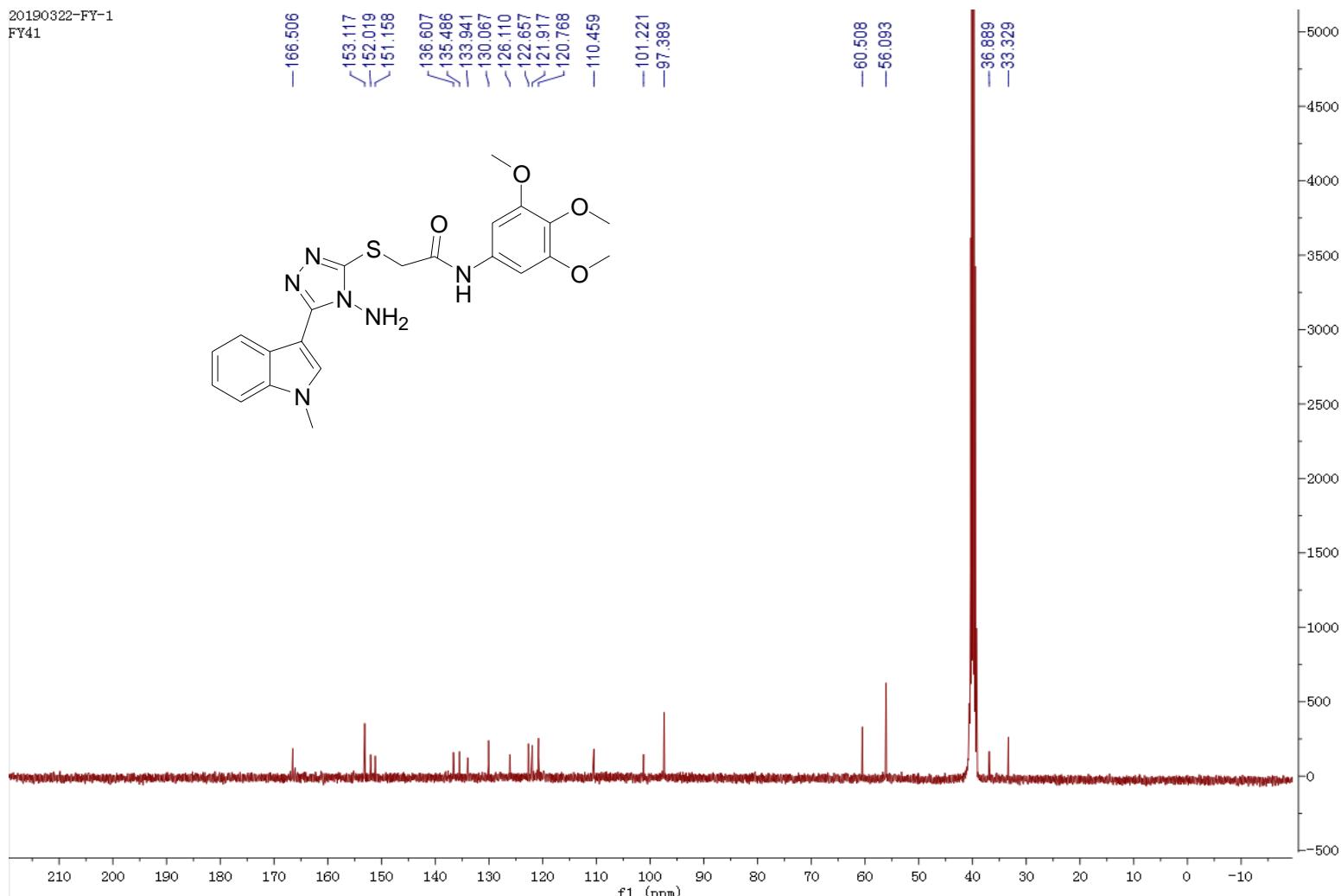


Figure 16. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9h**.

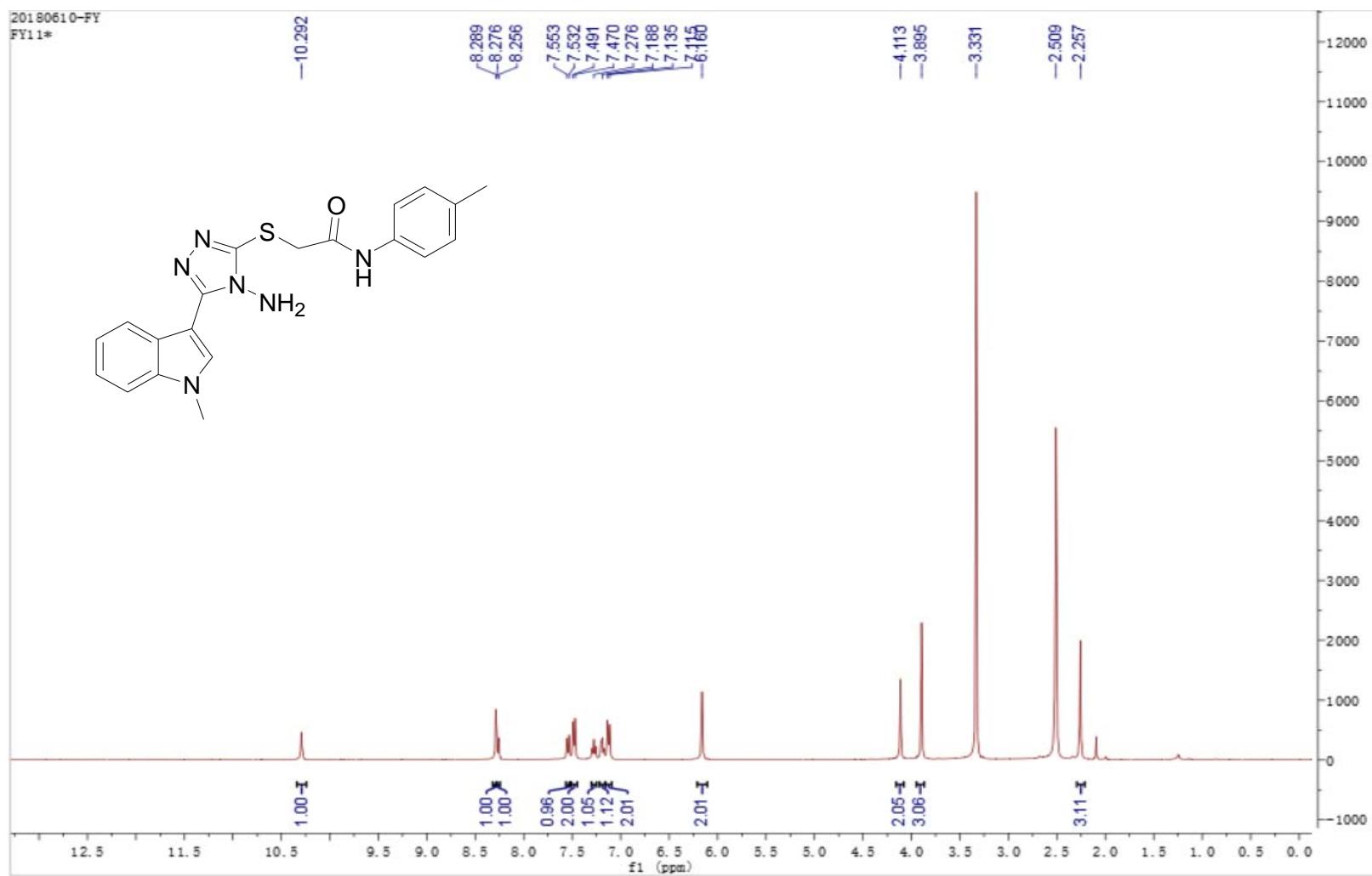


Figure 17. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound 9i.

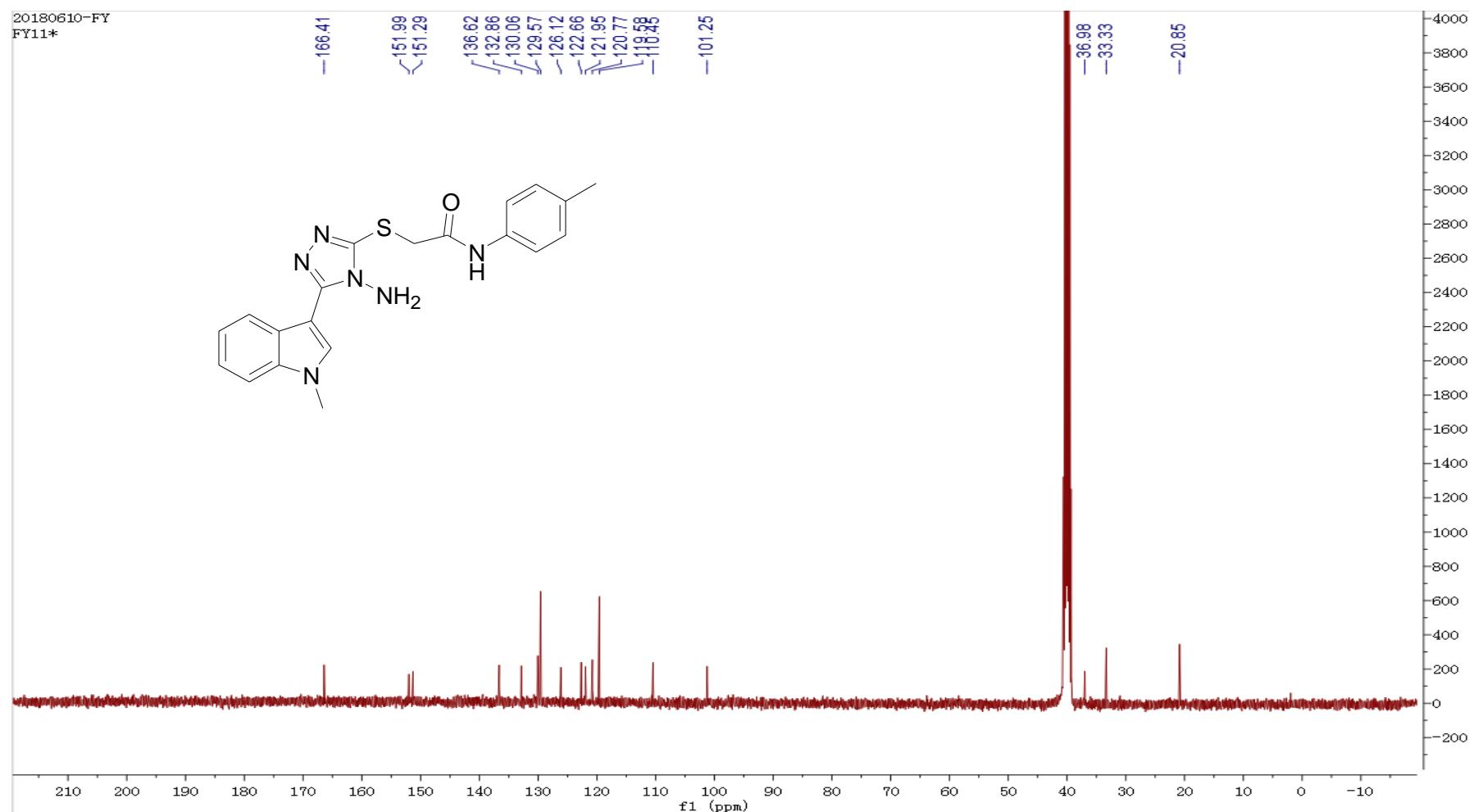


Figure 18. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9i**.

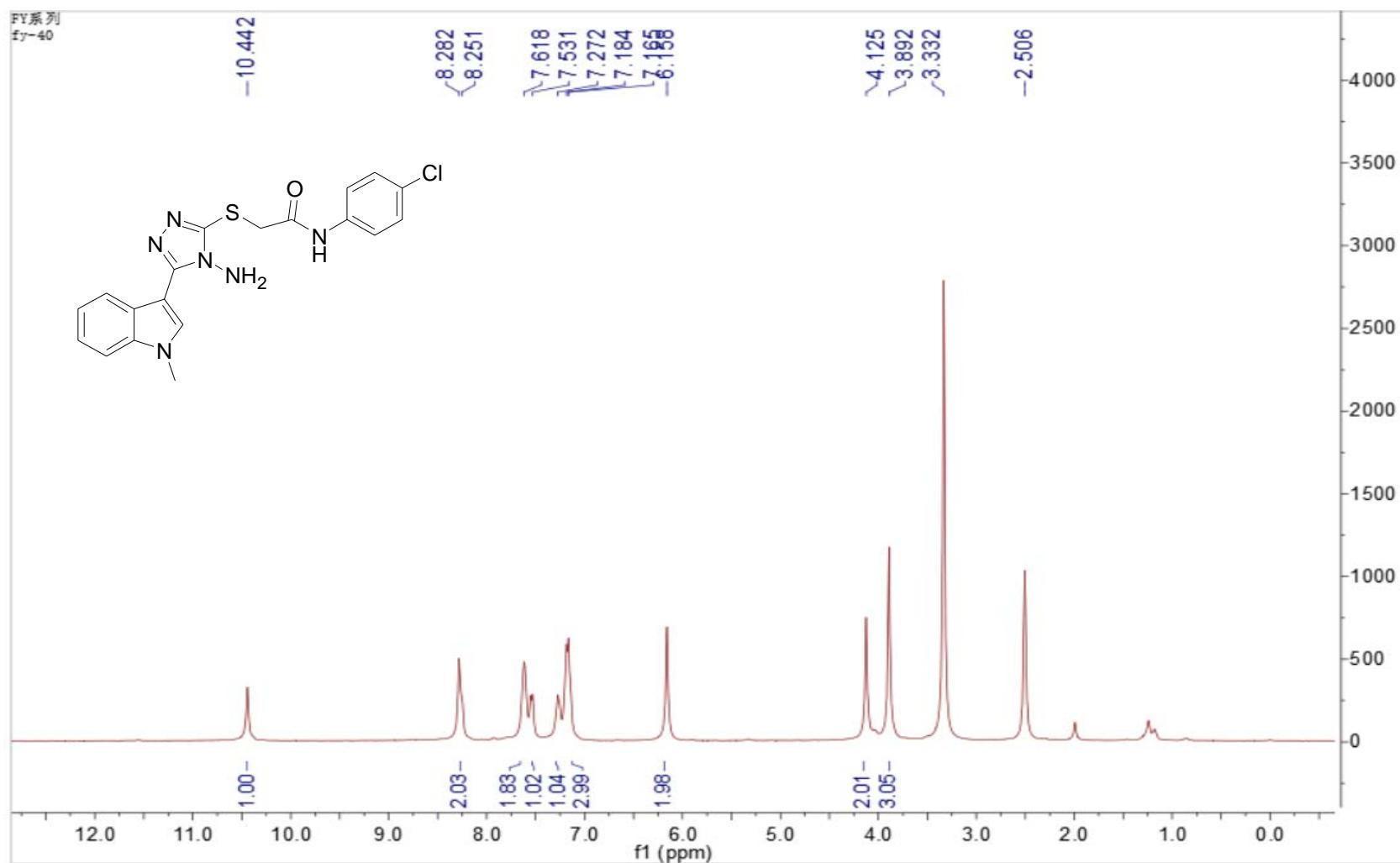


Figure 19. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 9j.

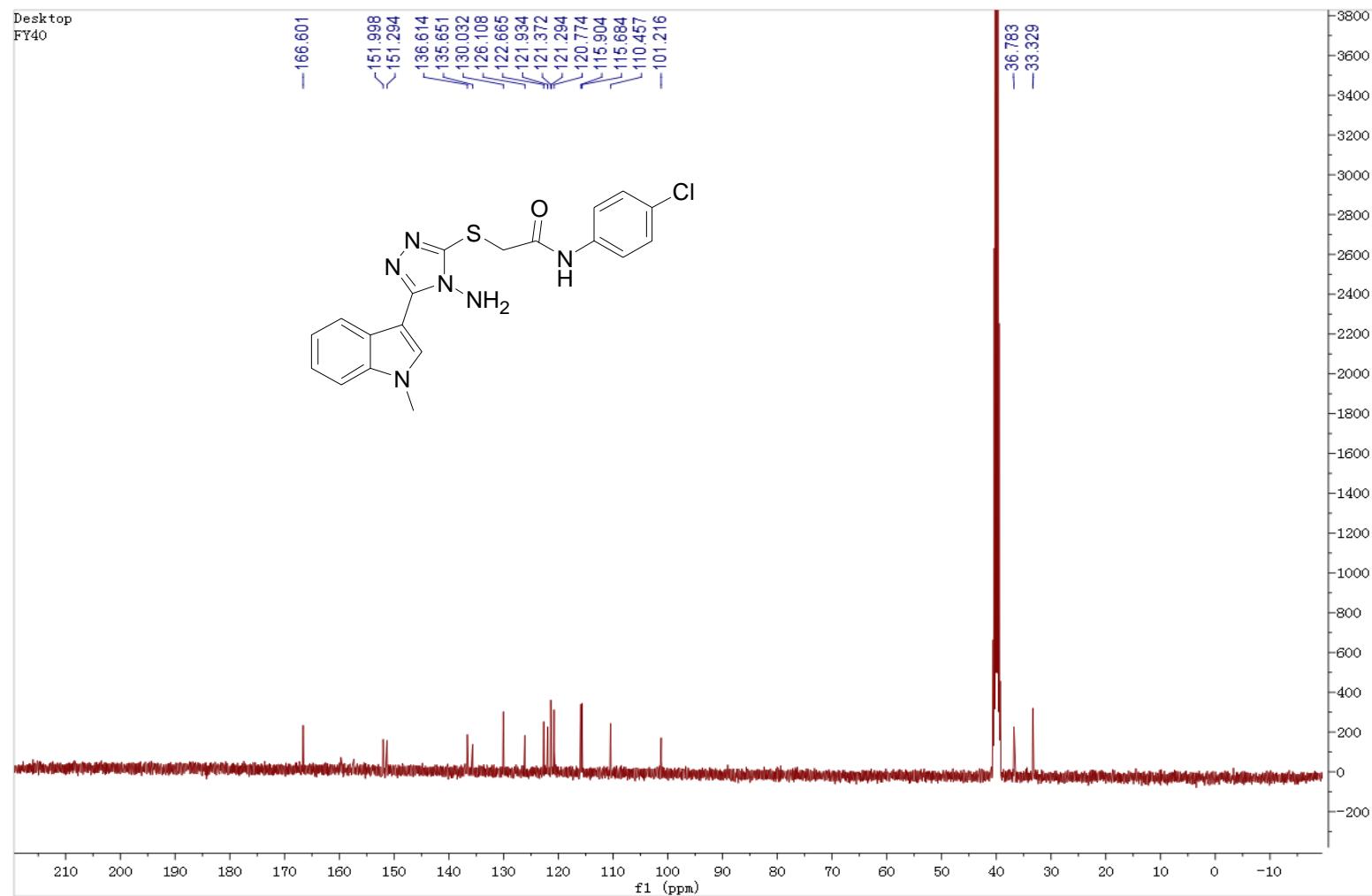


Figure 20. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9j**.

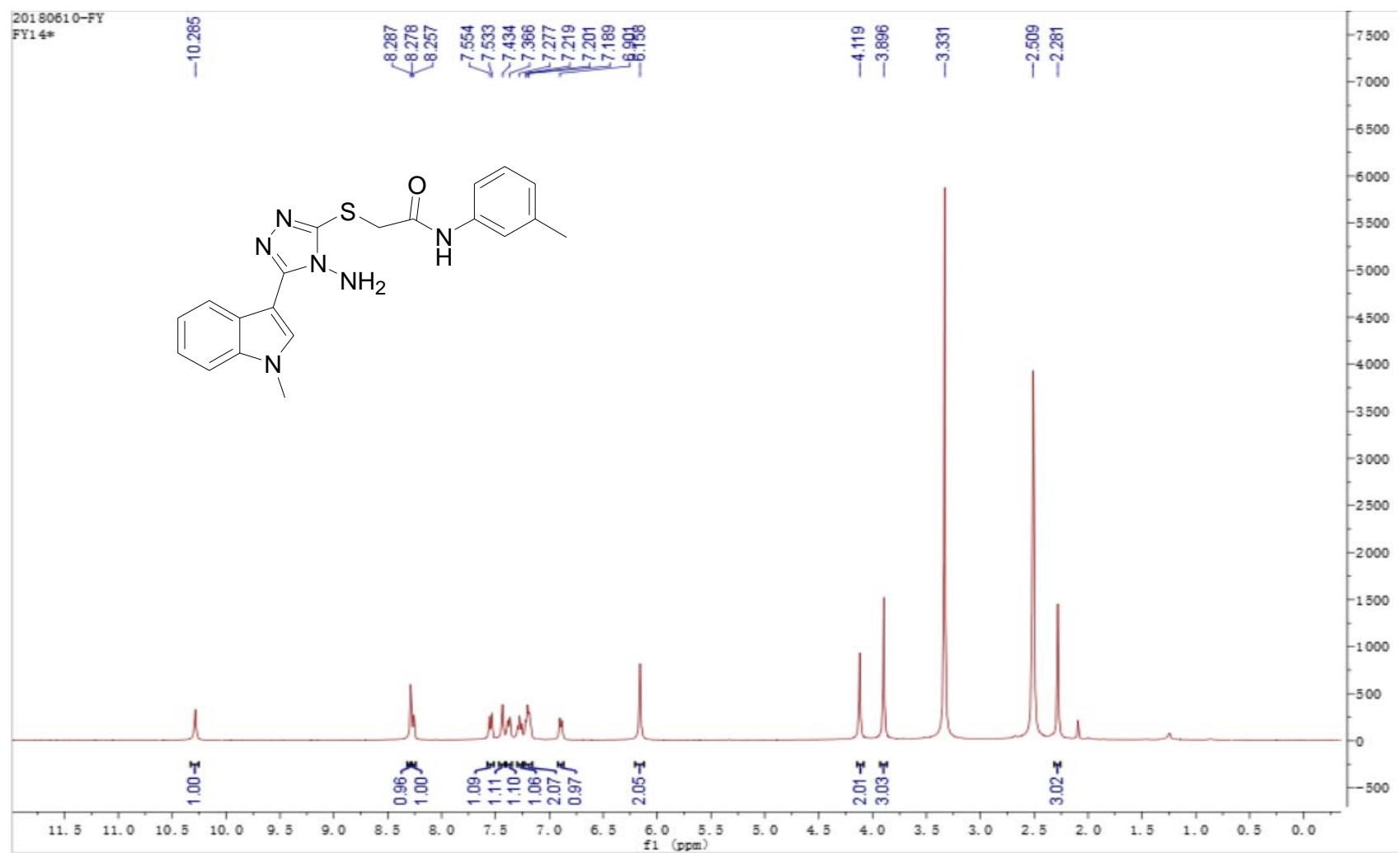


Figure 21. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **9k**.

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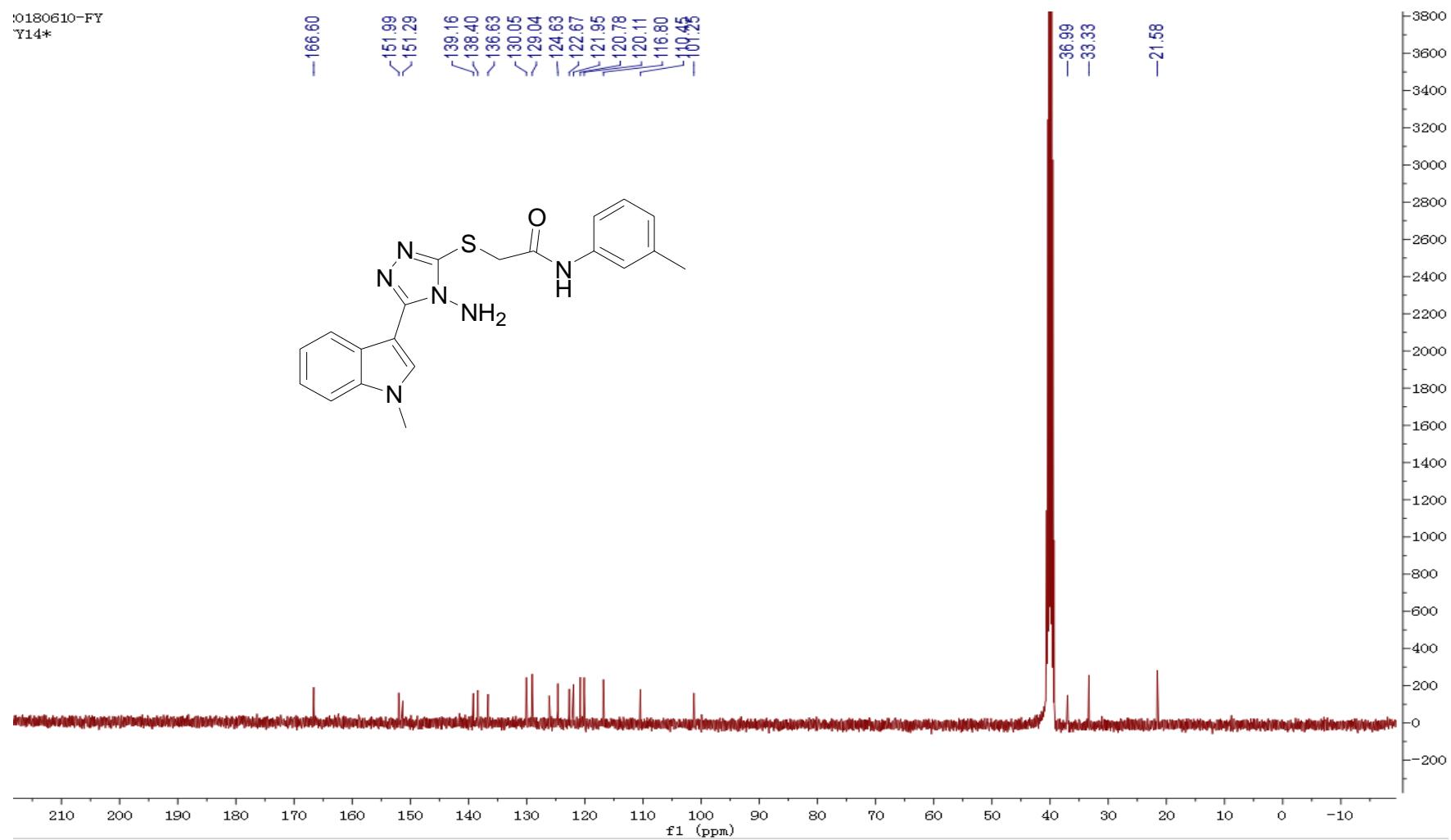


Figure 22. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **9k**.

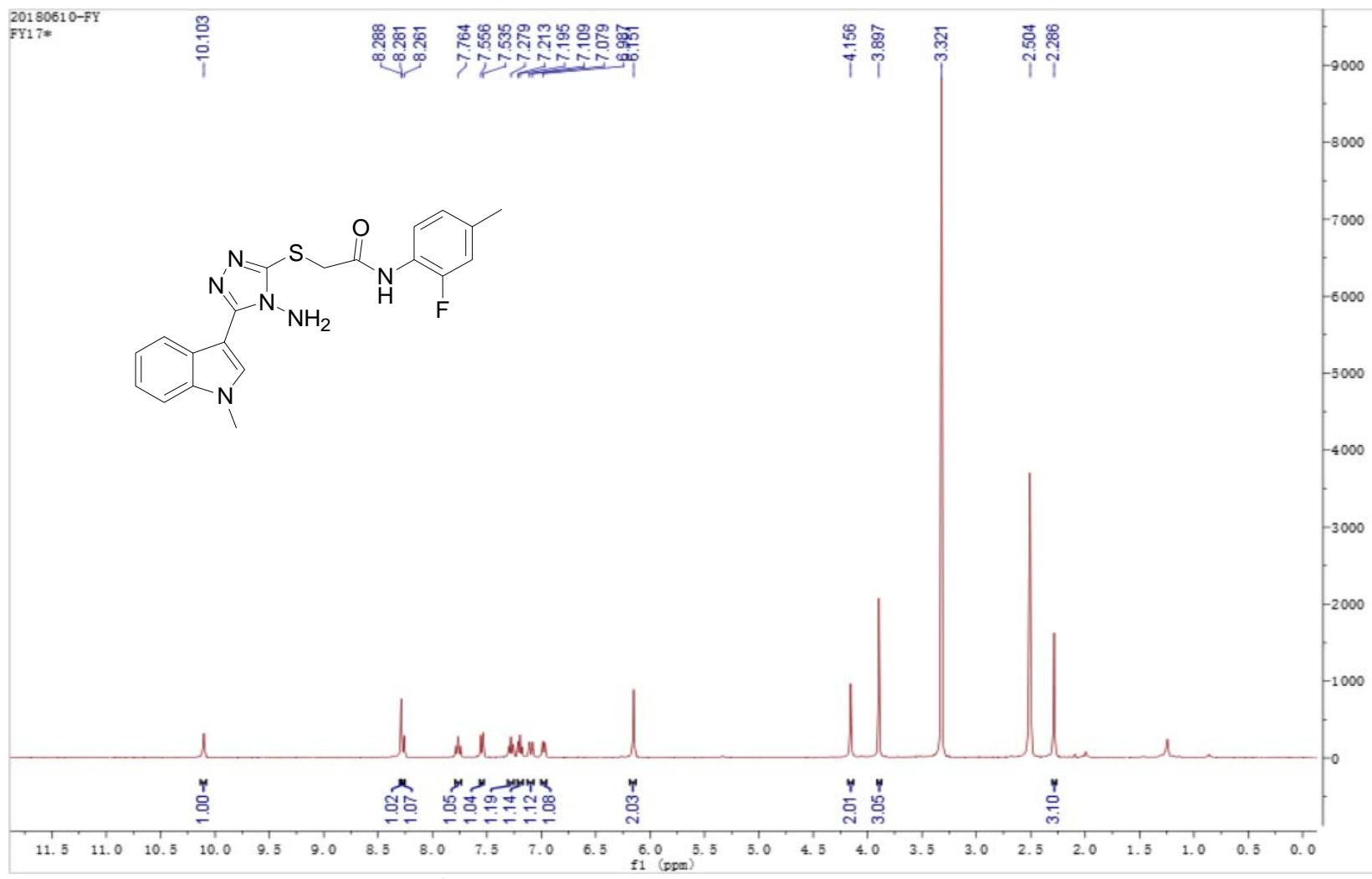


Figure 23. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 9l.

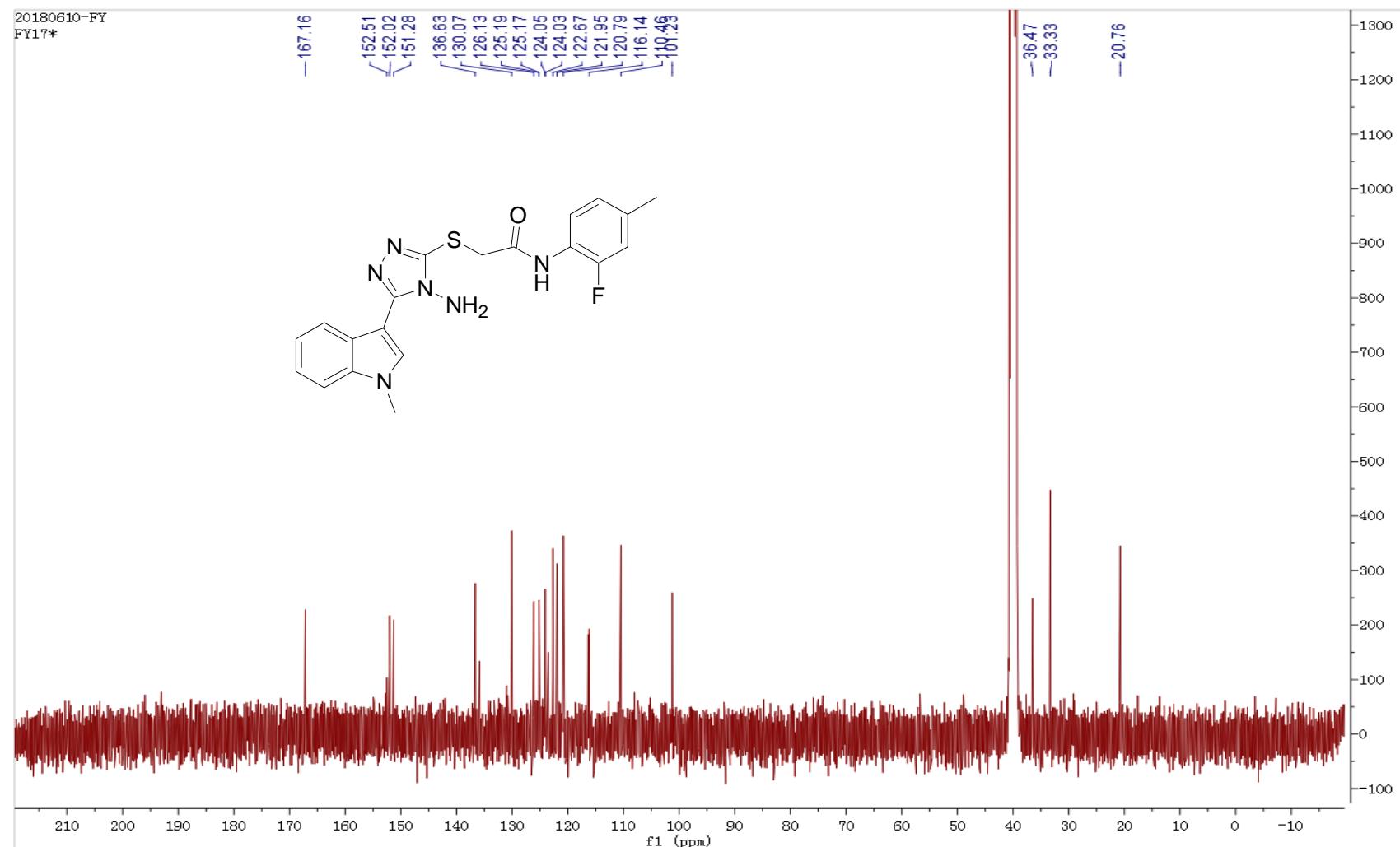


Figure 24. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9l**.

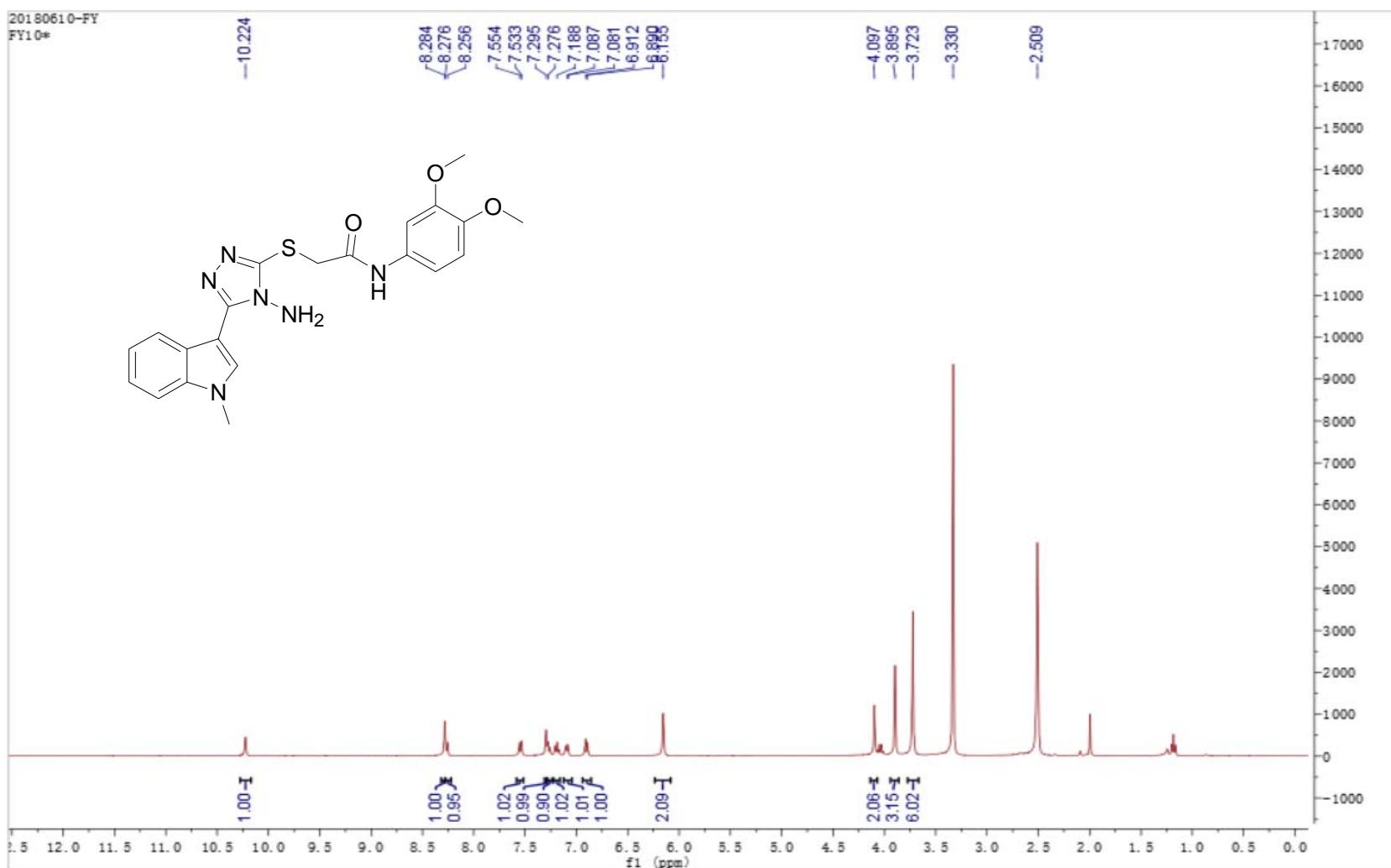


Figure 25. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **9m**.

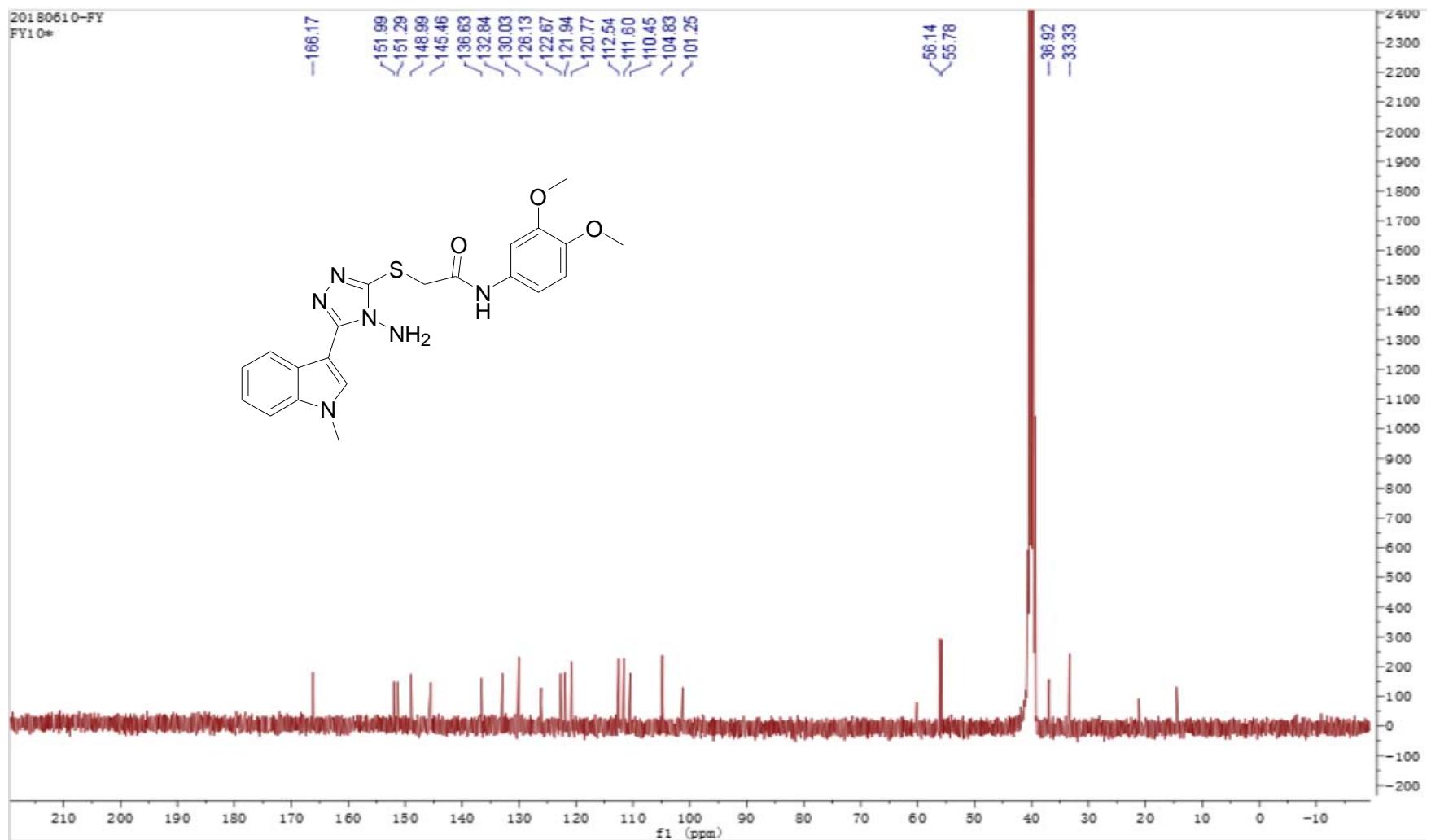


Figure 26. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9m**.

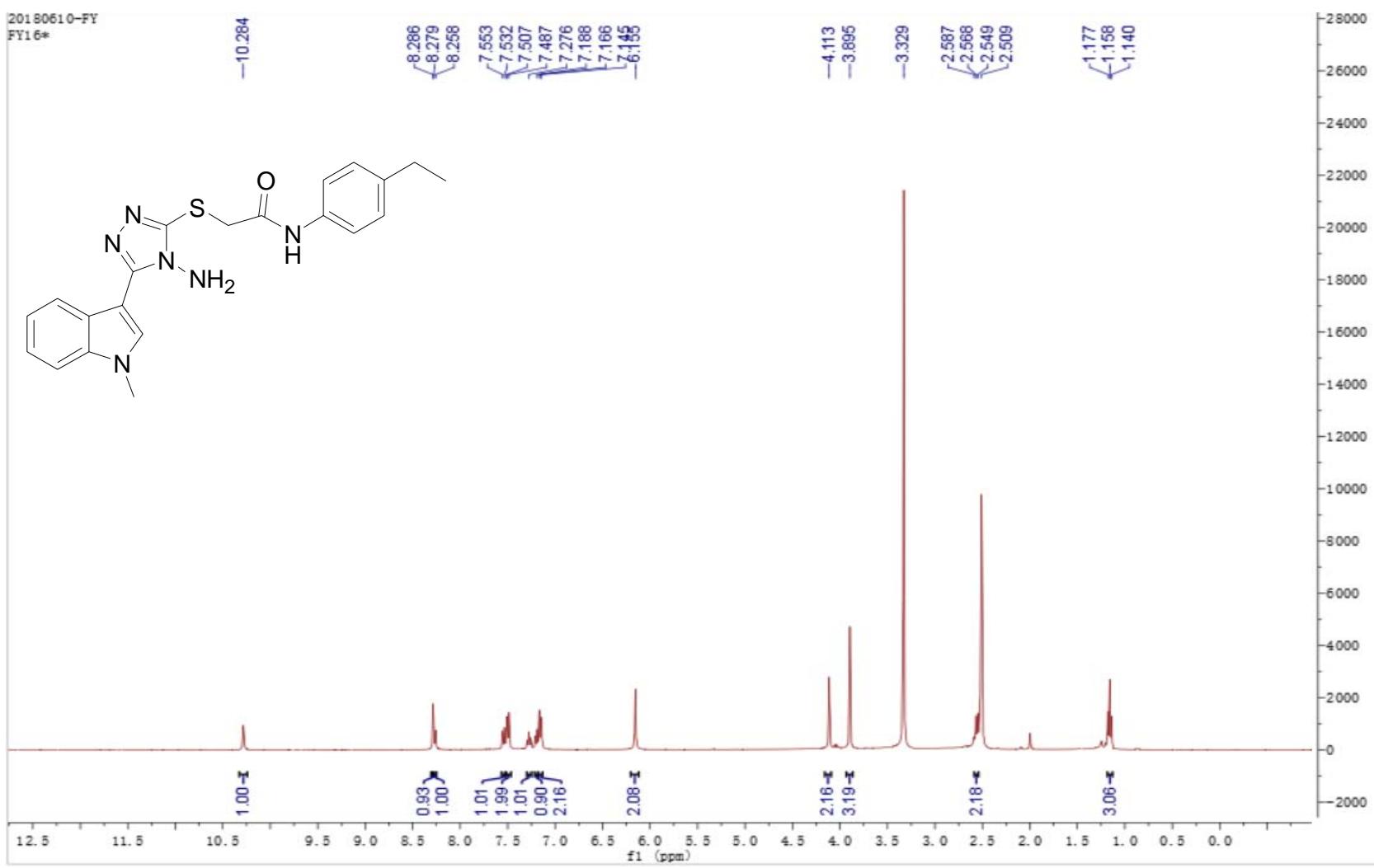


Figure 27. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 9n.

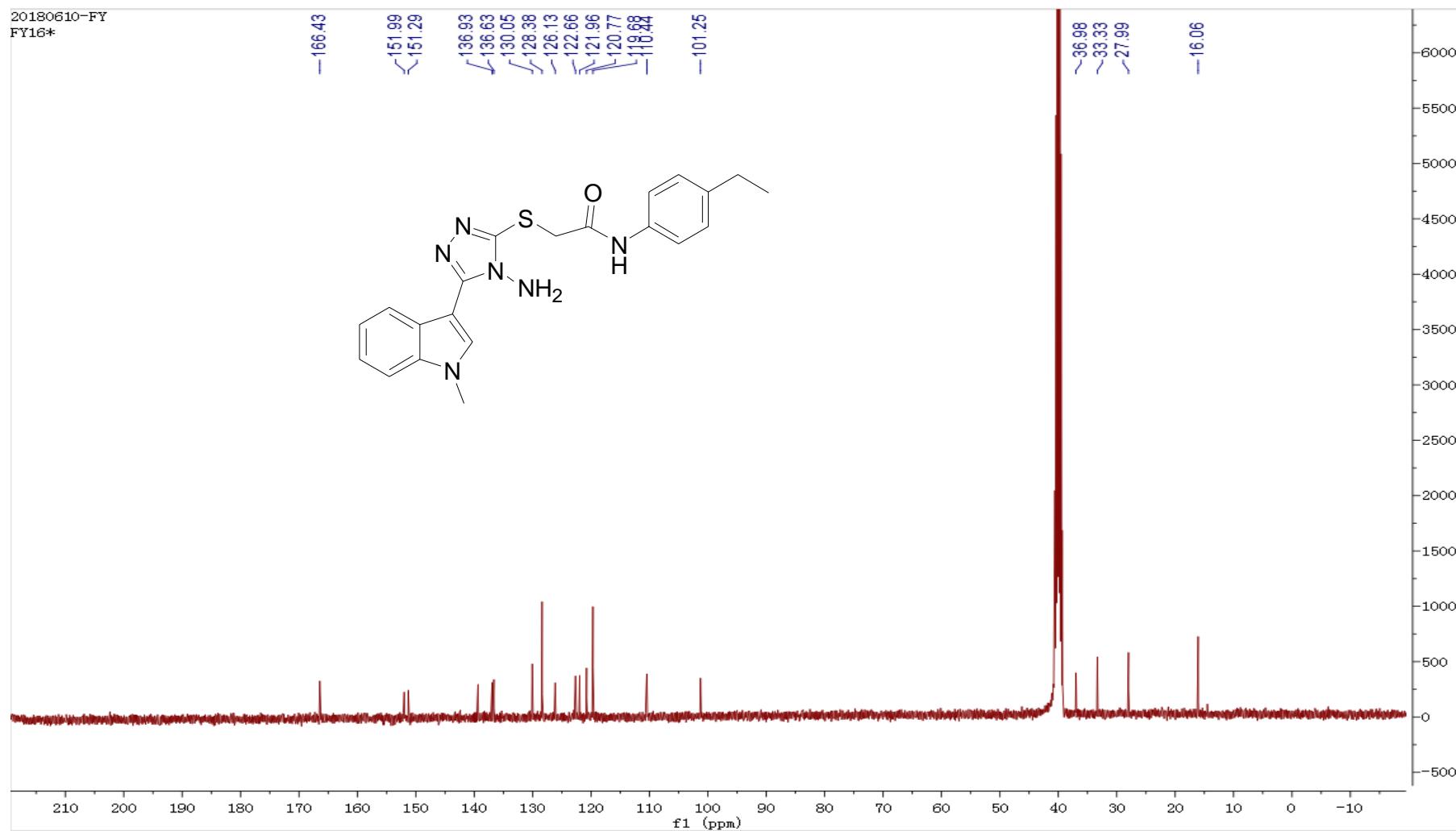


Figure 28. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9n**.

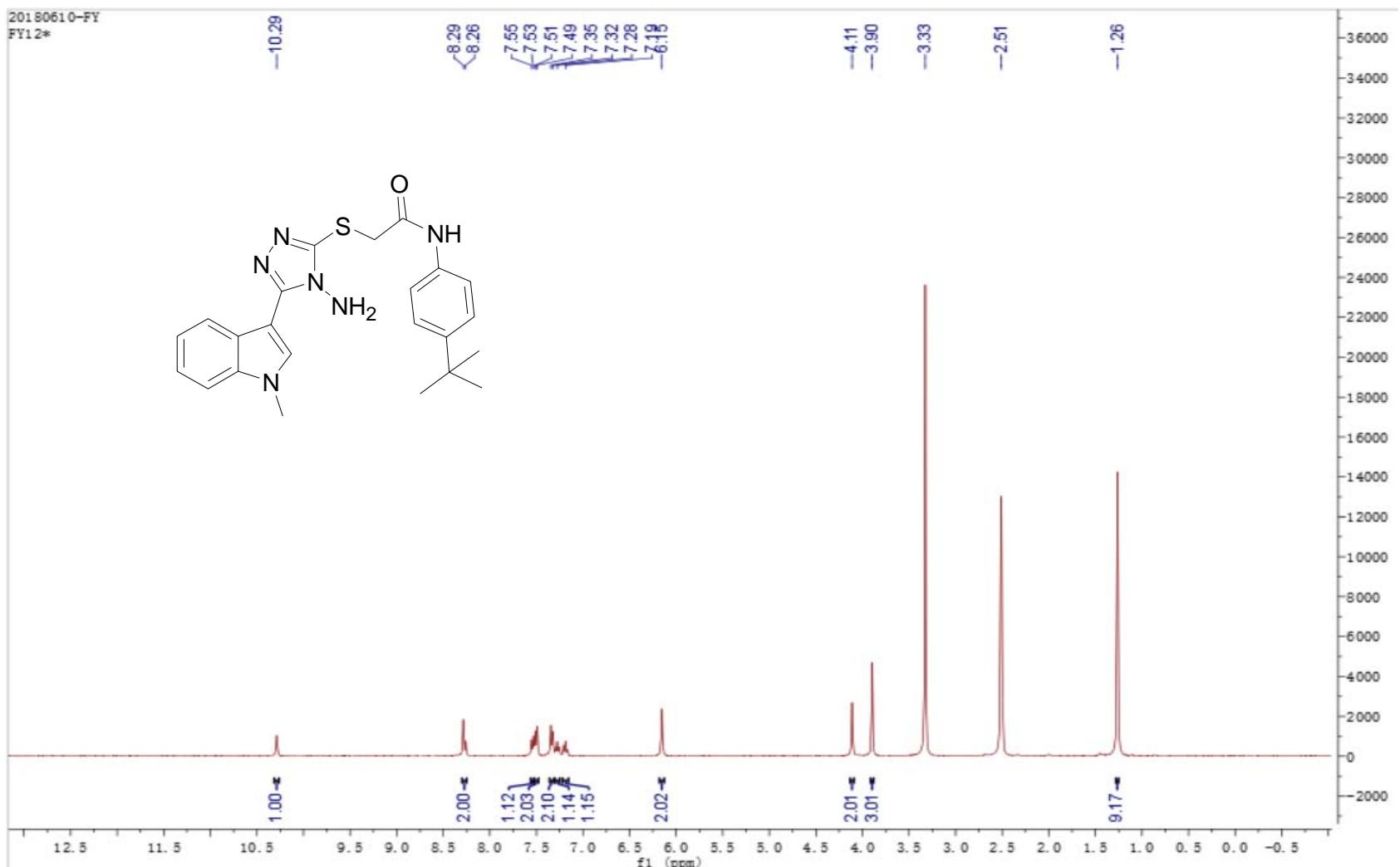


Figure 29. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 9o.

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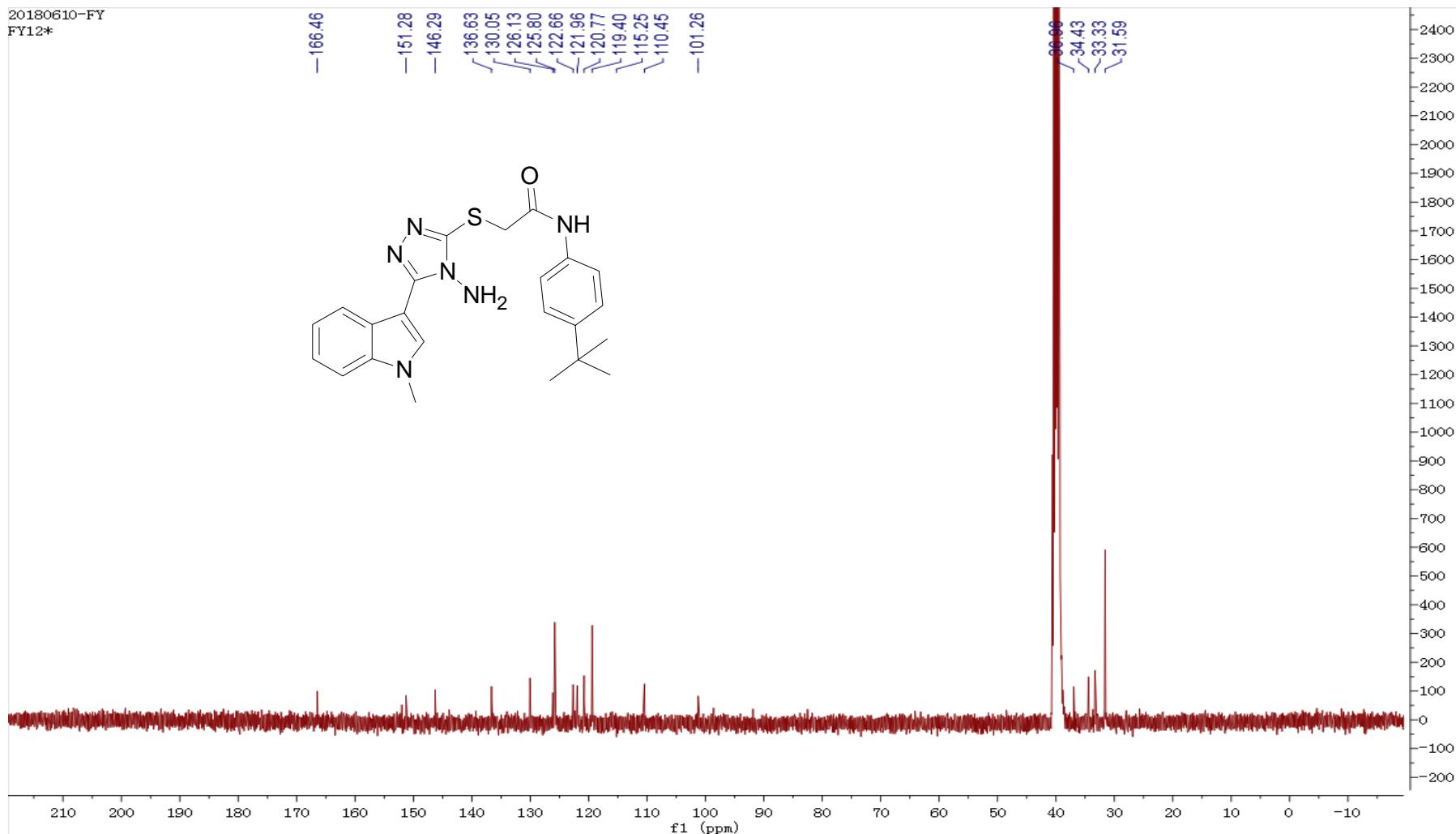


Figure 30. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9o**.

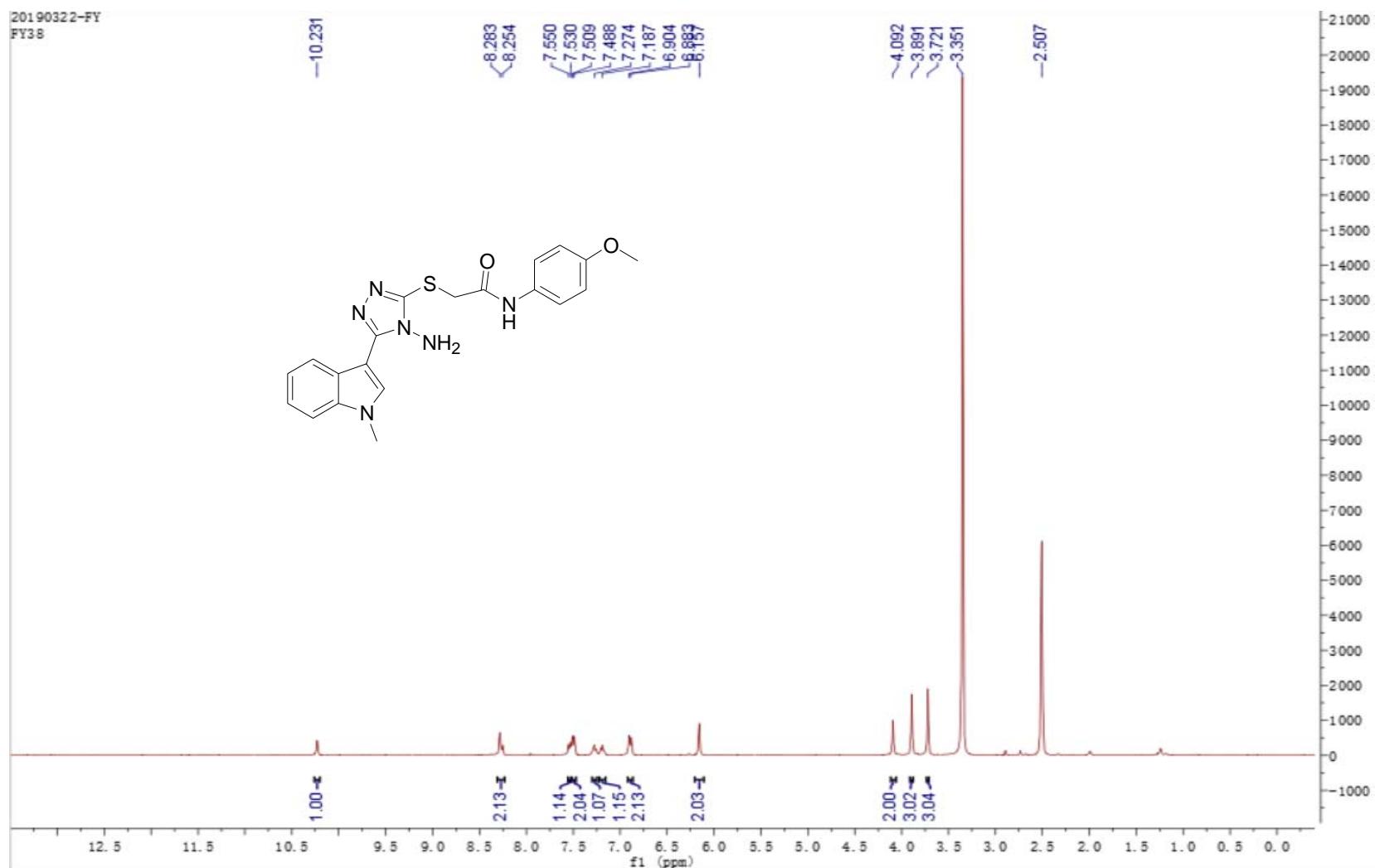


Figure 31. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 9p.

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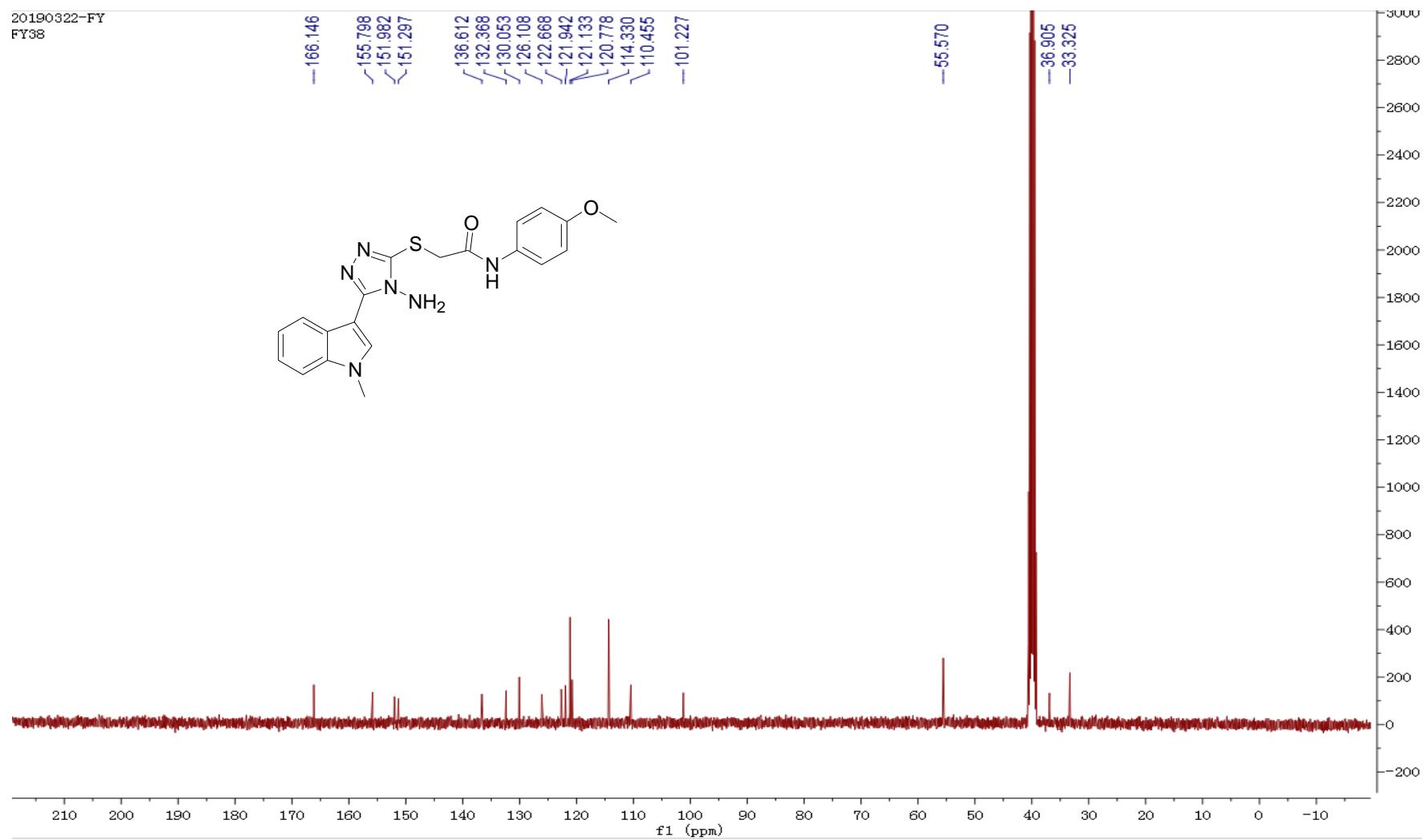


Figure 32. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9p**.

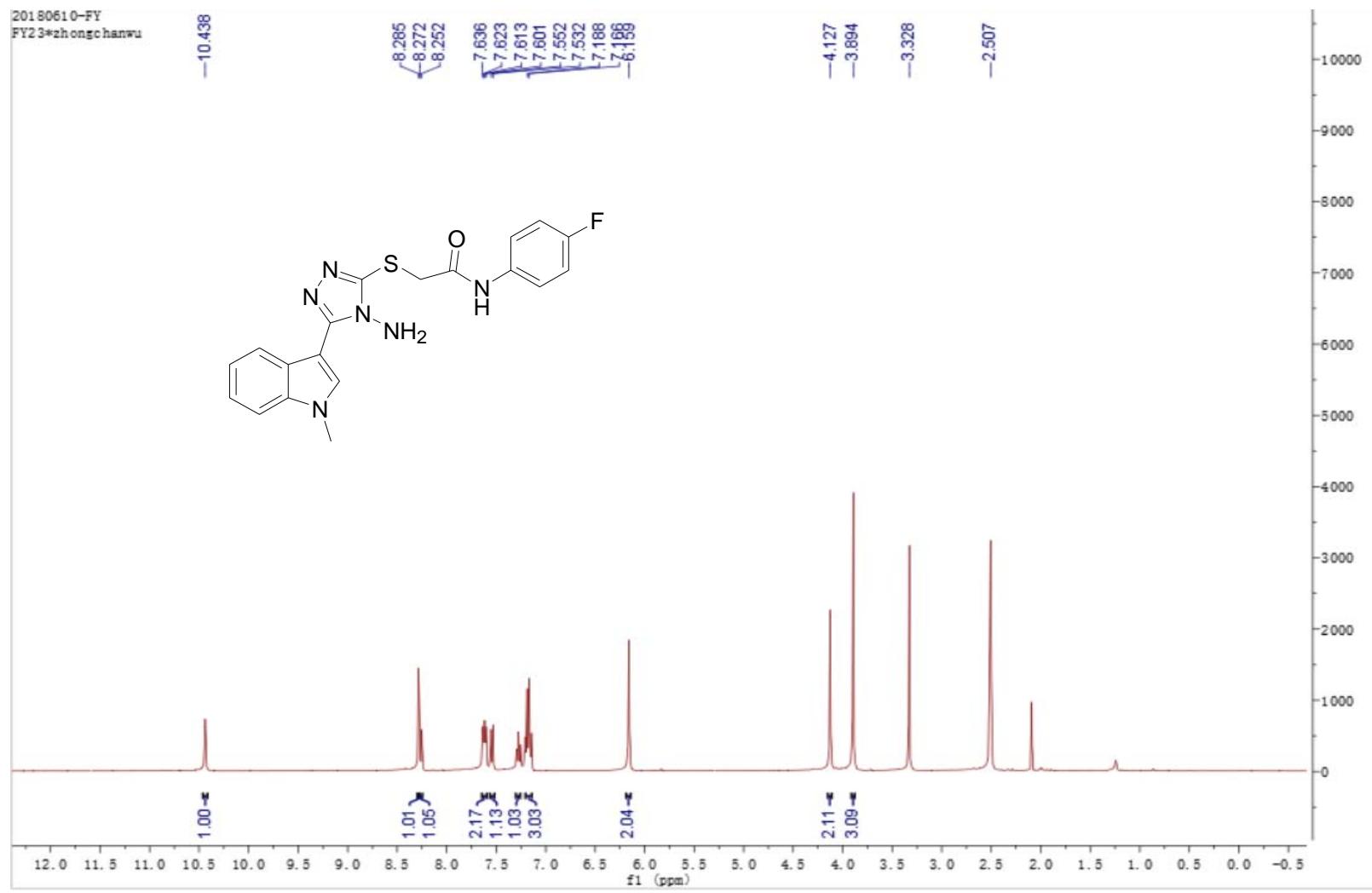


Figure 33. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound 9q.

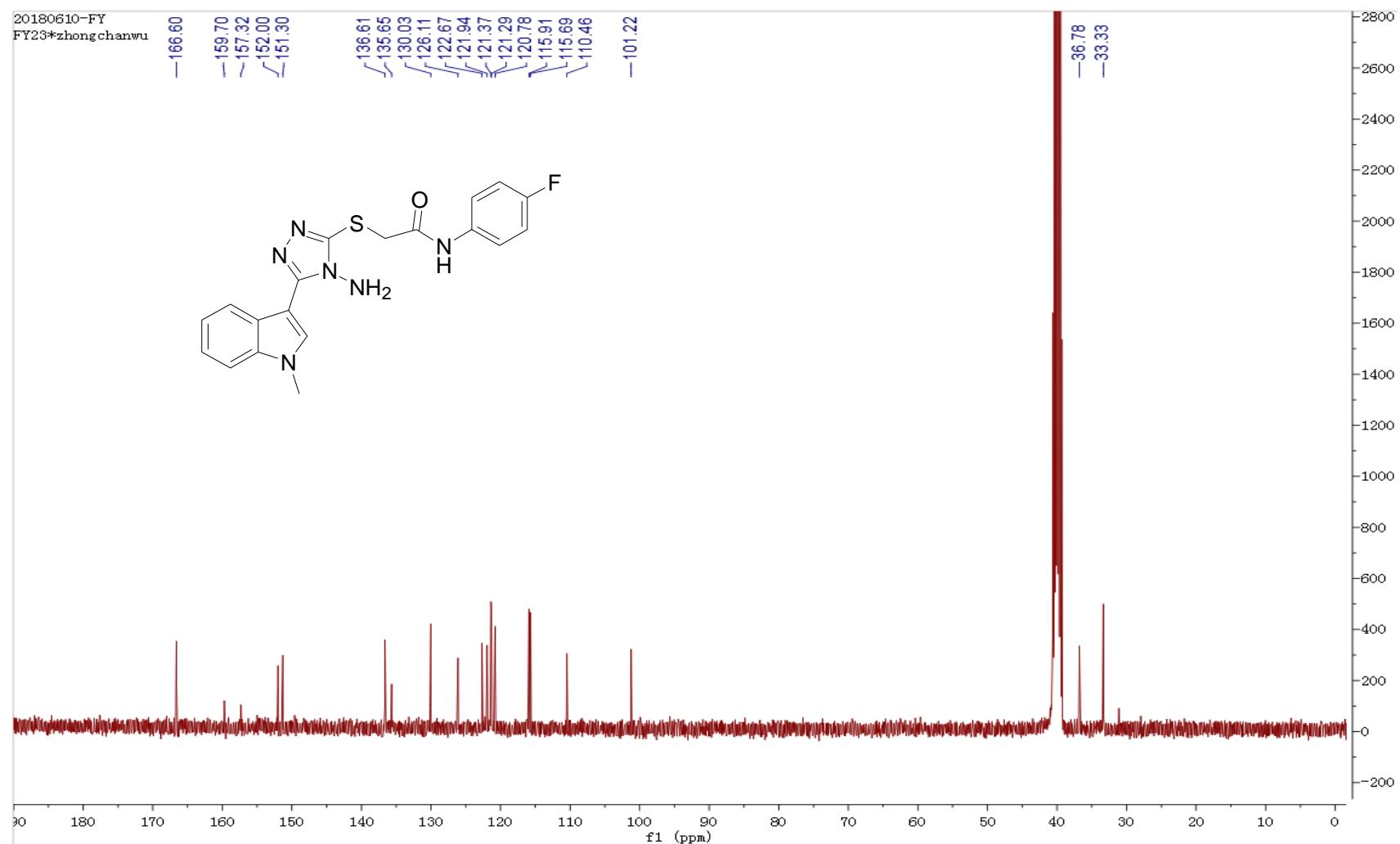


Figure 34. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9q**.

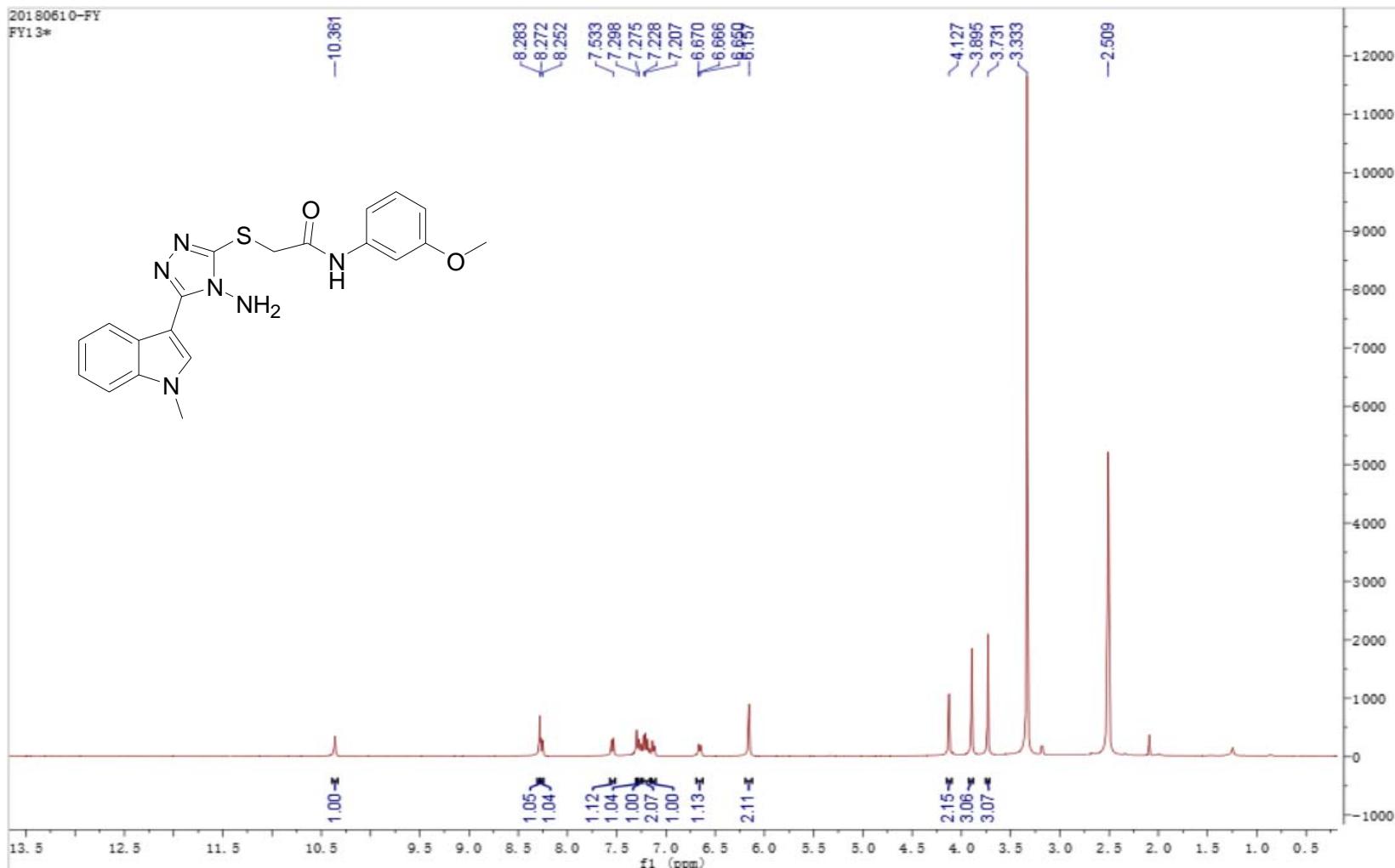


Figure 35. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **9r**.

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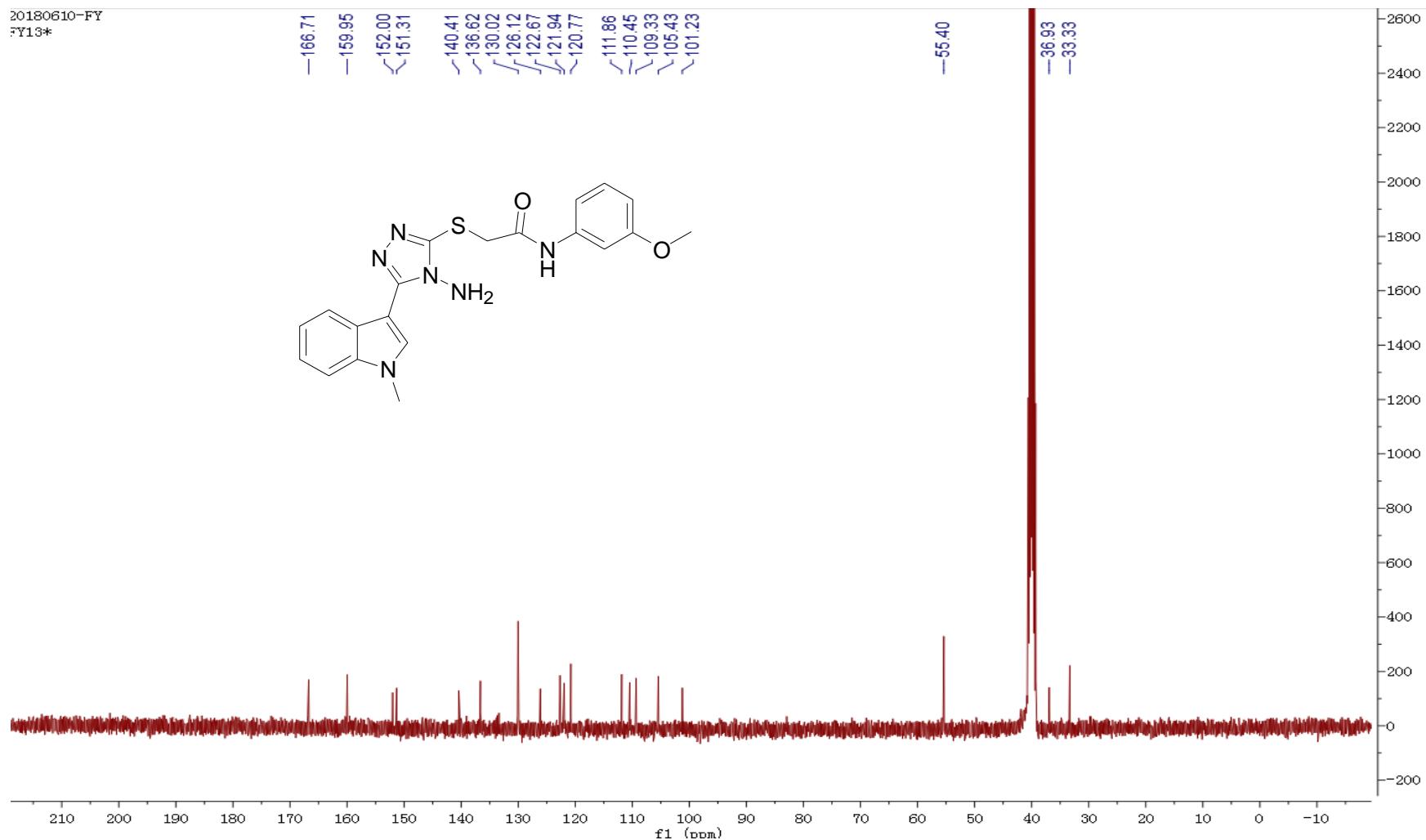


Figure 36. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9r**.

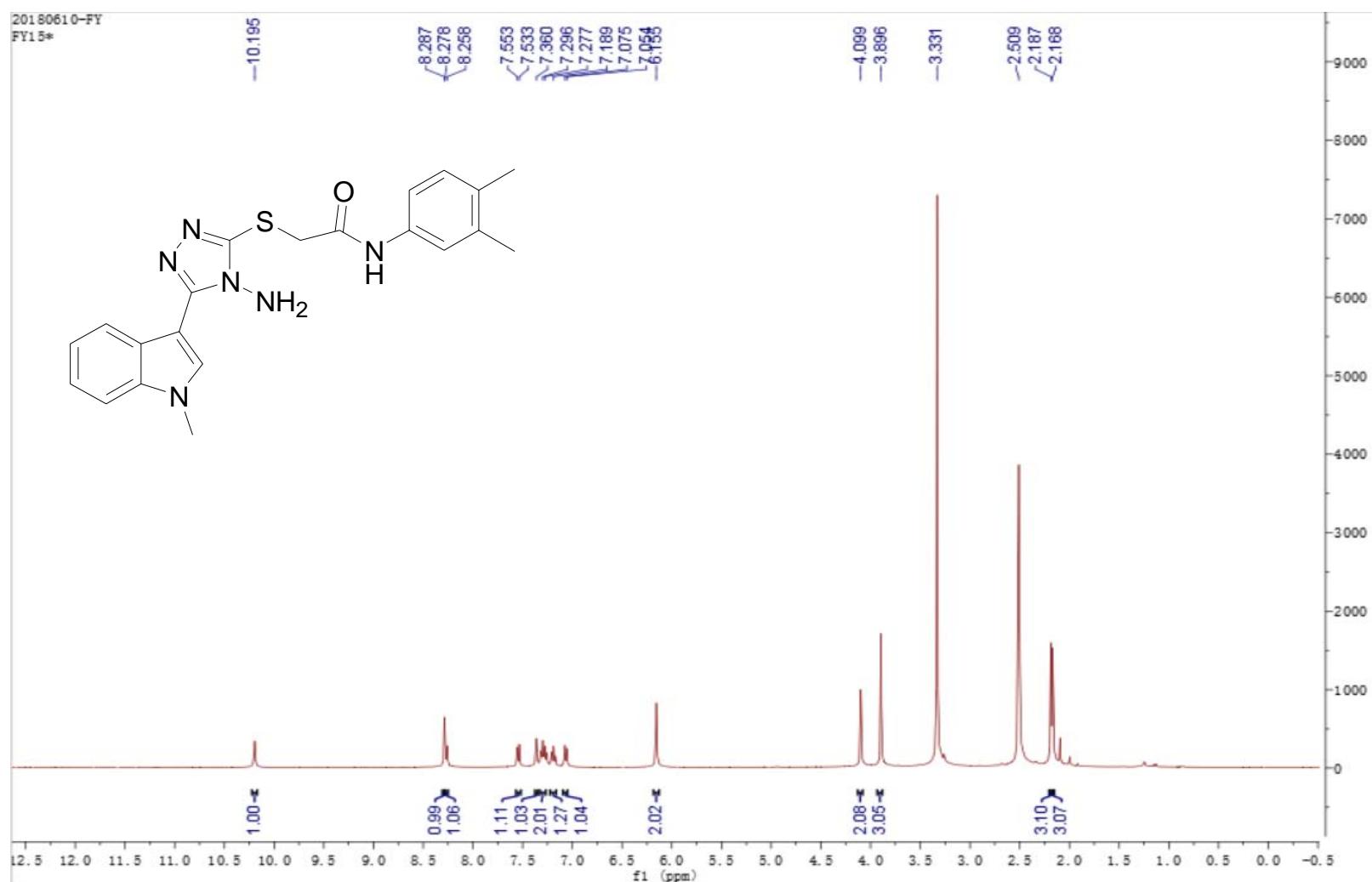


Figure 37. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **9s**.

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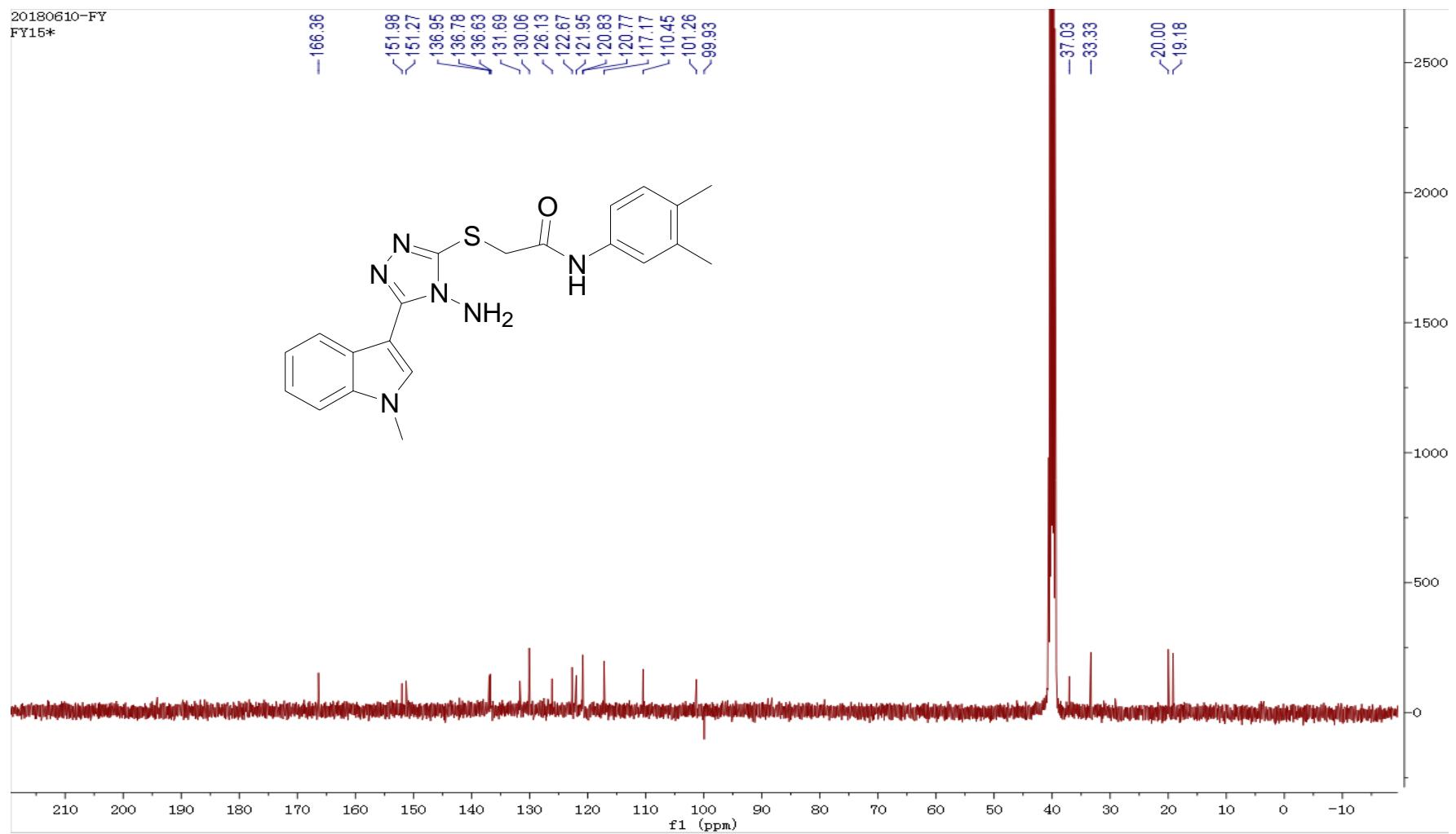


Figure 38. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **9s**.

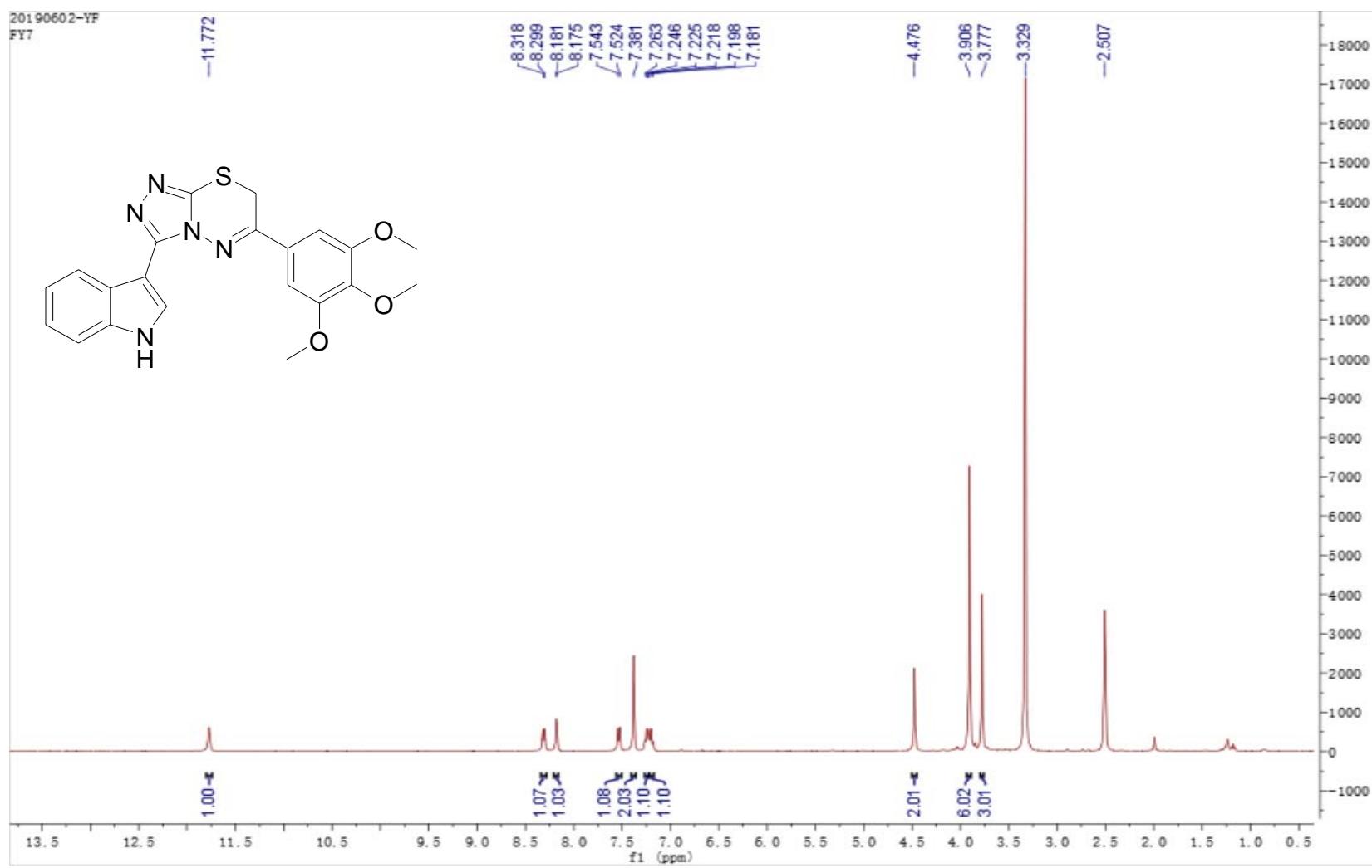


Figure 39. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **10a**.

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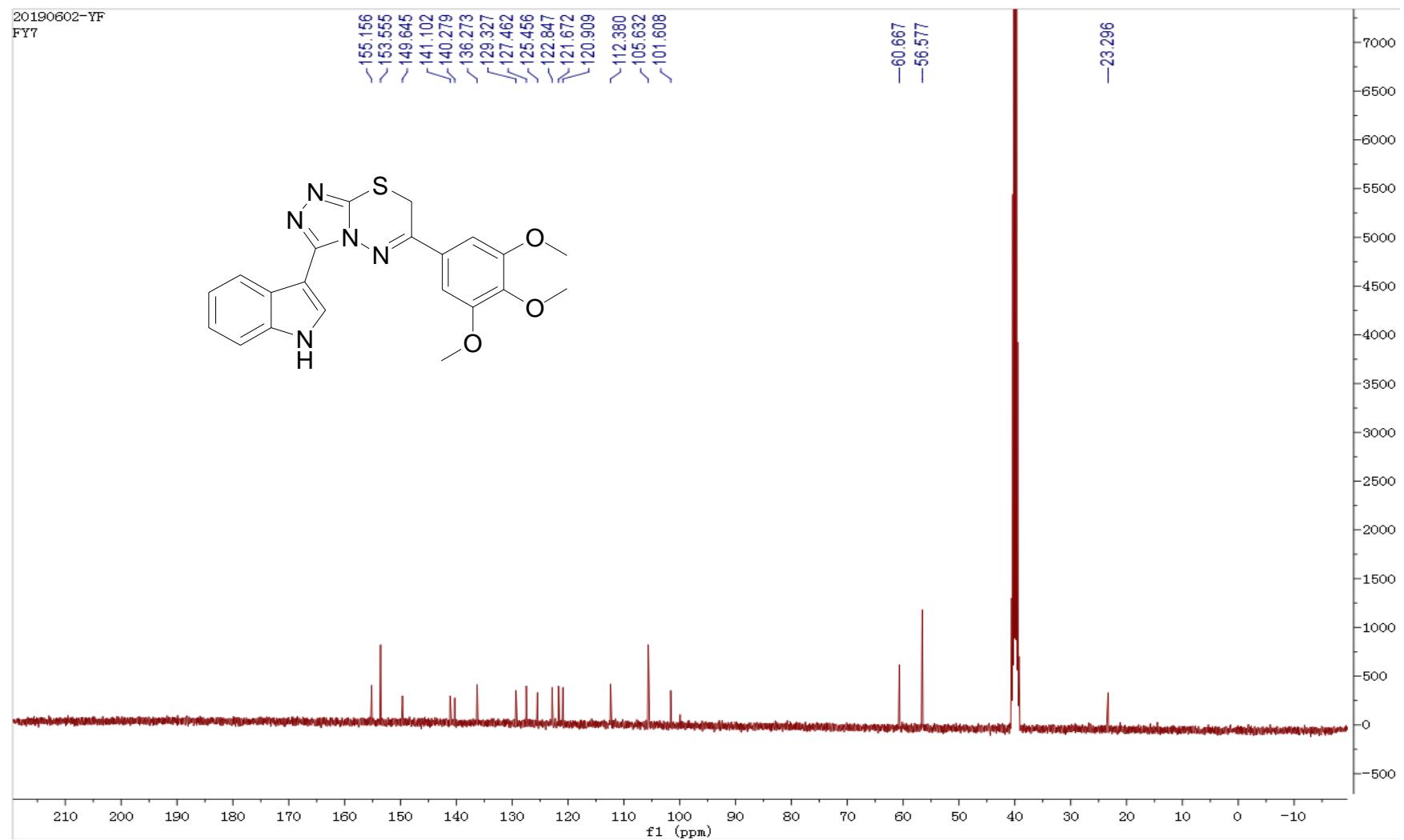
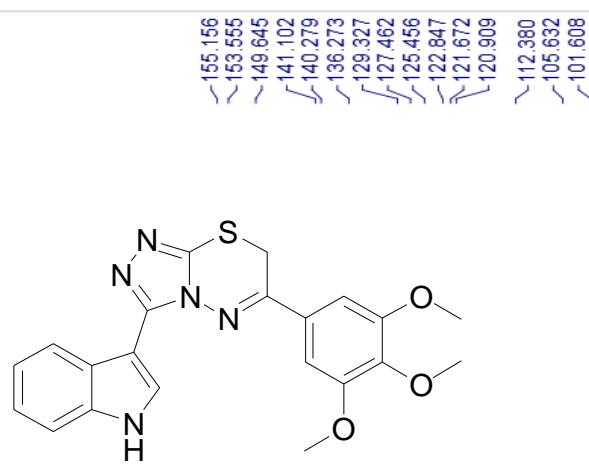


Figure 40. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound 10a.

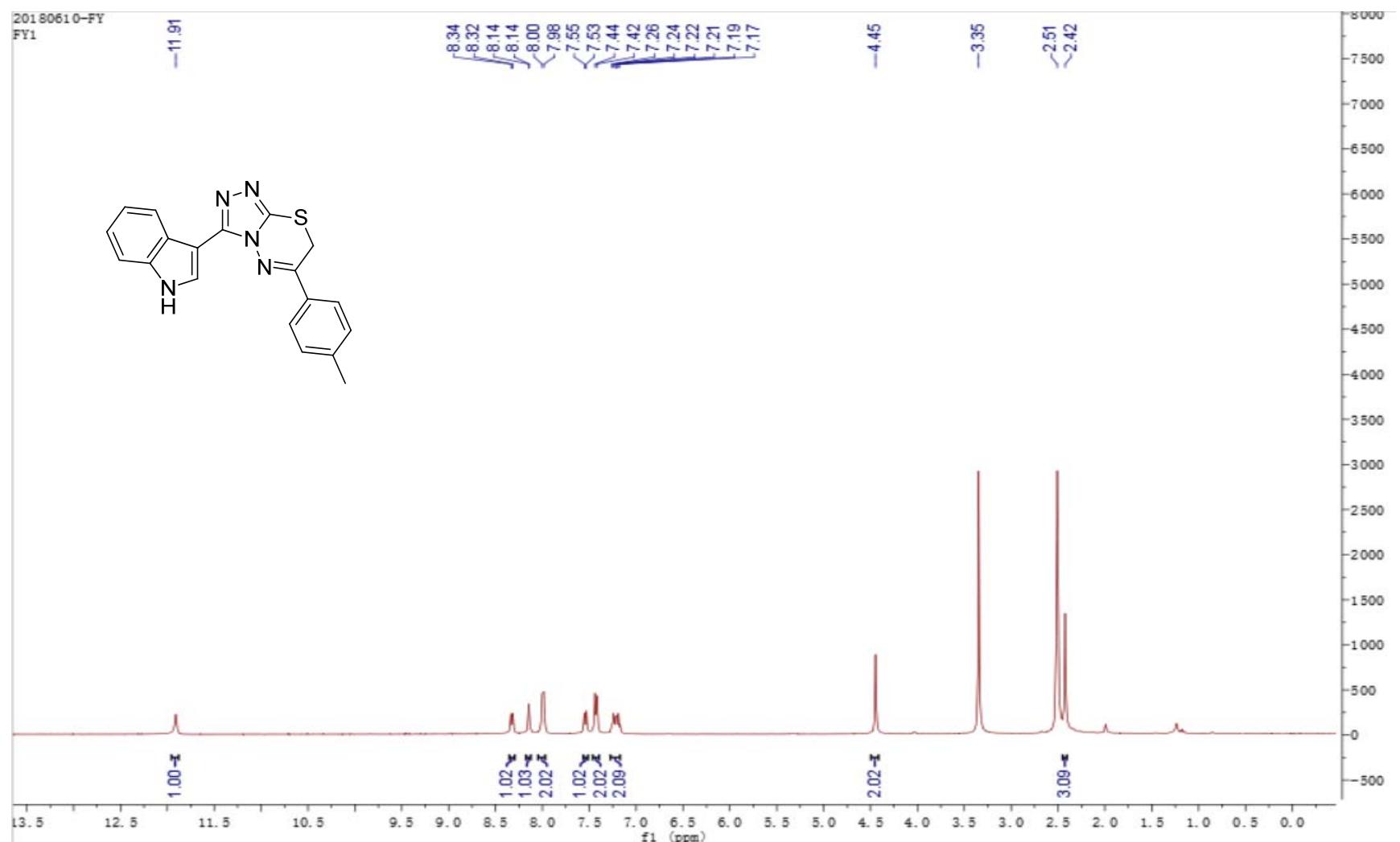


Figure 41. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **10b**.

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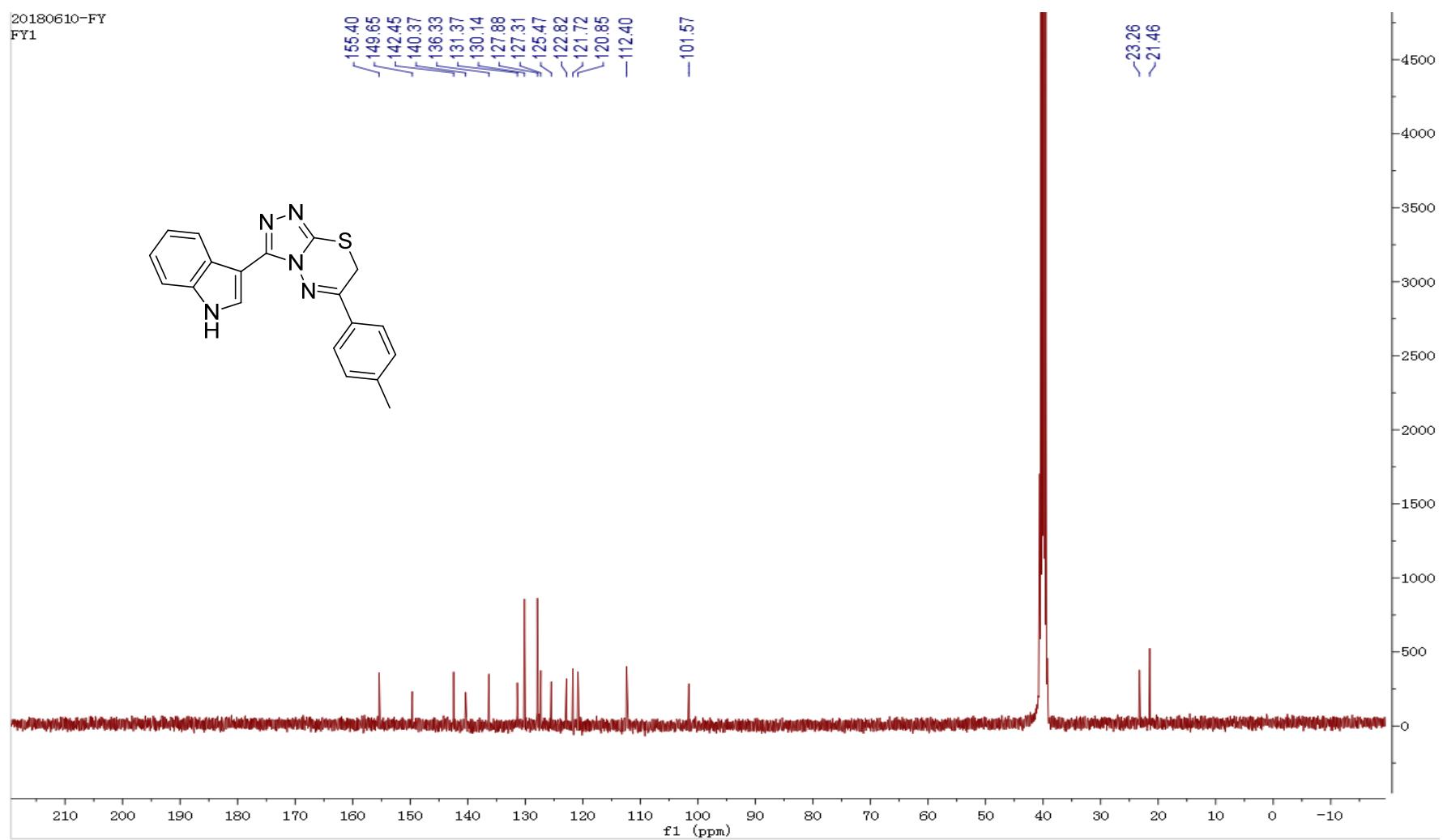


Figure 42. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10b**.

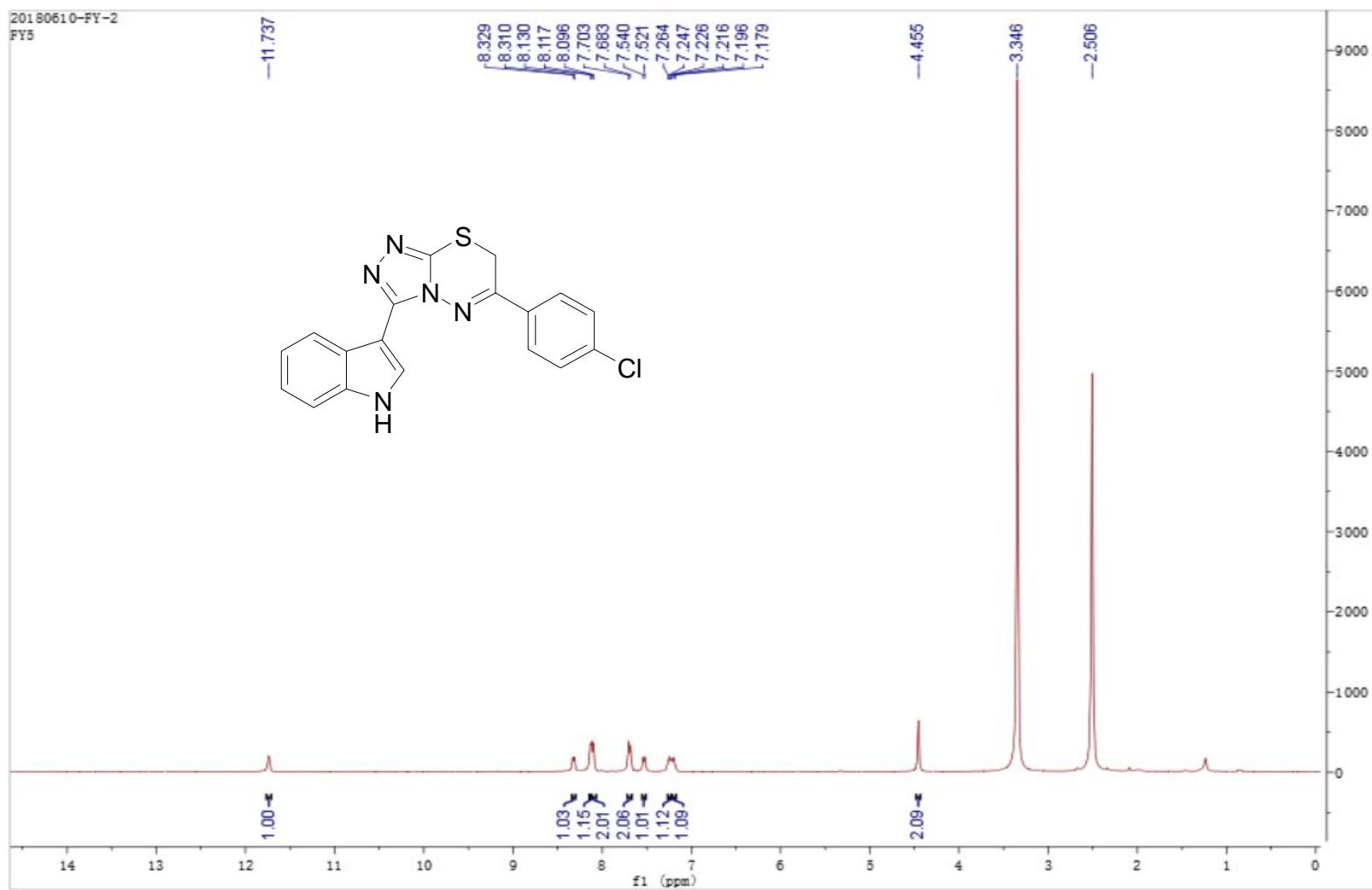


Figure 43. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **10c**.

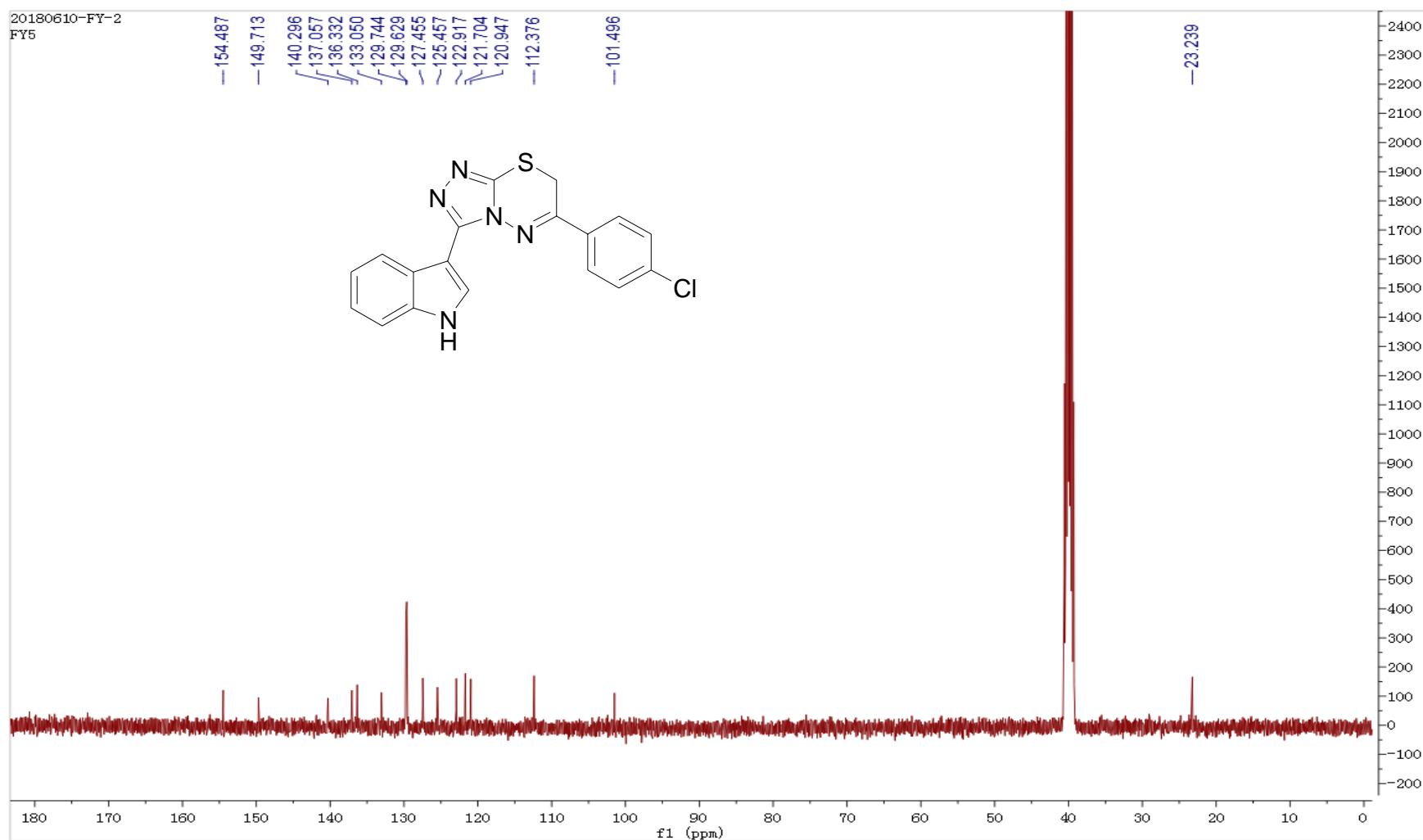


Figure 44. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10c**.

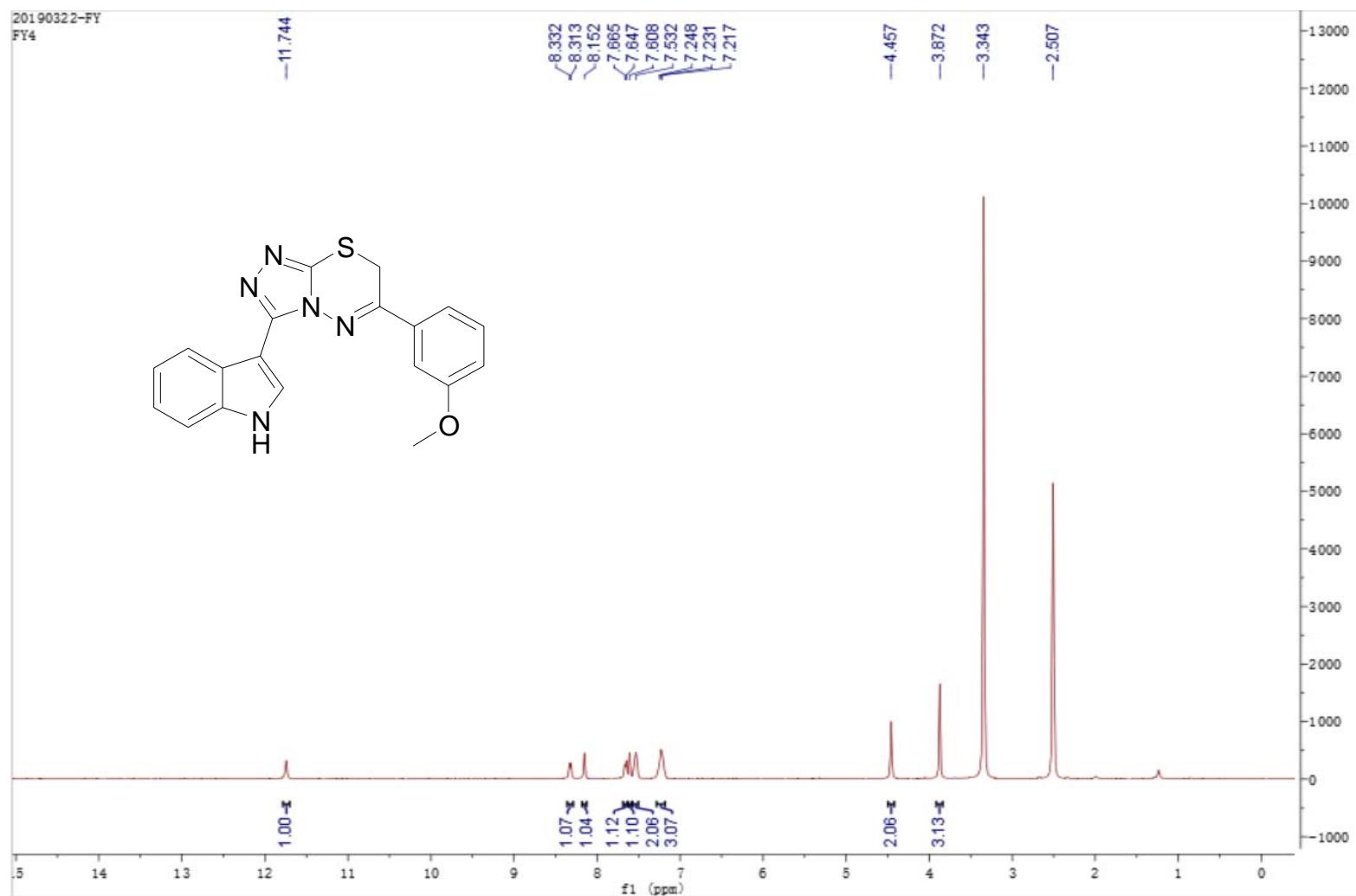


Figure 45. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound 10d.

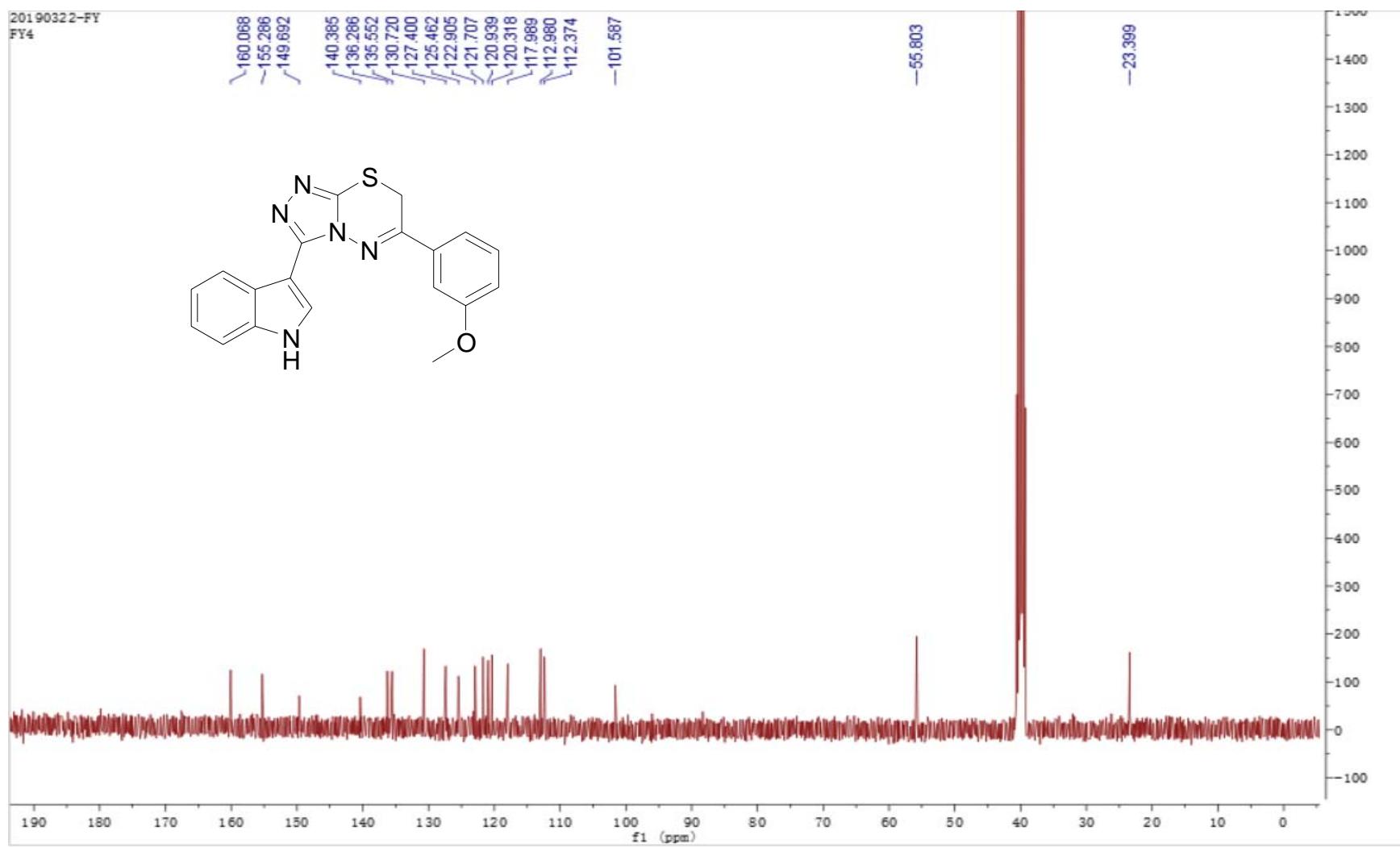


Figure 46. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of compound **10d**.

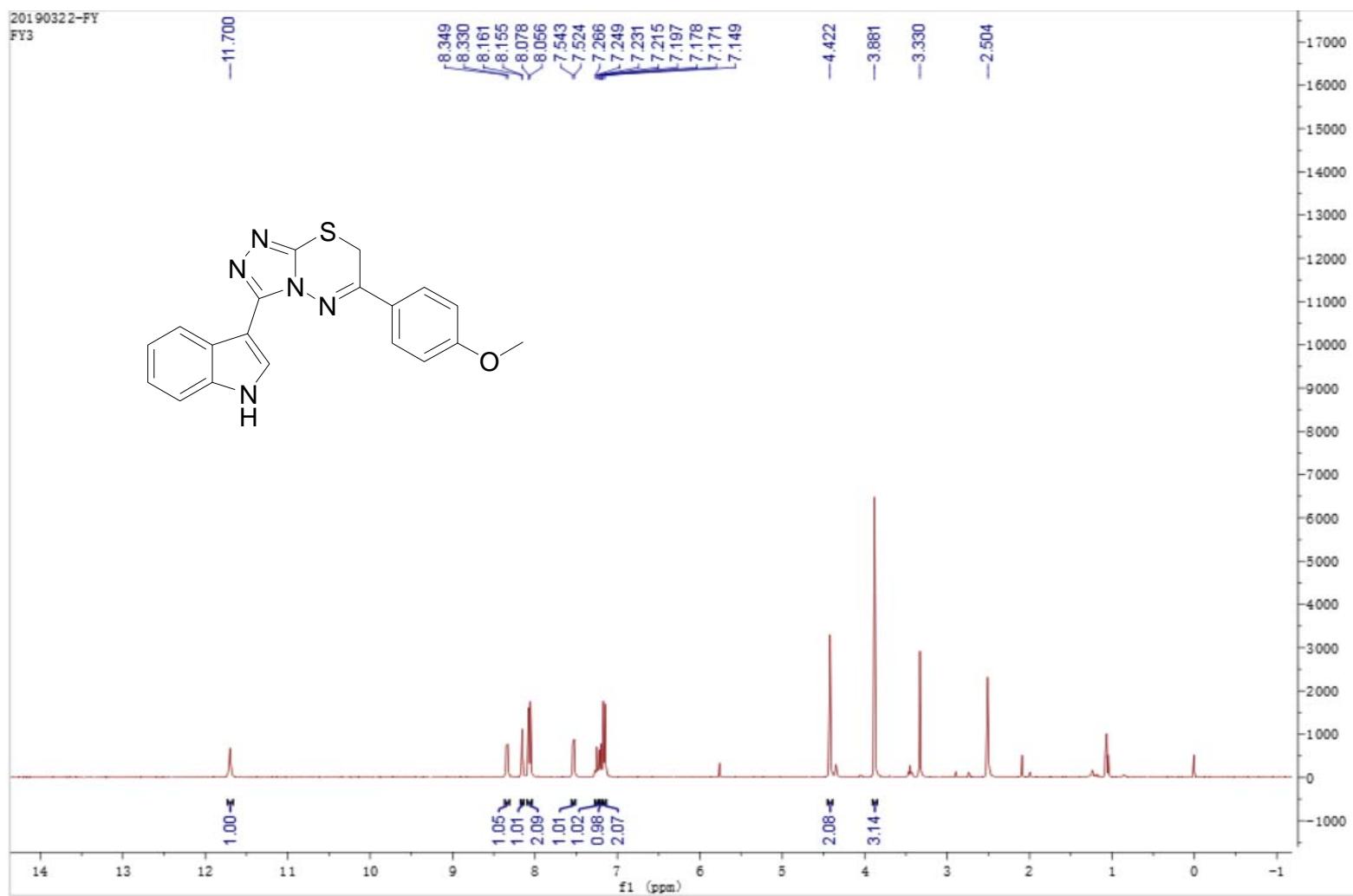


Figure 47. ¹H NMR spectrum (400 MHz, DMSO- *d*₆) of compound **10e**.

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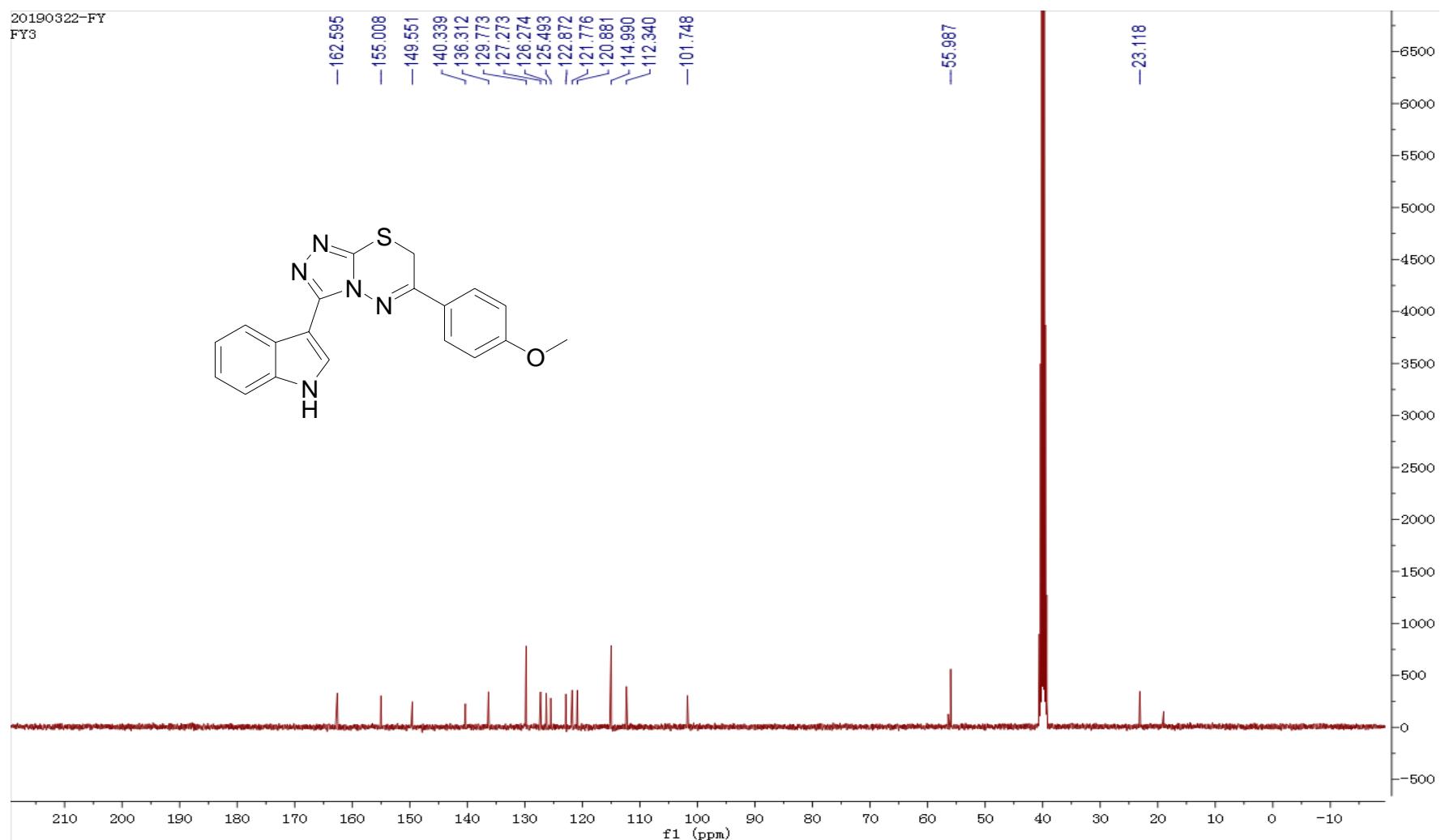


Figure 48. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10e**.

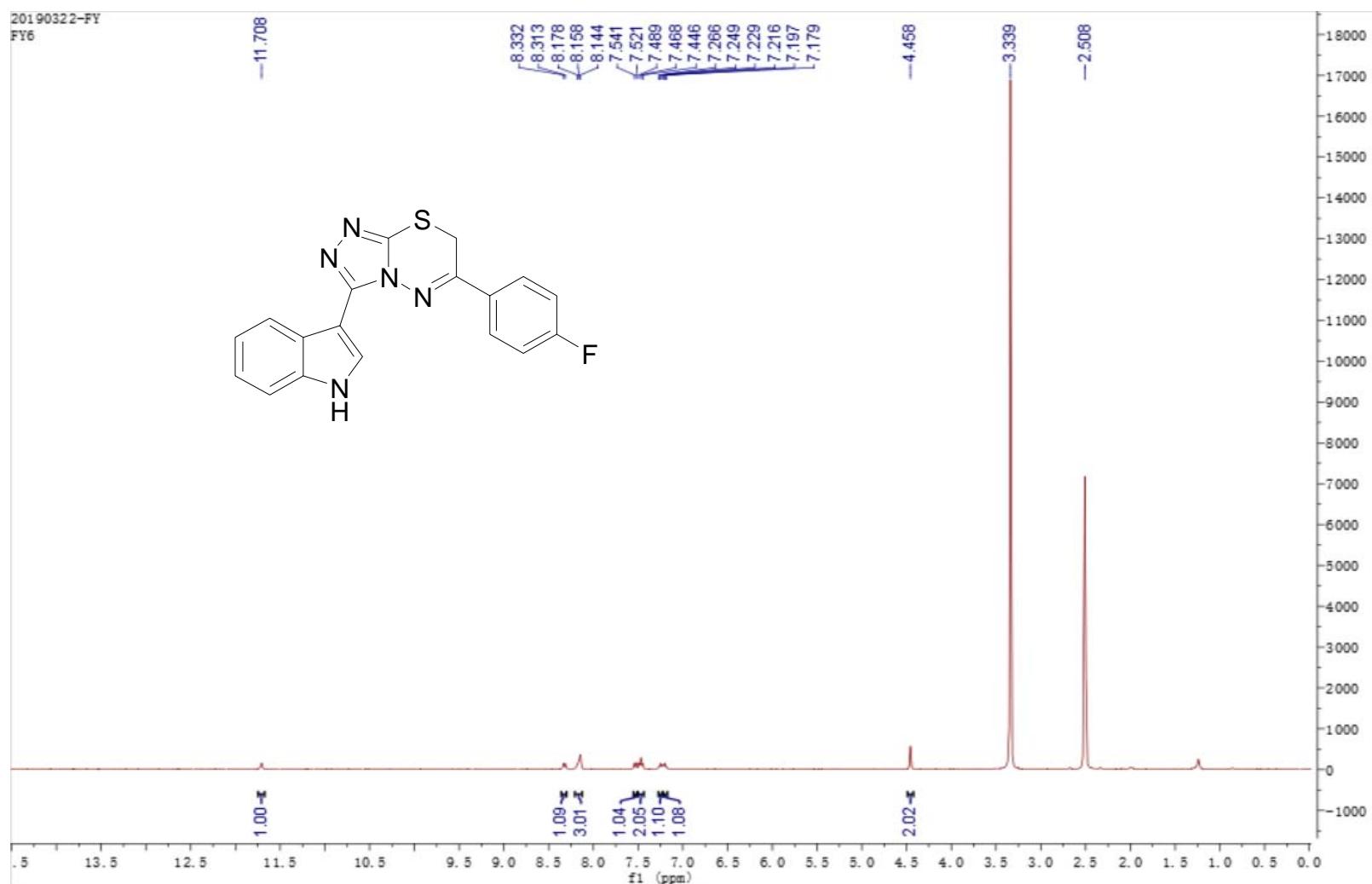


Figure 49. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound **10f**.

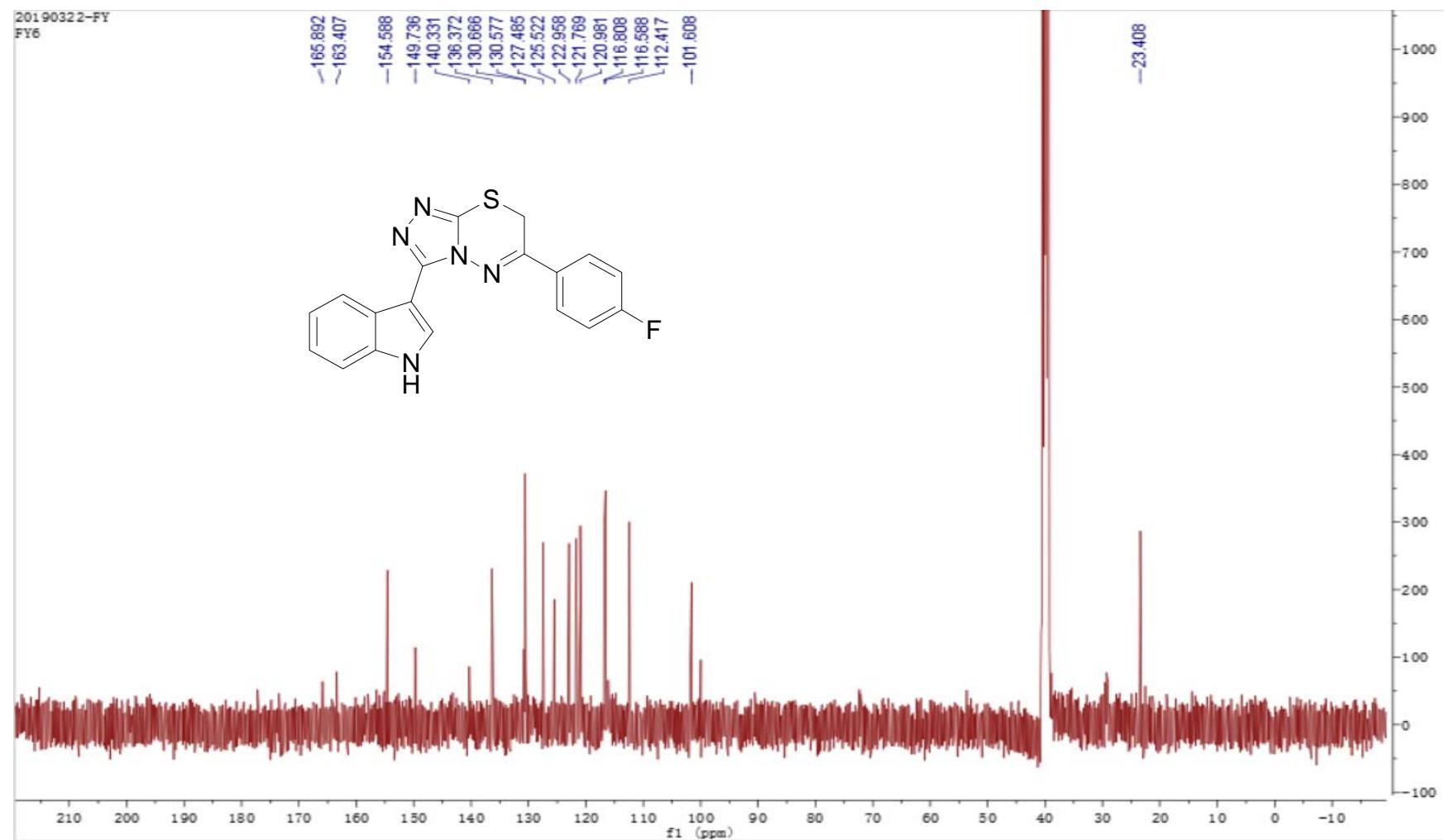


Figure 50. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10f**.

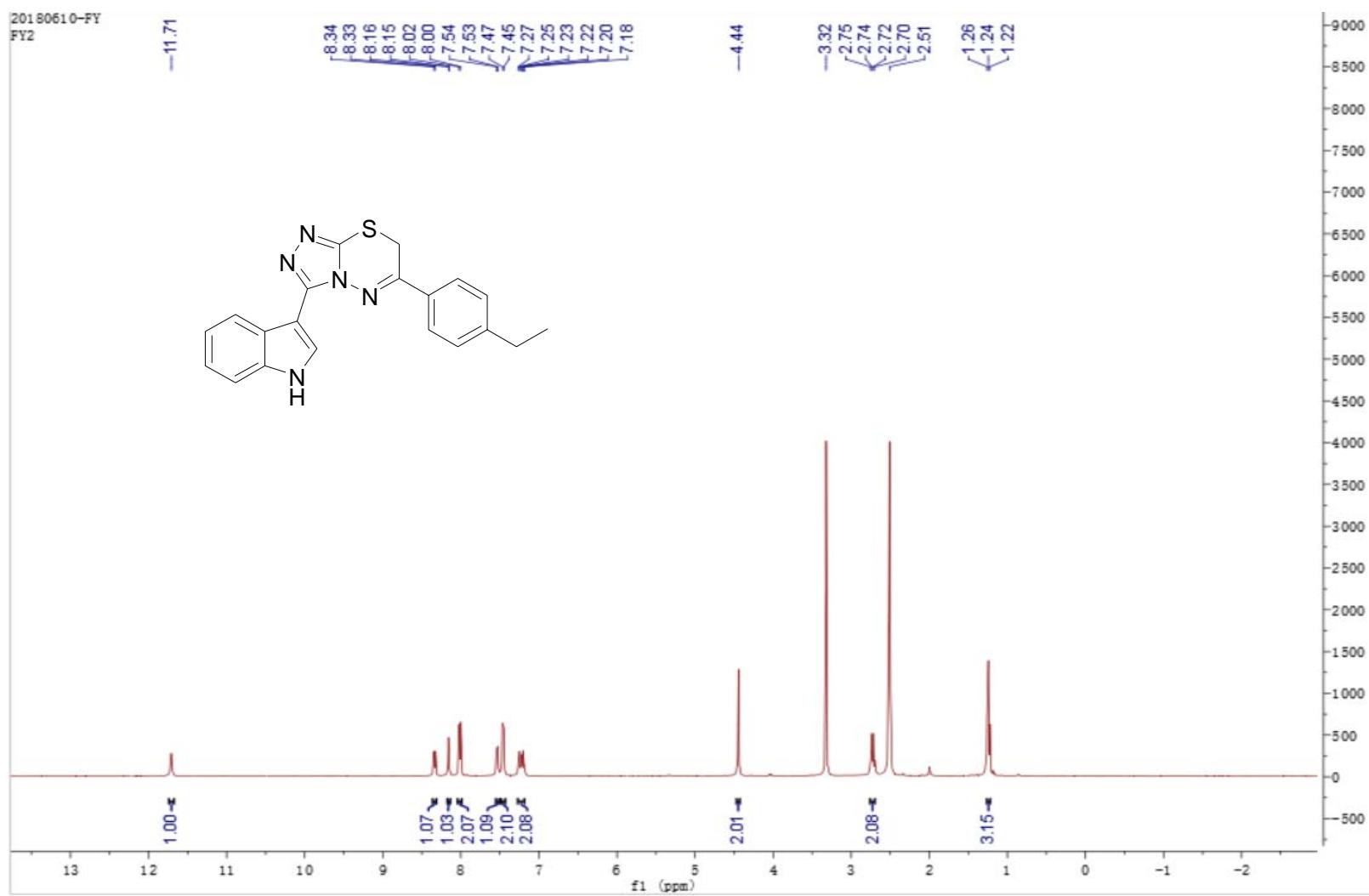


Figure 51. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **10g**.

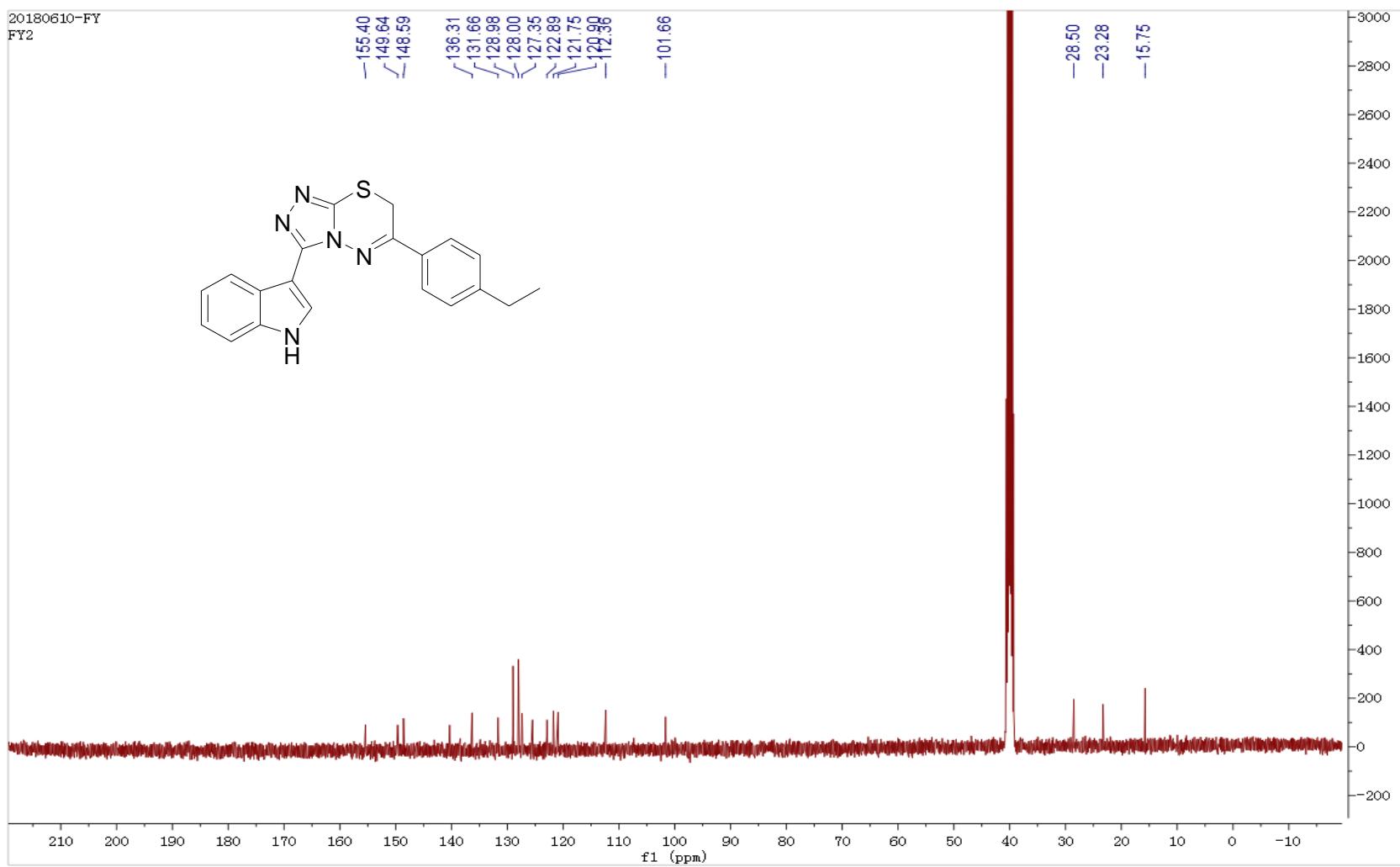


Figure 52. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10g**.

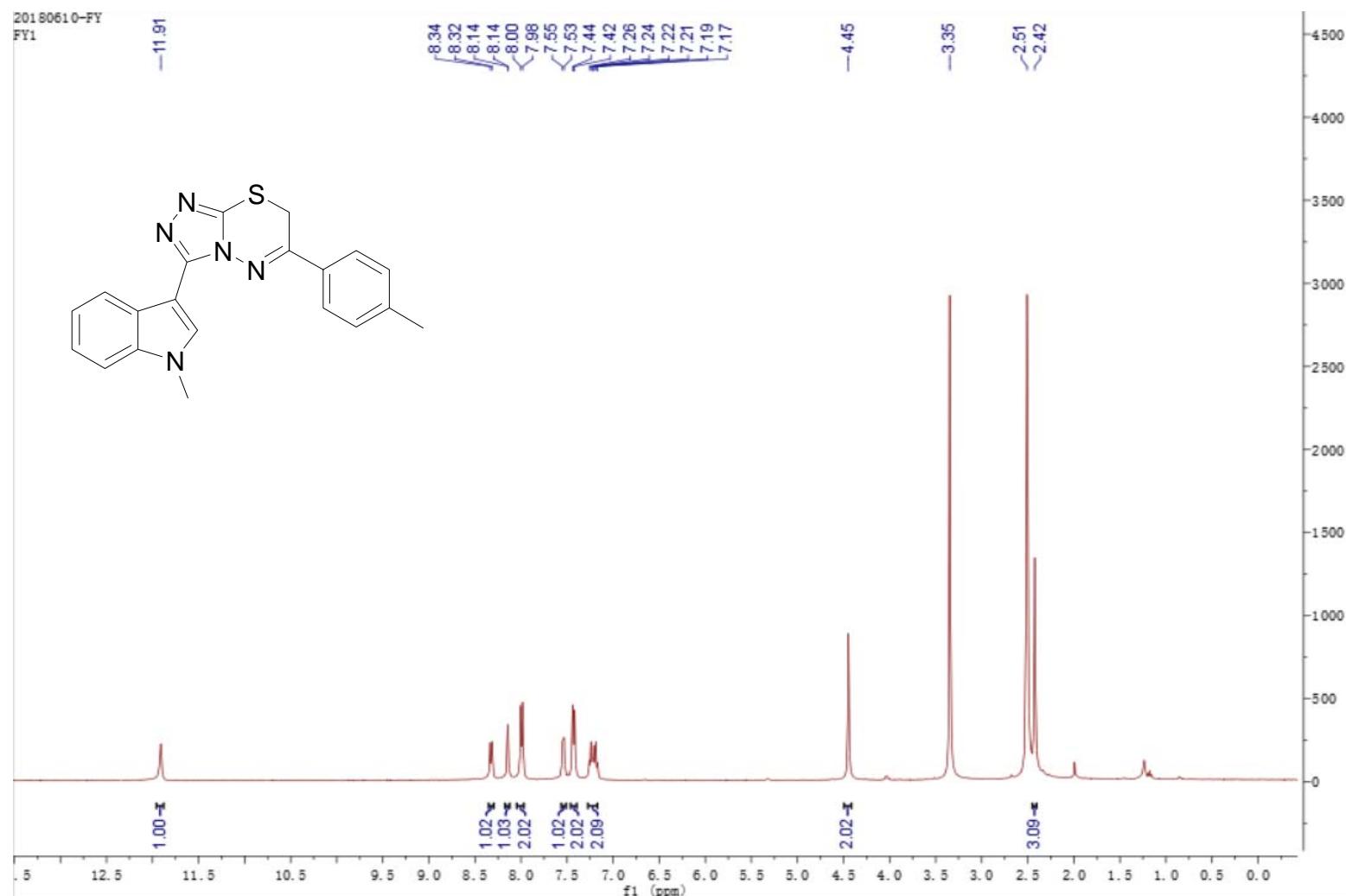


Figure 53. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **10h**.

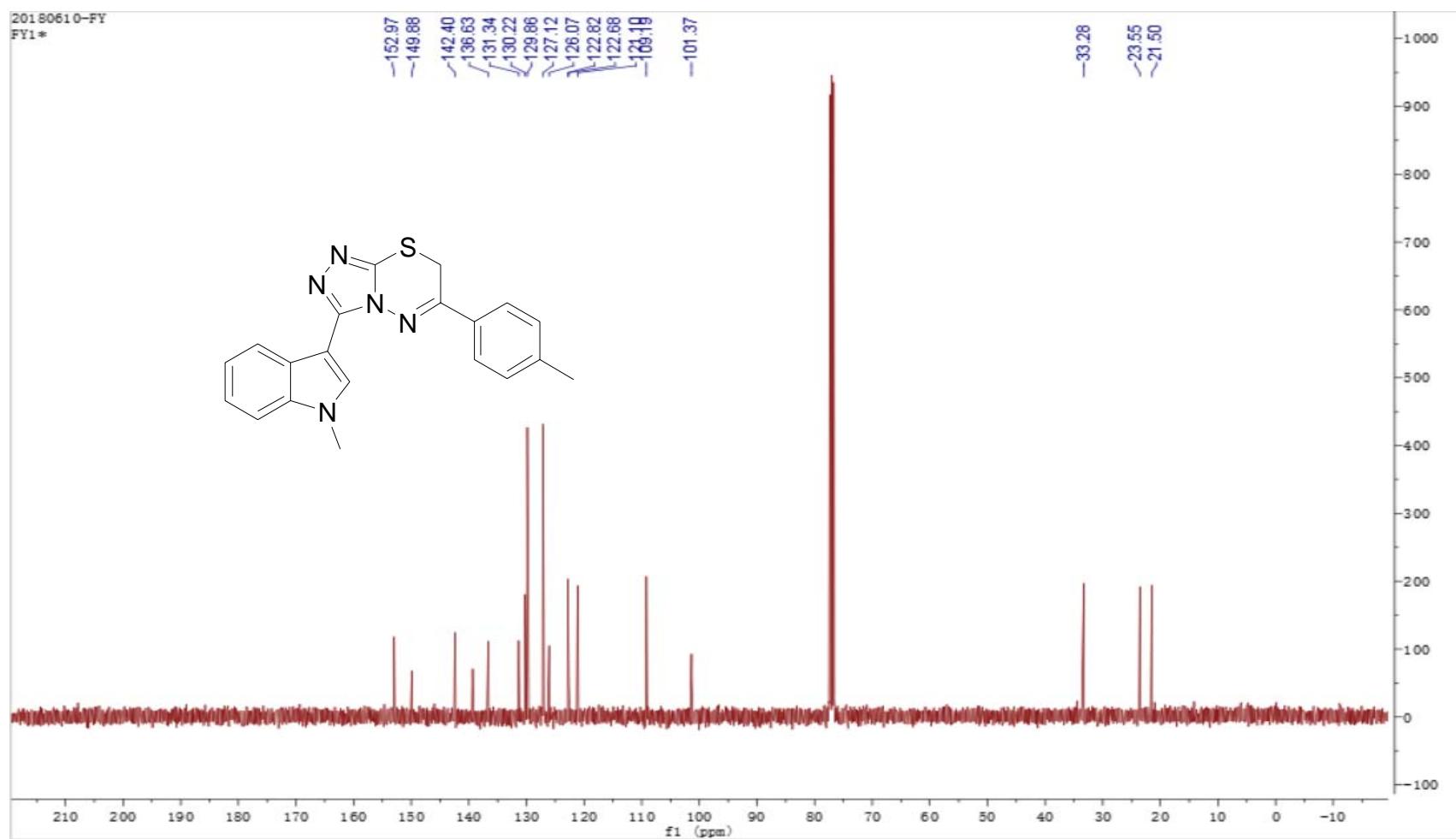


Figure 54. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **10h**.

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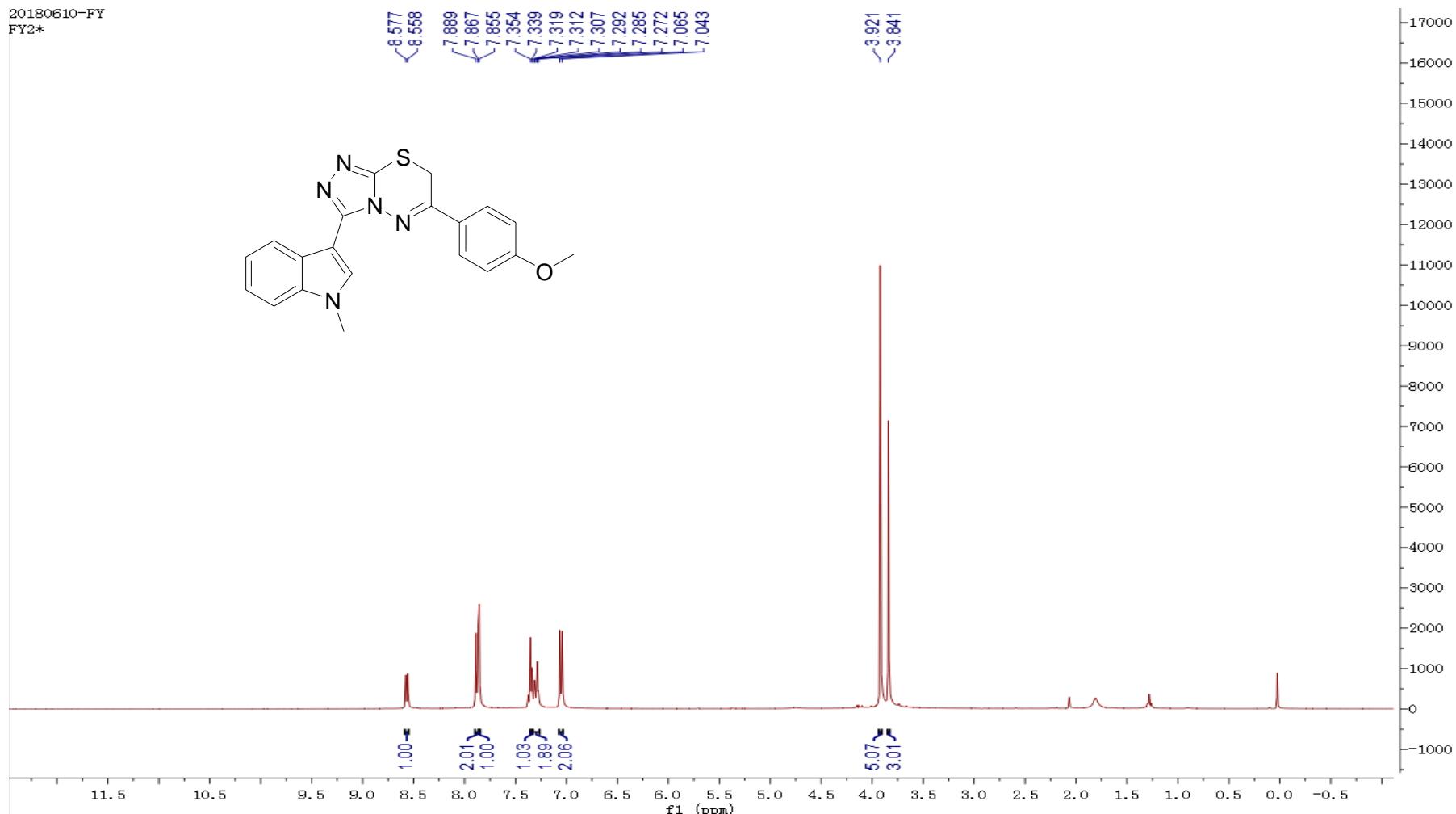
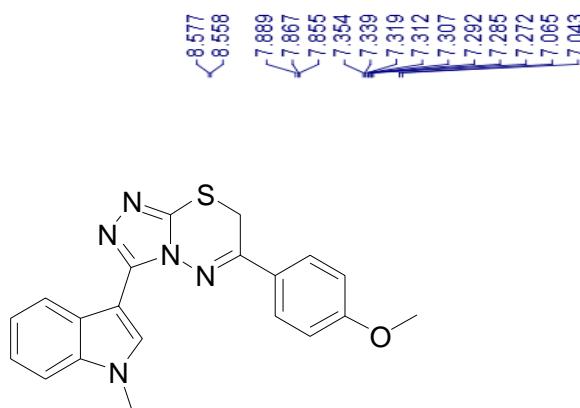


Figure 55. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **10i**.

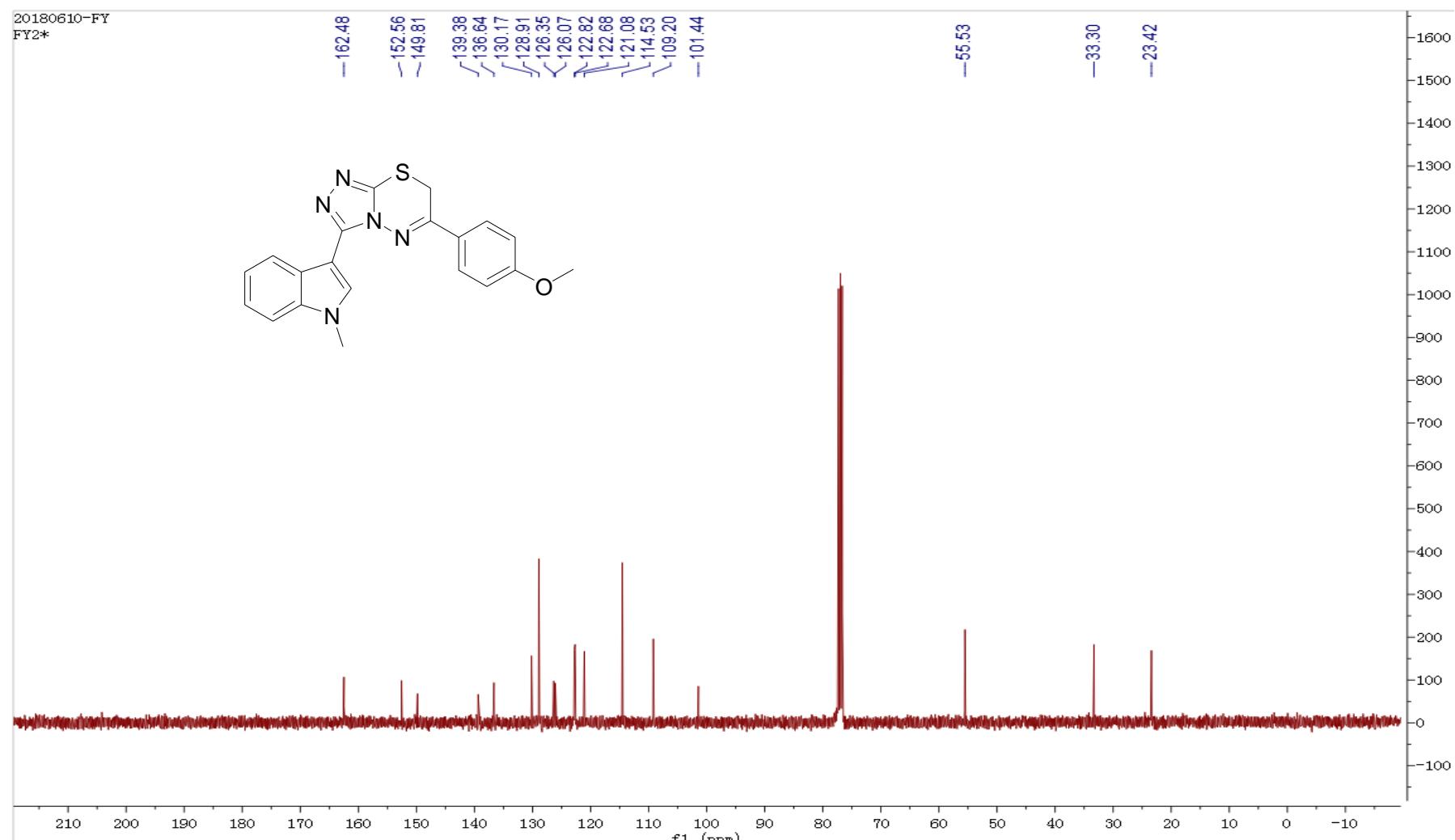


Figure 56. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **10i**.

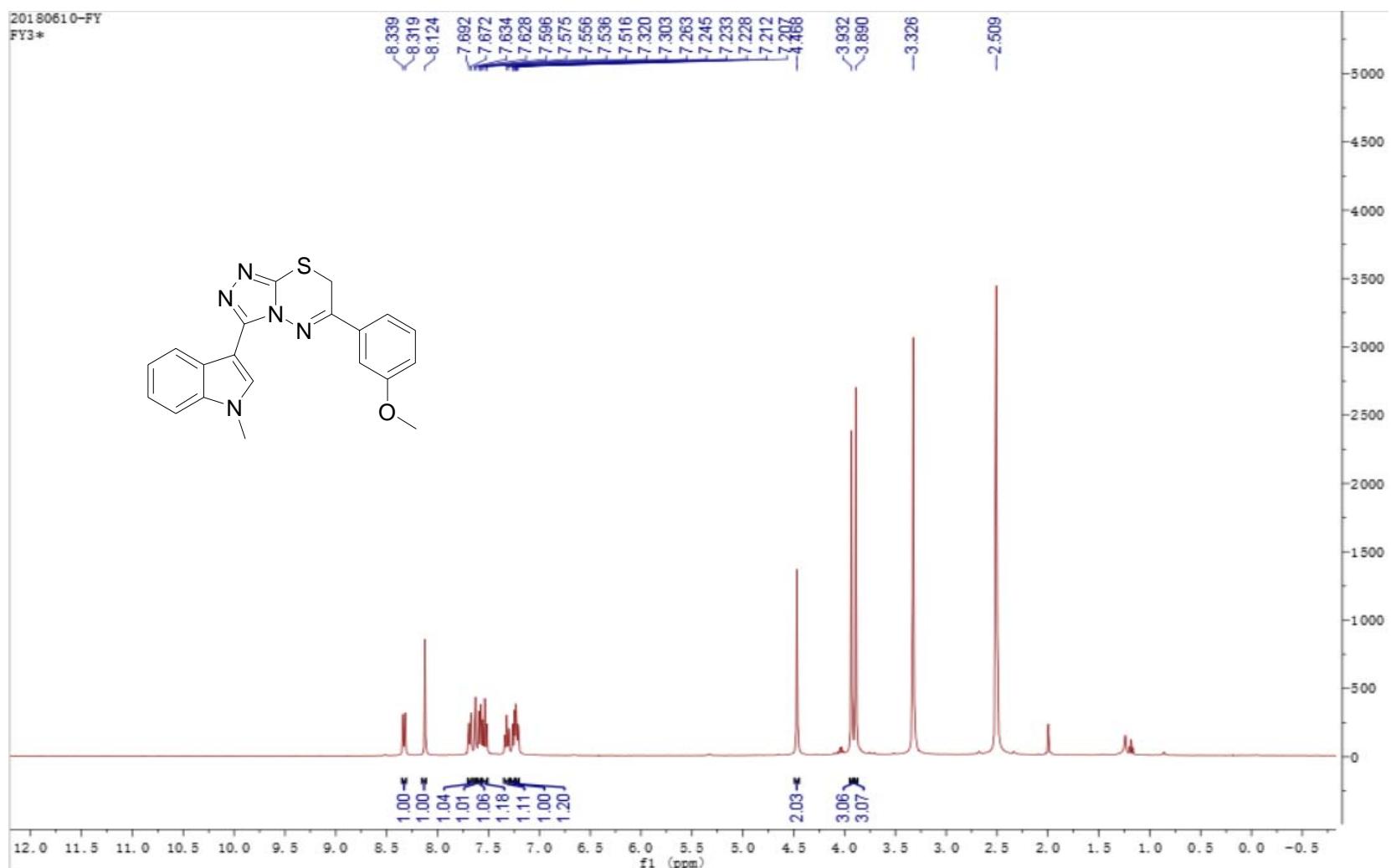


Figure 57. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 10j.

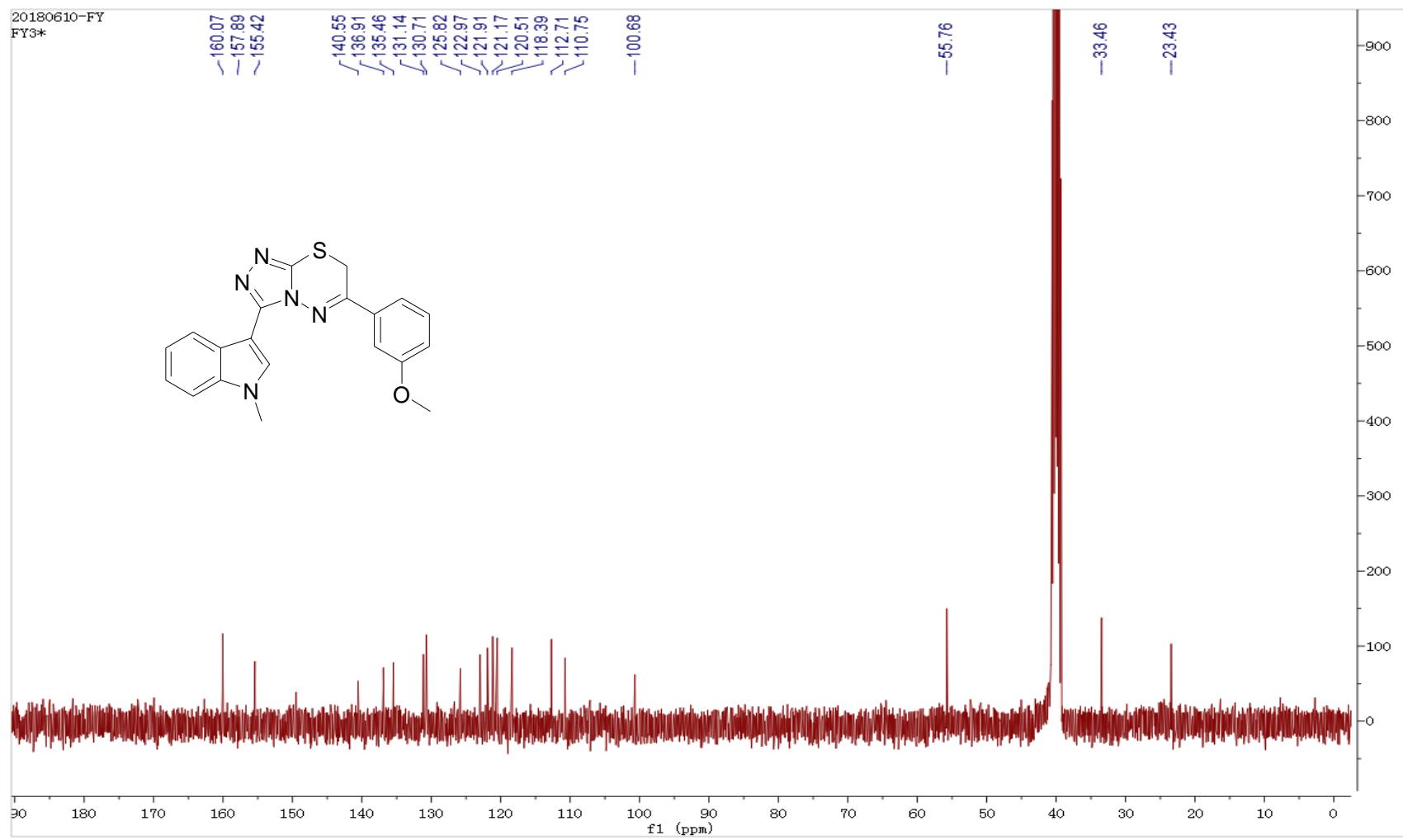


Figure 58. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **10j**.

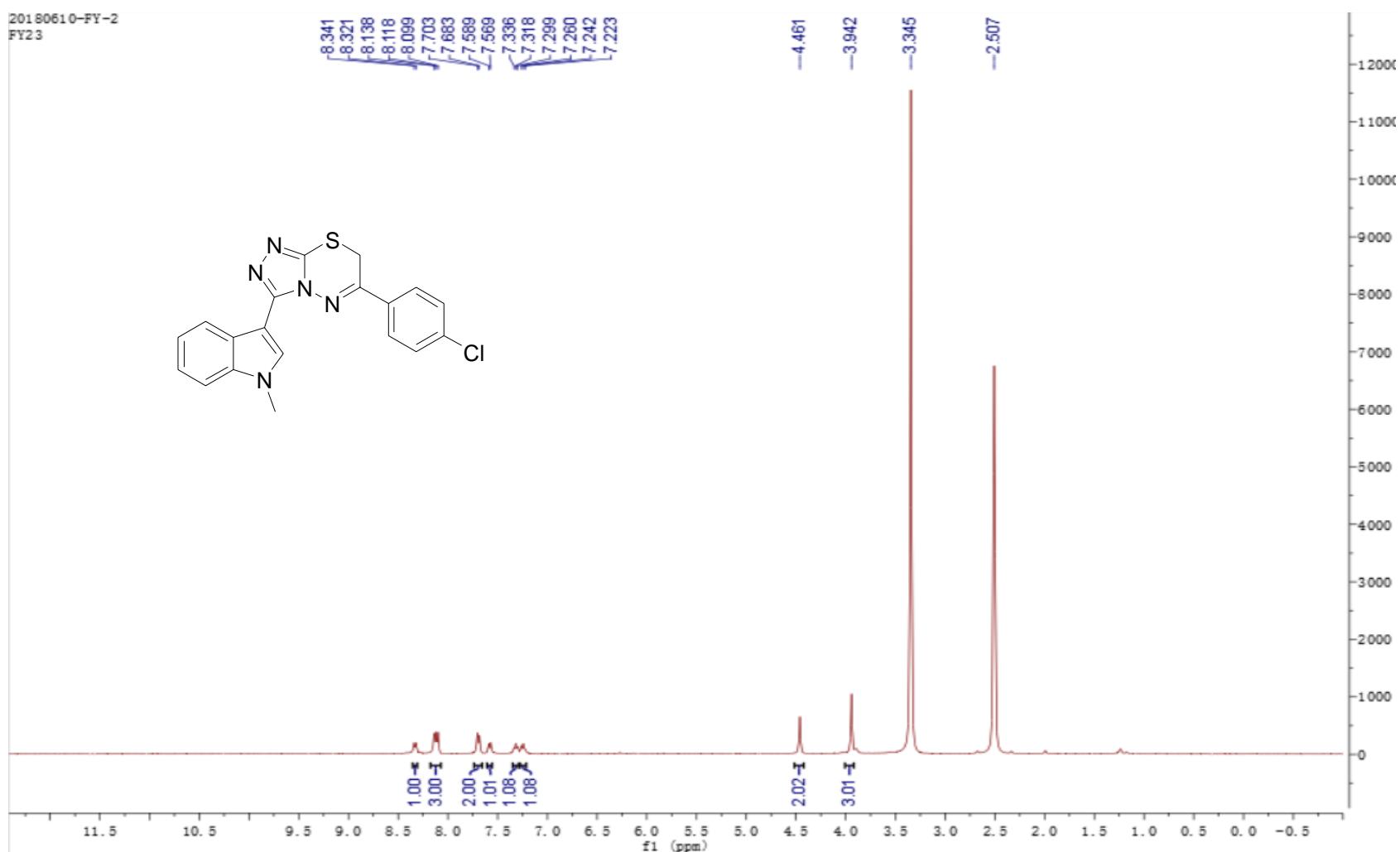


Figure 59. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **10k**.

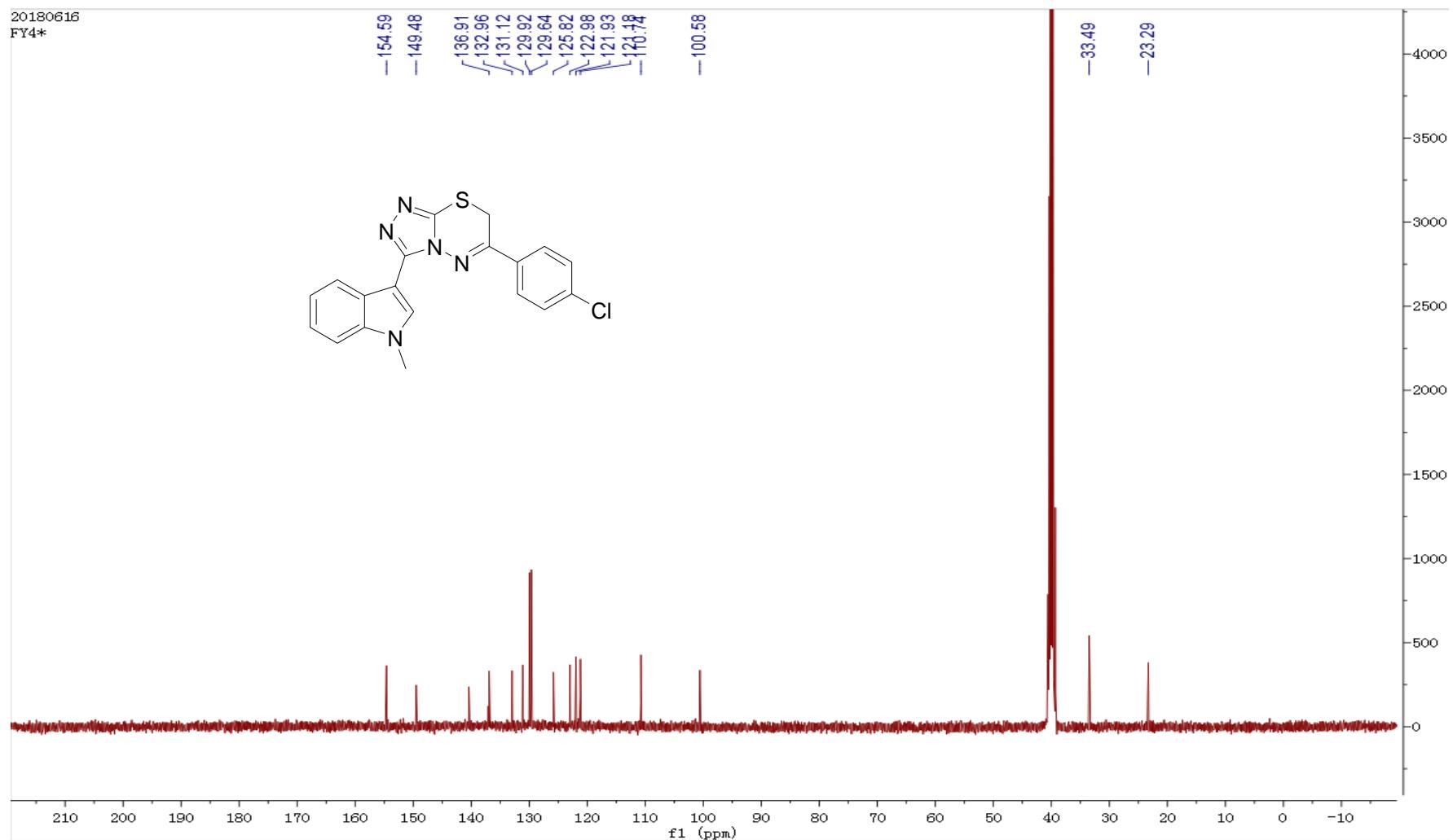


Figure 60. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10k**.

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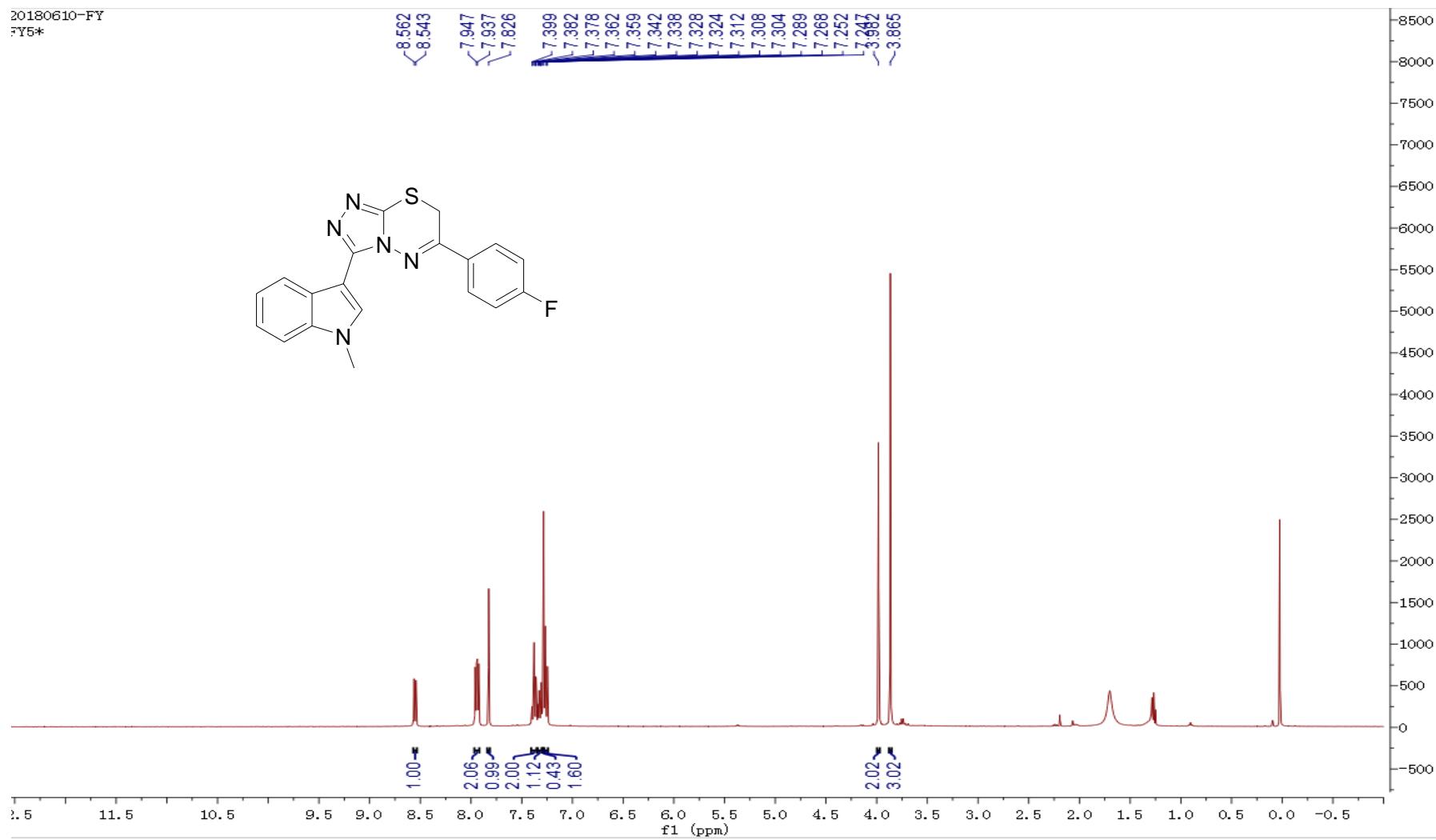
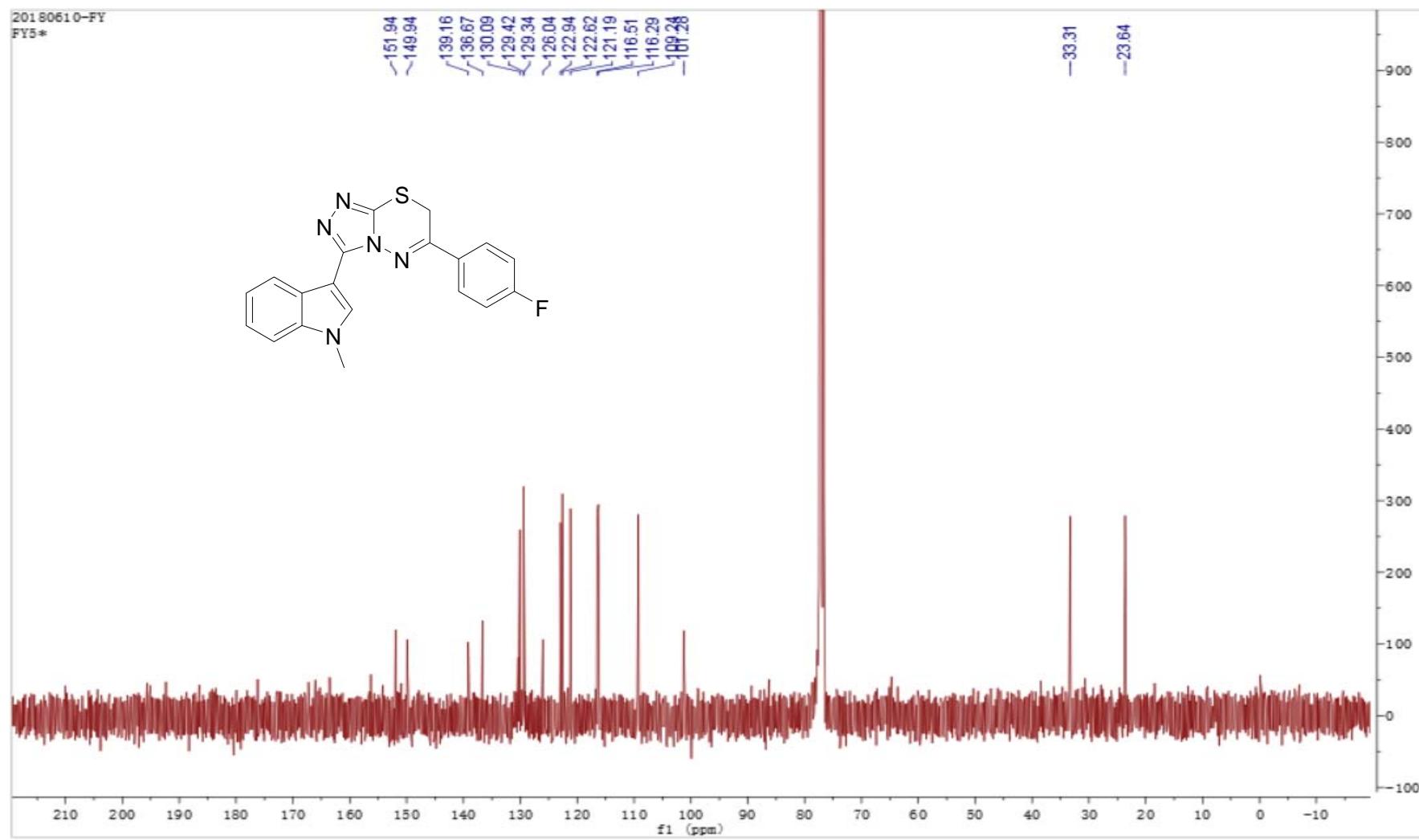


Figure 61. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 10l.



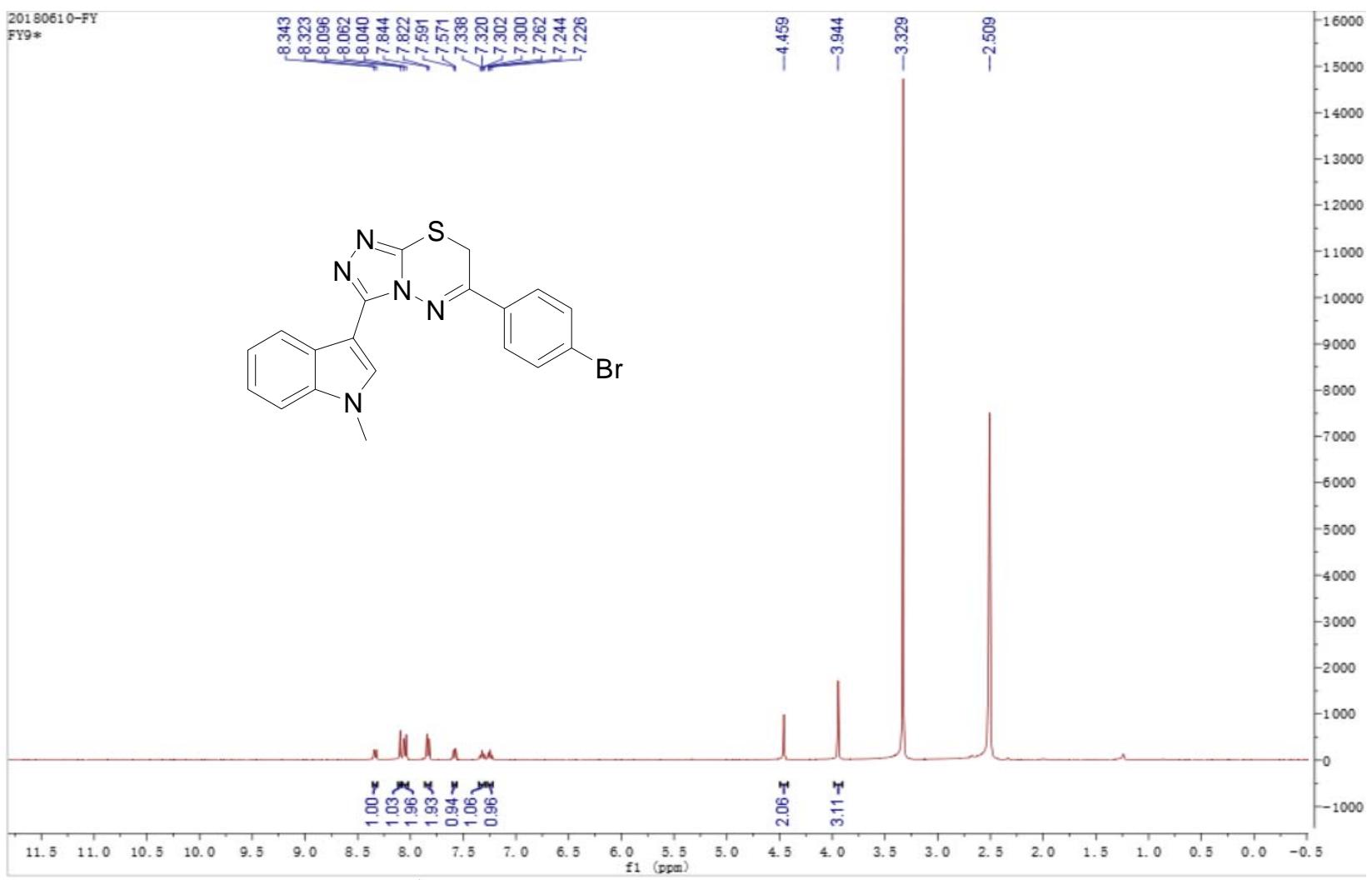


Figure 63. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound **10m**.

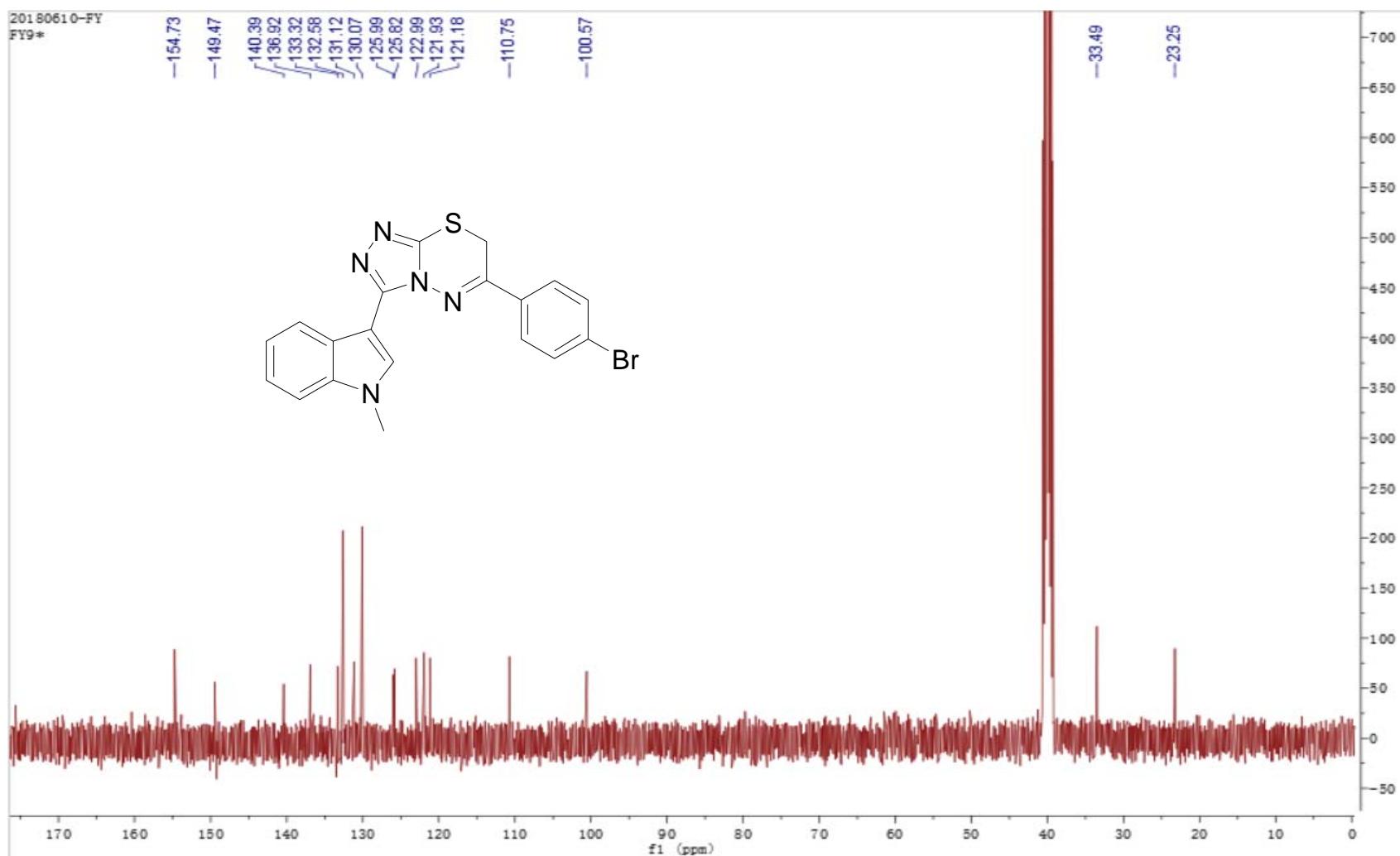


Figure 64. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **10m**.

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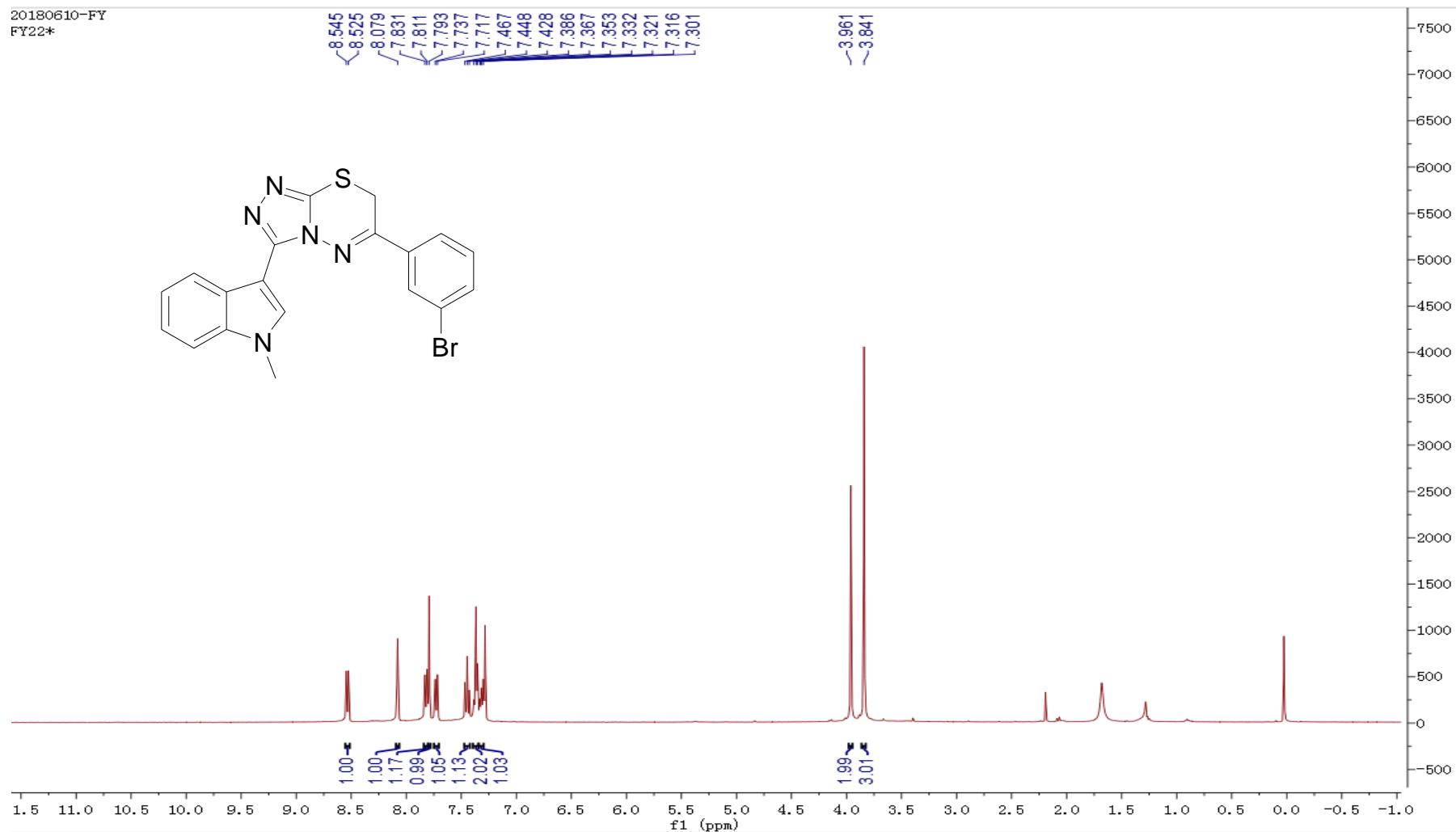


Figure 65. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 10n.

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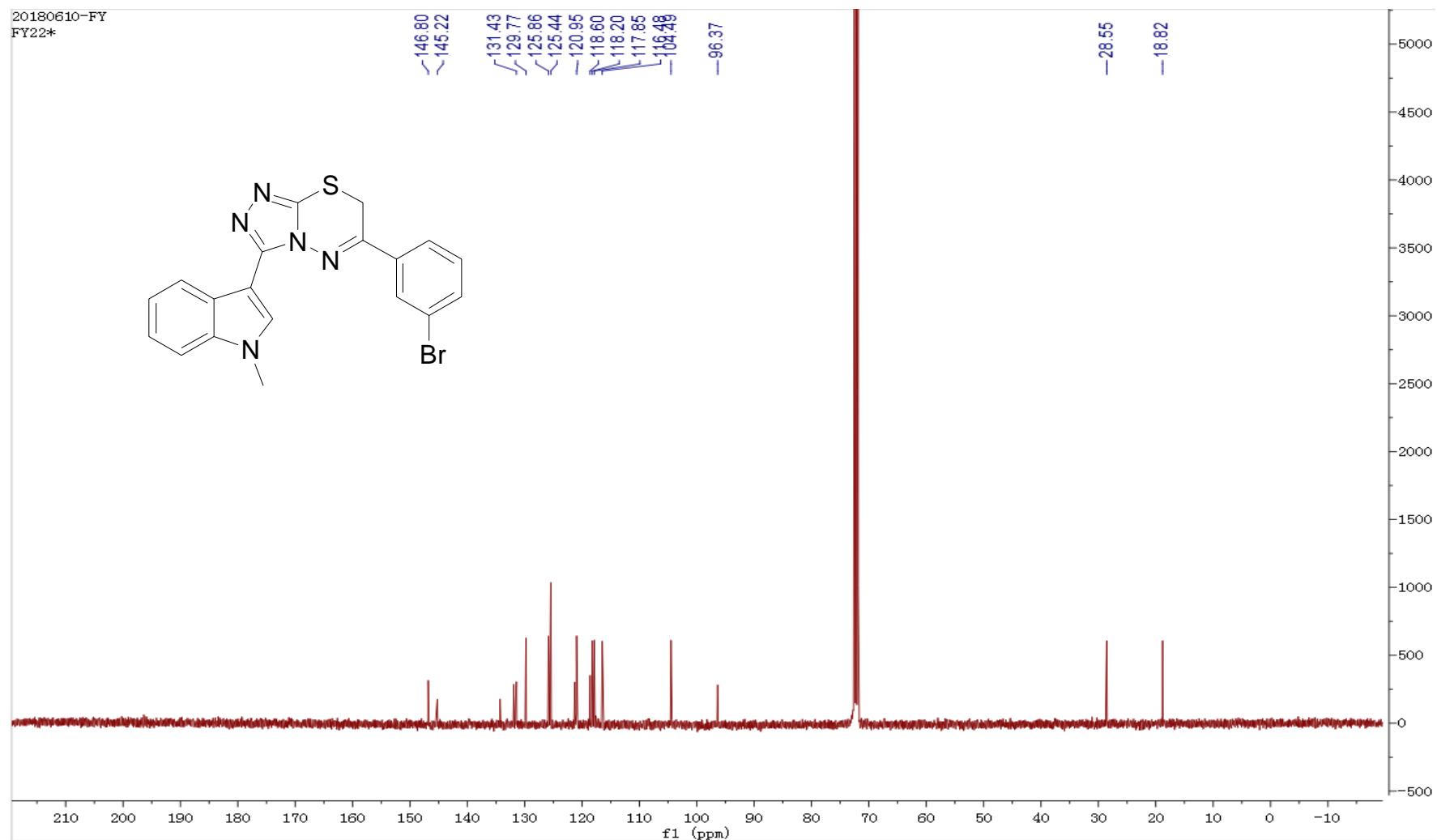


Figure 66. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **10n**.

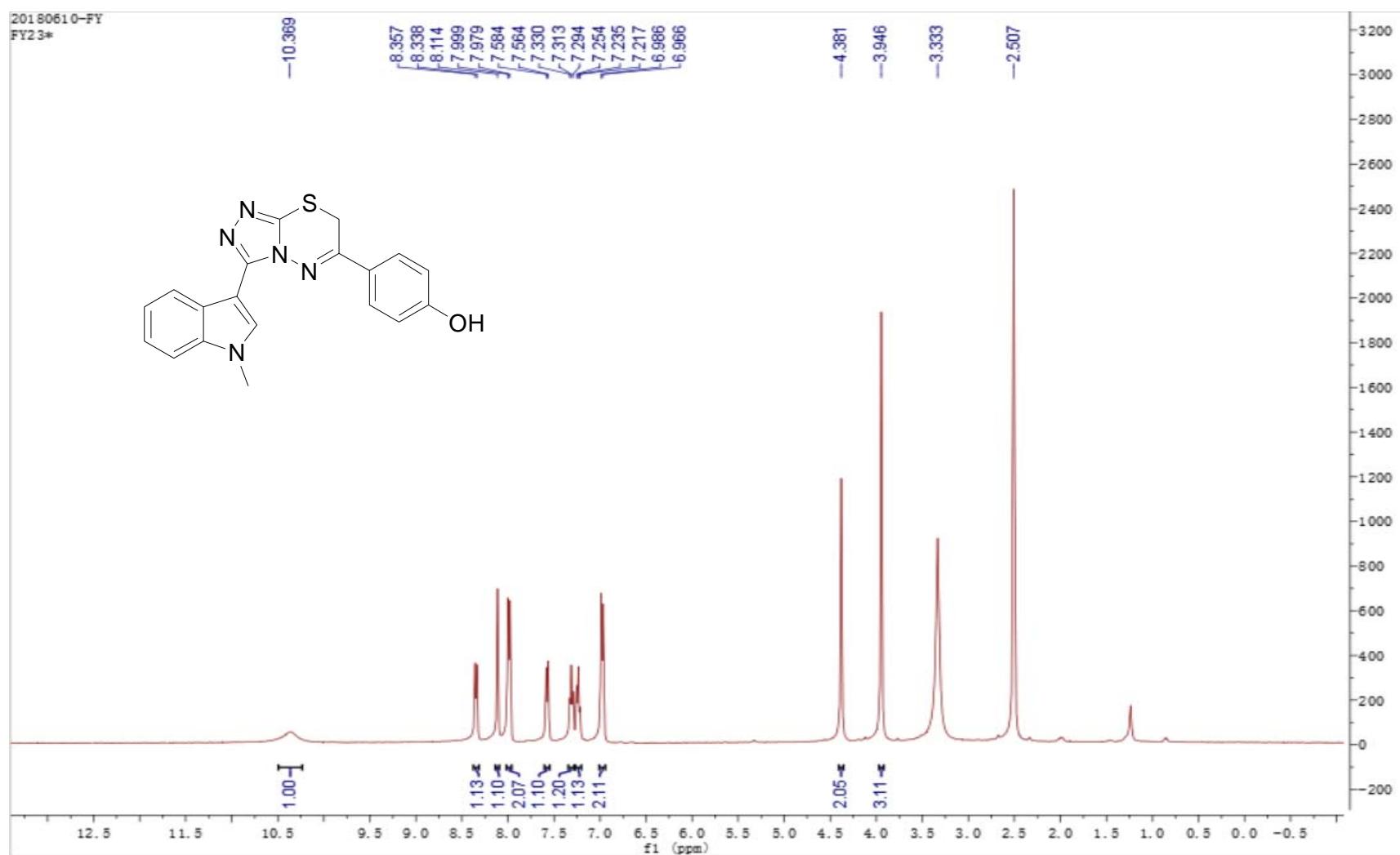


Figure 67. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **10o**.

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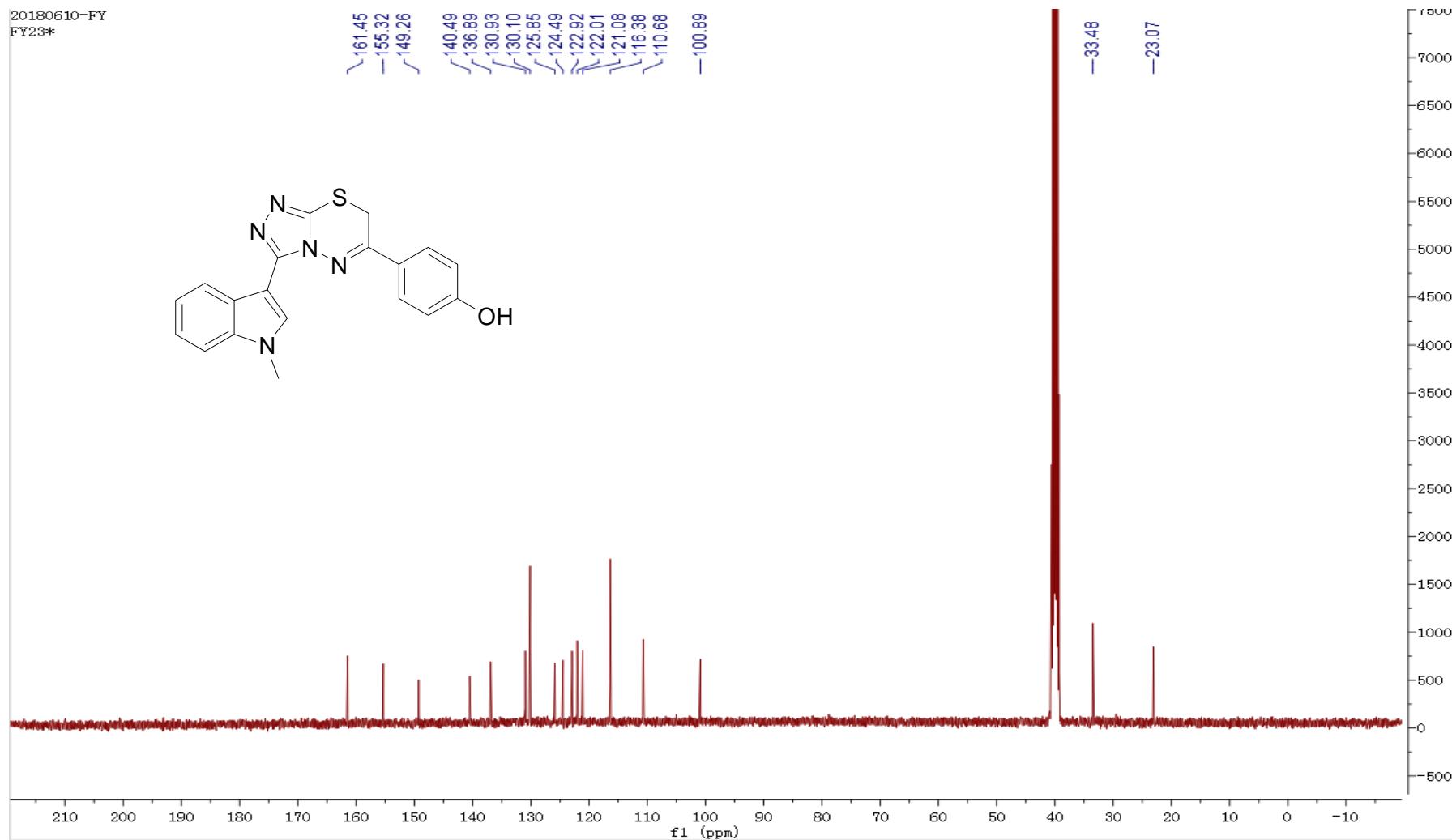
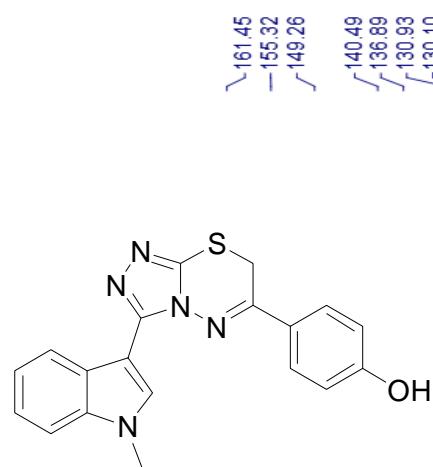


Figure 68. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10o**.

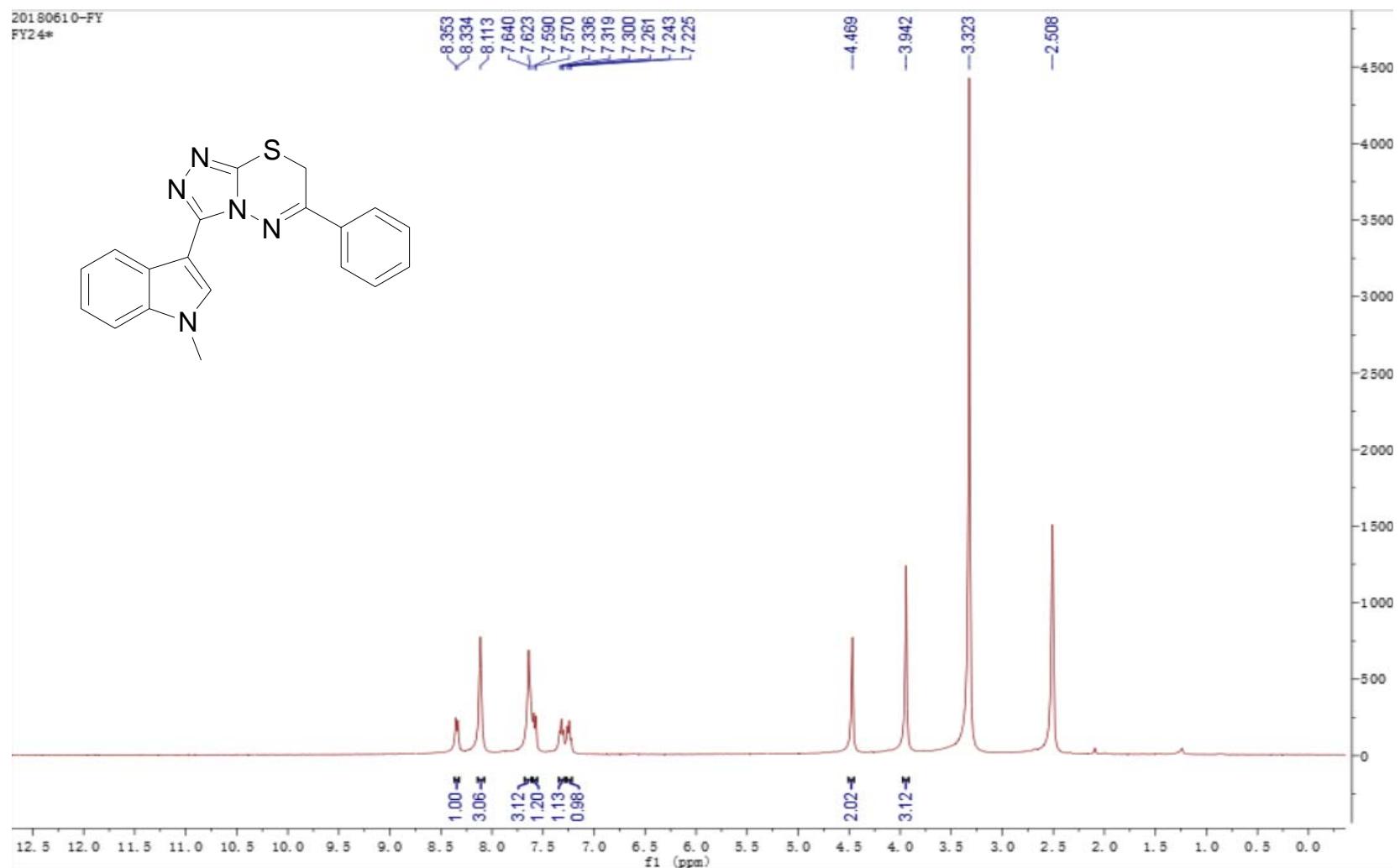


Figure 69. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound 10p.

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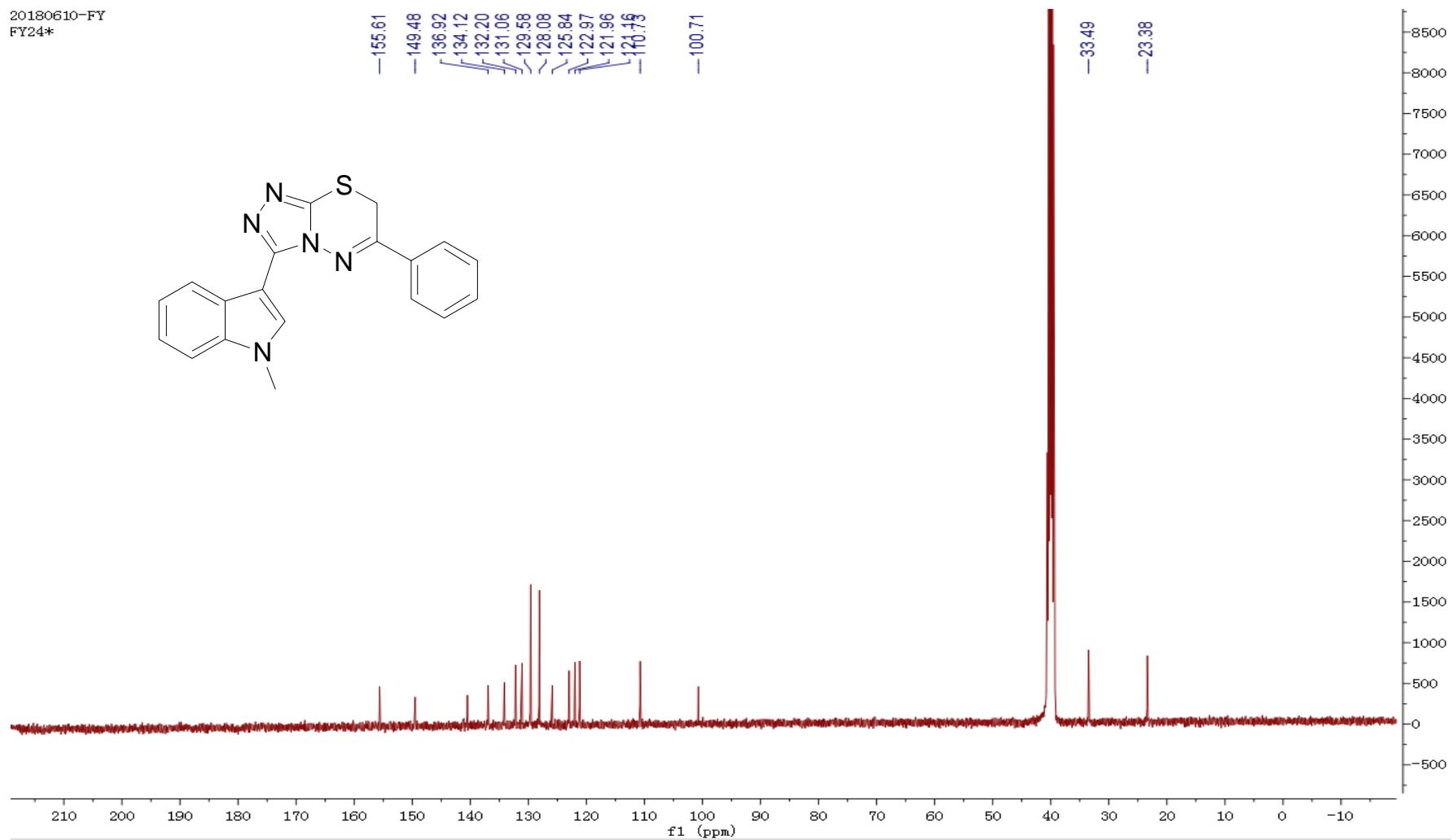


Figure 70. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10p**.

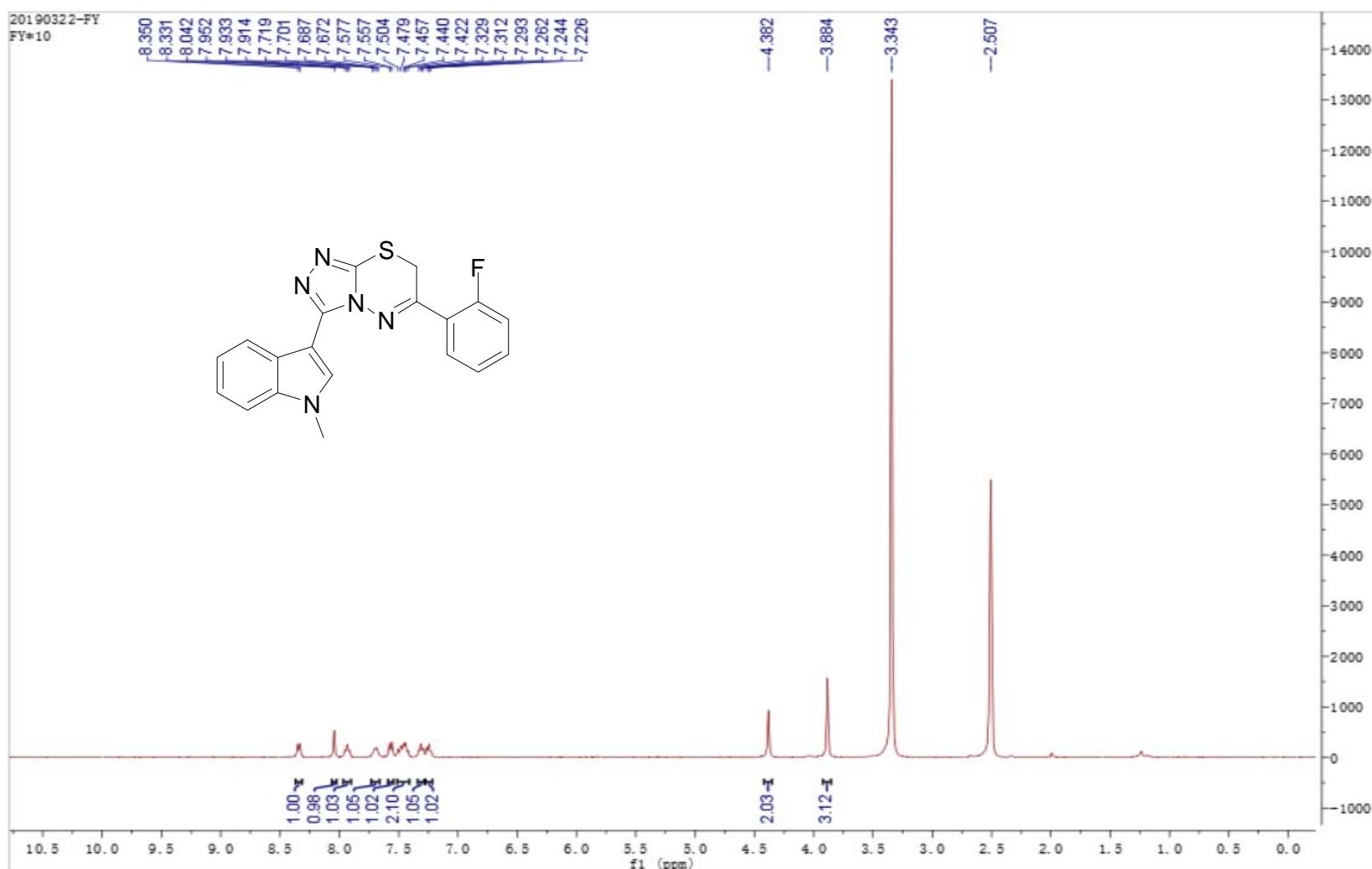


Figure 71. ¹H NMR spectrum (400 MHz, DMSO-d₆) of compound 10q.

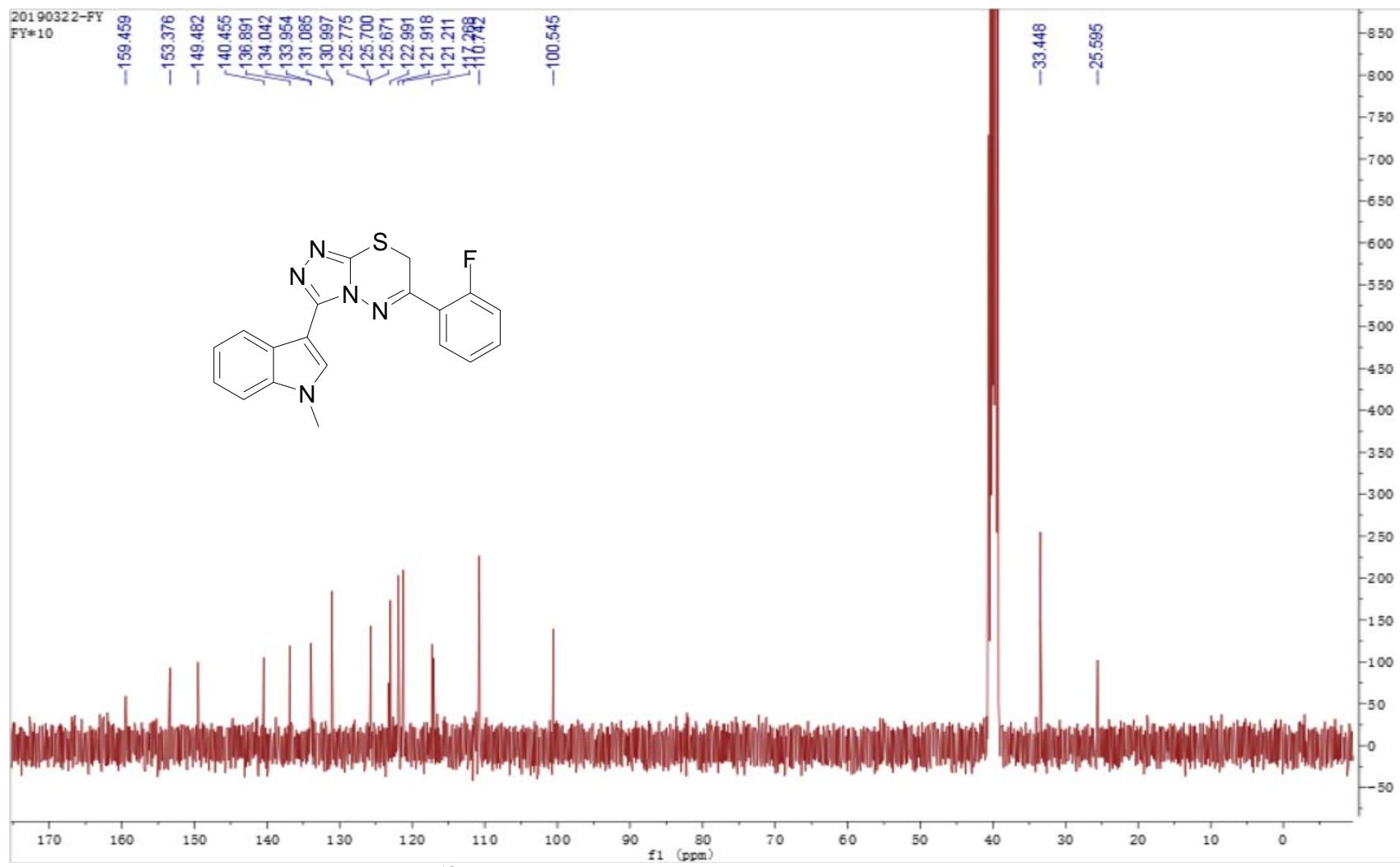


Figure 72. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **10q**.

Spectrum from FY17-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.665 to 0.674 min

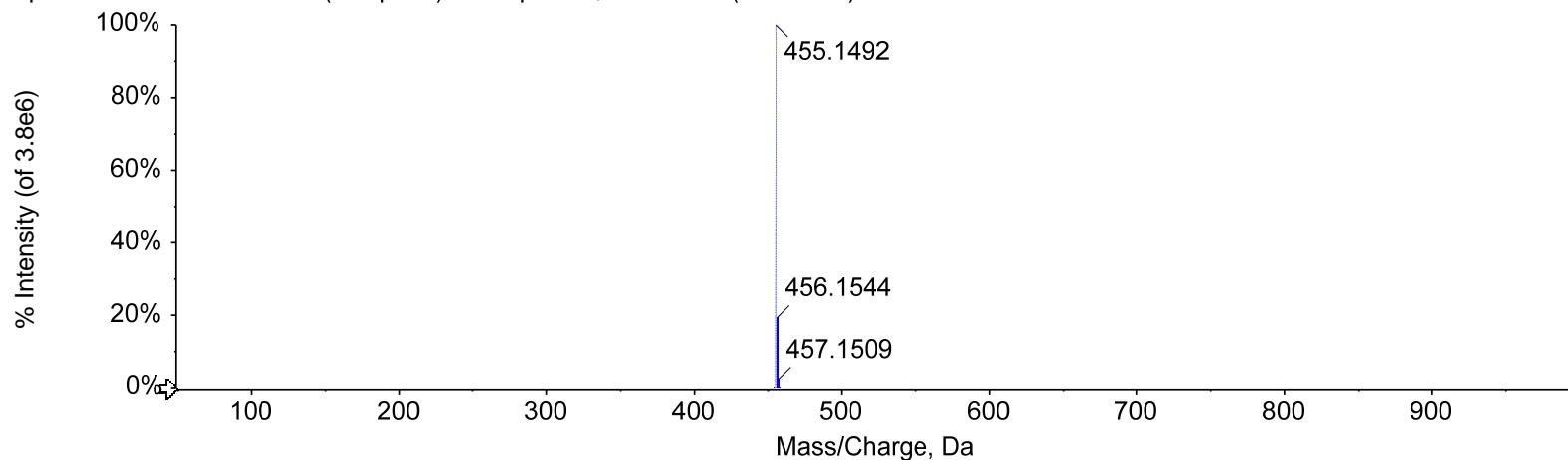


Figure 73. HRMS spectrum of compound **9a**.

Spectrum from FY15.wiff (sample 1) - Sample092, Experiment 1, -TOF MS (50 - 1250) from 0.695 to 0.733 min

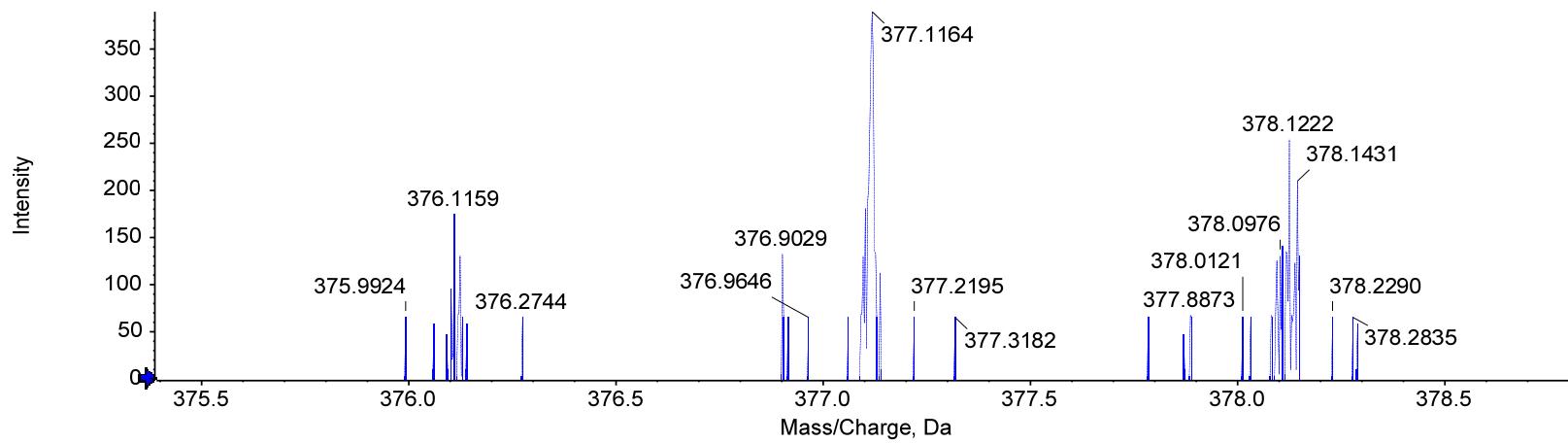


Figure 74. HRMS spectrum of compound **9b**.

Spectrum from FY10-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.702 to 0.712 min

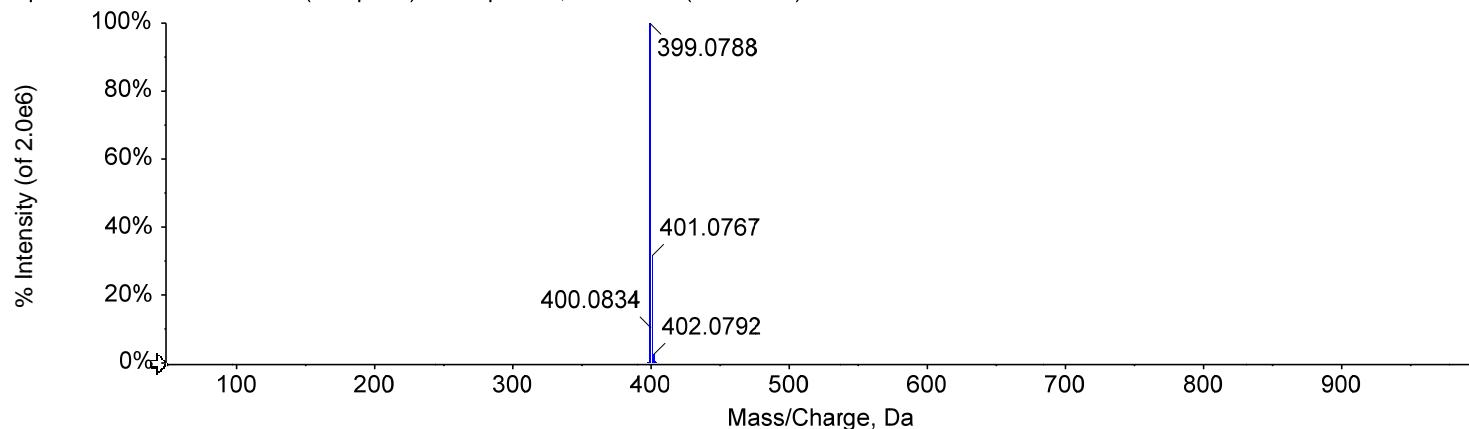


Figure 75. HRMS spectrum of compound **9c**.

Spectrum from FY15.wiff (sample 1) - sample001, Experiment 1, +TQF MS (50 – 1300) from 0.664 to 0.712 min

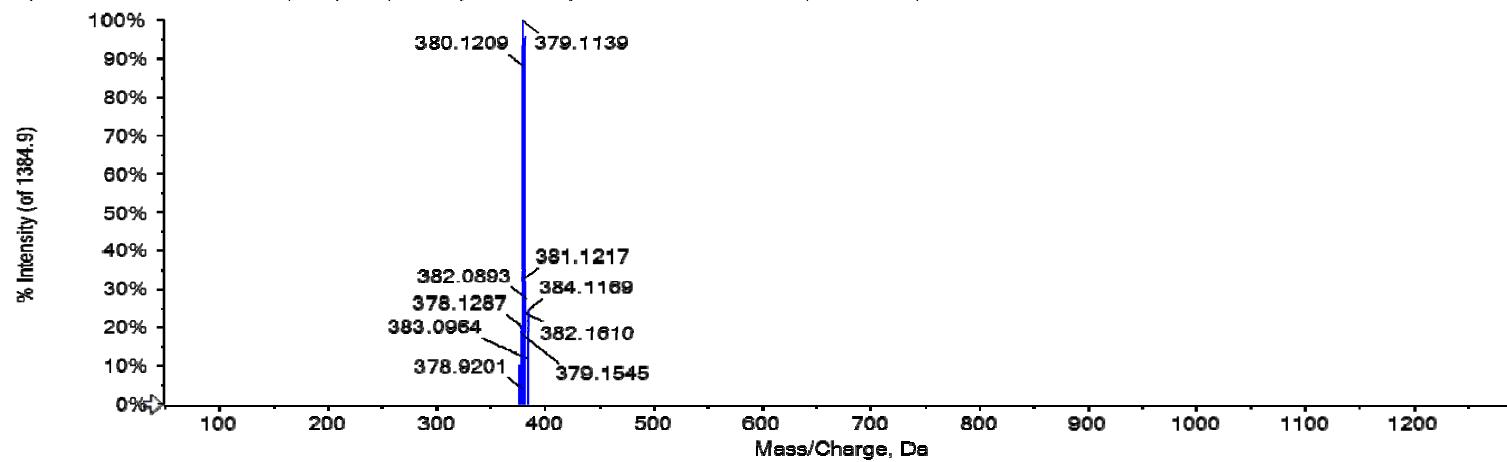


Figure 76. HRMS spectrum of compound **9d**.

Spectrum from YF11.wiff (sample 1) - Sample012, Experiment 1, +TOF MS (50 - 1000) from 0.881 min

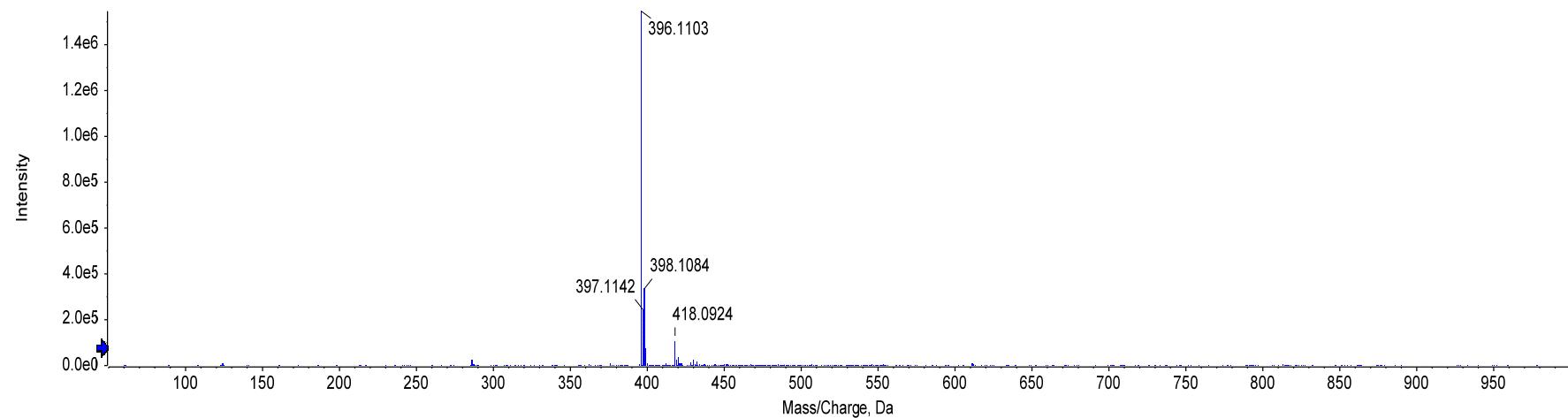


Figure 77. HRMS spectrum of compound **9e**.

Spectrum from FY8-1.wiff (sample 1) - Sample002, -TOF MS (50 - 1000) from 0.674 to 0.684 min

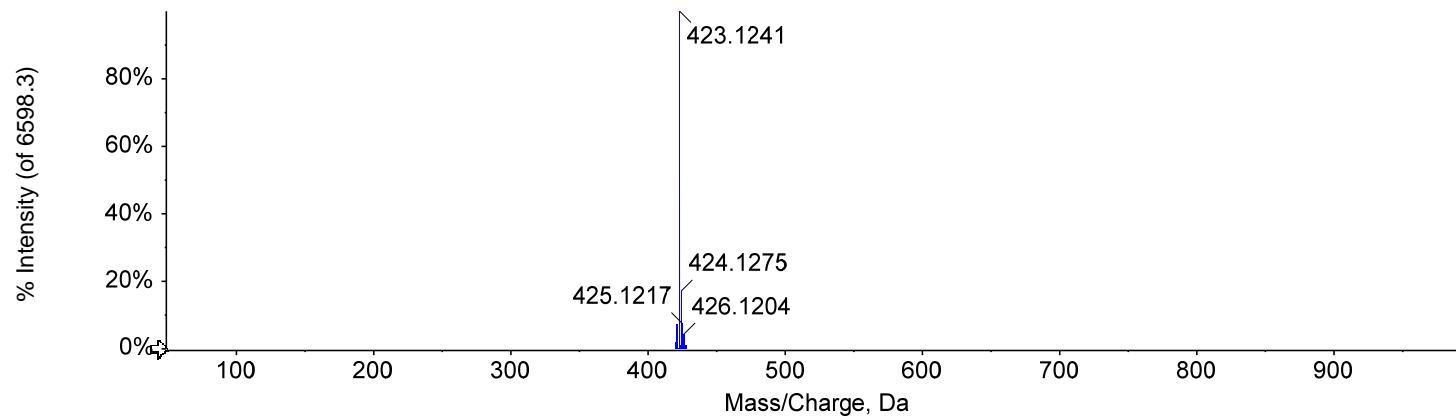


Figure 78. HRMS spectrum of compound **9f**.

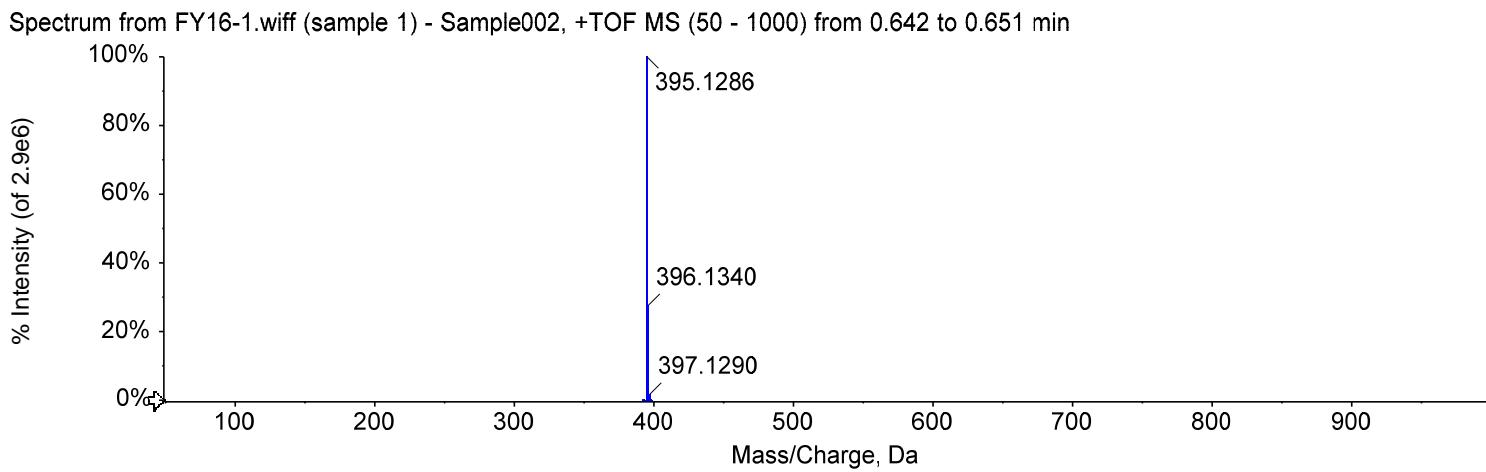


Figure 79. HRMS spectrum of compound **9g**.

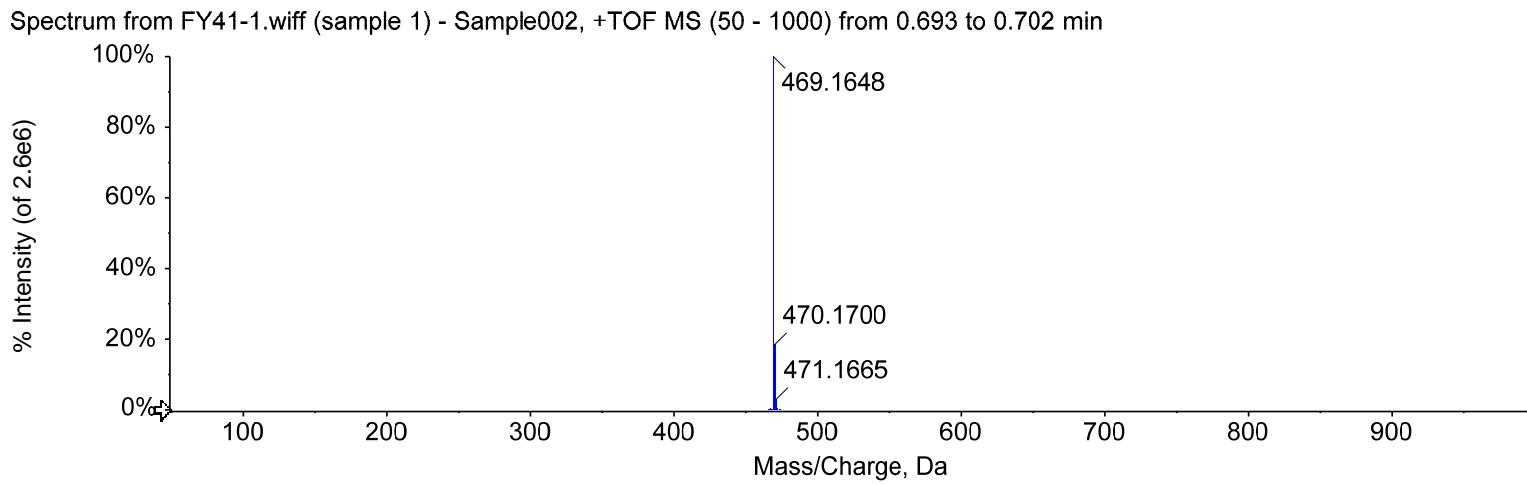


Figure 80. HRMS spectrum of compound **9h**.

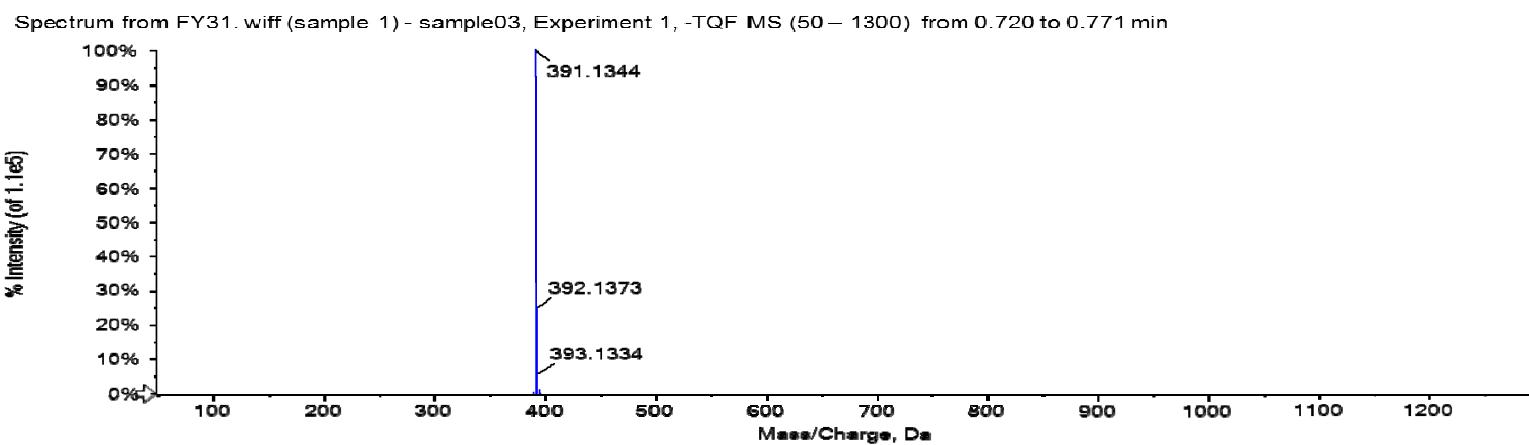


Figure 81. HRMS spectrum of compound **9i**.

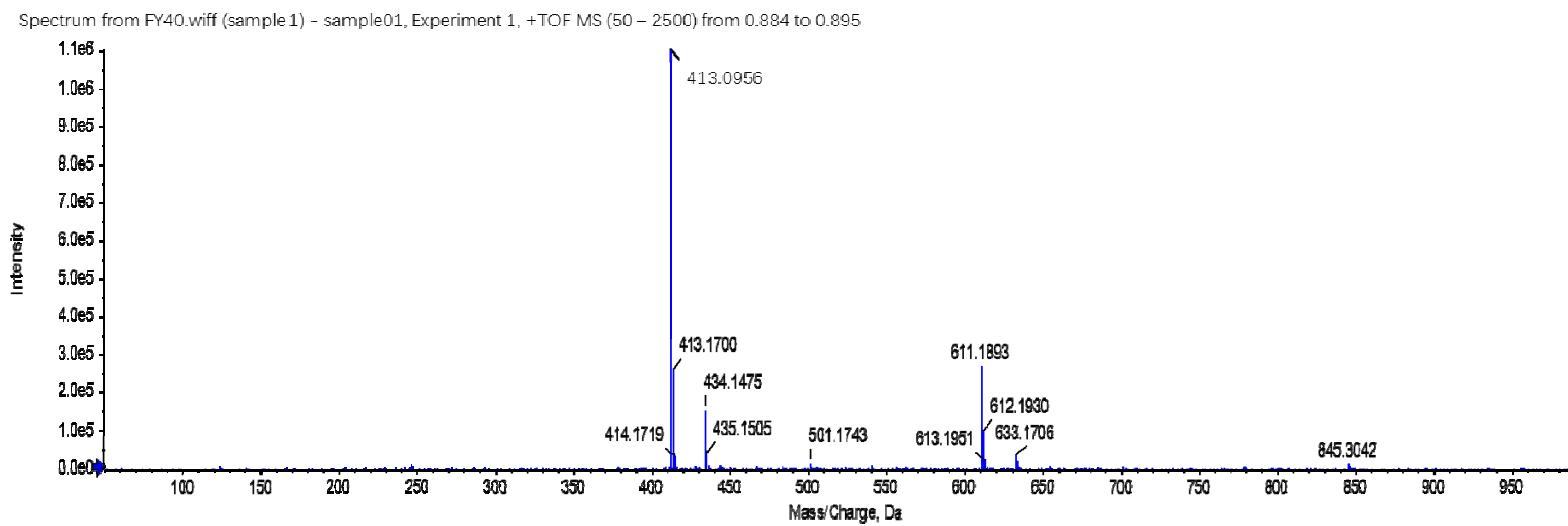


Figure 82. HRMS spectrum of compound **9j**.

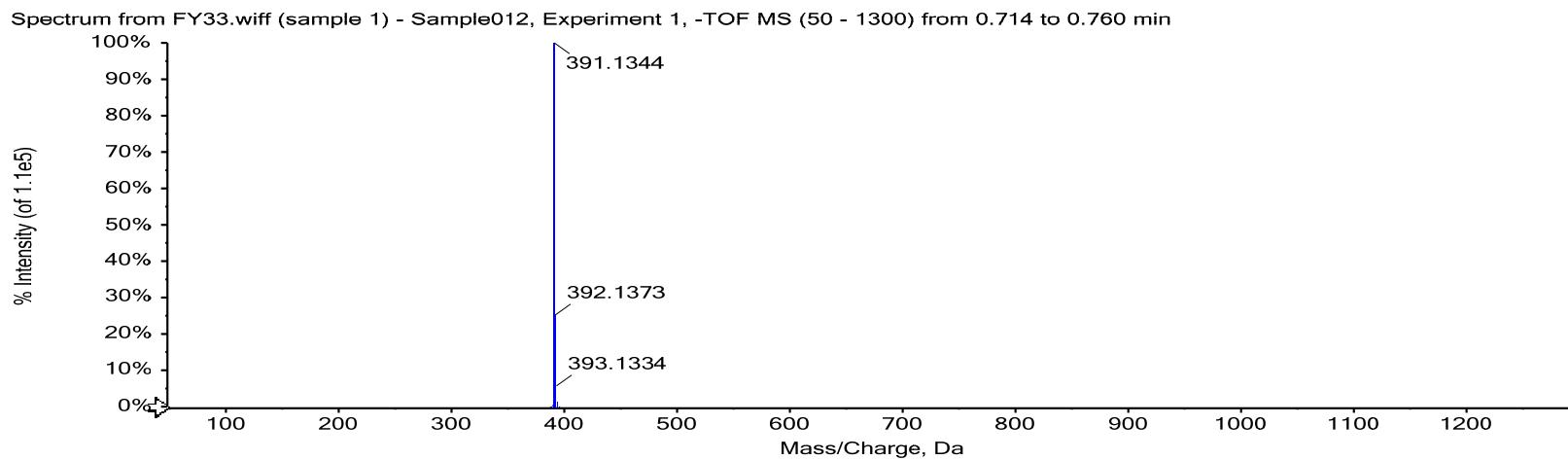


Figure 83. HRMS spectrum of compound **9k**.

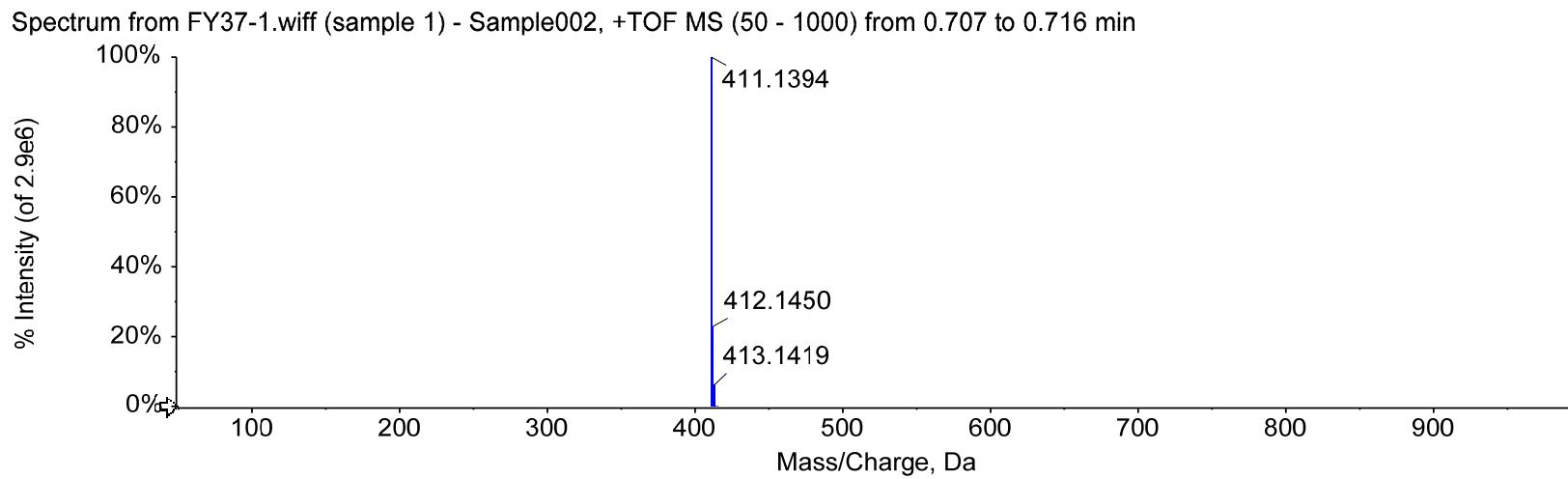


Figure 84. HRMS spectrum of compound **9l**.

Spectrum from FY30-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.716 to 0.725 min

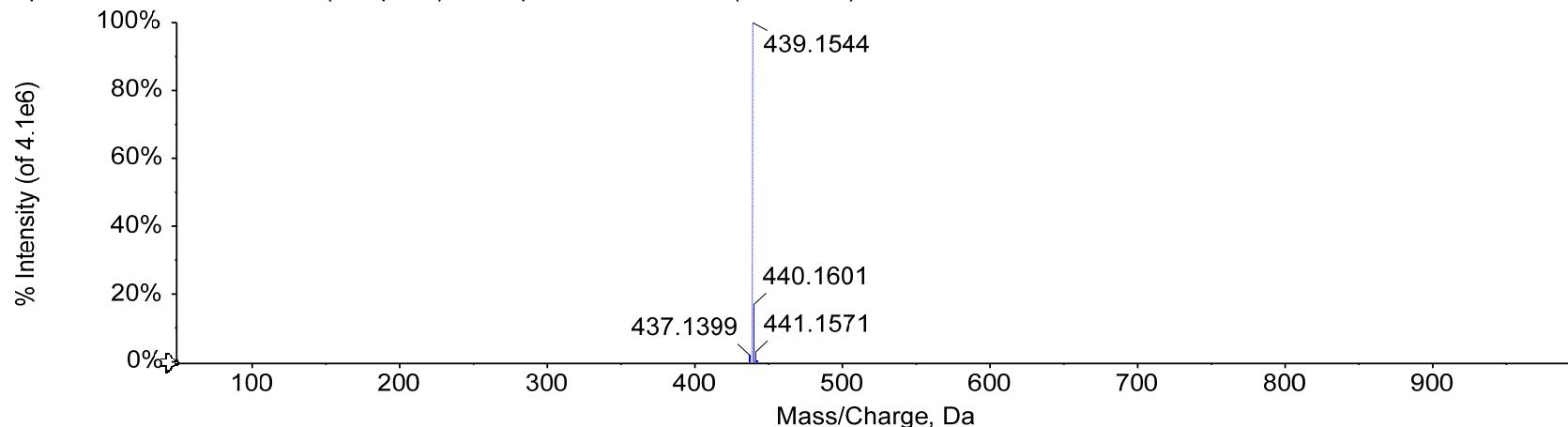


Figure 85. HRMS spectrum of compound **9m**.

Spectrum from FY36-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.809 to 0.818 min

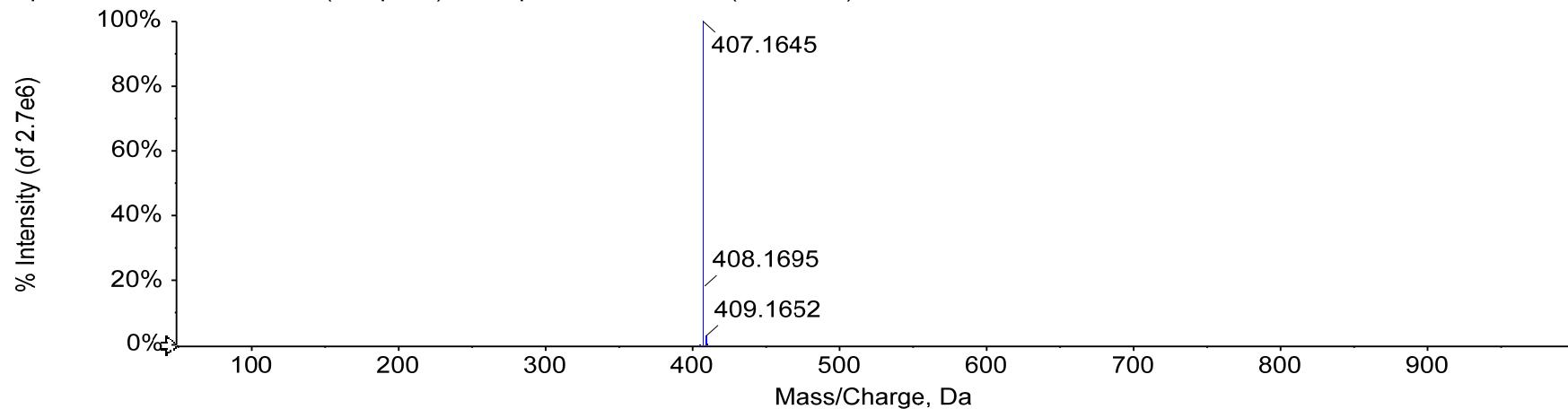


Figure 86. HRMS spectrum of compound **9n**.

Spectrum from FY32-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.795 to 0.804 min

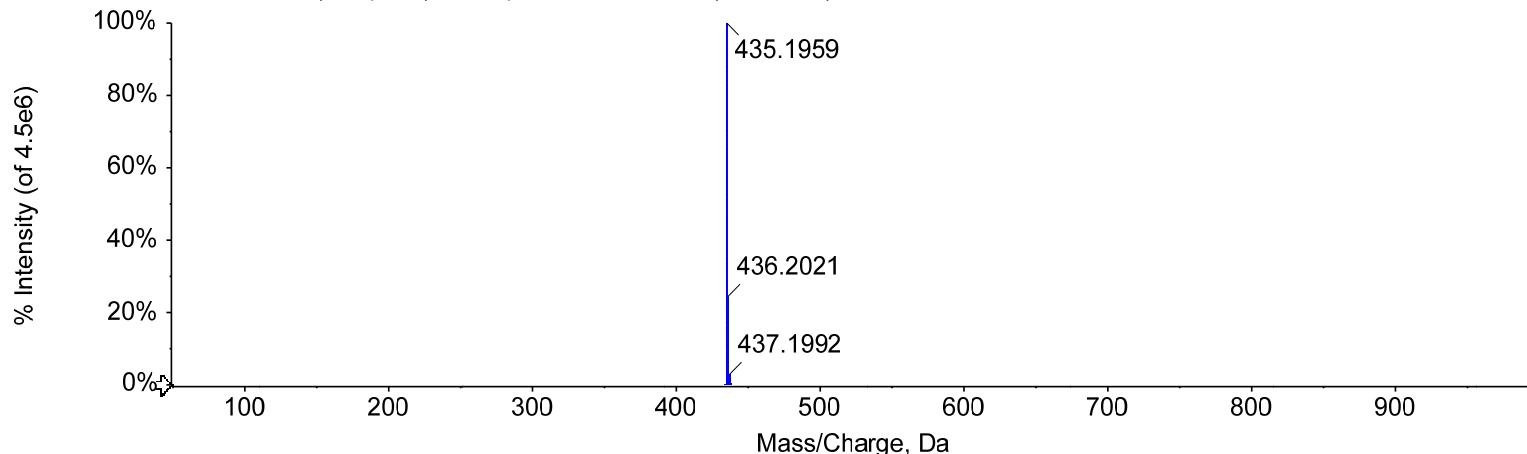


Figure 87. HRMS spectrum of compound **9o**.

Spectrum from FY38.wiff (sample 1)- sample016; Experiment1, +TQFMS (50–1300) from 0.804 to 0.852 min

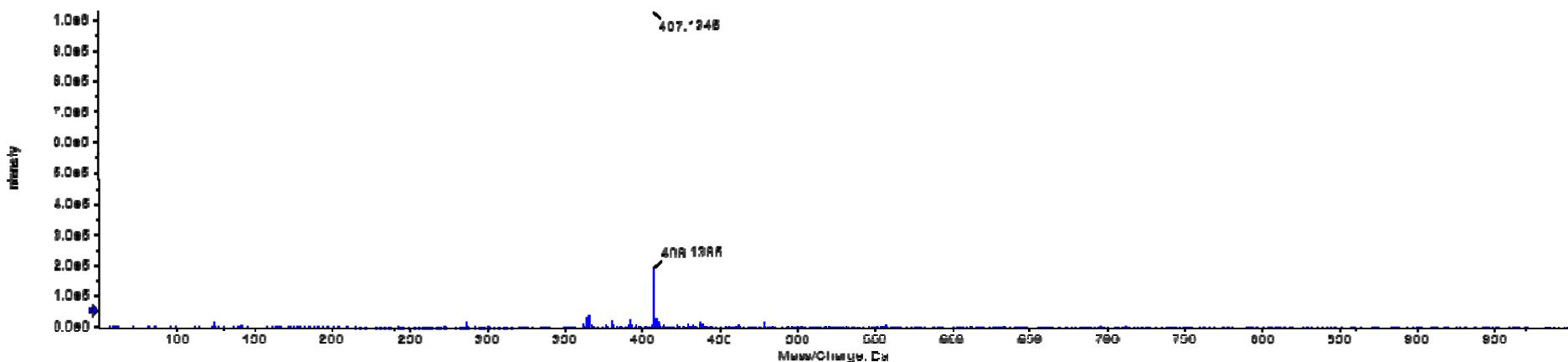


Figure 88. HRMS spectrum of compound **9p**.

Spectrum from YF4.wiff (sample 1) - Sample005, Experiment 1, +TOF MS (50 - 1000) from 0.688 min

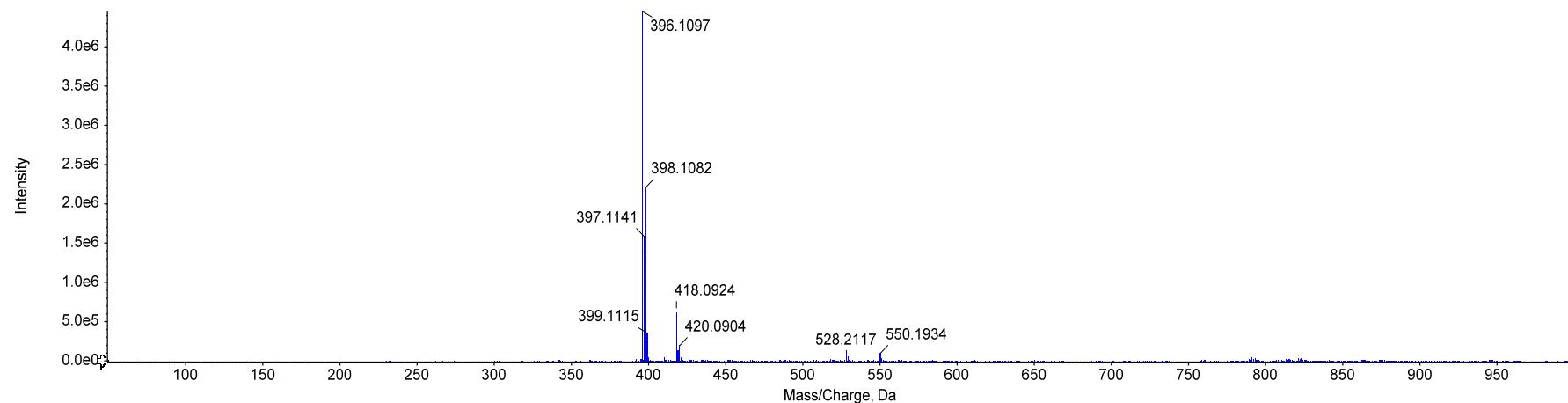


Figure 89. HRMS spectrum of compound **9q**.

Spectrum from FY8.wiff (sample 1) - Sample085, Experiment 1, +TOF MS (50 - 1250) from 0.682 to 0.721 min

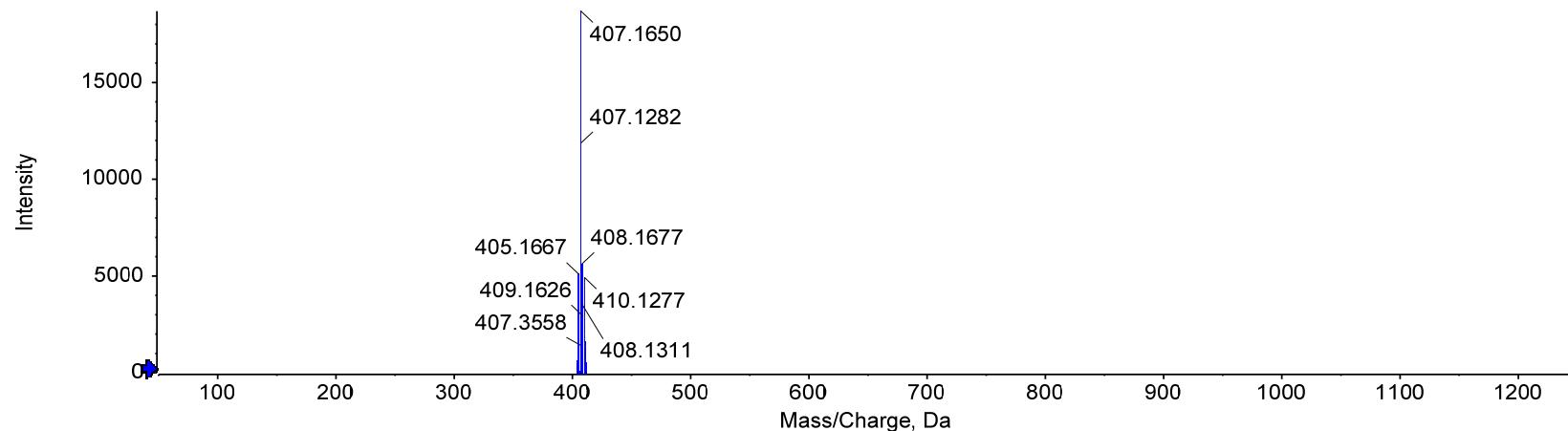


Figure 90. HRMS spectrum of compound **9r**.

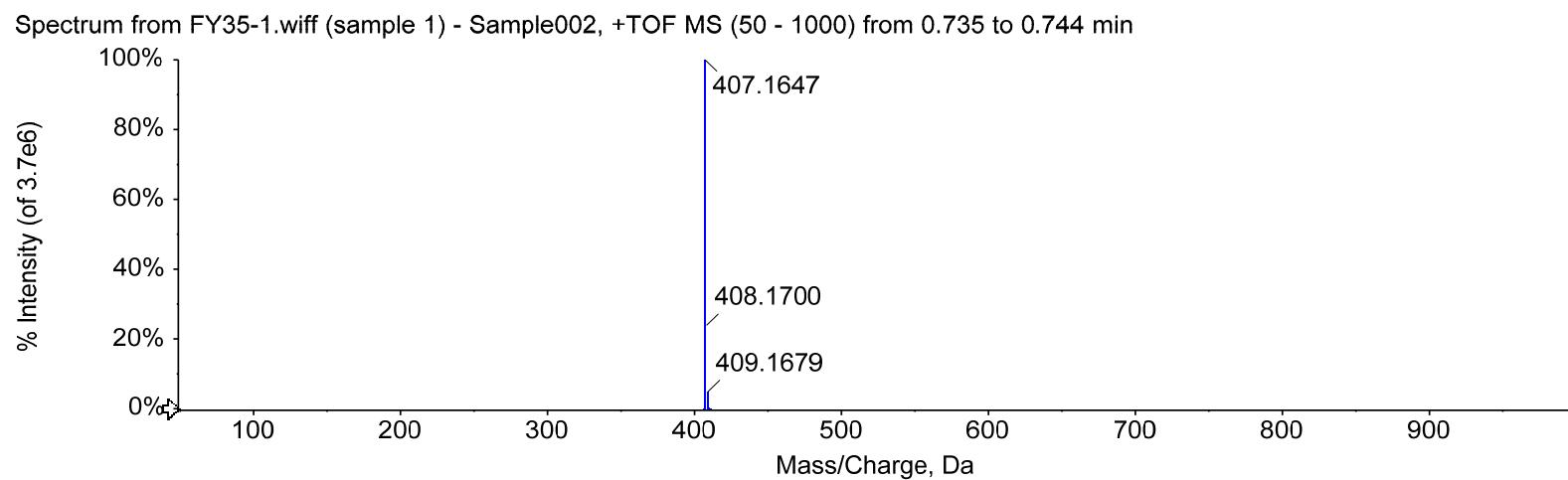


Figure 91. HRMS spectrum of compound **9s**.

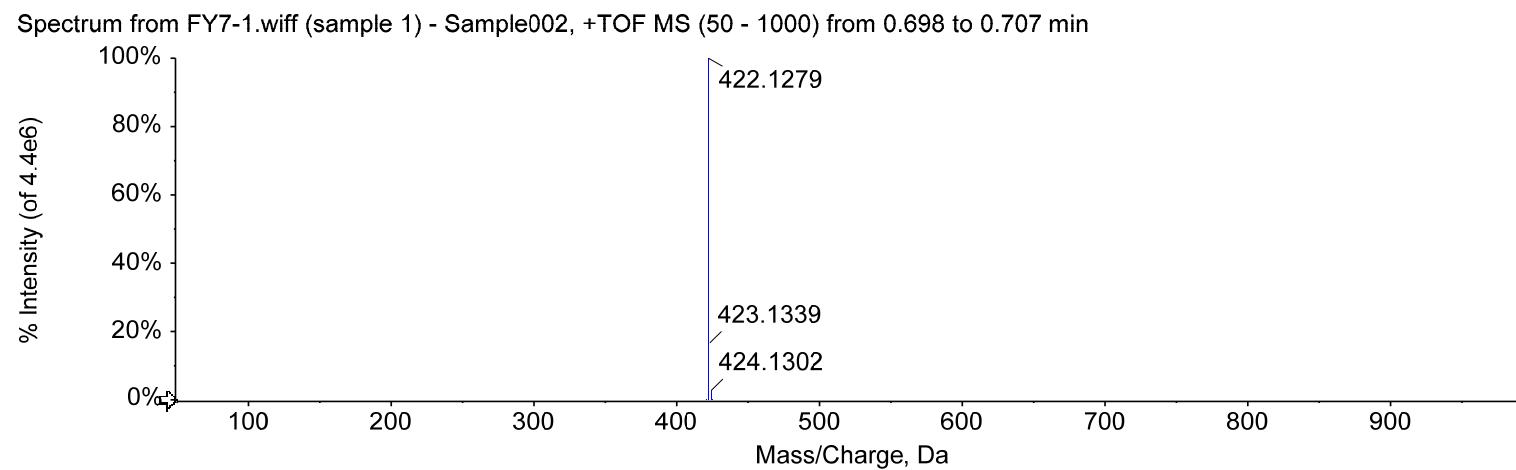


Figure 92. HRMS spectrum of compound **10a**.

Spectrum from FY1.wiff (sample 1) - Sample078, Experiment 1, -TOF MS (50 - 1250) from 0.756 to 0.794 min

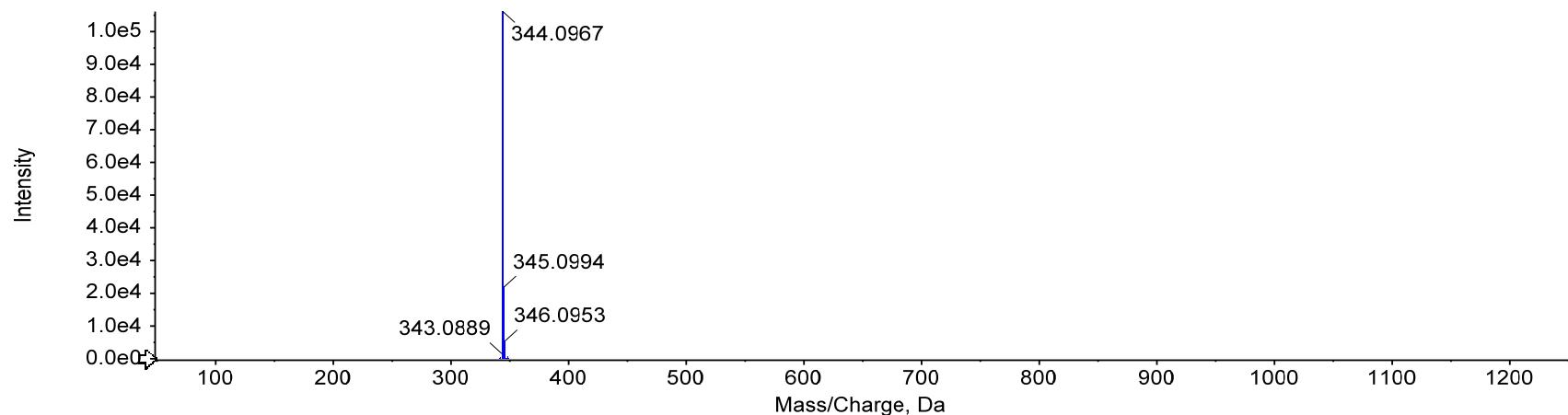


Figure 93. HRMS spectrum of compound **10b**.

Spectrum from FY5-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.674 to 0.749 min

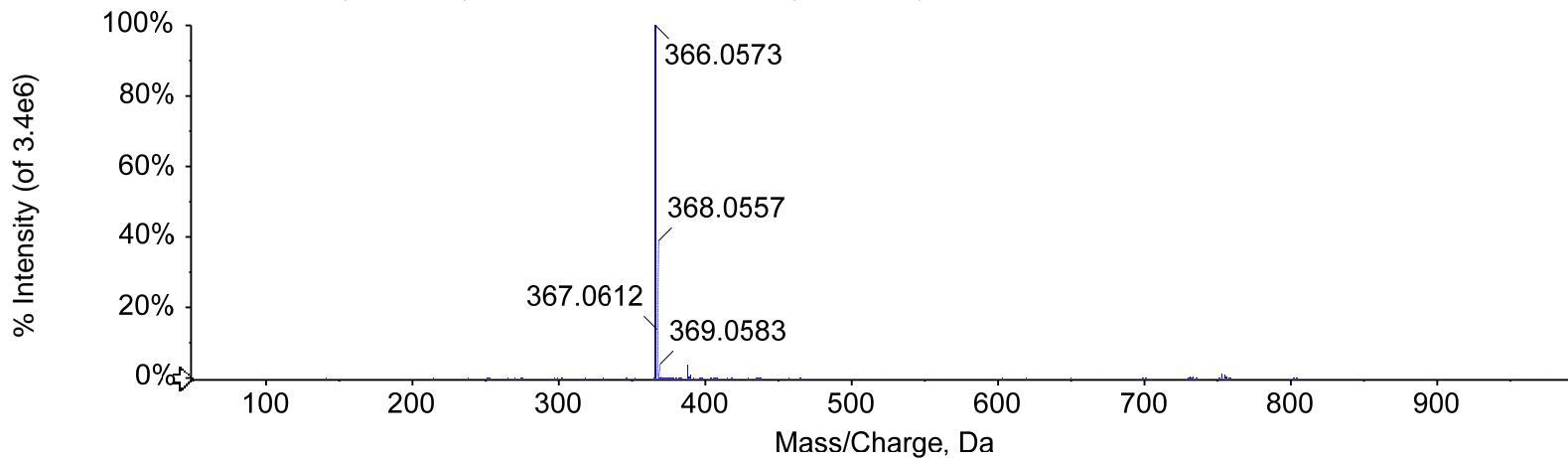


Figure 94. HRMS spectrum of compound **10c**.

Spectrum from FY4.wiff (sample 1) - Sample081, Experiment 1, -TOF MS (50 - 1250) from 0.754 to 0.792 min

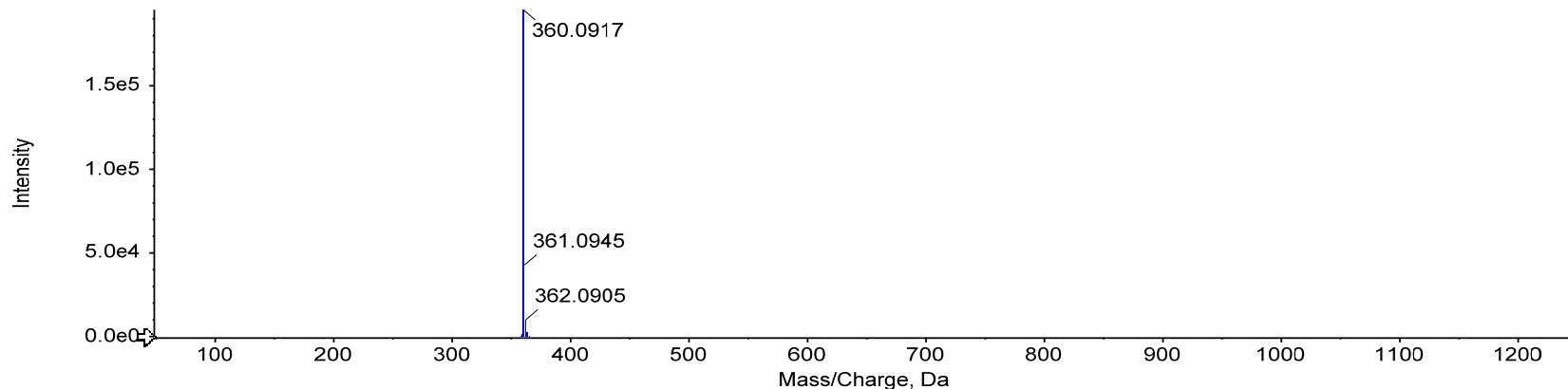


Figure 95. HRMS spectrum of compound **10d**.

Spectrum from FY3-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.702 to 0.711 min

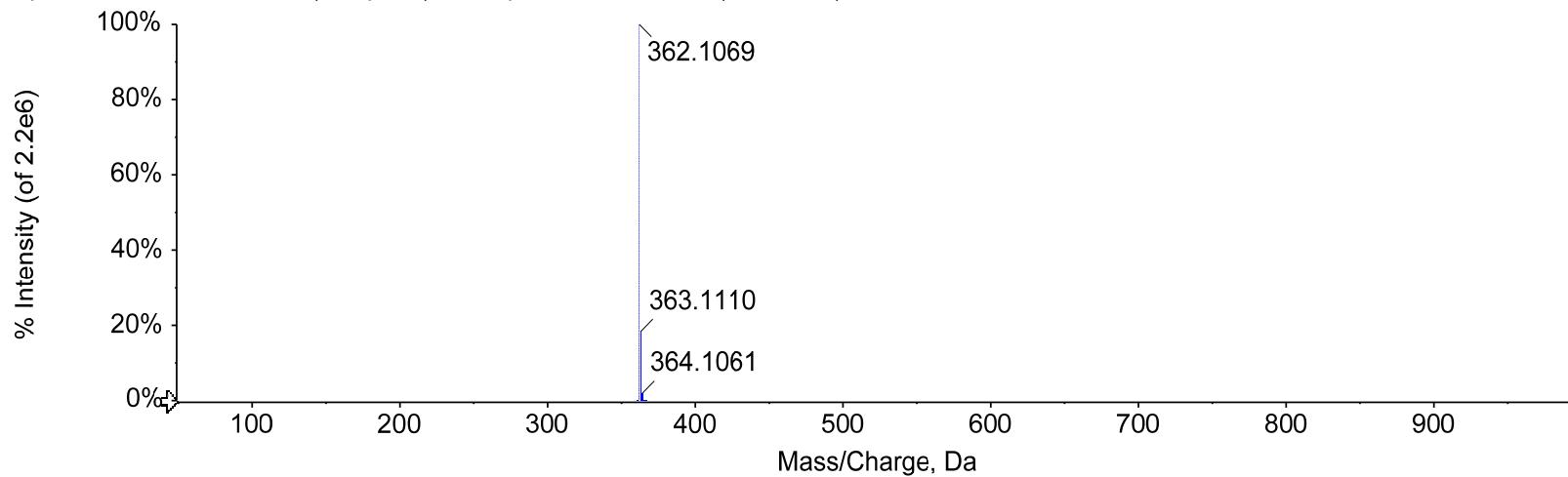


Figure 96. HRMS spectrum of compound **10e**.

Spectrum from FY6.wiff (sample 1) - Sample083, Experiment 1, -TOF MS (50 - 1250) from 0.723 to 0.761 min

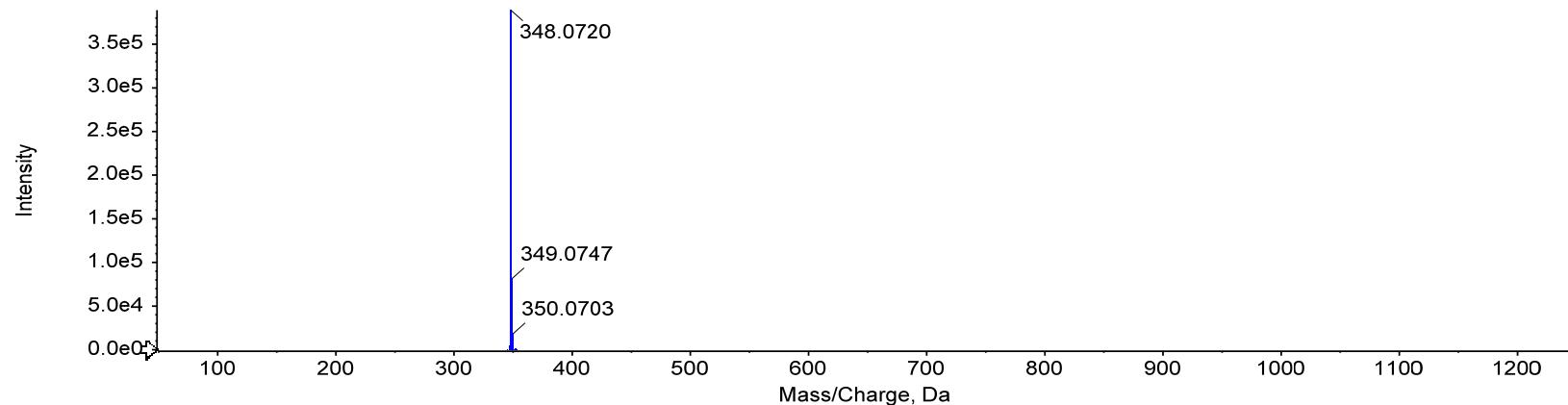


Figure 97. HRMS spectrum of compound **10f**.

Spectrum from FY2.wiff (sample 1) - Sample079, Experiment 1, -TOF MS (50 - 1250) from 0.784 to 0.822 min

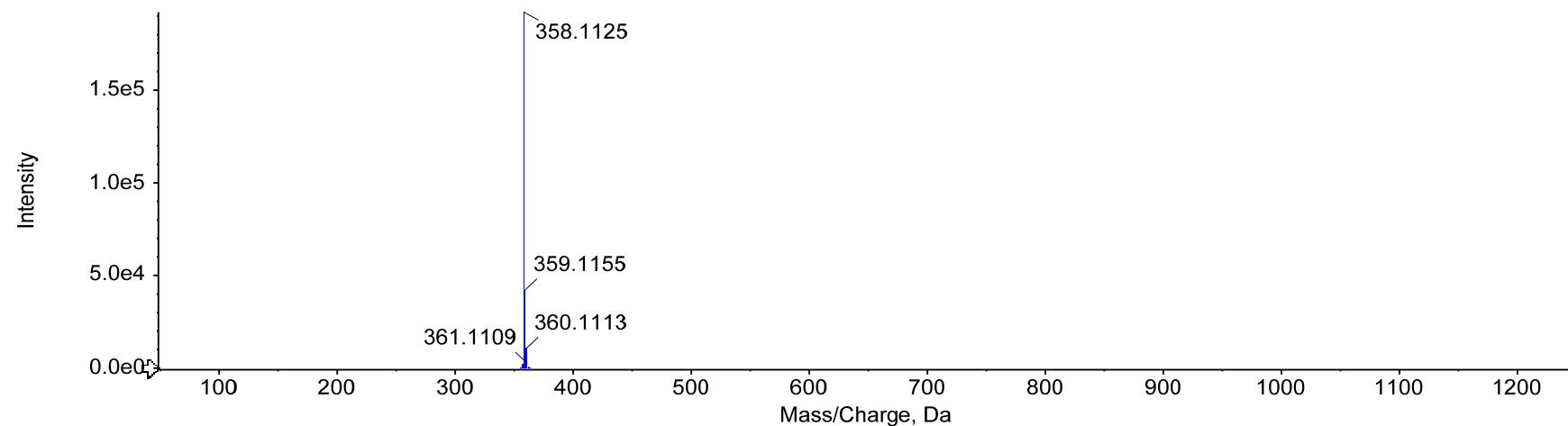


Figure 98. HRMS spectrum of compound **9g**.

Spectrum from FY20.wiff (sample 1) - Sample097, Experiment 1, -TOF MS (50 - 1250) from 0.818 to 0.856 min

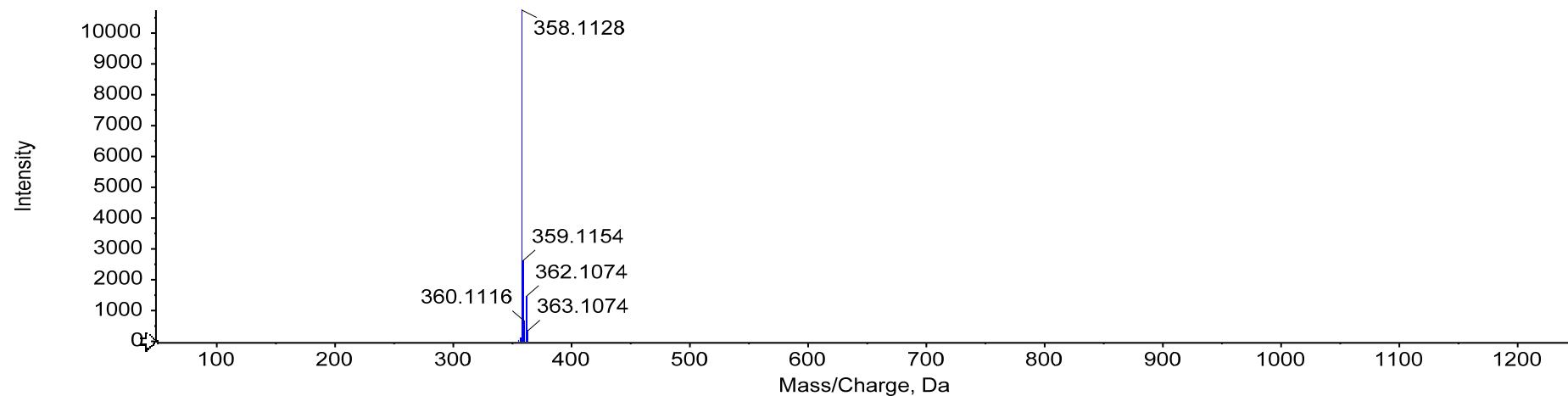


Figure 99. HRMS spectrum of compound **10h**.

Spectrum from FY21.wiff (sample 1) - Sample098, Experiment 1, -TOF MS (50 - 1250) from 0.796 to 0.834 min

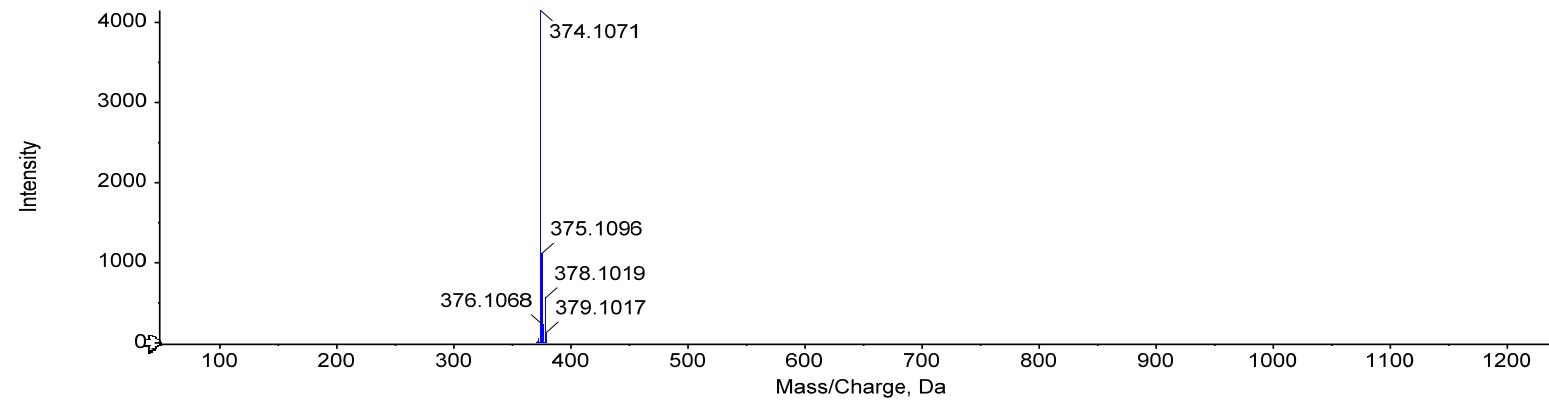


Figure 100. HRMS spectrum of compound **10i**.

Spectrum from FY22.wiff (sample 1) - Sample099, Experiment 1, -TOF MS (50 - 1250) from 0.735 to 0.773 min

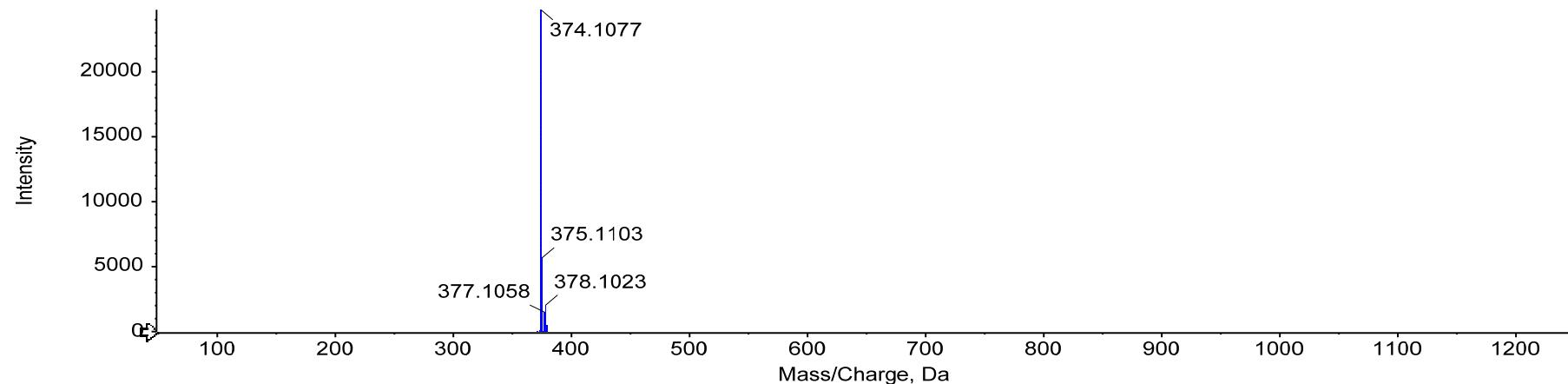


Figure 101. HRMS spectrum of compound **10j**.

Spectrum from FY23-1.wiff (sample 1) - Sample002, +TOF MS (50 - 1000) from 0.711 to 0.777 min

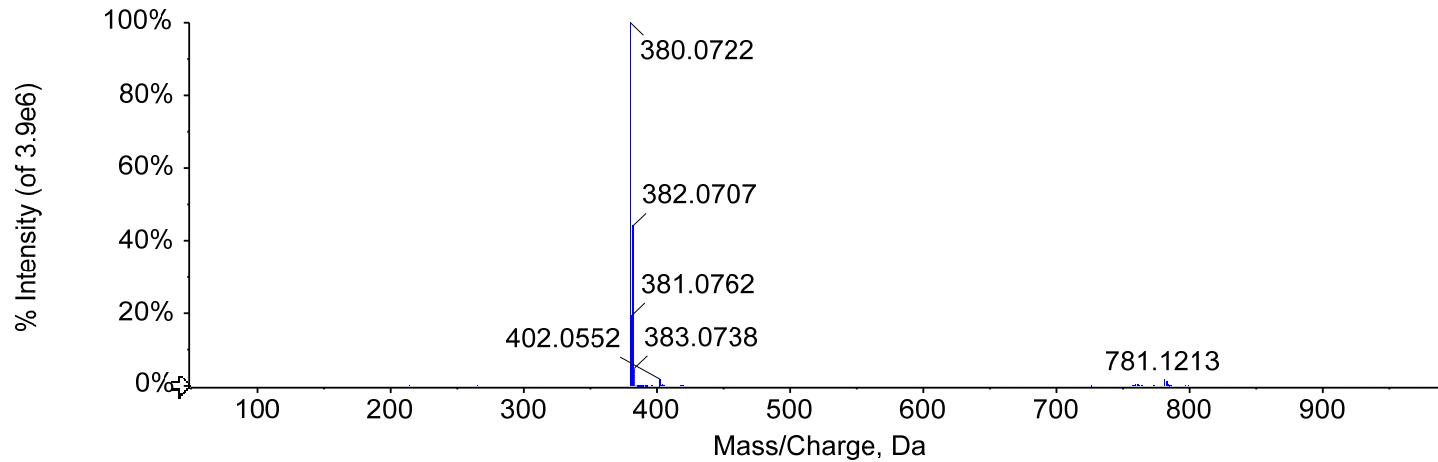


Figure 102. HRMS spectrum of compound **10k**.

Spectrum from FY24.wiff (sample 1) - Sample101, Experiment 1, -TOF MS (50 - 1250) from 0.756 to 0.794 min

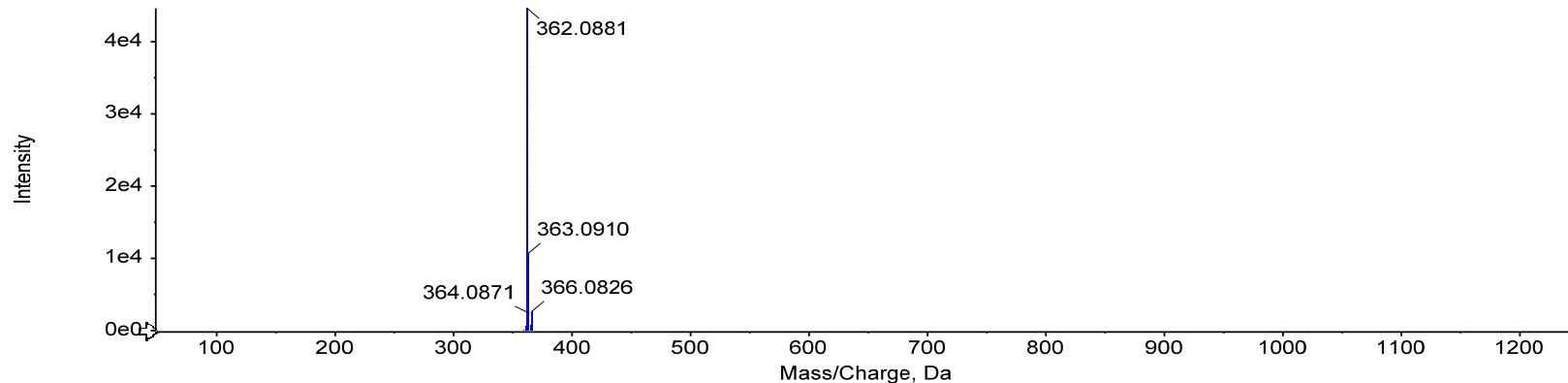


Figure 103. HRMS spectrum of compound **10l**.

Spectrum from FY25.wiff (sample 1) - Sample102, Experiment 1, -TOF MS (50 - 1250) from 0.833 to 0.871 min

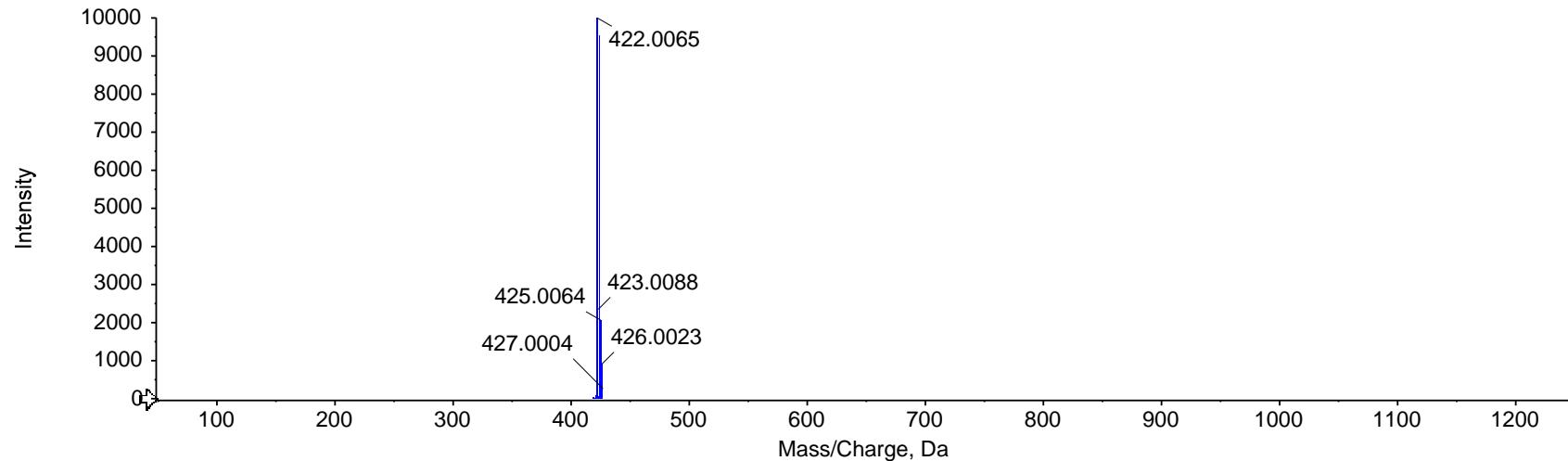


Figure 104. HRMS spectrum of compound **10m**.

Spectrum from FY26.wiff (sample 1) - Sample103, Experiment 1, -TOF MS (50 - 1250) from 0.804 to 0.843 min

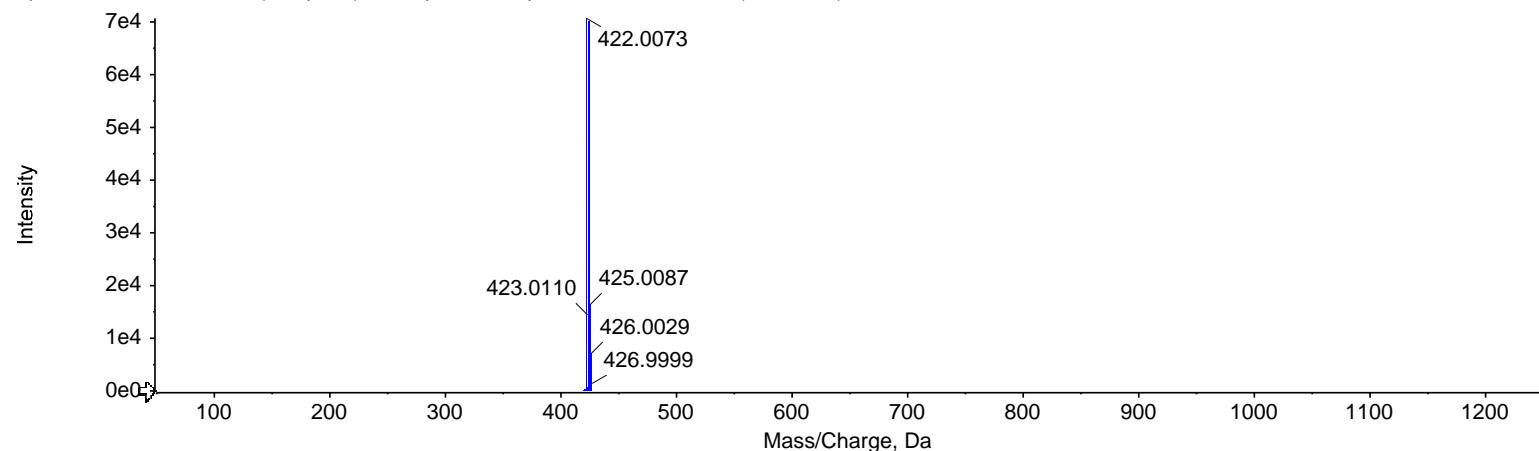


Figure 105. HRMS spectrum of compound **10n**.

Spectrum from FY27.wiff (sample 1) - Sample104, Experiment 1, -TOF MS (50 - 1250) from 0.709 to 0.747 min

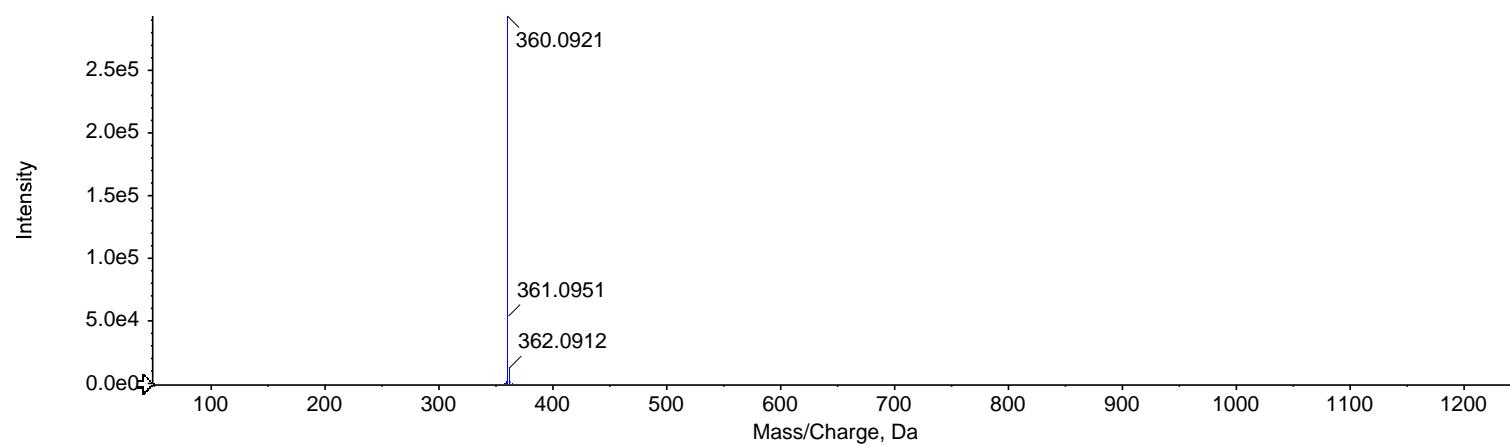


Figure 106. HRMS spectrum of compound **10o**.

Spectrum from FY28.wiff (sample 1) - Sample105, Experiment 1, -TOF MS (50 - 1250) from 0.745 to 0.783 min

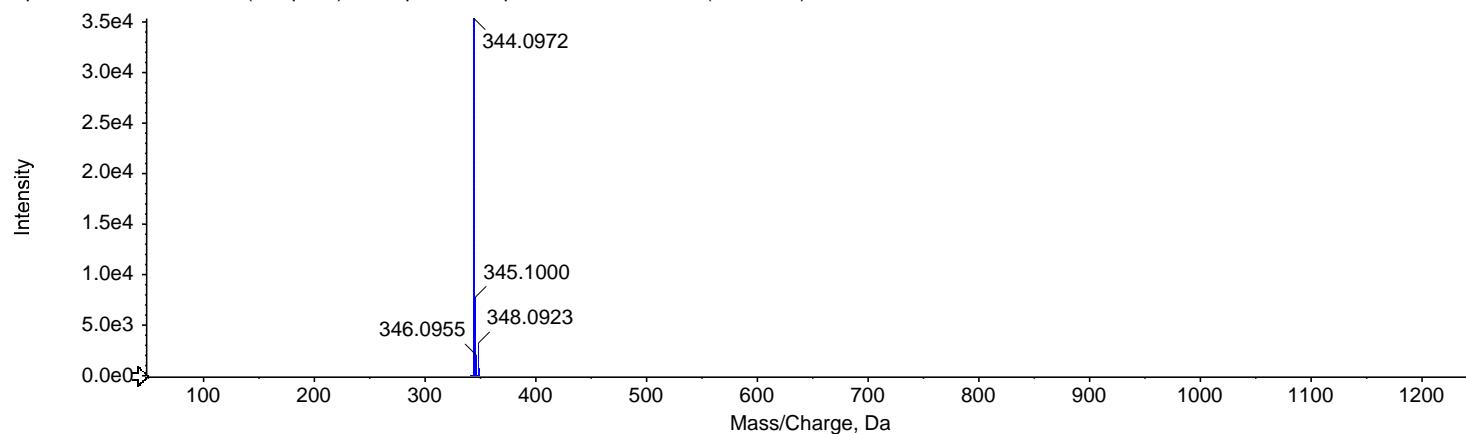


Figure 107. HRMS spectrum of compound **10p**.

Spectrum from FY29.wiff (sample 1) - Sample106, Experiment 1, -TOF MS (50 - 1250) from 0.787 to 0.825 min

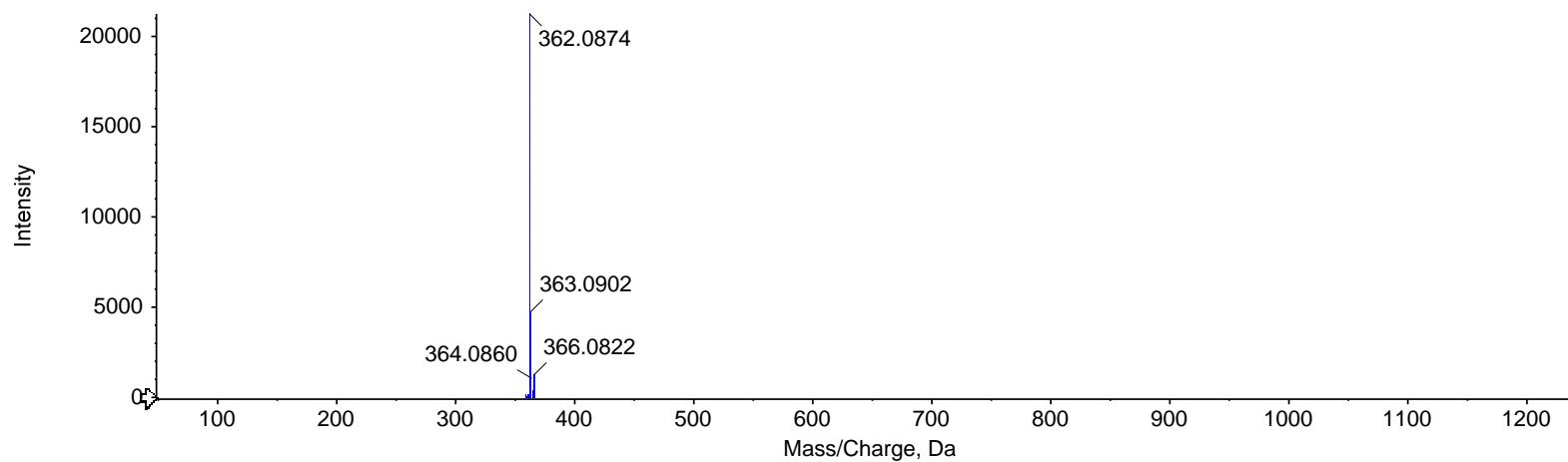


Figure 108. HRMS spectrum of compound **10q**.