

# **An expedient synthesis of novel spiro[indenoquinoxaline-pyrrolizidine]–pyrazole conjugates with anticancer activity from 1,5-diarylpent-4-ene-1,3-diones through 1,3-dipolar cycloaddition/cyclocondensation sequence**

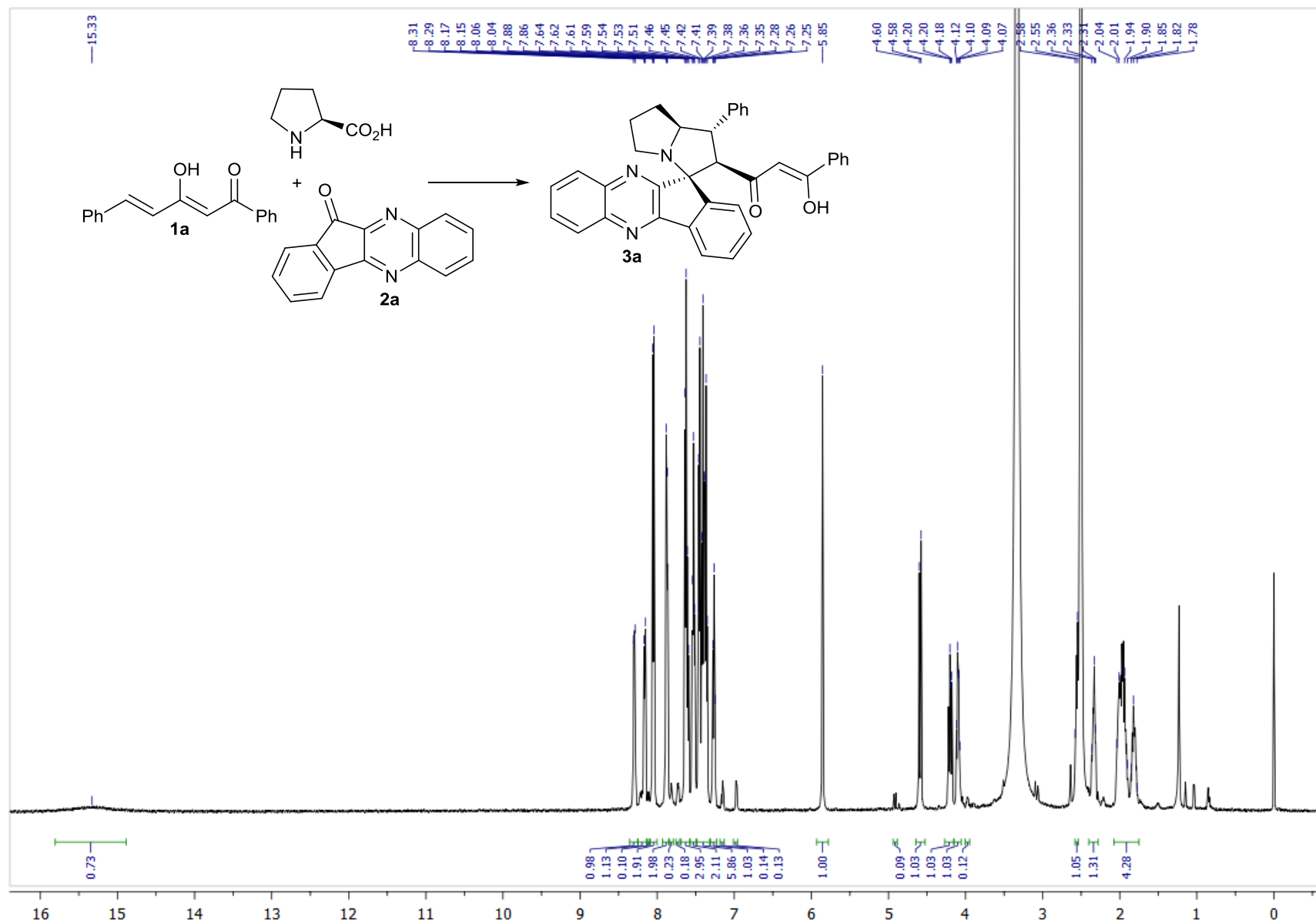
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Vladislav Yu. Korotaev,\* Vyacheslav Ya. Sosnovskikh

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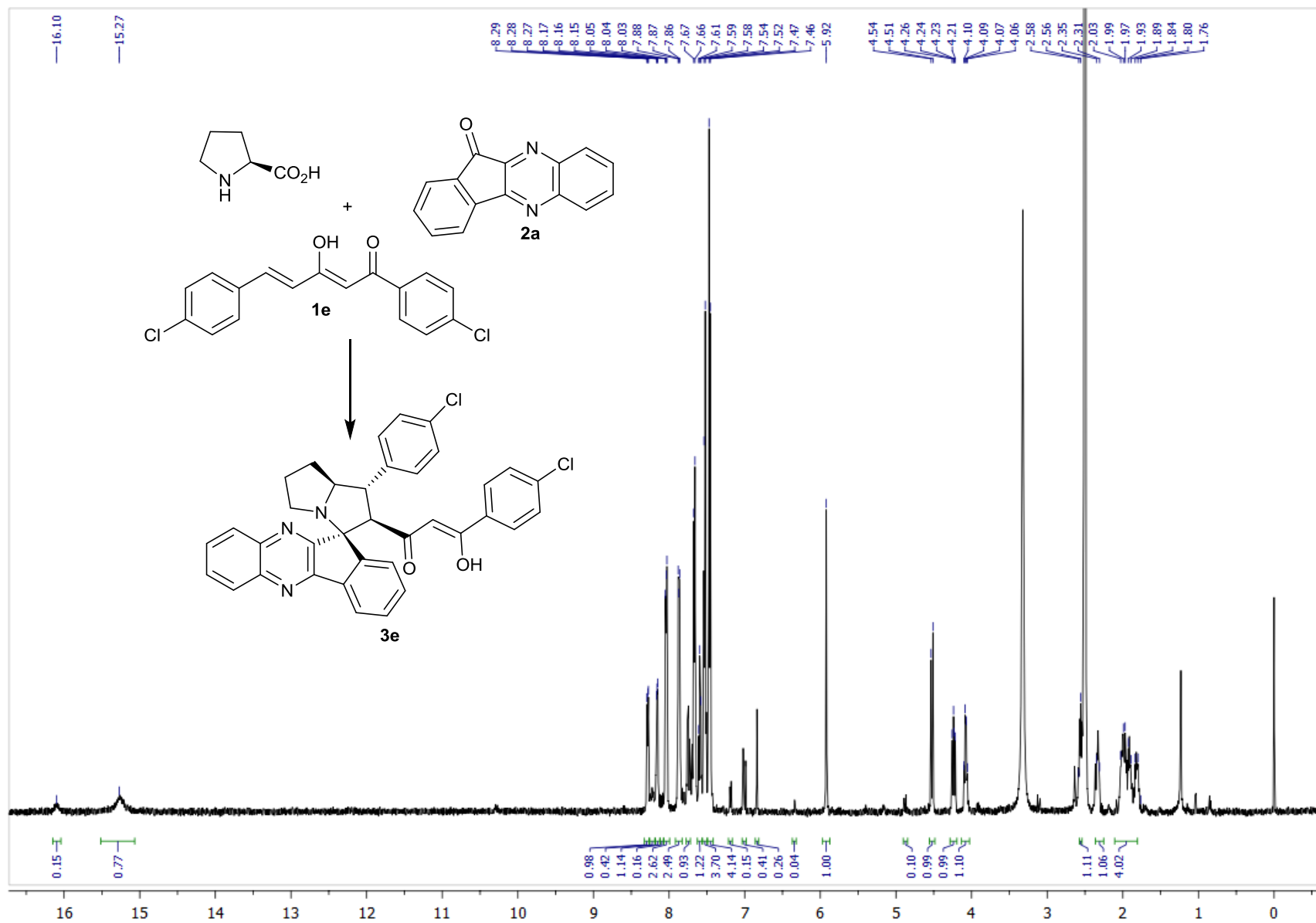
## **Supporting Information**

### **Table of Contents**

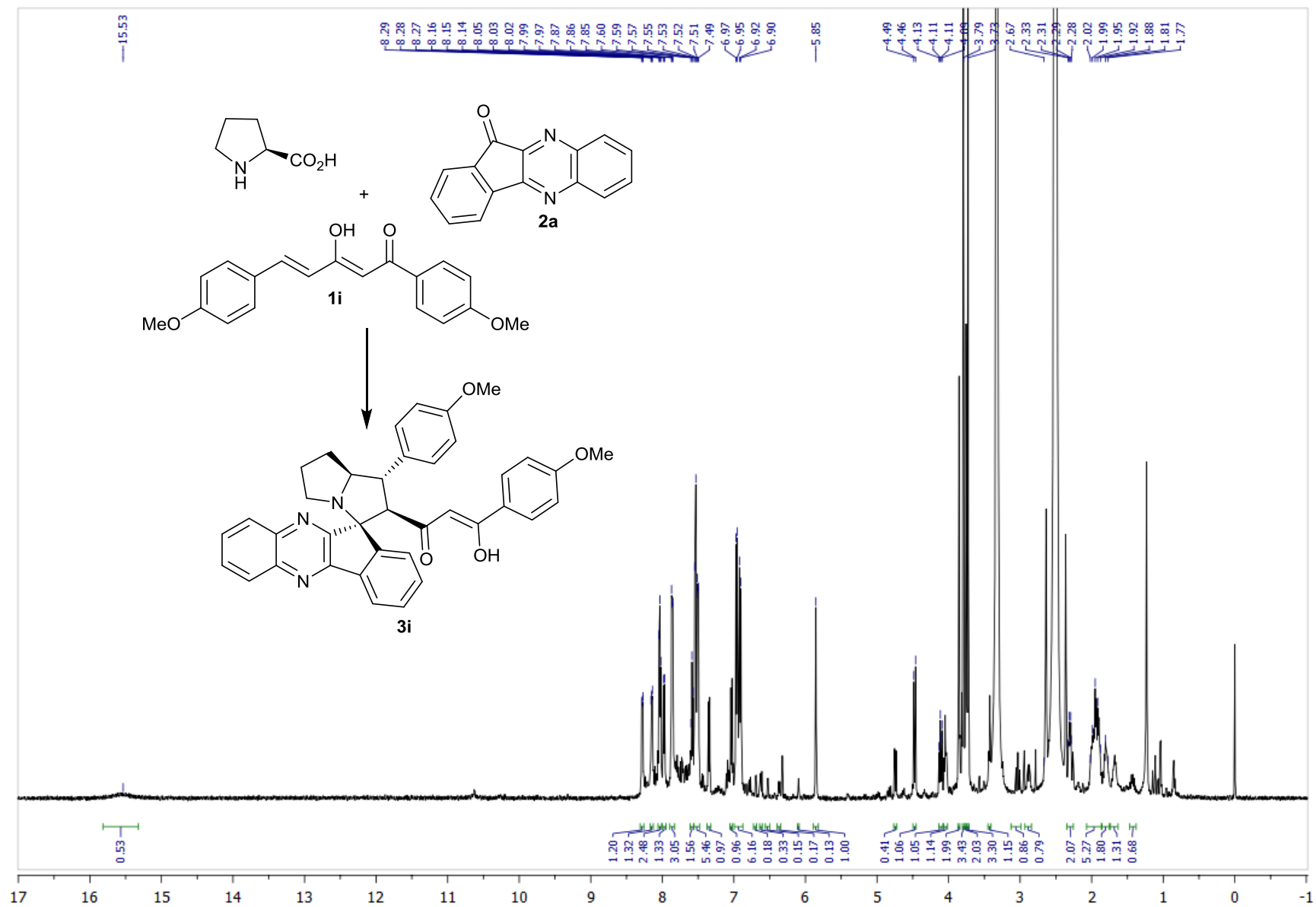
1. <sup>1</sup> H NMR spectra of crude products <b>3a</b> , <b>3e</b> , <b>3i</b>	S2–S4
2. NMR spectra of compounds <b>3</b>	S5–S48
3. NMR spectra of compounds <b>4</b>	S49–S58
4. NMR spectra of compounds <b>5</b>	S59–S76
5. NMR spectra of compounds <b>6</b>	S77–S88
6. NMR spectra of compounds <b>7</b>	S89–S92



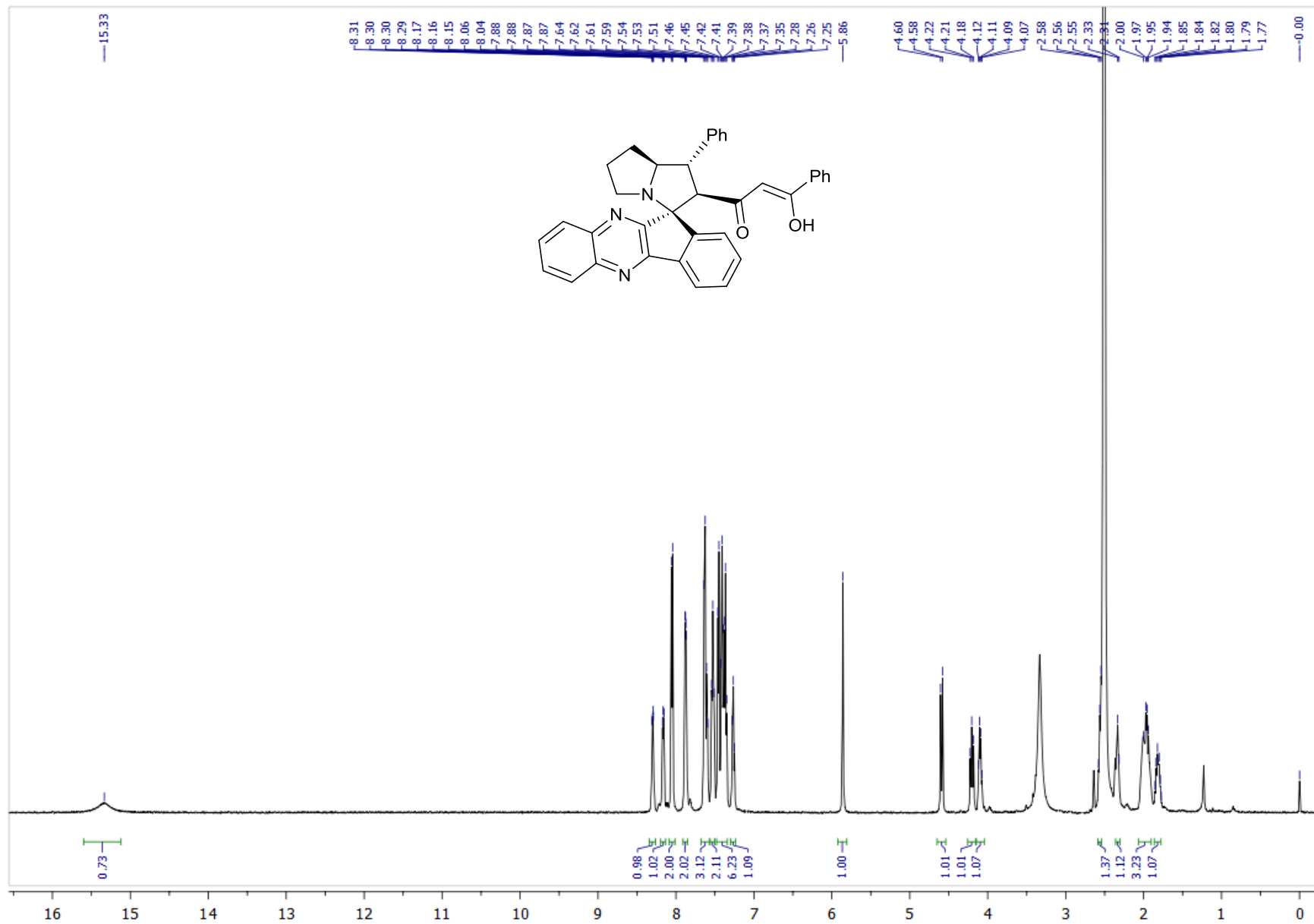
**Figure S1.** Copy of  $^1\text{H}$  NMR spectrum of the three-component reaction between **1a**, **2a** and proline in  $\text{DMSO-}d_6$  (reaction mixture)



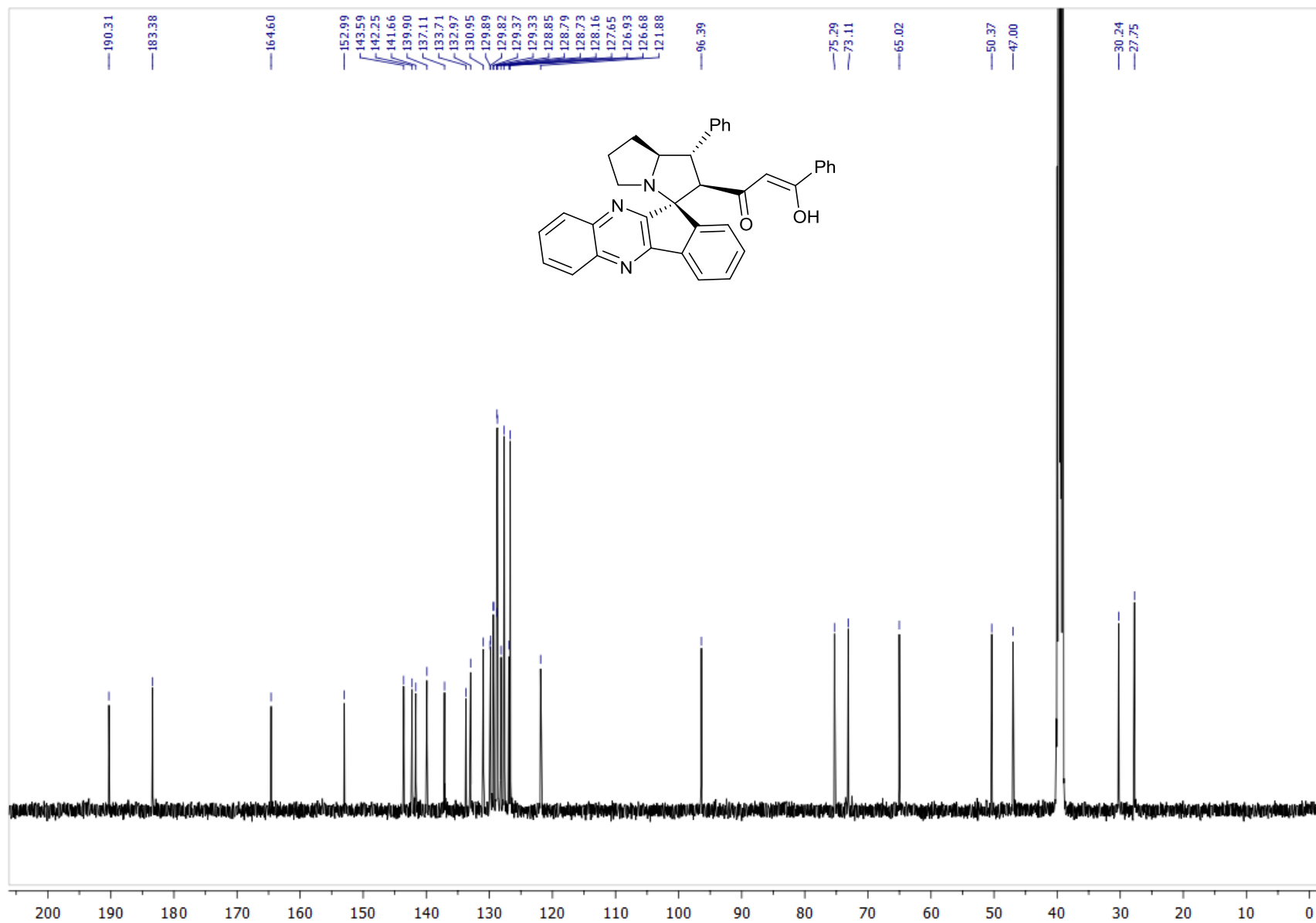
**Figure S2.** Copy of  $^1\text{H}$  NMR spectrum of the three-component reaction between **1e**, **2a** and proline in  $\text{DMSO-}d_6$  (reaction mixture)



**Figure S3.** Copy of  $^1\text{H}$  NMR spectrum of the three-component reaction between **1i**, **2a** and proline in  $\text{DMSO-}d_6$  (reaction mixture)



**Figure S4.** Copy of  $^1\text{H}$  NMR spectrum of **3a** in  $\text{DMSO-}d_6$



**Figure S5.** Copy of  $^{13}\text{C}$  NMR spectrum of **3a** in  $\text{DMSO-}d_6$

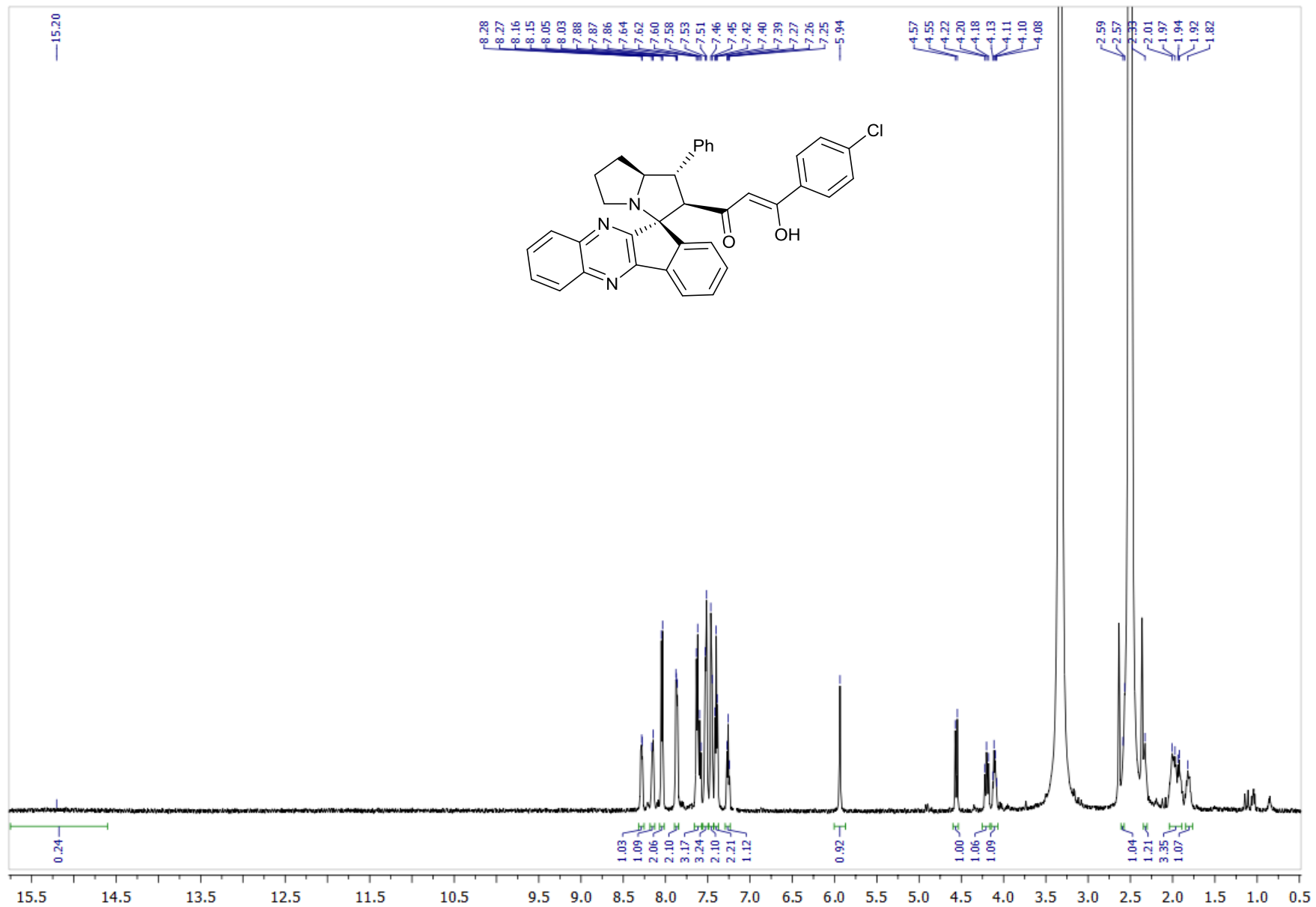


Figure S6. Copy of  $^1\text{H}$  NMR spectrum of **3b** in  $\text{DMSO}-d_6$

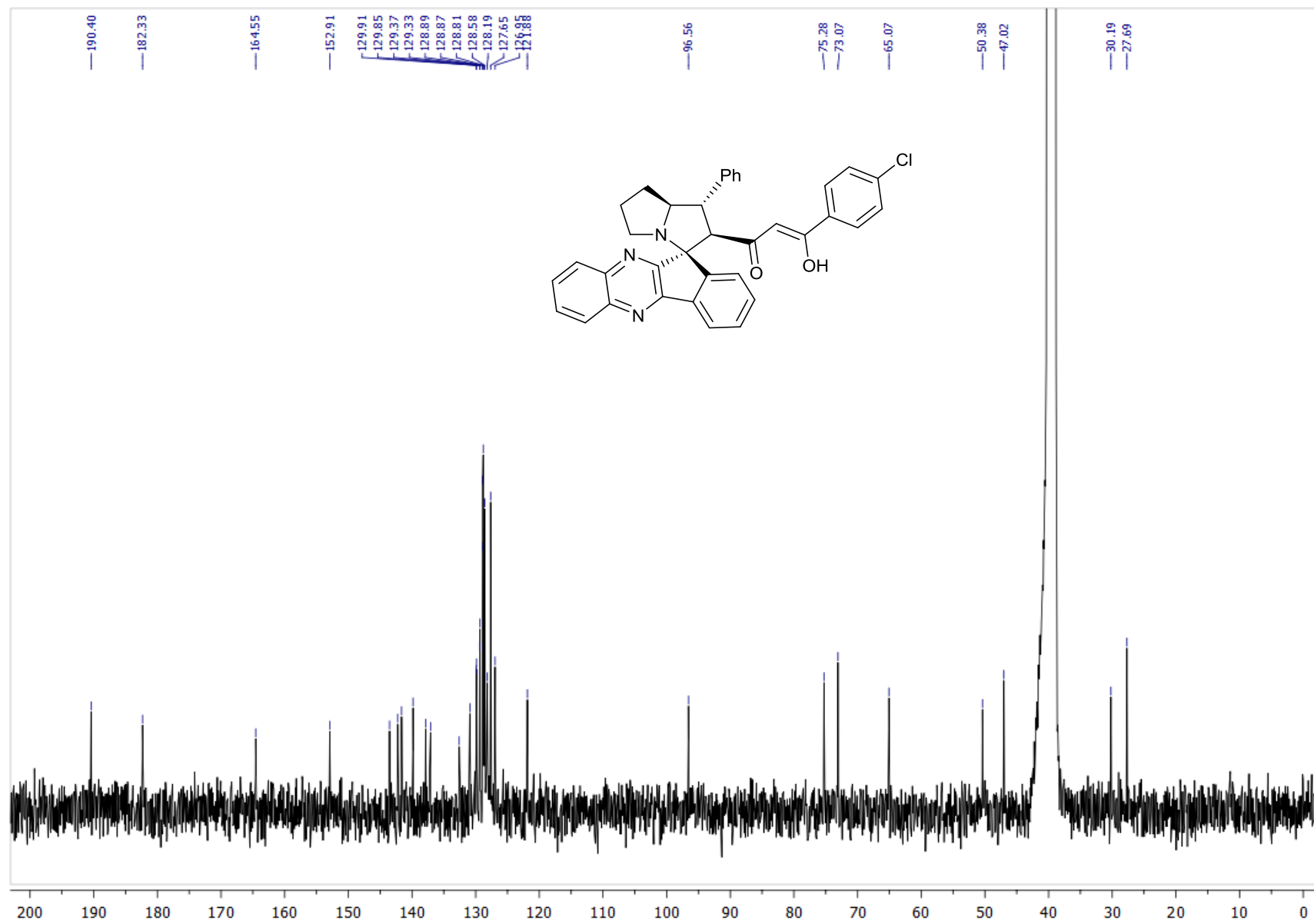
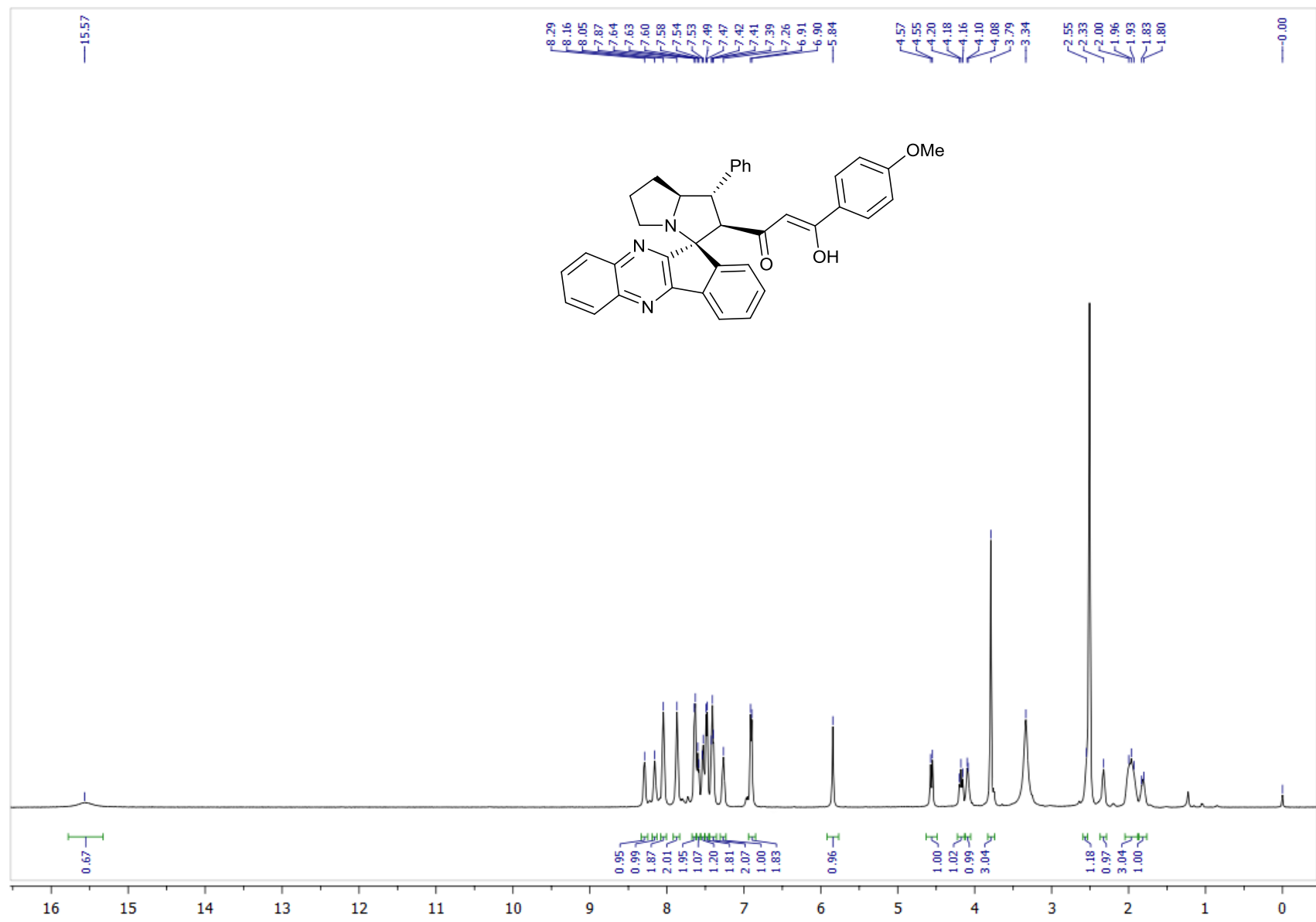


Figure S7. Copy of  $^{13}\text{C}$  NMR spectrum of **3b** in  $\text{DMSO-}d_6$





**Figure S8.** Copy of <sup>1</sup>H NMR spectrum of **3c** in DMSO-*d*<sub>6</sub>

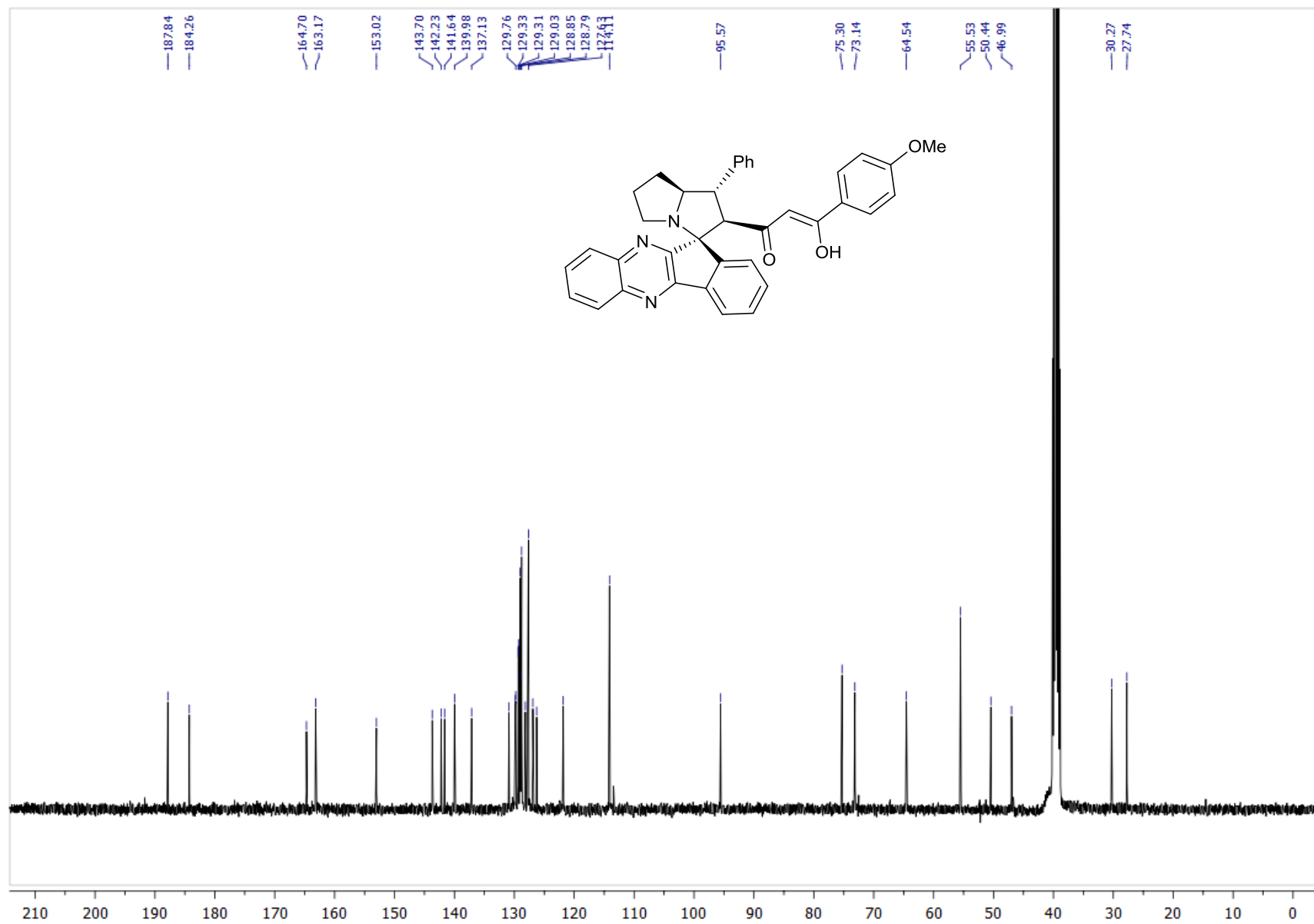


Figure S9. Copy of  $^{13}\text{C}$  NMR spectrum of **3c** in  $\text{DMSO-}d_6$

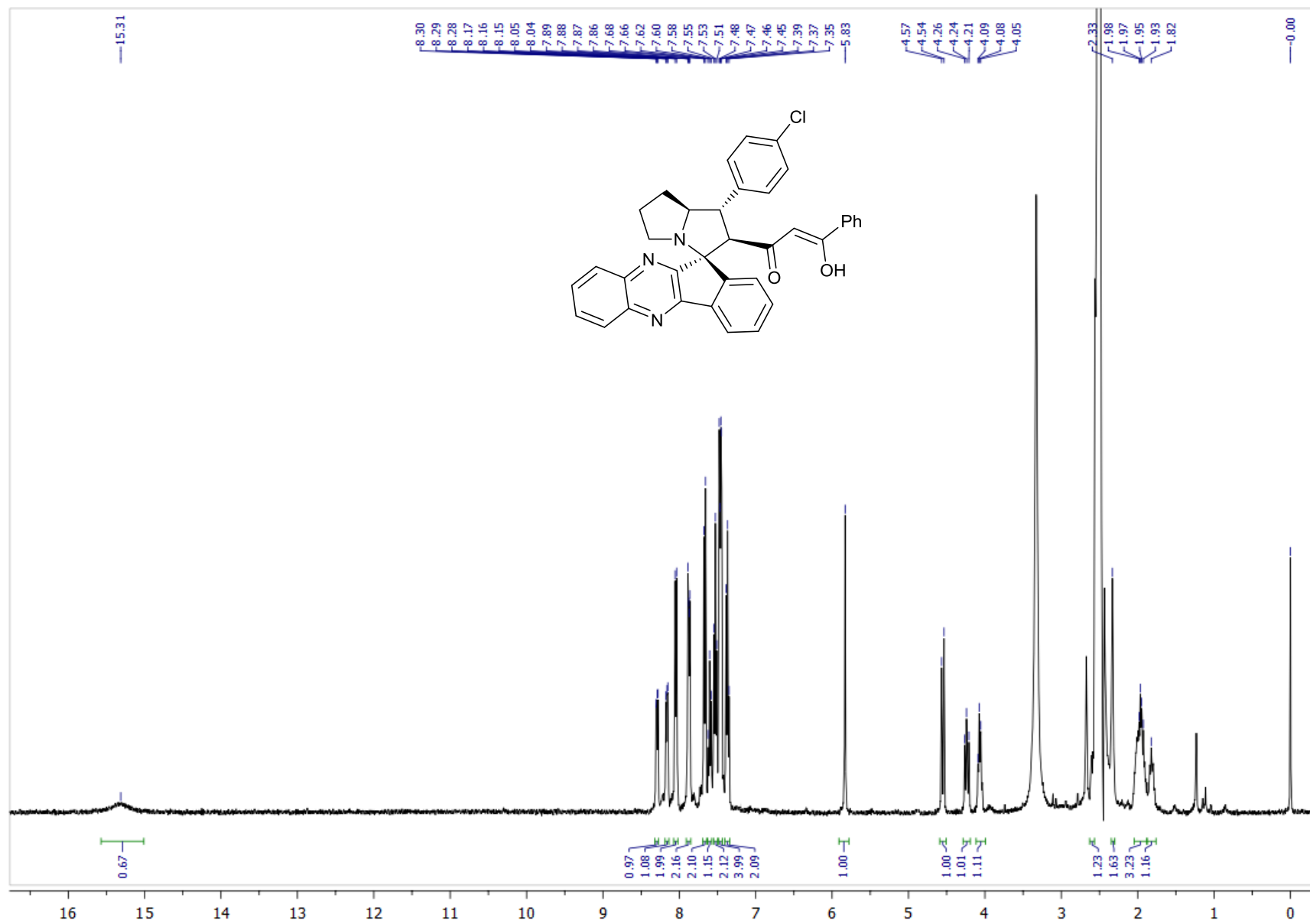
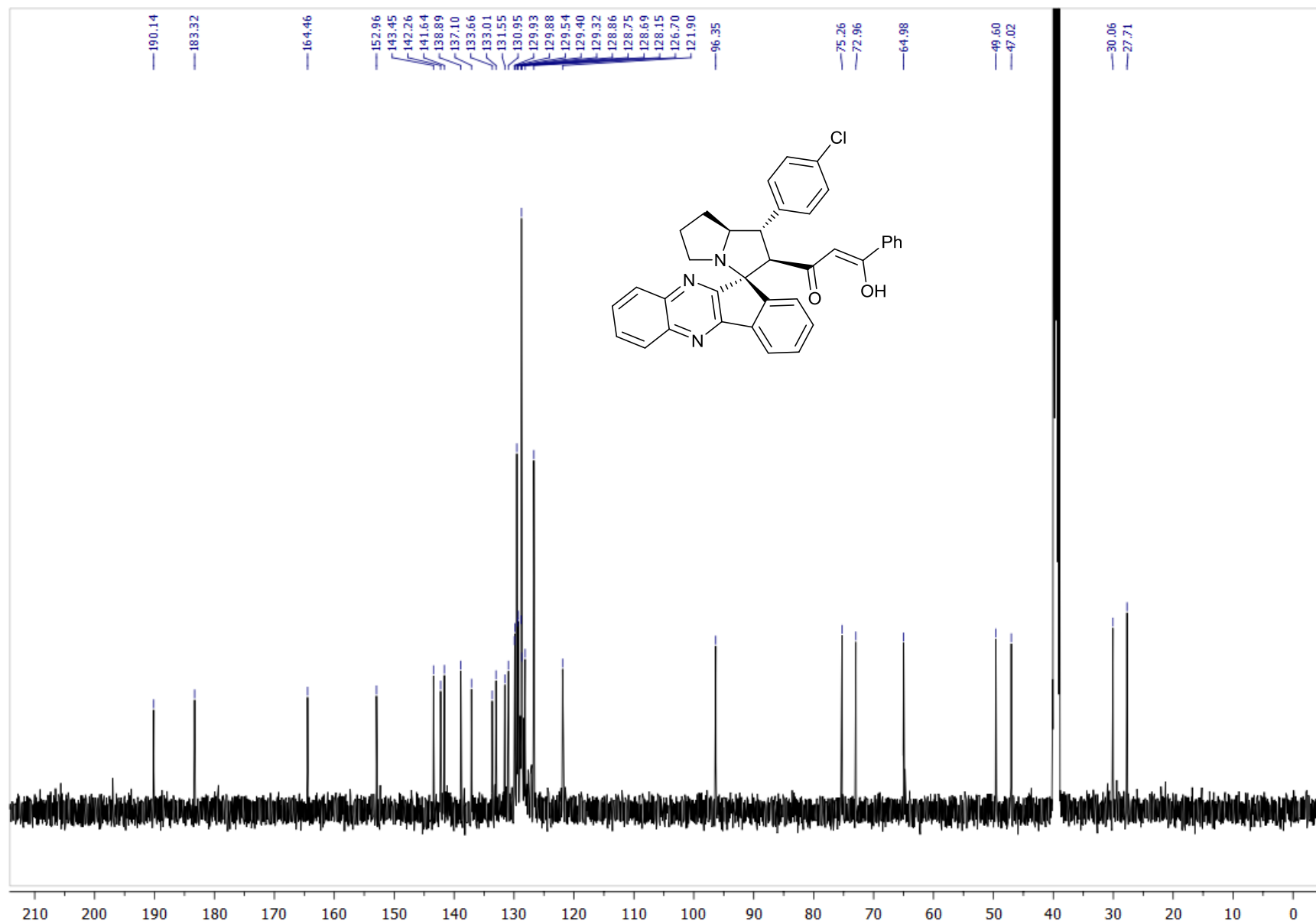
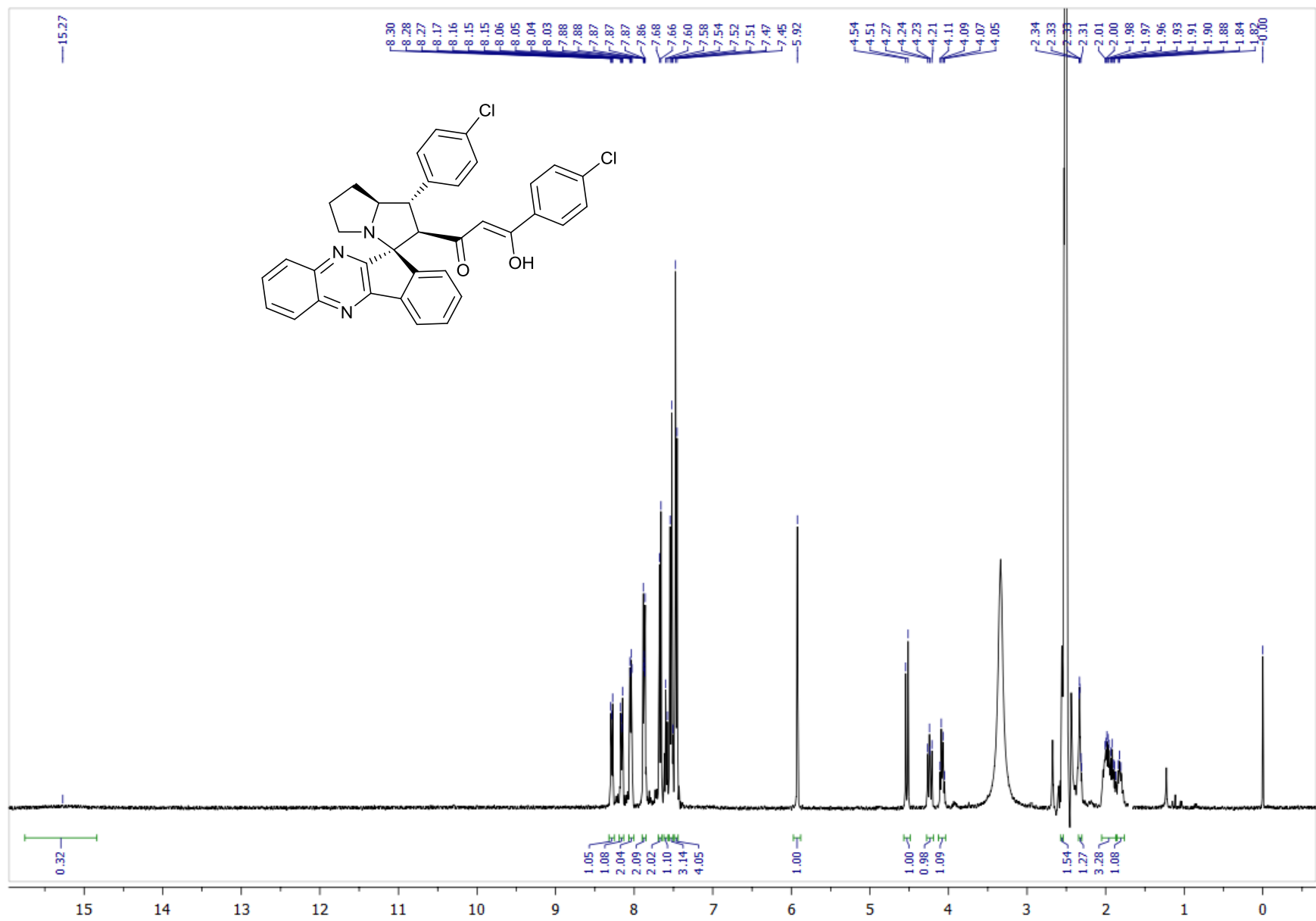


Figure S10. Copy of  $^1\text{H}$  NMR spectrum of **3d** in DMSO- $d_6$



**Figure S11.** Copy of  $^{13}\text{C}$  NMR spectrum of **3d** in  $\text{DMSO-}d_6$



**Figure S12.** Copy of  $^1\text{H}$  NMR spectrum of **3e** in DMSO- $d_6$

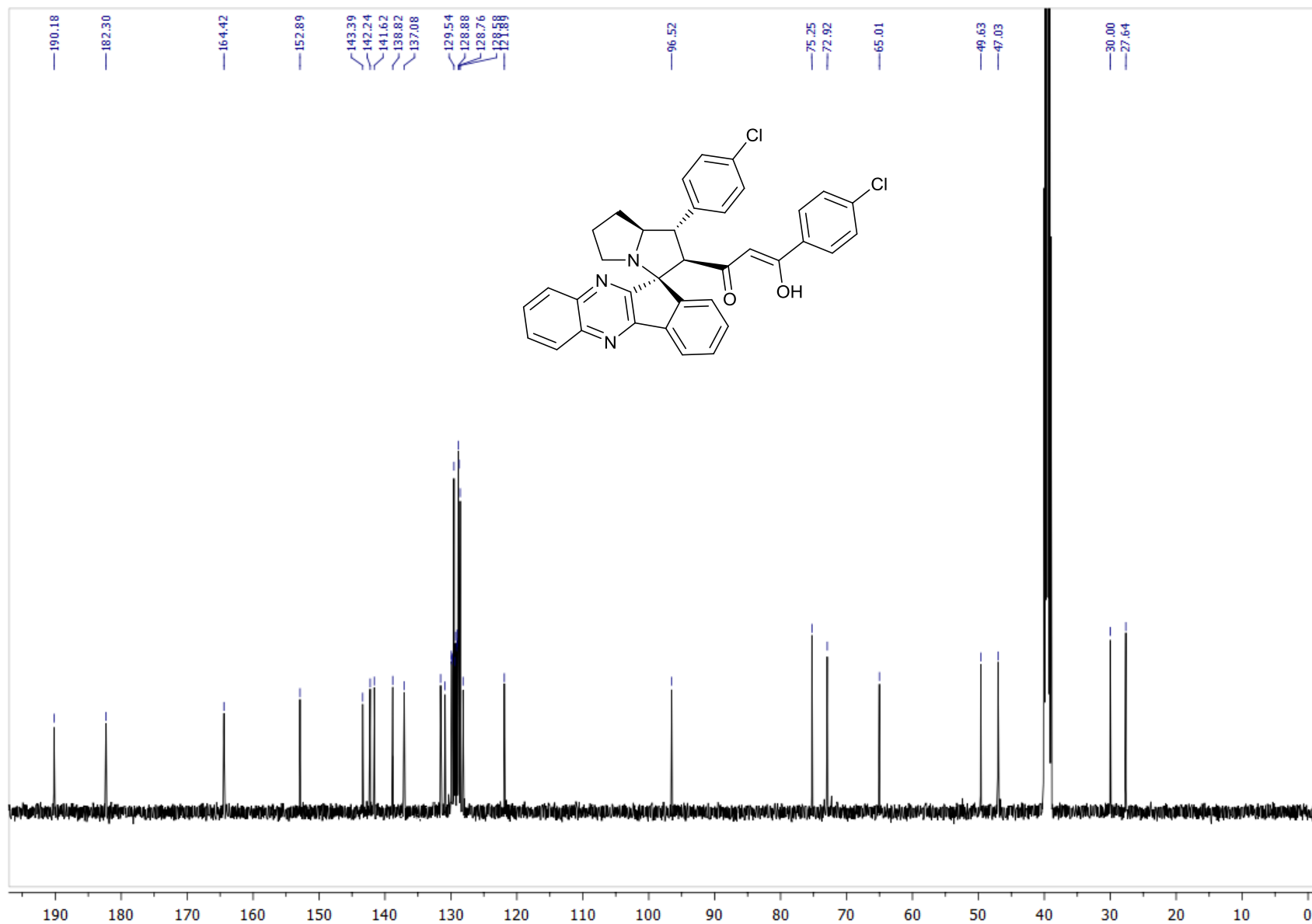
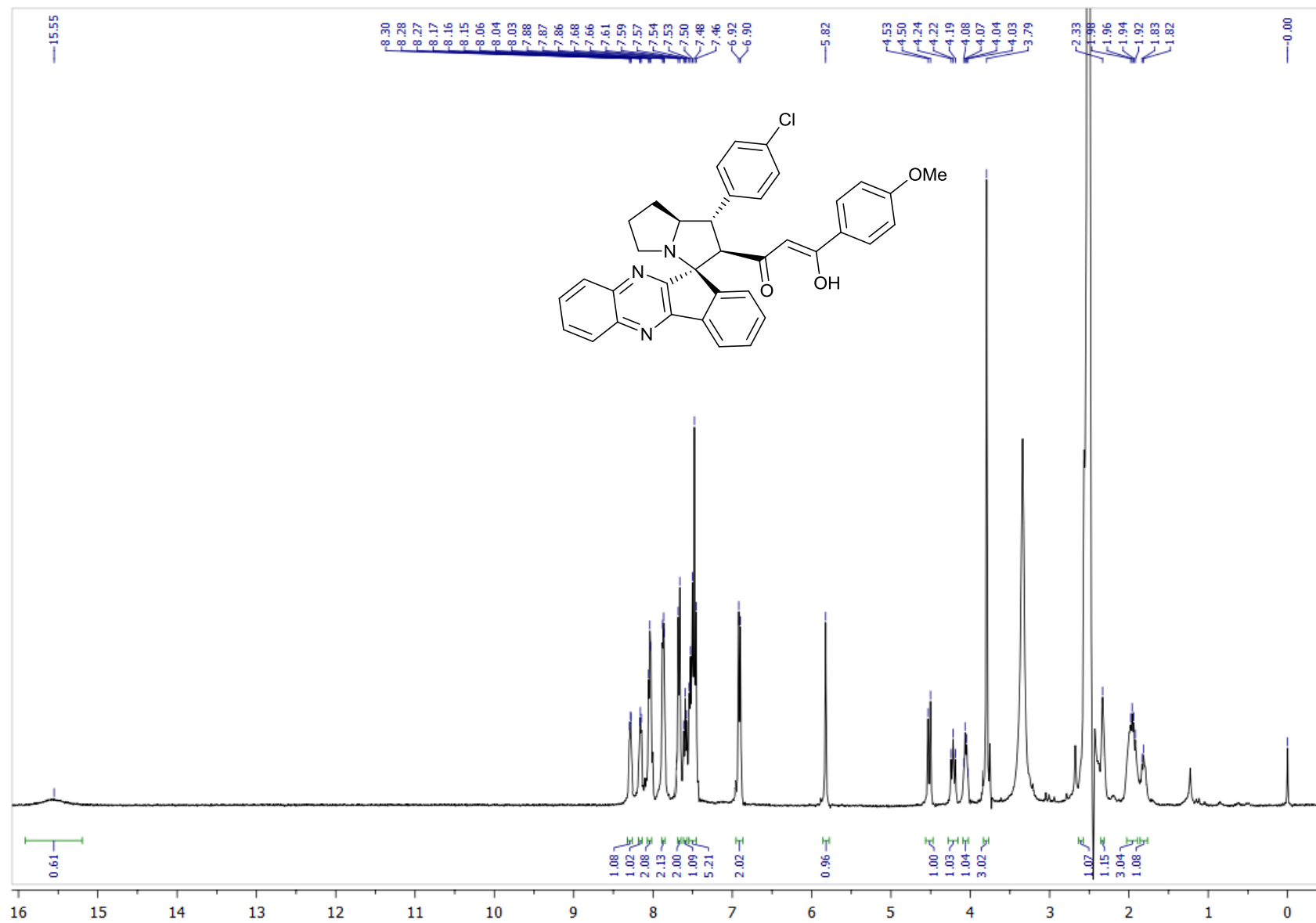


Figure S13. Copy of  $^{13}\text{C}$  NMR spectrum of **3e** in  $\text{DMSO-}d_6$



**Figure S14.** Copy of  $^1\text{H}$  NMR spectrum of **3f** in  $\text{DMSO-}d_6$

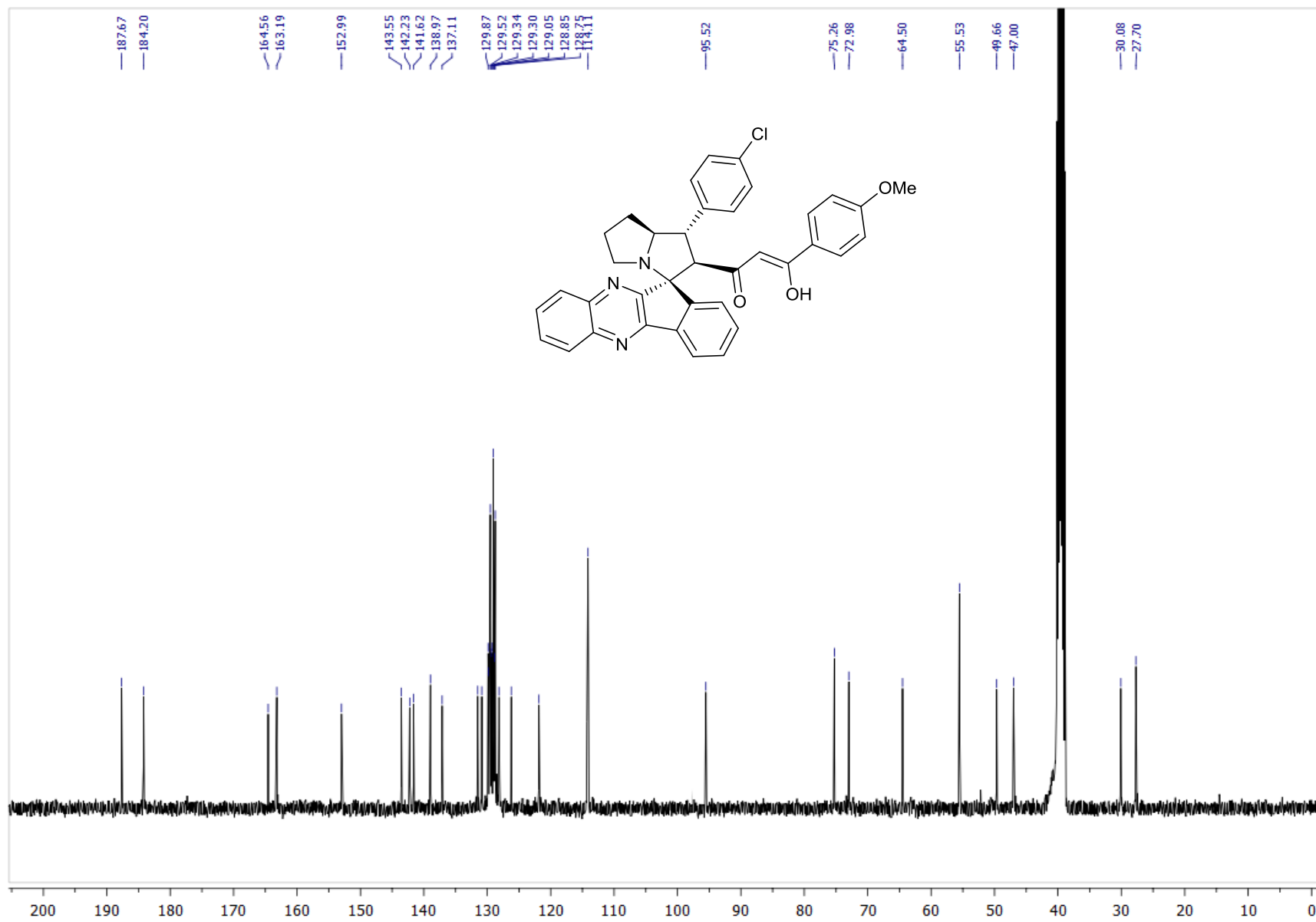


Figure S15. Copy of  $^{13}\text{C}$  NMR spectrum of **3f** in  $\text{DMSO-}d_6$



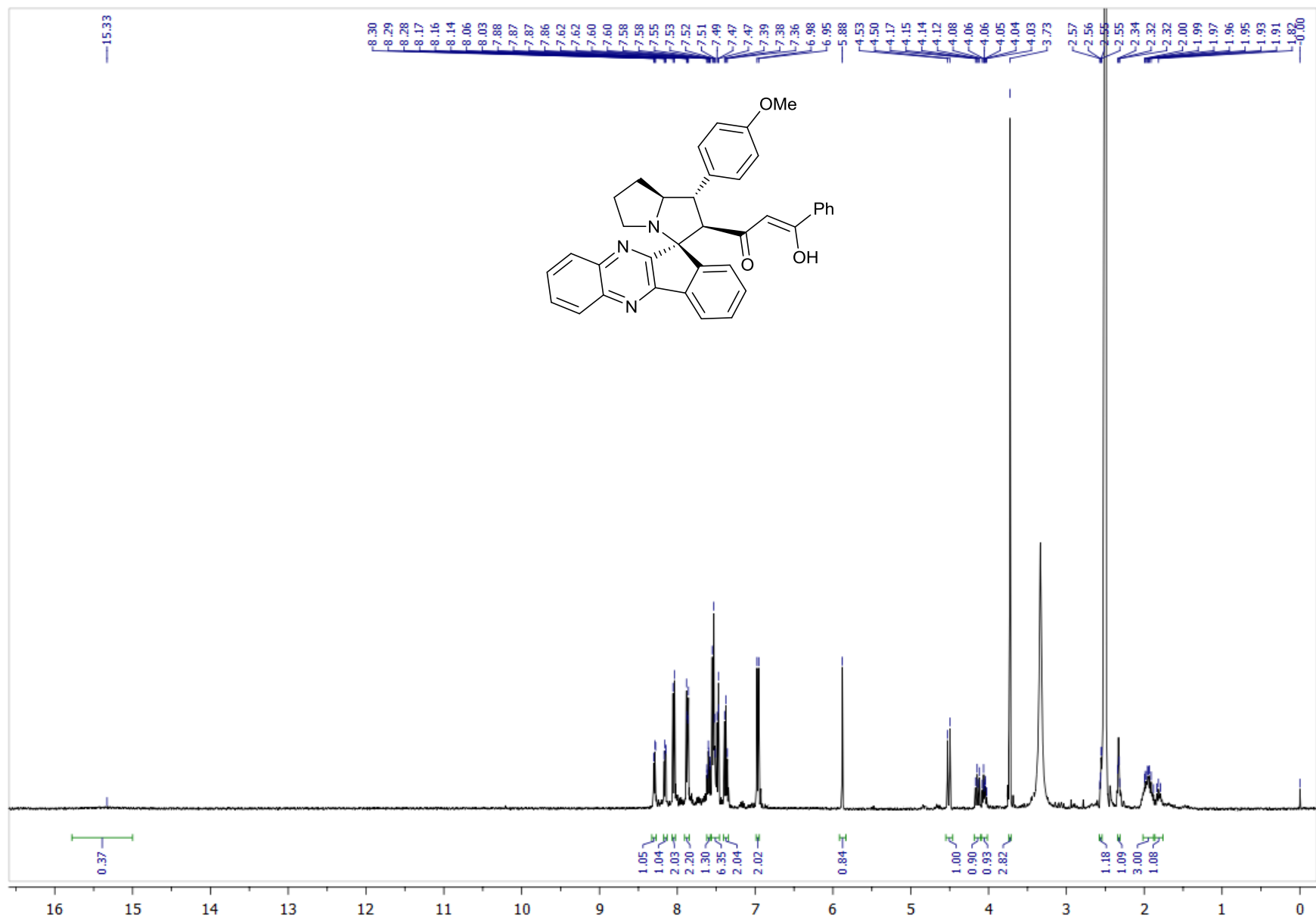


Figure S16. Copy of  $^1\text{H}$  NMR spectrum of **3g** in  $\text{DMSO}-d_6$

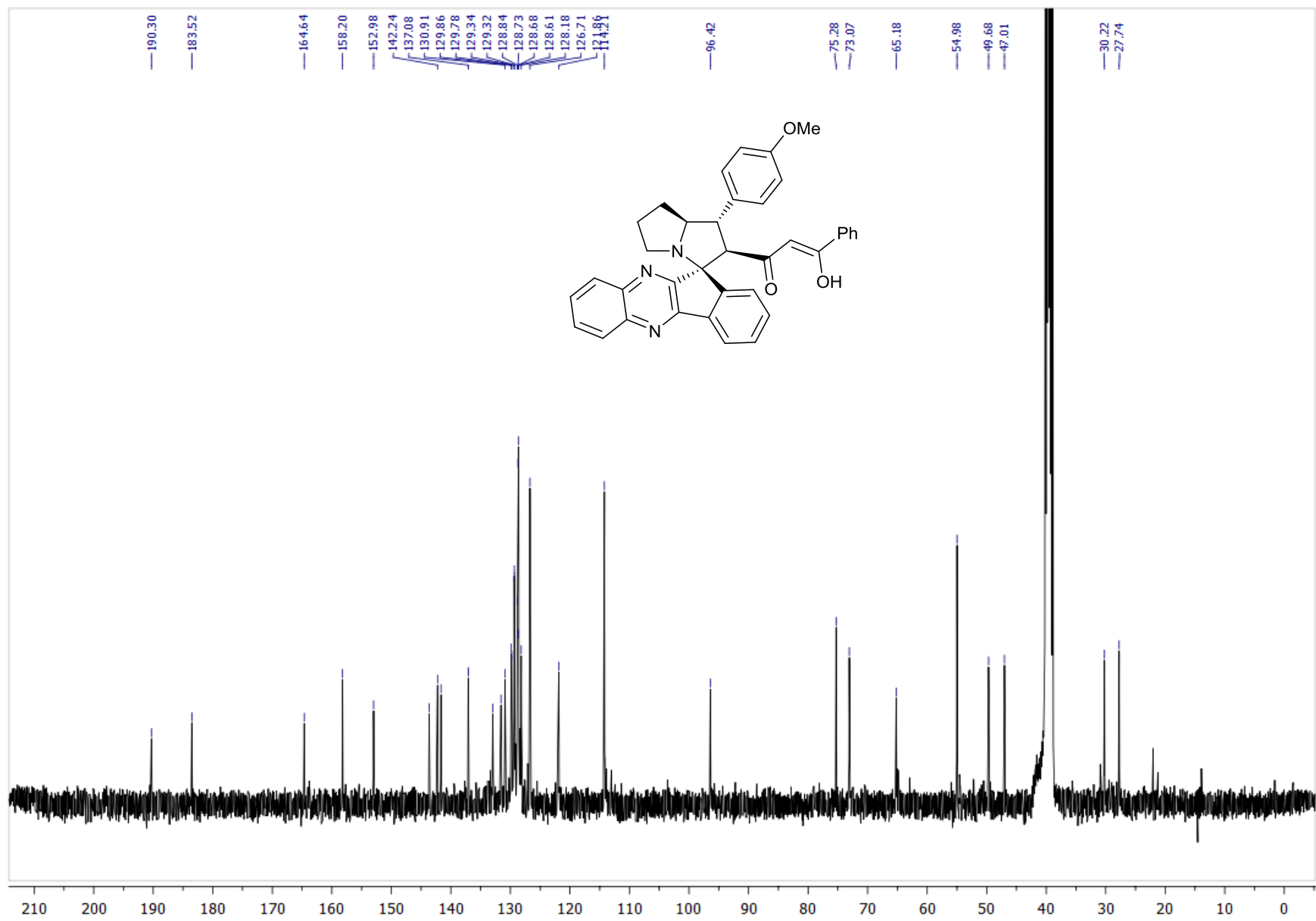
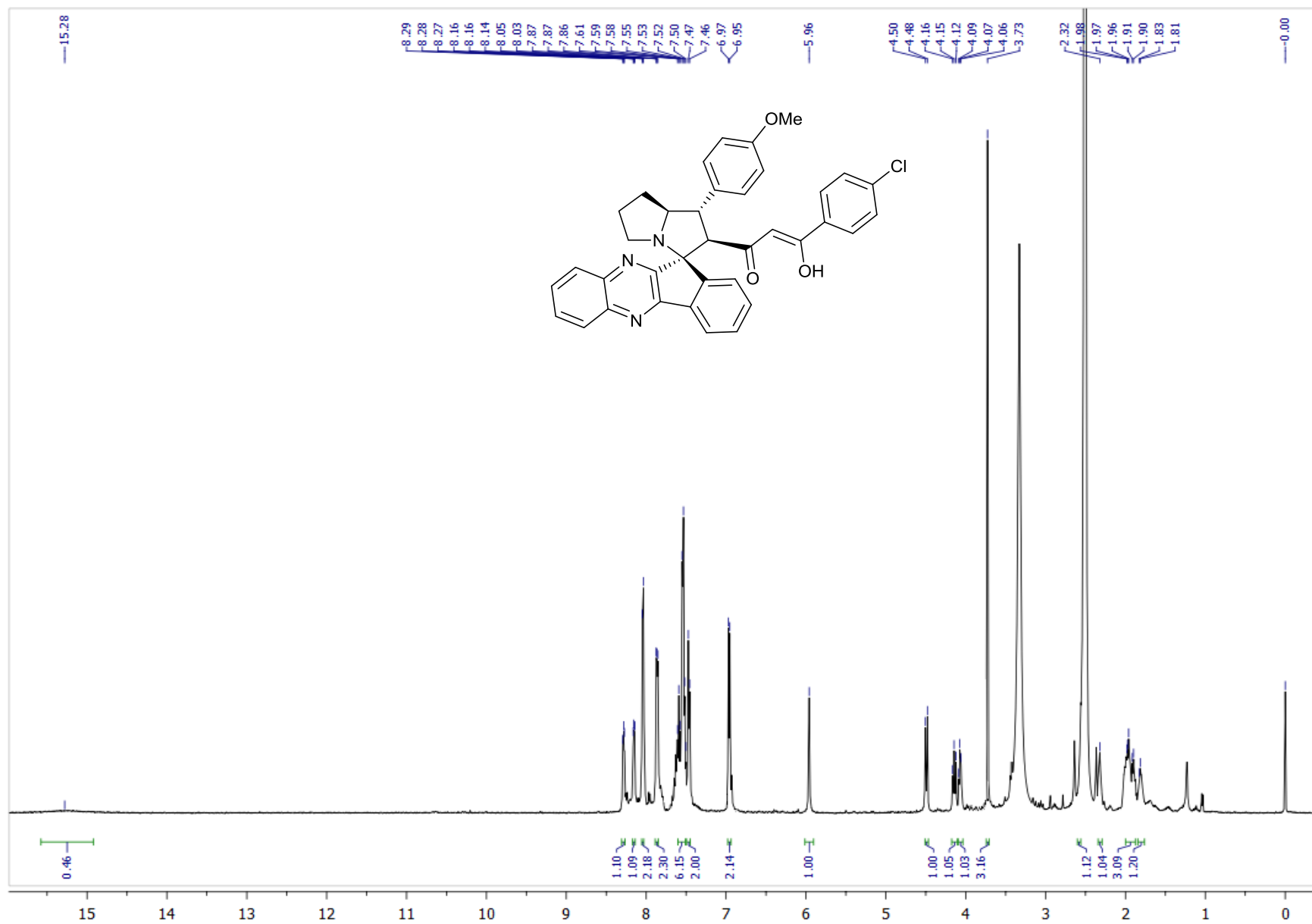
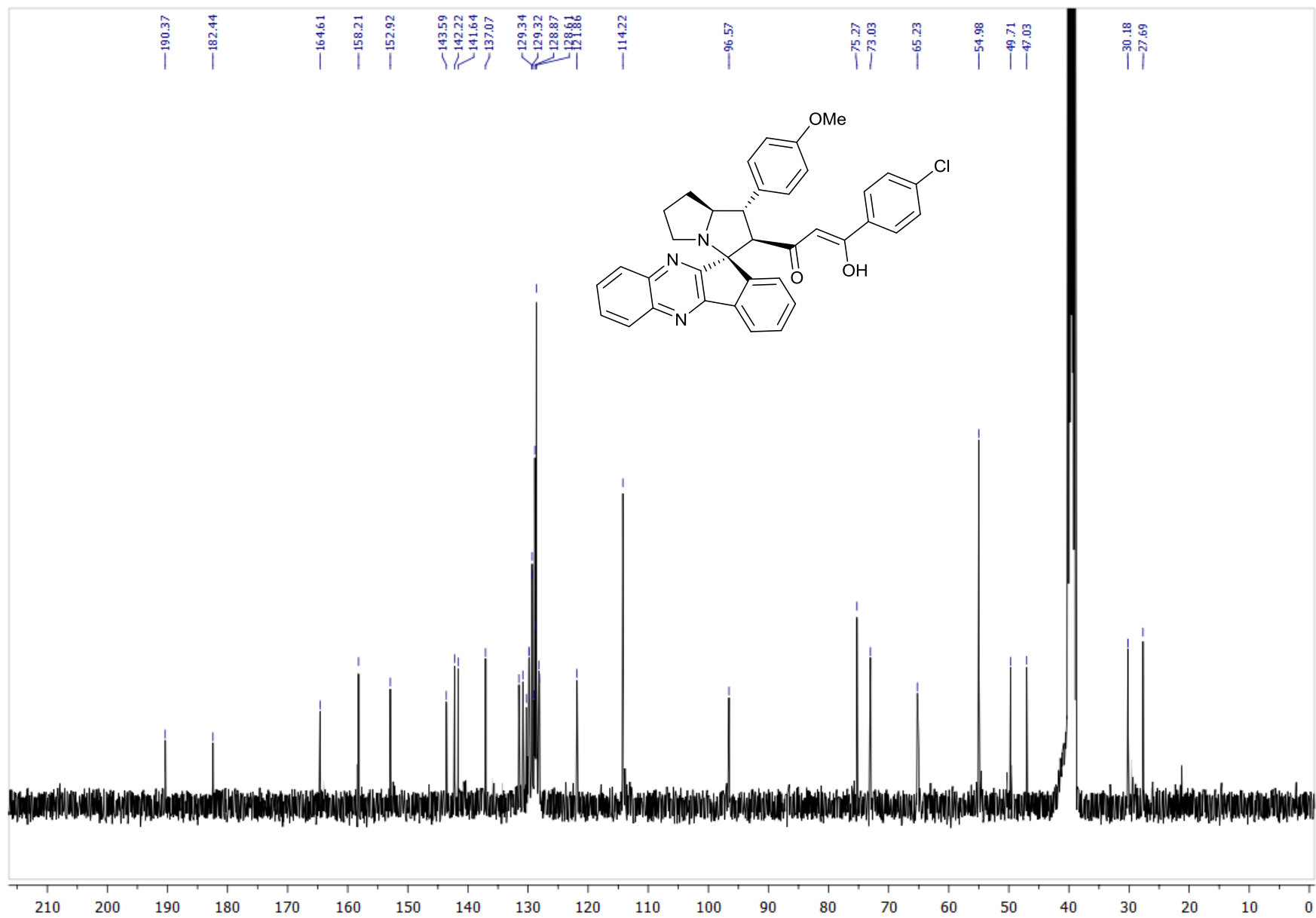


Figure S17. Copy of  $^{13}\text{C}$  NMR spectrum of **3g** in  $\text{DMSO-}d_6$



**Figure S18.** Copy of <sup>1</sup>H NMR spectrum of **3h** in DMSO-*d*<sub>6</sub>



**Figure S19.** Copy of  $^{13}\text{C}$  NMR spectrum of **3h** in  $\text{DMSO-}d_6$

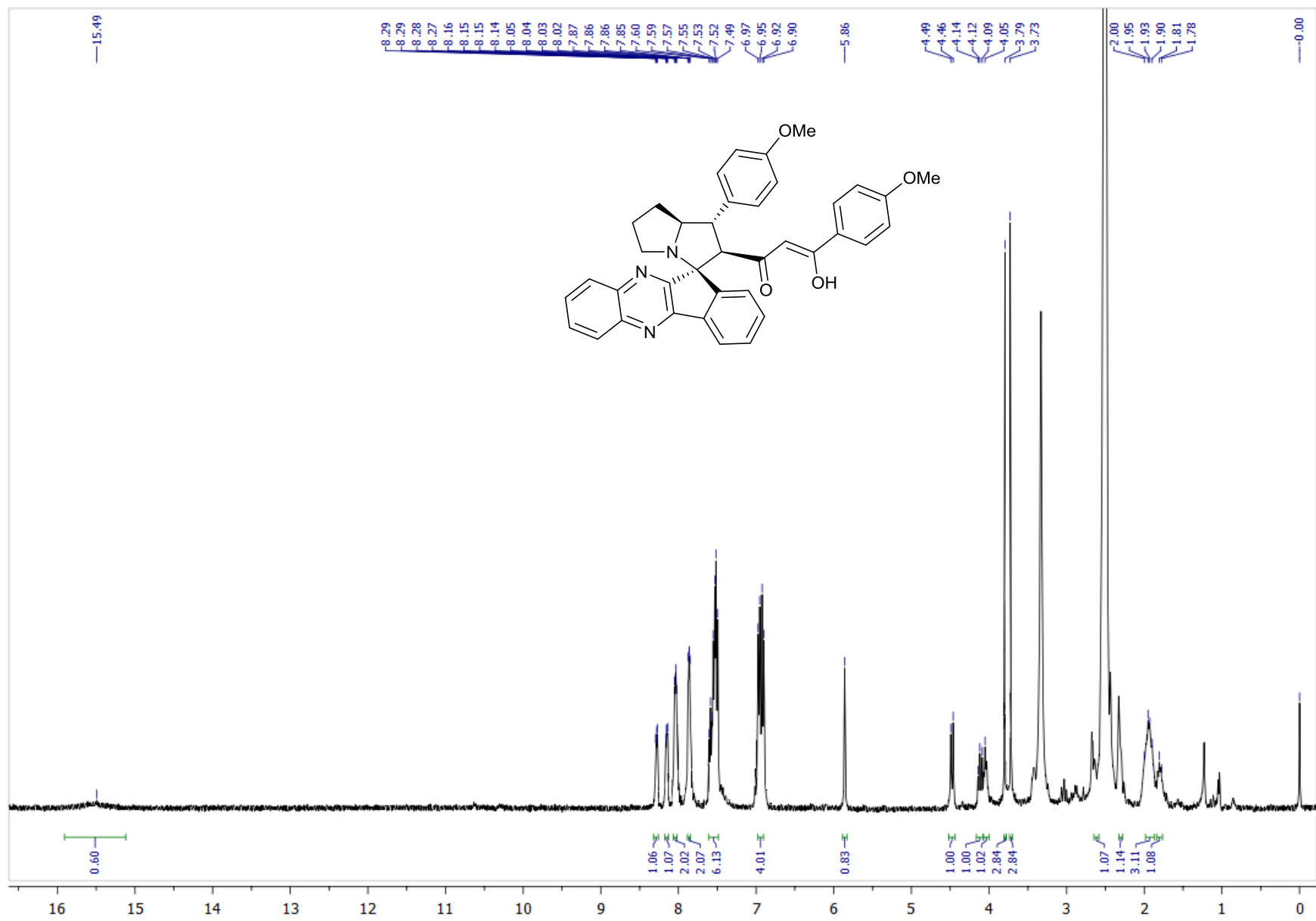


Figure S20. Copy of <sup>1</sup>H NMR spectrum of **3i** in DMSO-*d*<sub>6</sub>

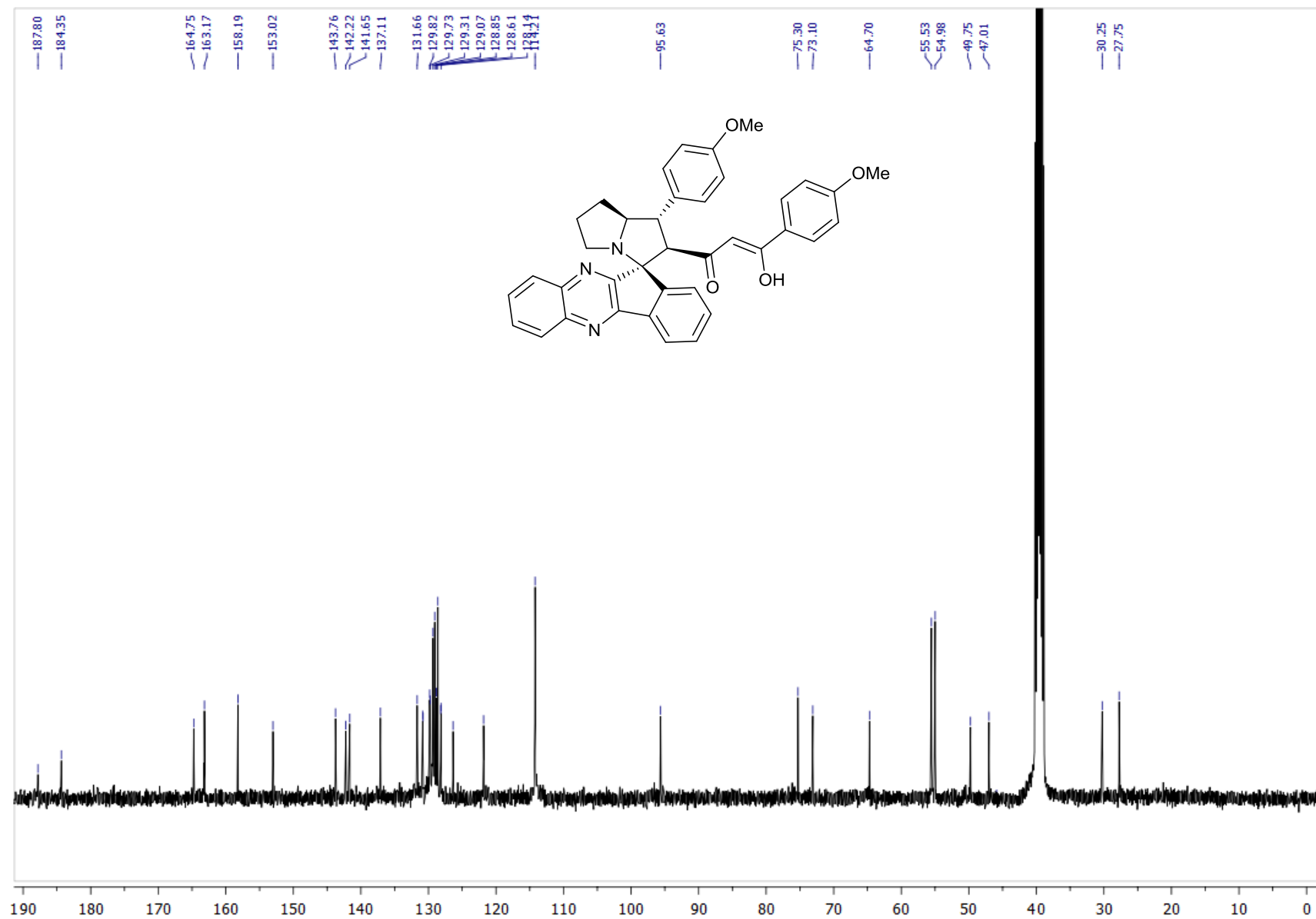


Figure S21. Copy of  $^{13}\text{C}$  NMR spectrum of **3i** in  $\text{DMSO-}d_6$

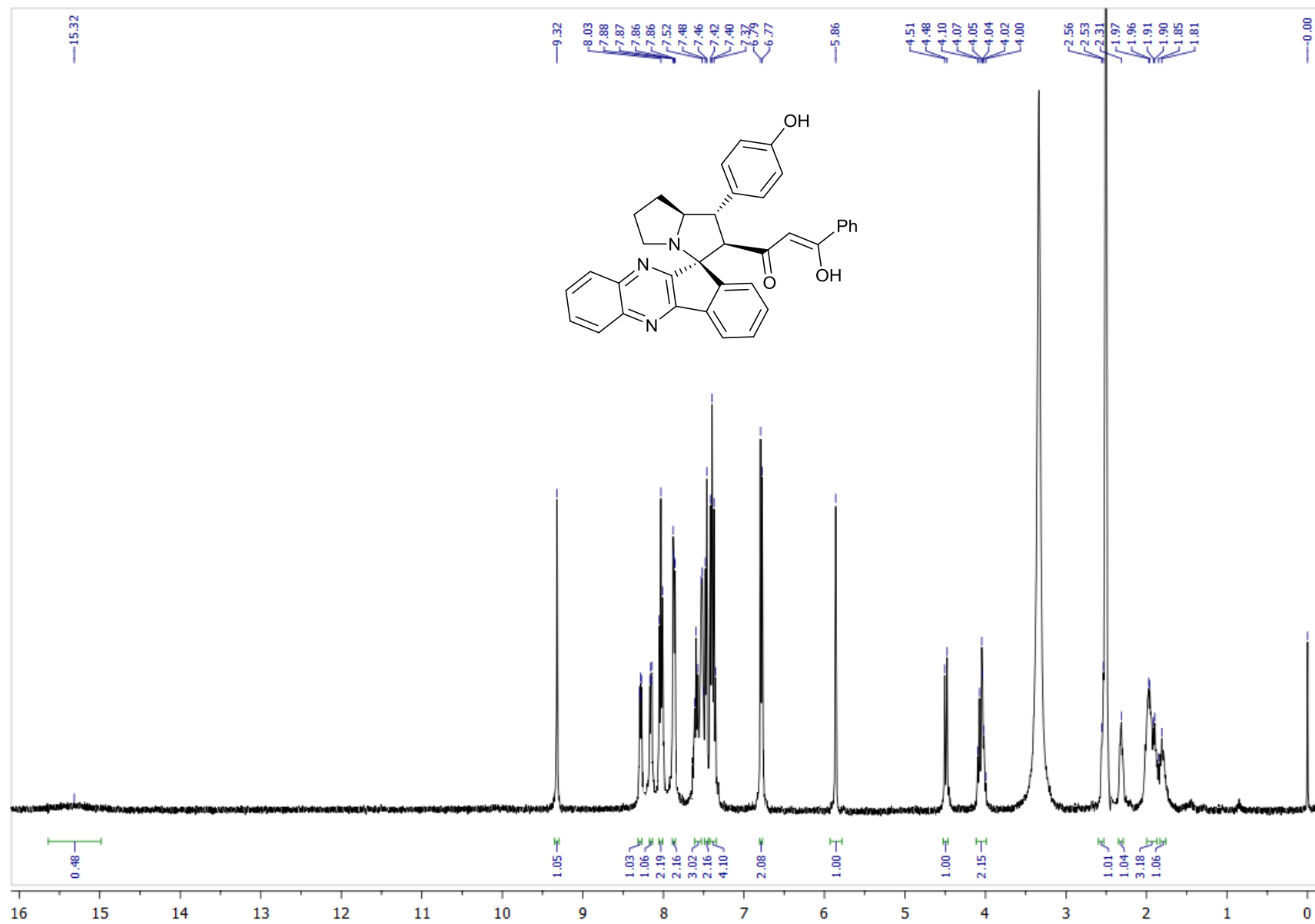


Figure S22. Copy of <sup>1</sup>H NMR spectrum of **3j** in DMSO-*d*<sub>6</sub>

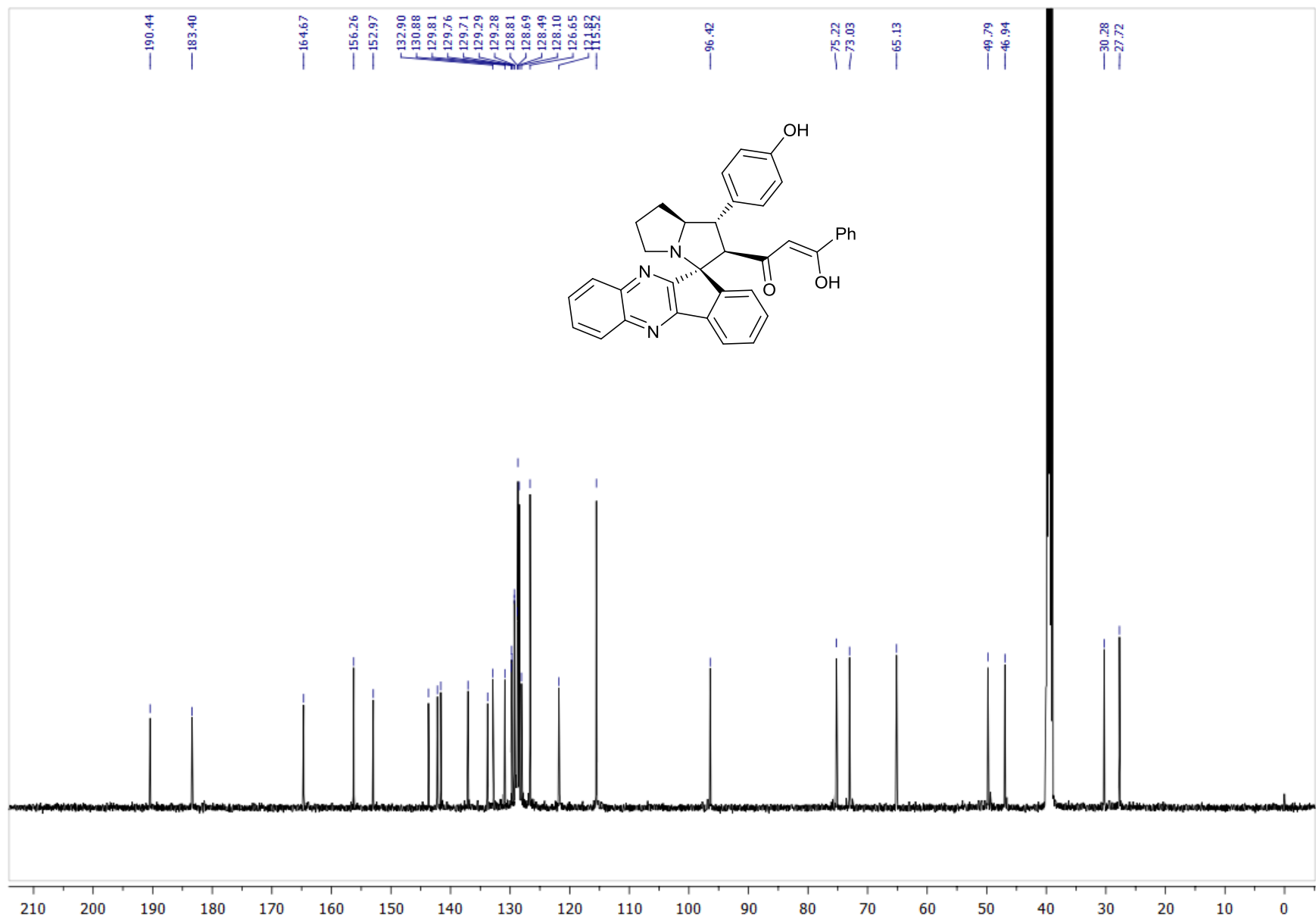


Figure S23. Copy of  $^{13}\text{C}$  NMR spectrum of **3j** in  $\text{DMSO-}d_6$



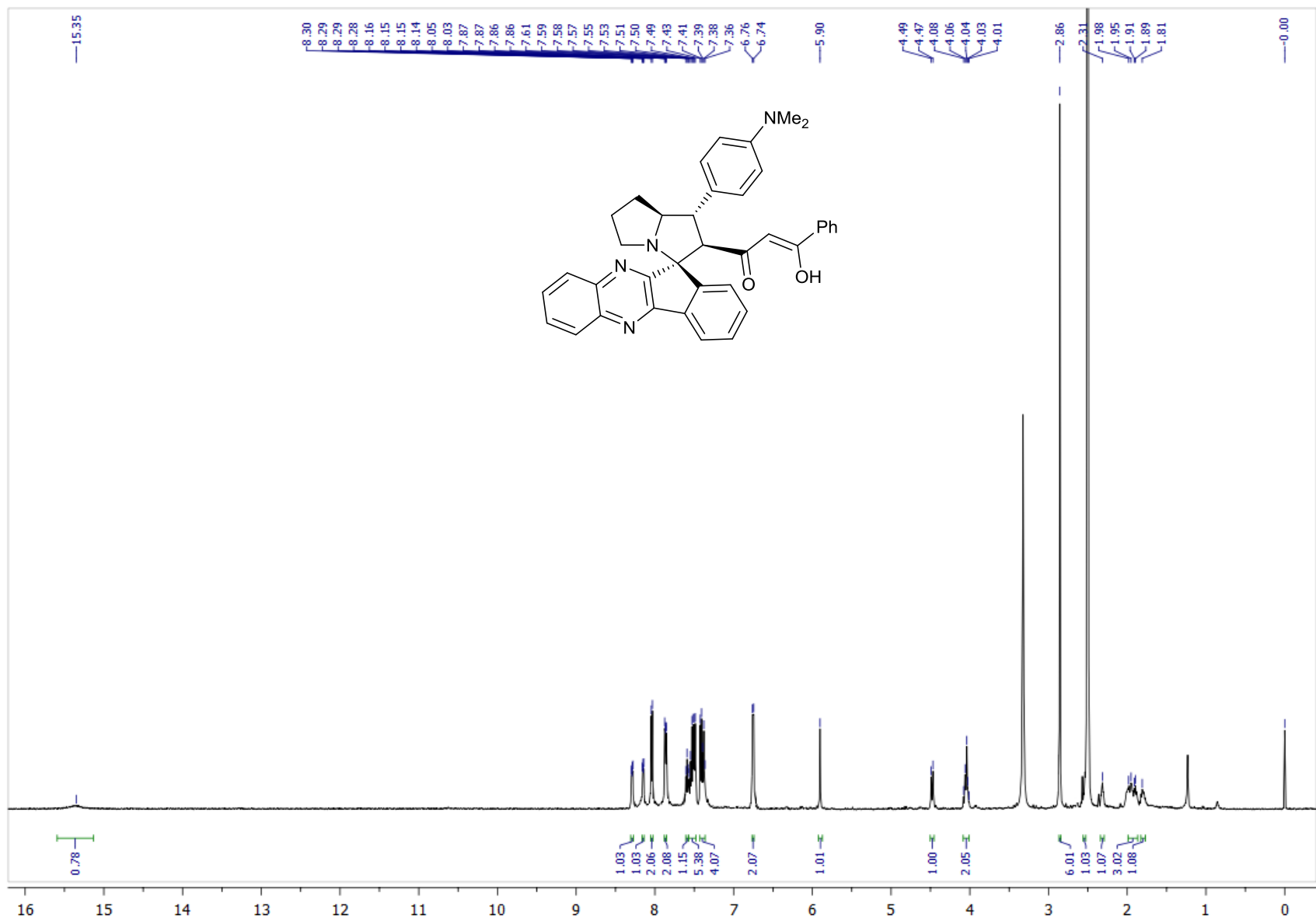
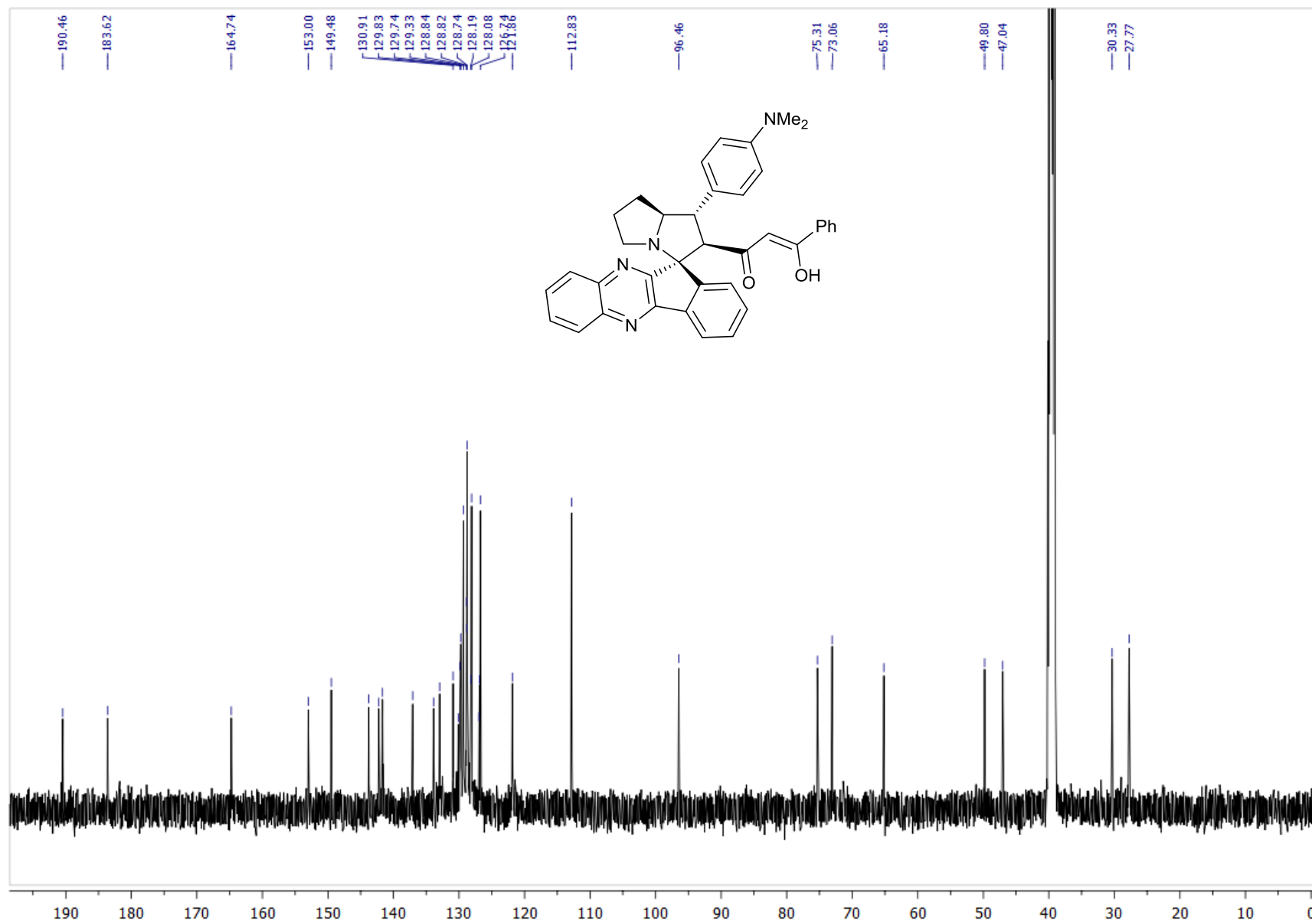


Figure S24. Copy of <sup>1</sup>H NMR spectrum of **3k** in DMSO-*d*<sub>6</sub>



**Figure S25.** Copy of  $^{13}\text{C}$  NMR spectrum of **3k** in  $\text{DMSO-}d_6$

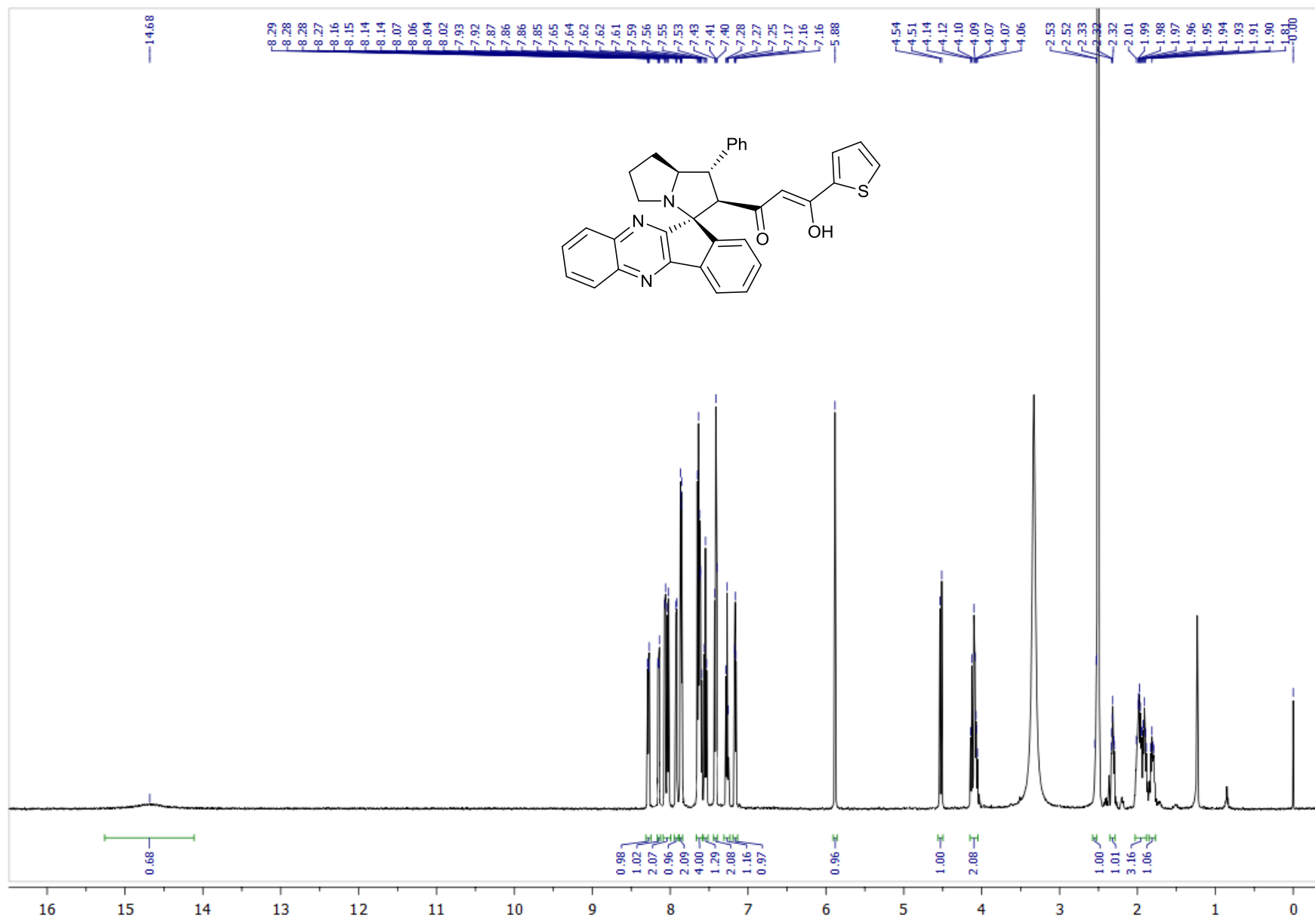


Figure S26. Copy of  $^1\text{H}$  NMR spectrum of **31** in  $\text{DMSO-}d_6$

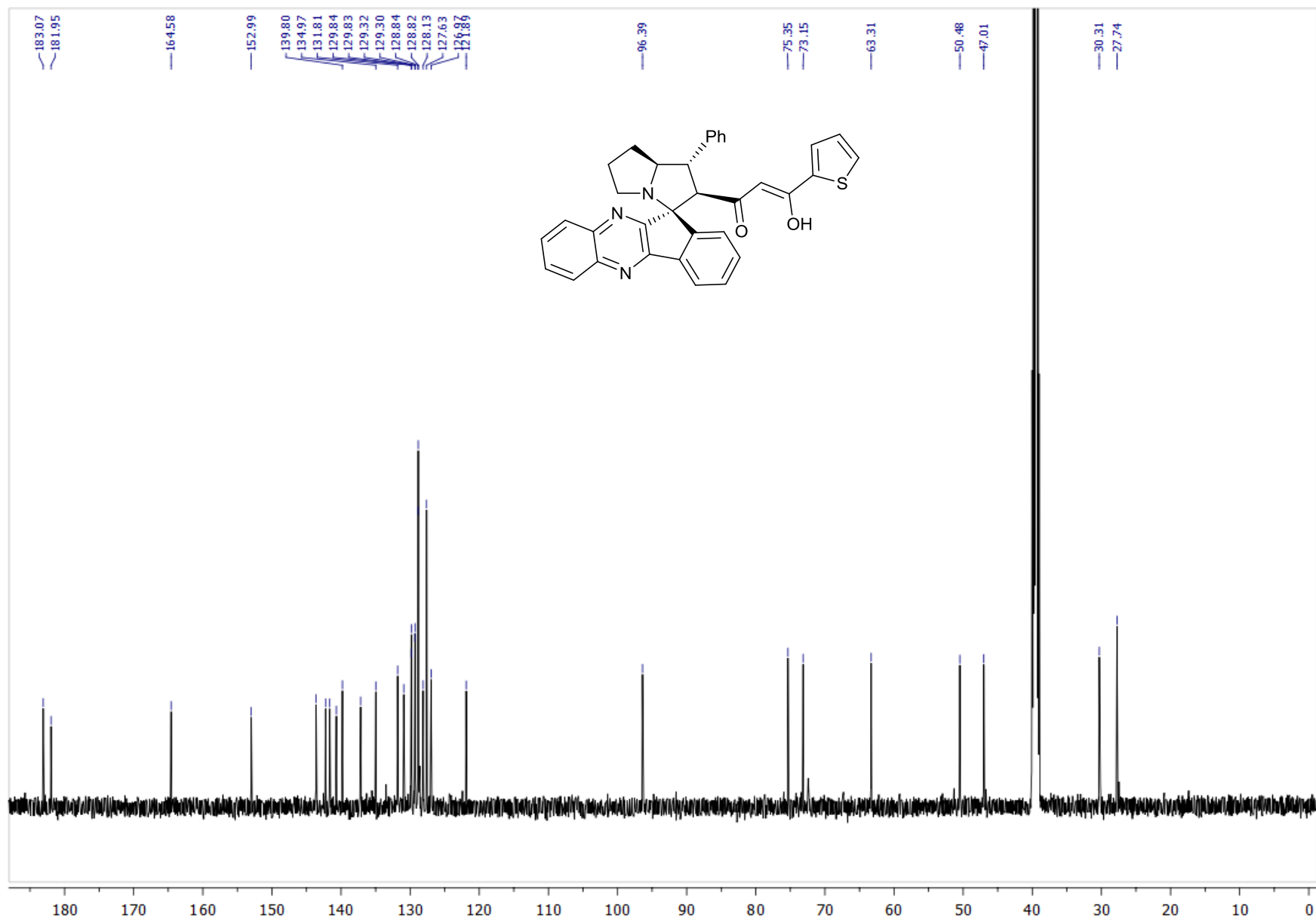


Figure S27. Copy of  $^{13}\text{C}$  NMR spectrum of **31** in  $\text{DMSO-}d_6$

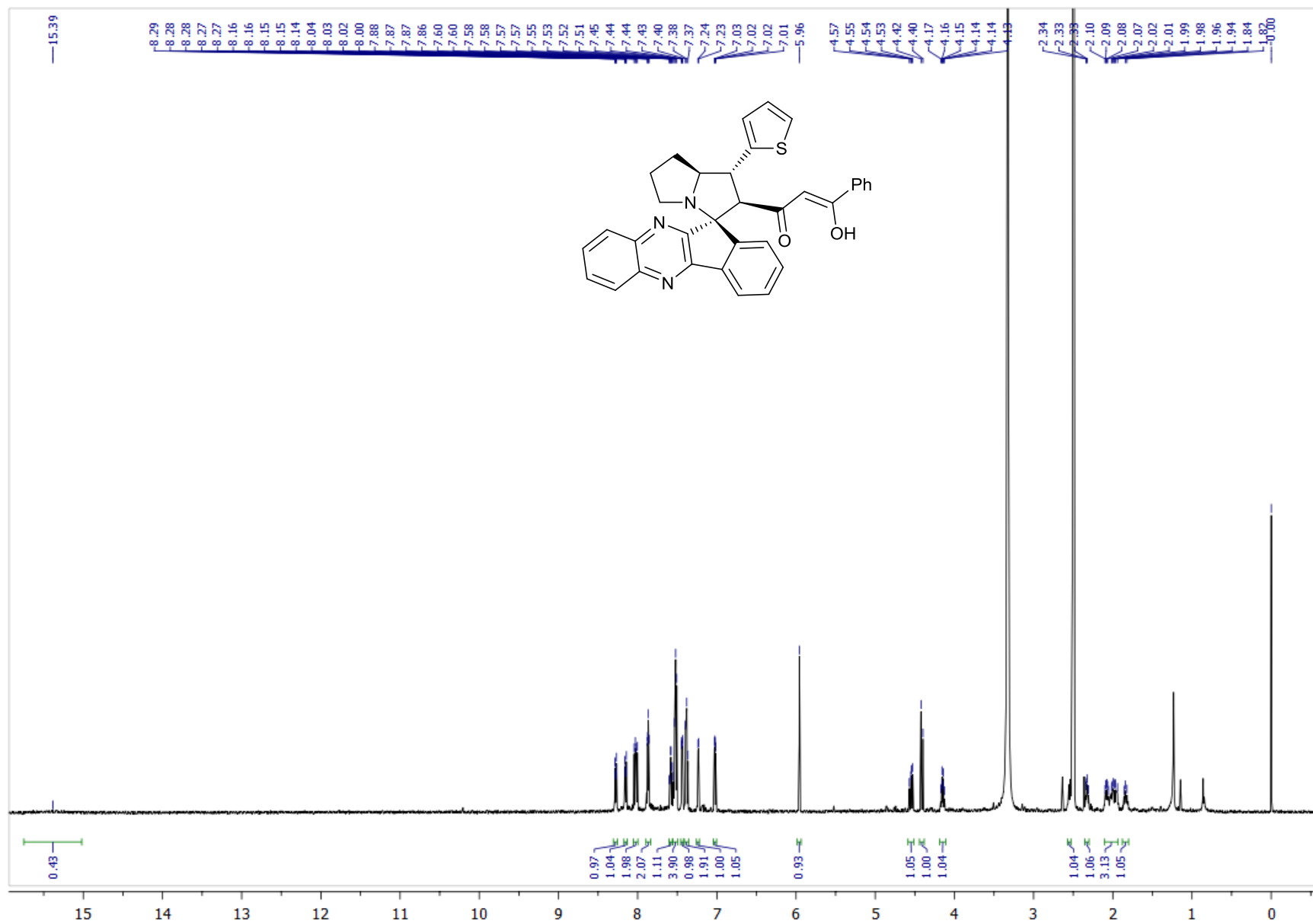


Figure S28. Copy of  $^1\text{H}$  NMR spectrum of **3m** in  $\text{DMSO-}d_6$

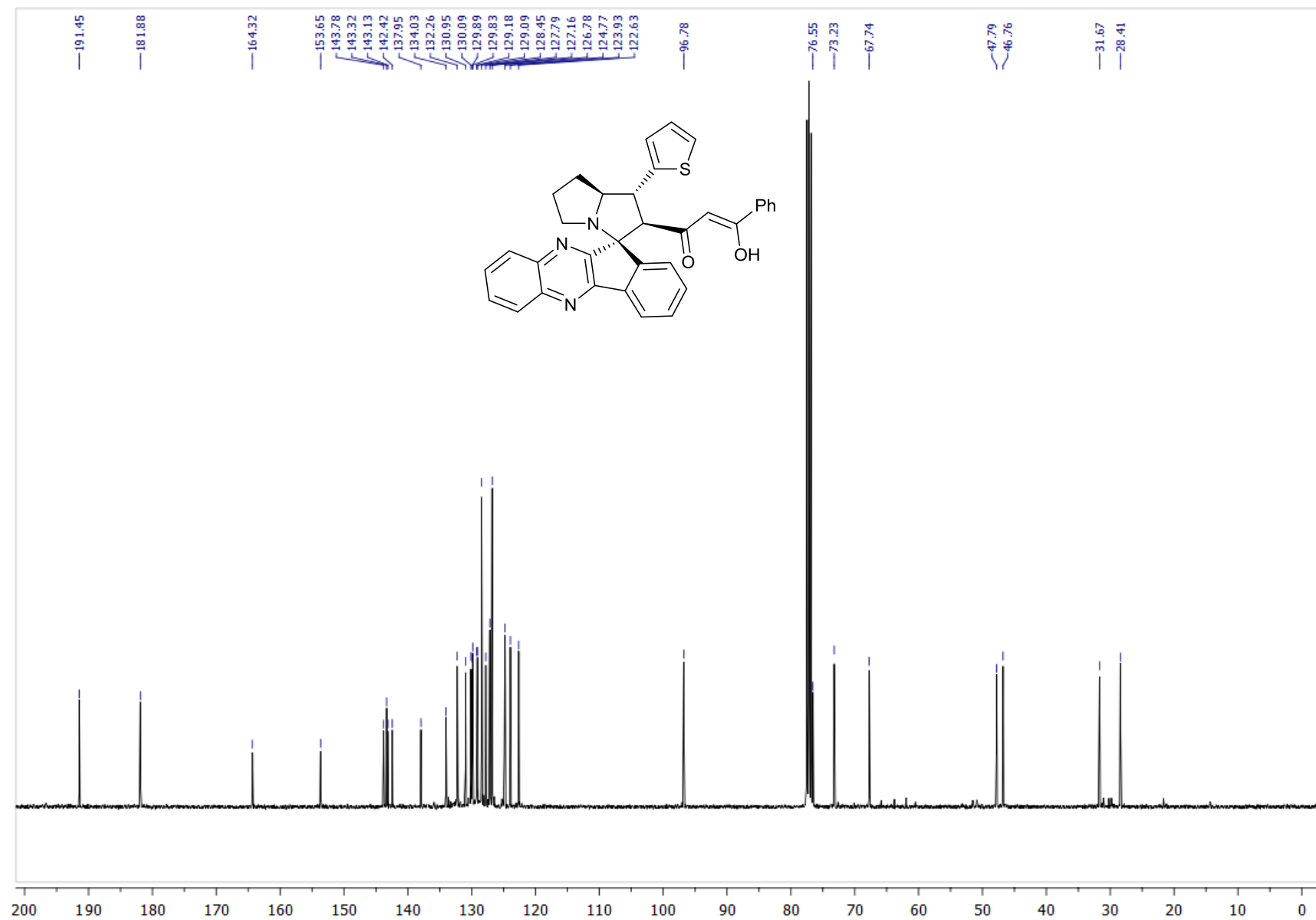
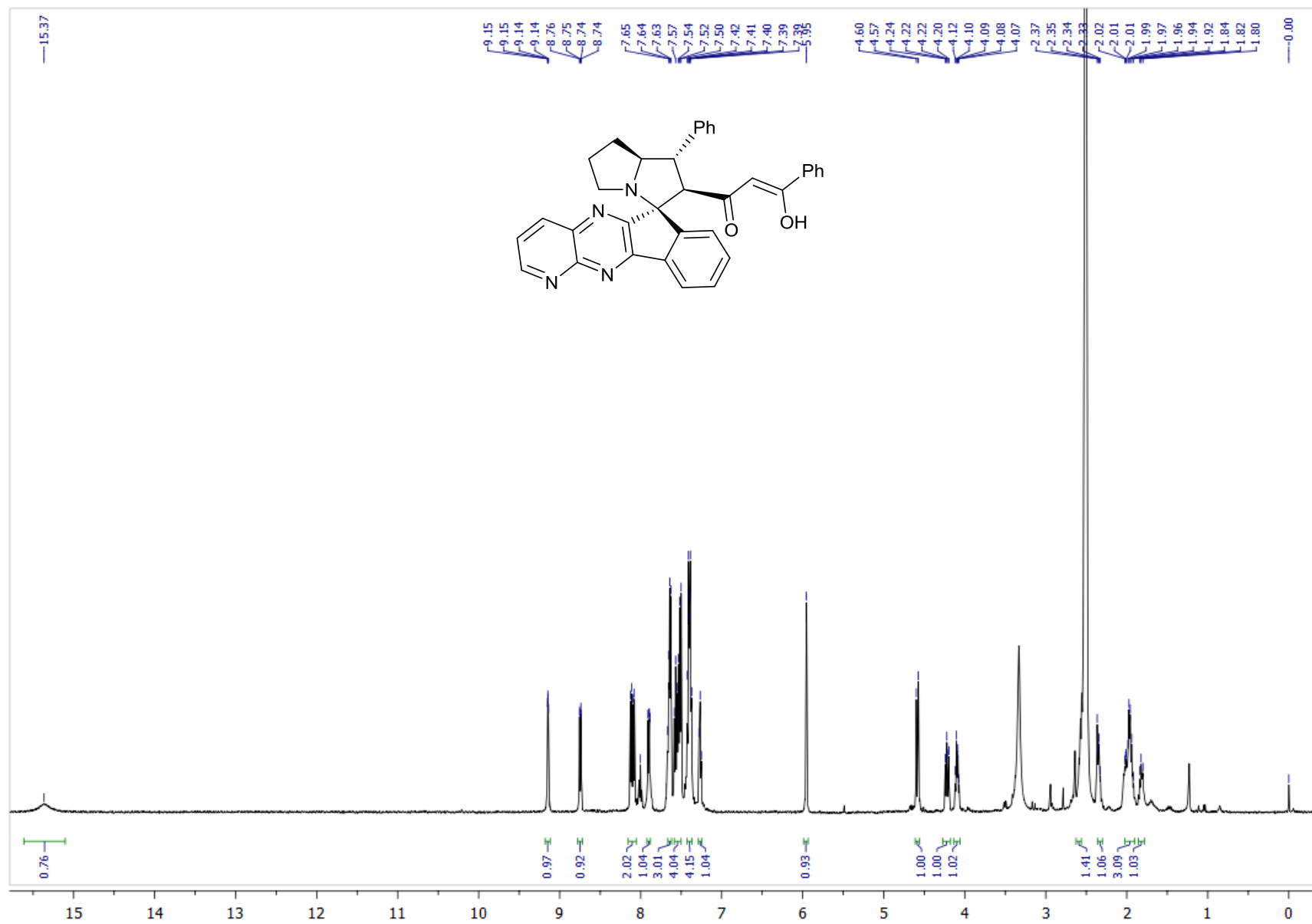


Figure S29. Copy of  $^{13}\text{C}$  NMR spectrum of **3m** in  $\text{CDCl}_3-d_6$



**Figure S30.** Copy of  $^1\text{H}$  NMR spectrum of **3n** in DMSO- $d_6$

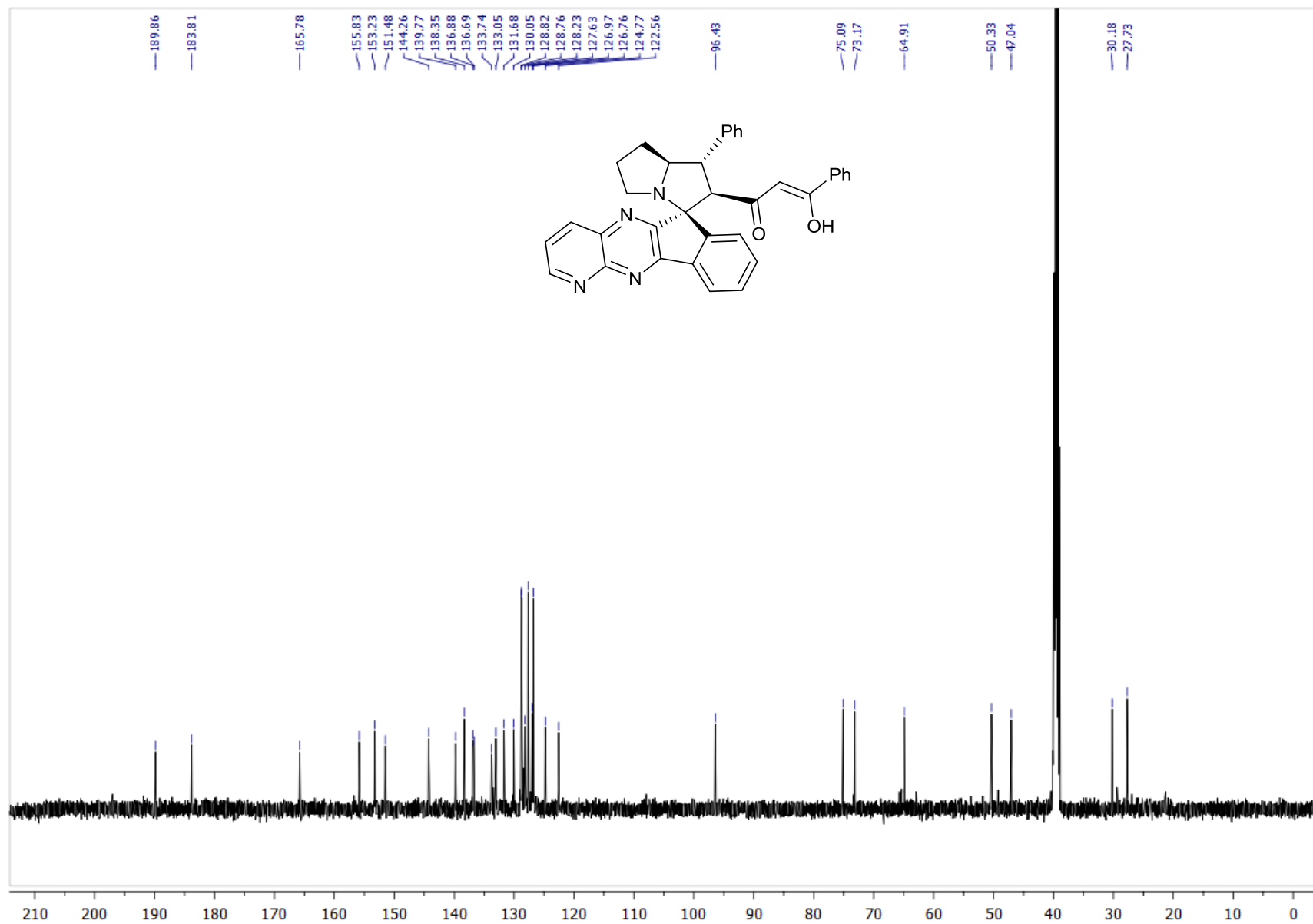
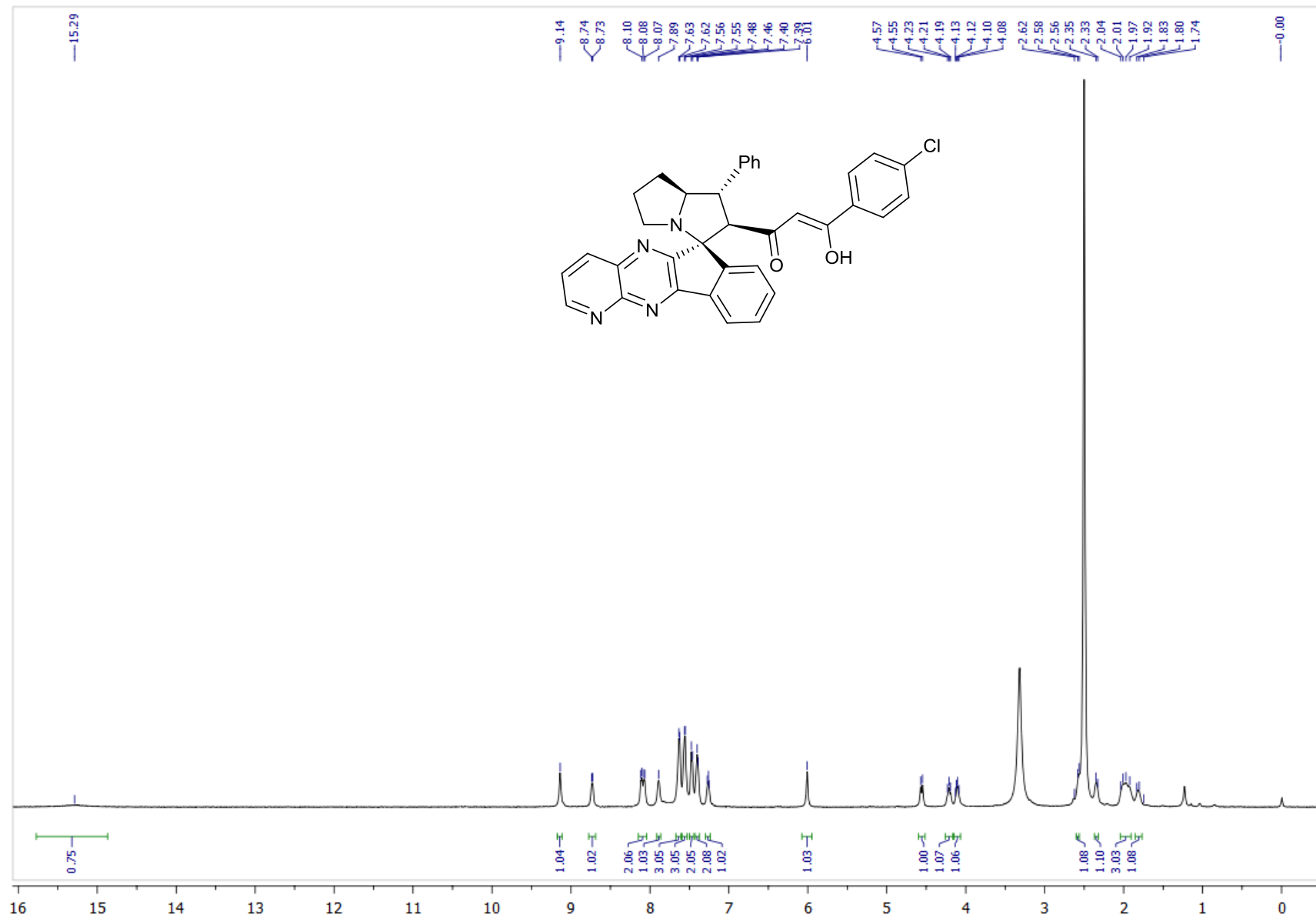


Figure S31. Copy of  $^{13}\text{C}$  NMR spectrum of **3n** in  $\text{DMSO-}d_6$





**Figure S32.** Copy of <sup>1</sup>H NMR spectrum of **30** in DMSO-*d*<sub>6</sub>

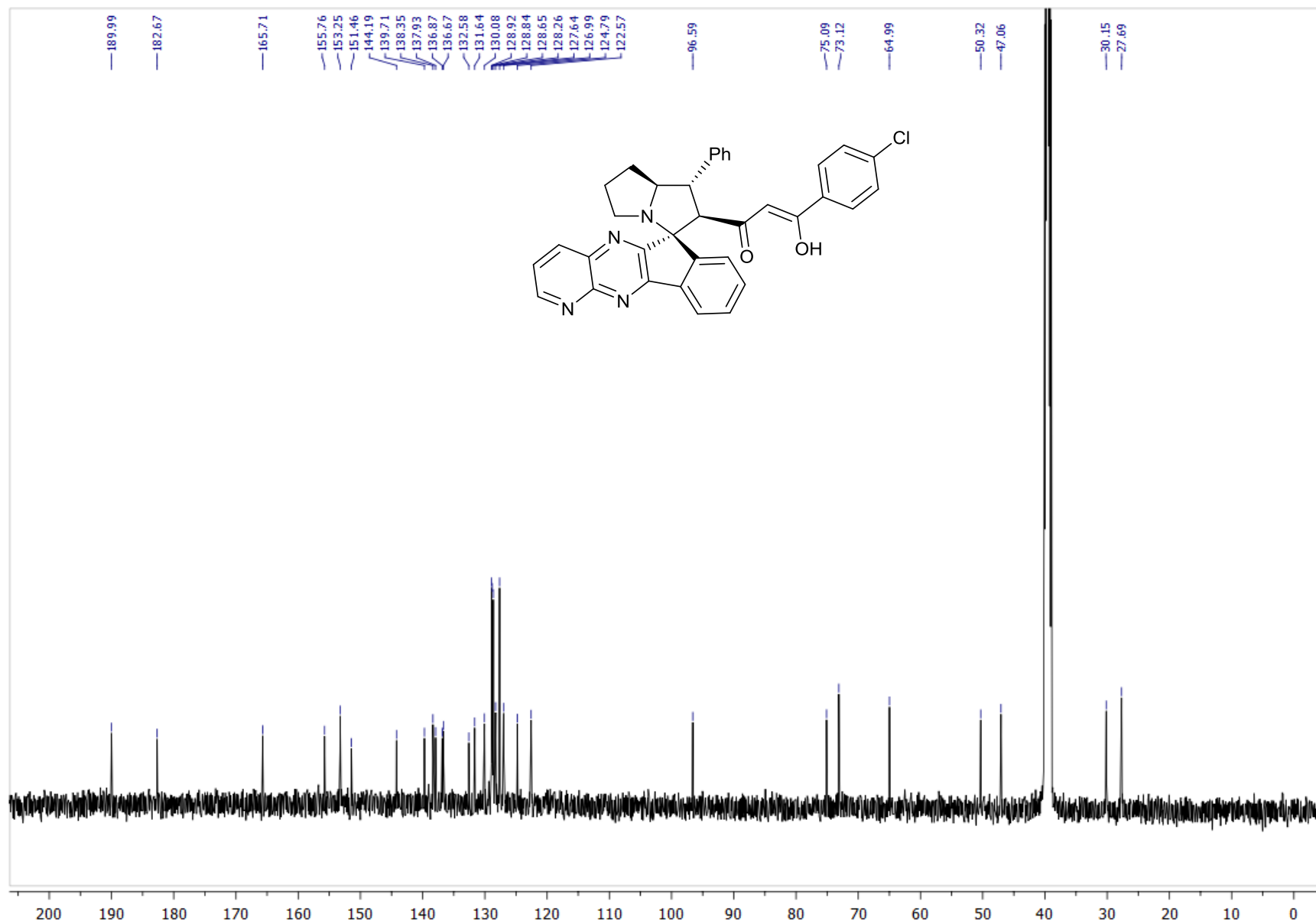
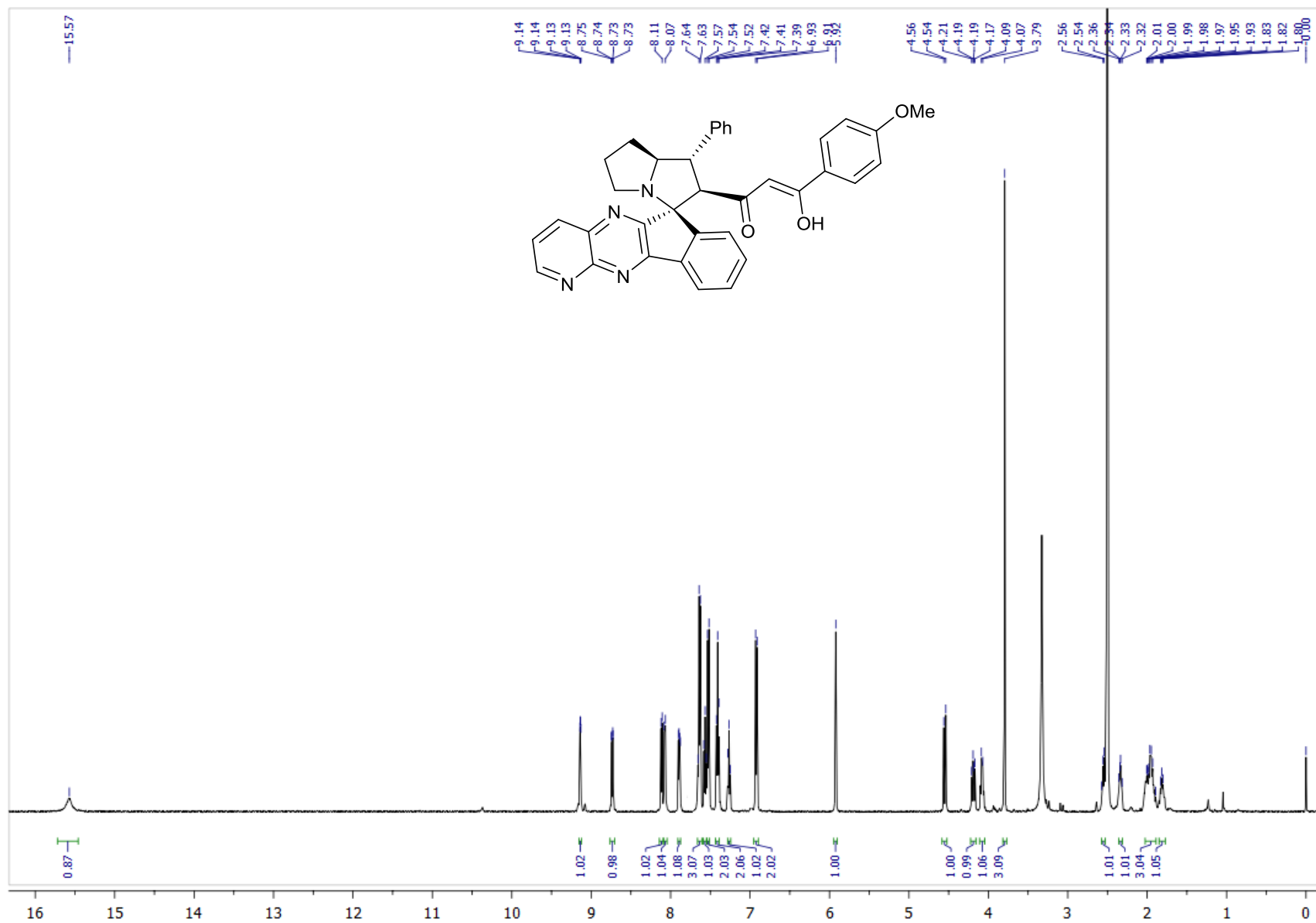


Figure S33. Copy of  $^{13}\text{C}$  NMR spectrum of **3o** in  $\text{DMSO-}d_6$



**Figure S34.** Copy of  $^1\text{H}$  NMR spectrum of **3p** in DMSO- $d_6$

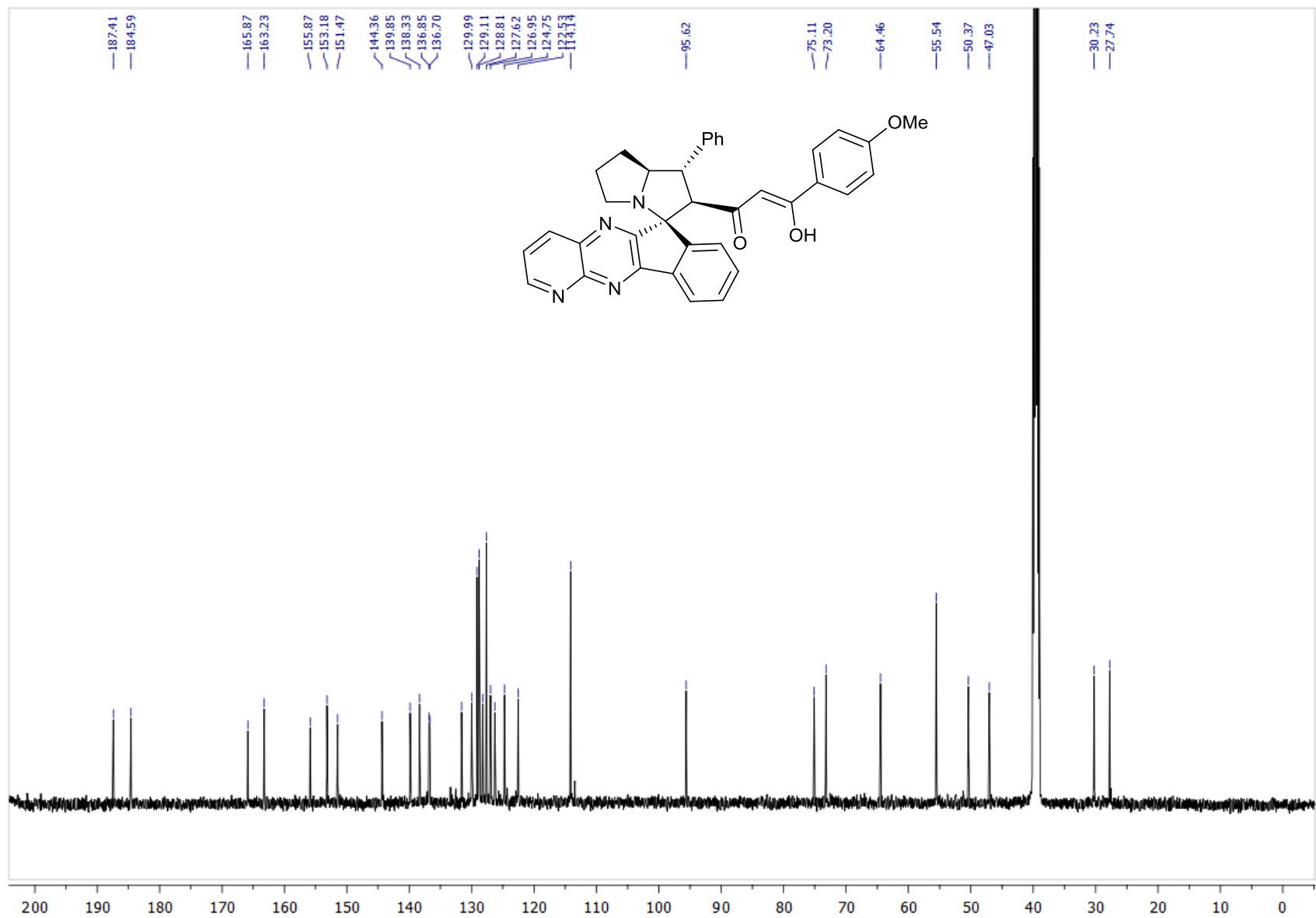


Figure S35. Copy of  $^{13}\text{C}$  NMR spectrum of **3p** in  $\text{DMSO-}d_6$

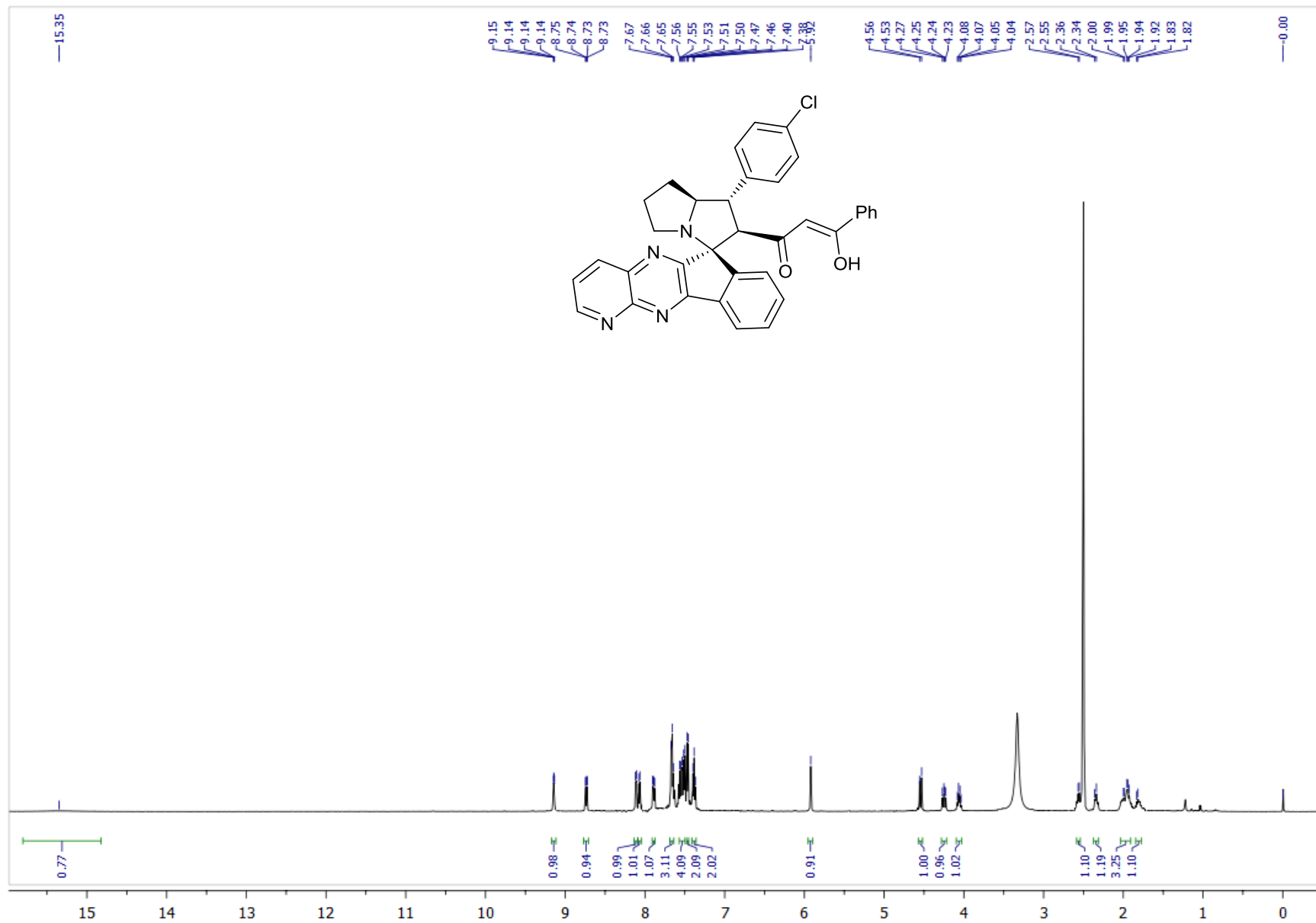


Figure S36. Copy of  $^1\text{H}$  NMR spectrum of **3q** in  $\text{DMSO-}d_6$

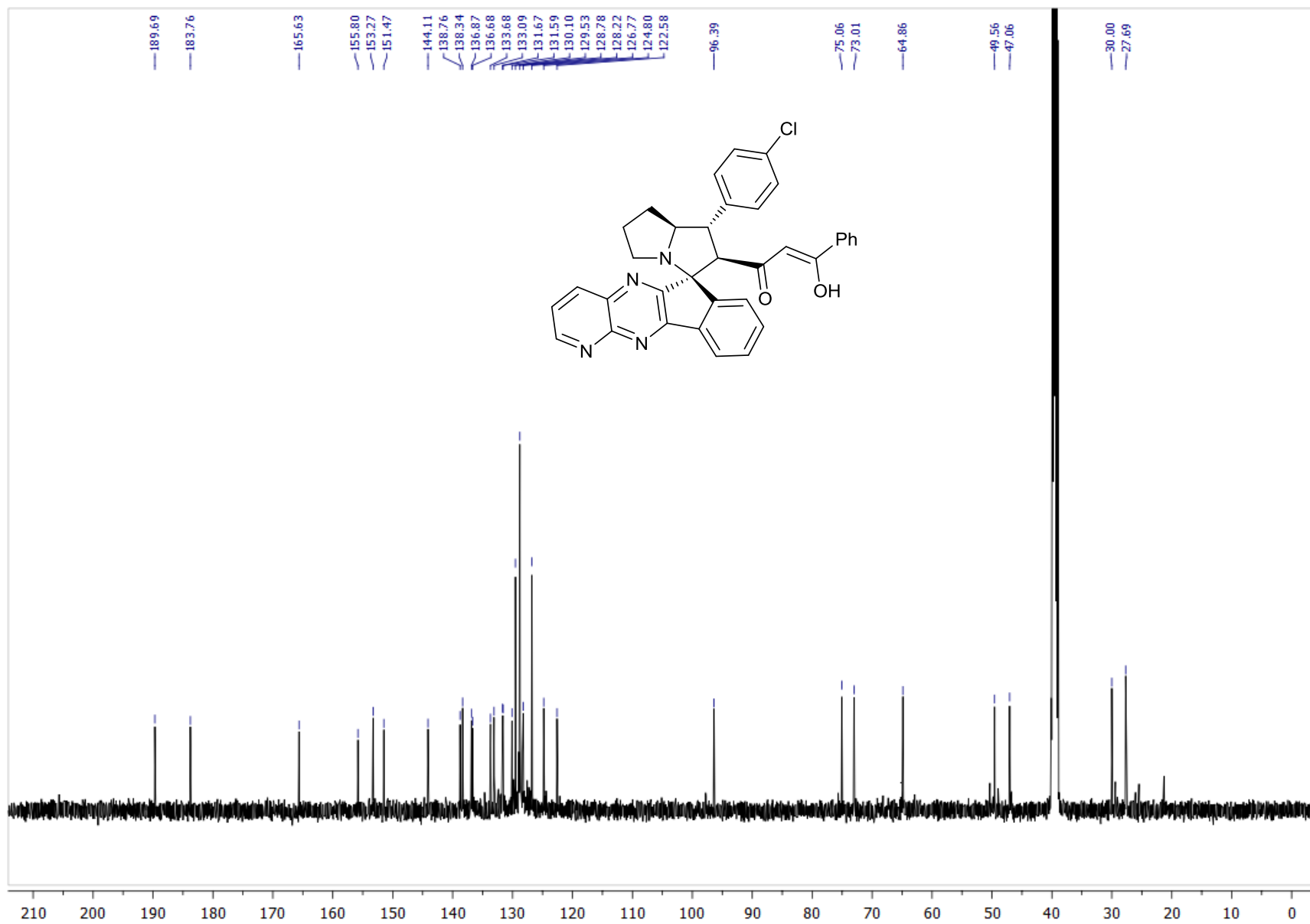
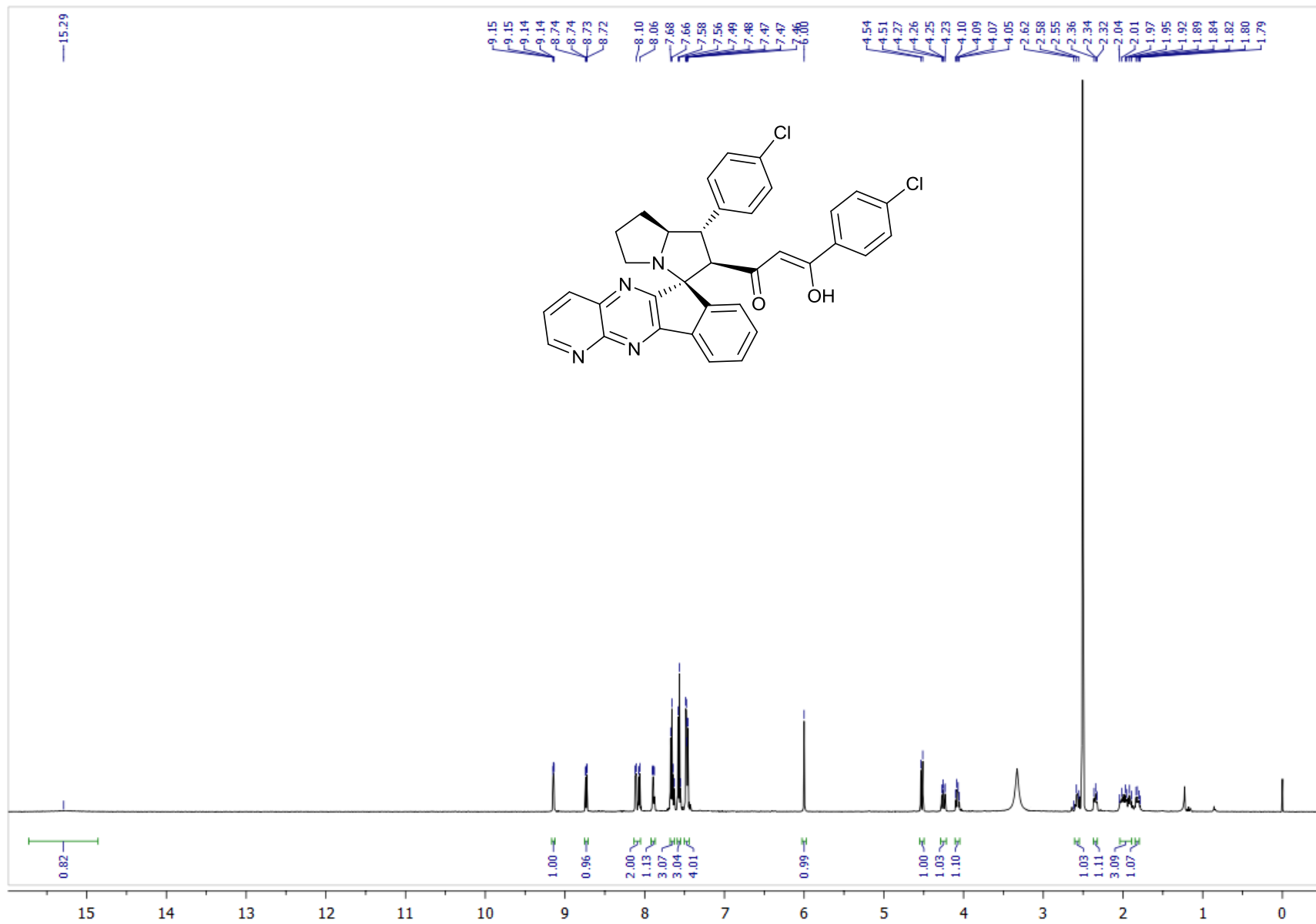


Figure S37. Copy of  $^{13}\text{C}$  NMR spectrum of **3q** in  $\text{DMSO-}d_6$



**Figure S38.** Copy of <sup>1</sup>H NMR spectrum of **3r** in DMSO-*d*<sub>6</sub>

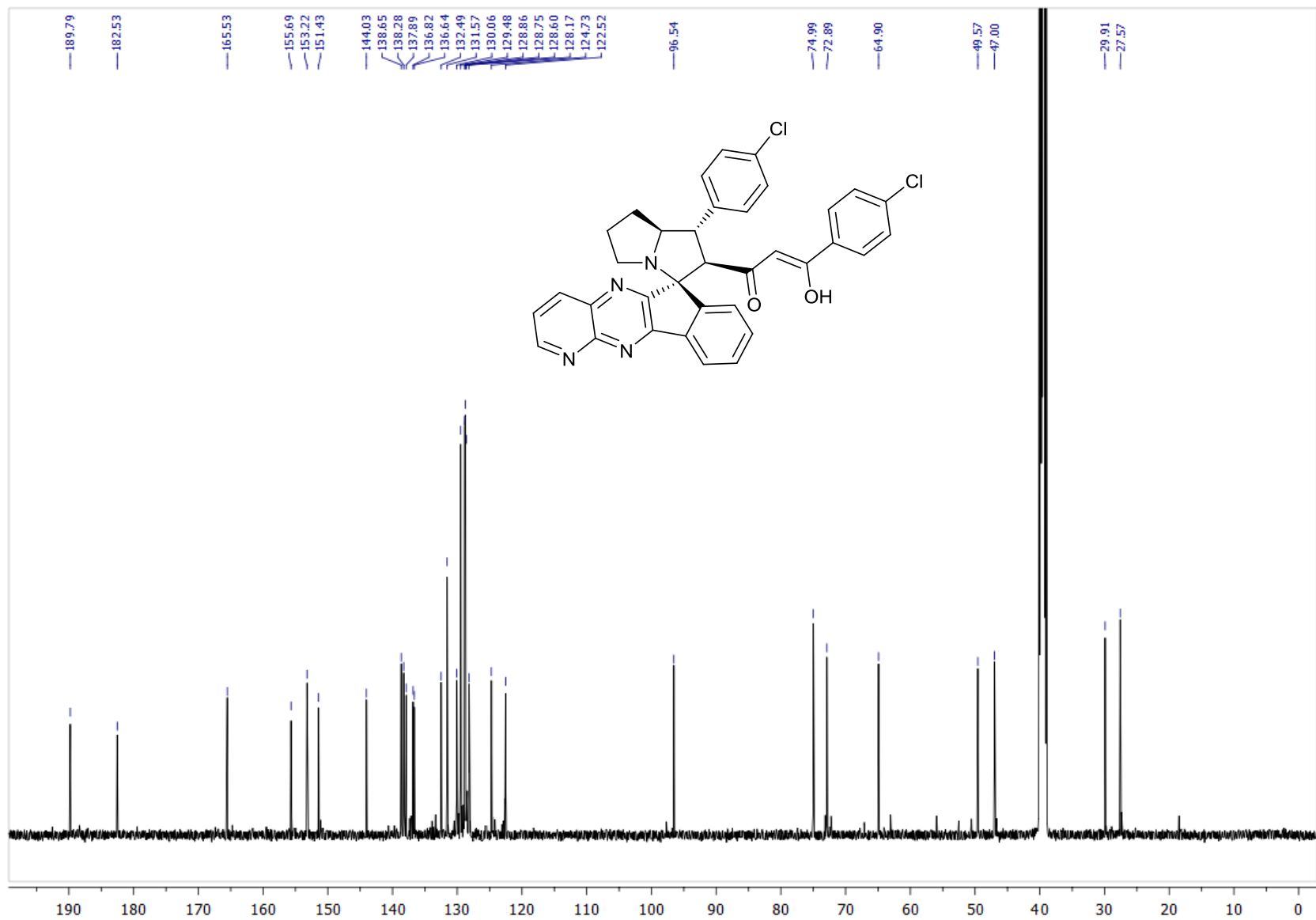


Figure S39. Copy of  $^{13}\text{C}$  NMR spectrum of **3r** in  $\text{DMSO-}d_6$



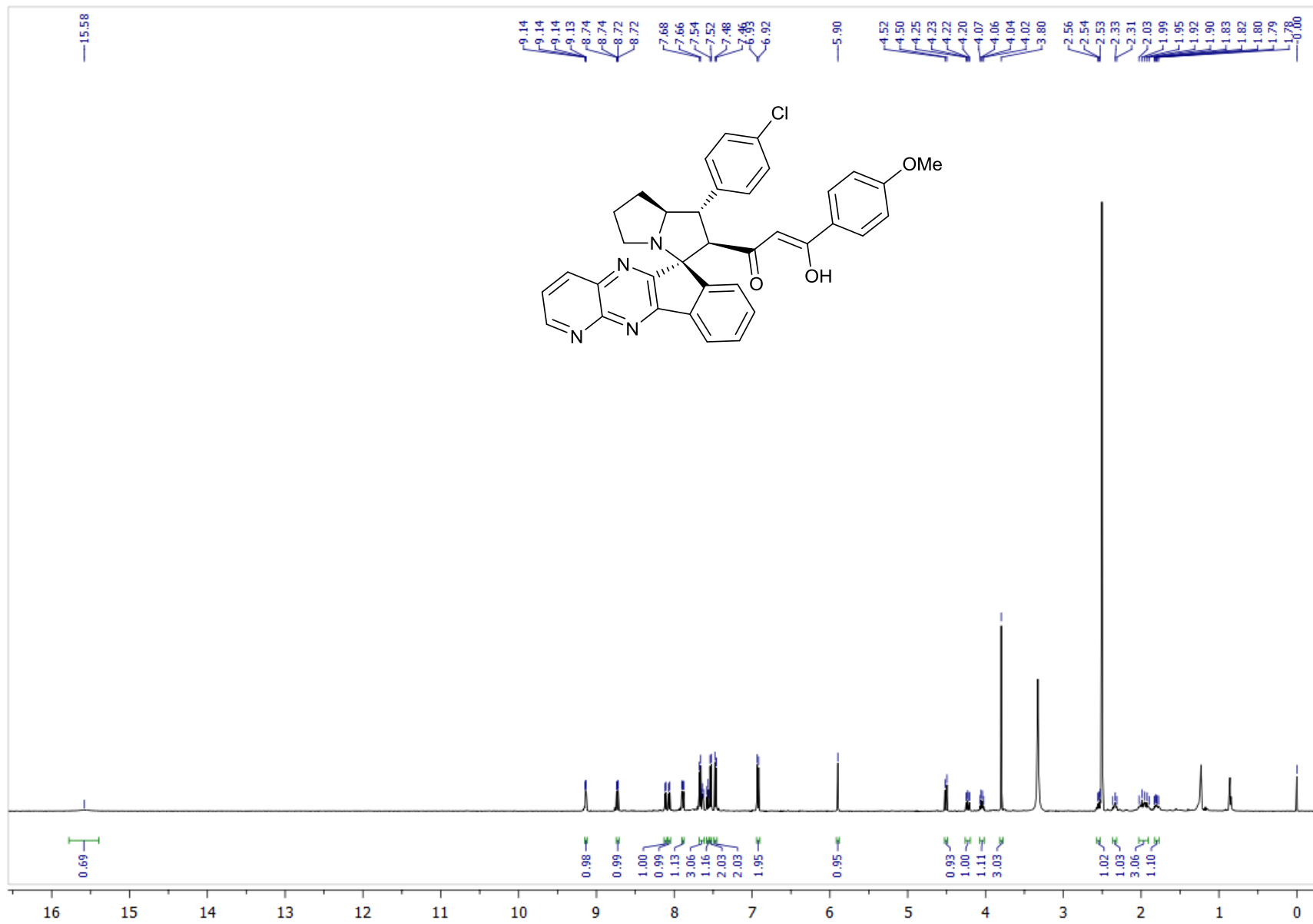


Figure S40. Copy of <sup>1</sup>H NMR spectrum of 3s in DMSO-d<sub>6</sub>

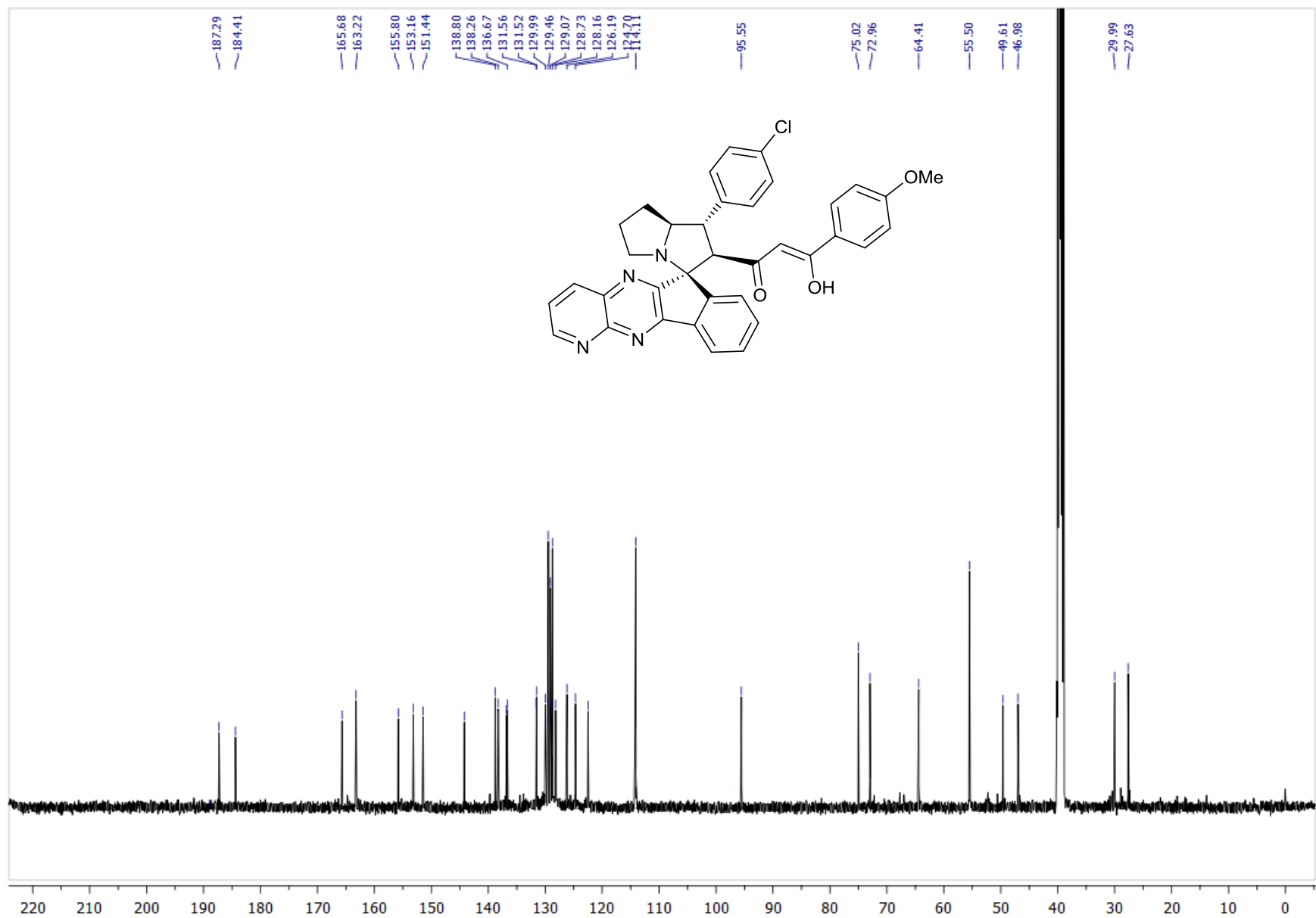


Figure S41. Copy of  $^{13}\text{C}$  NMR spectrum of **3s** in DMSO- $d_6$

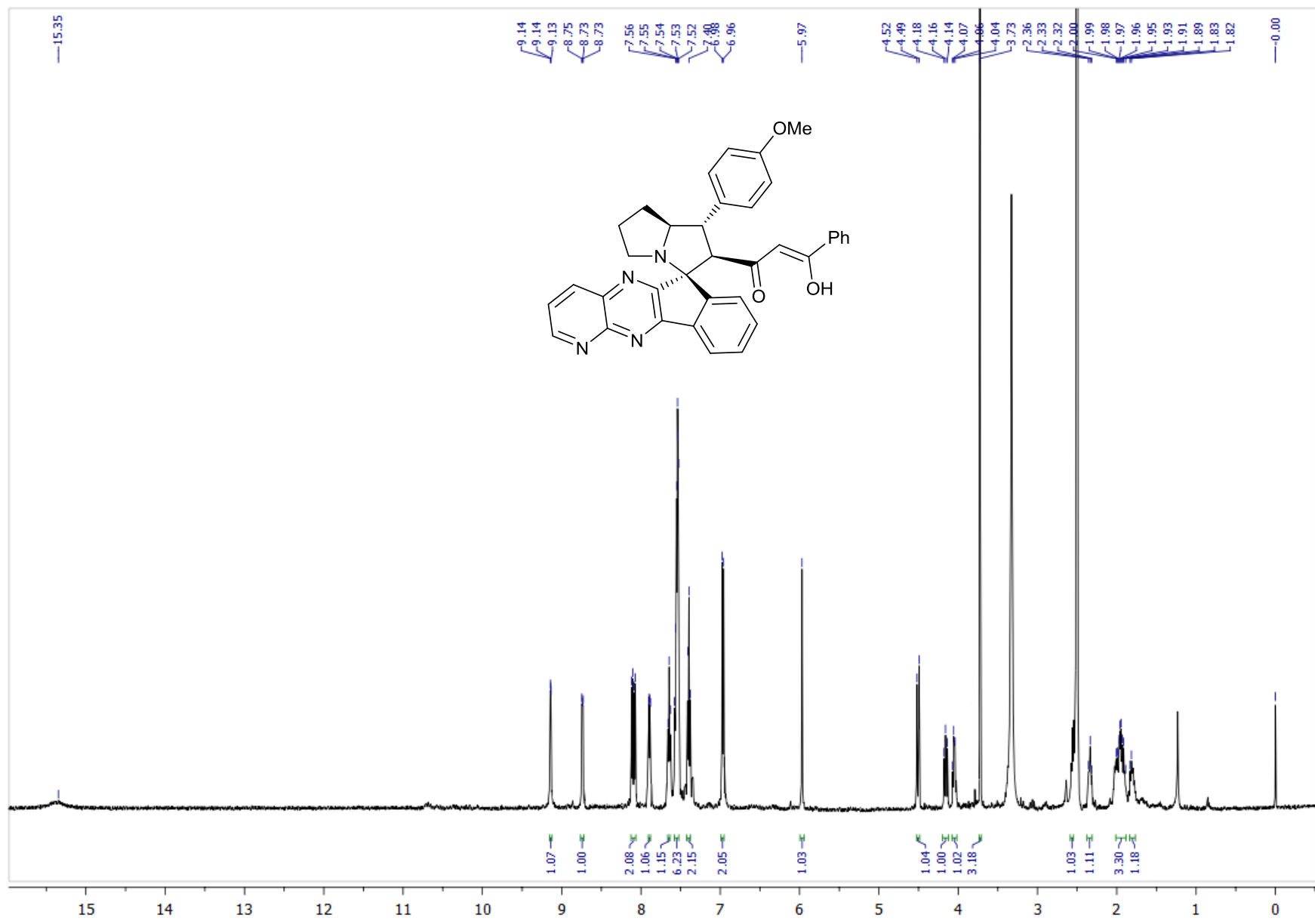
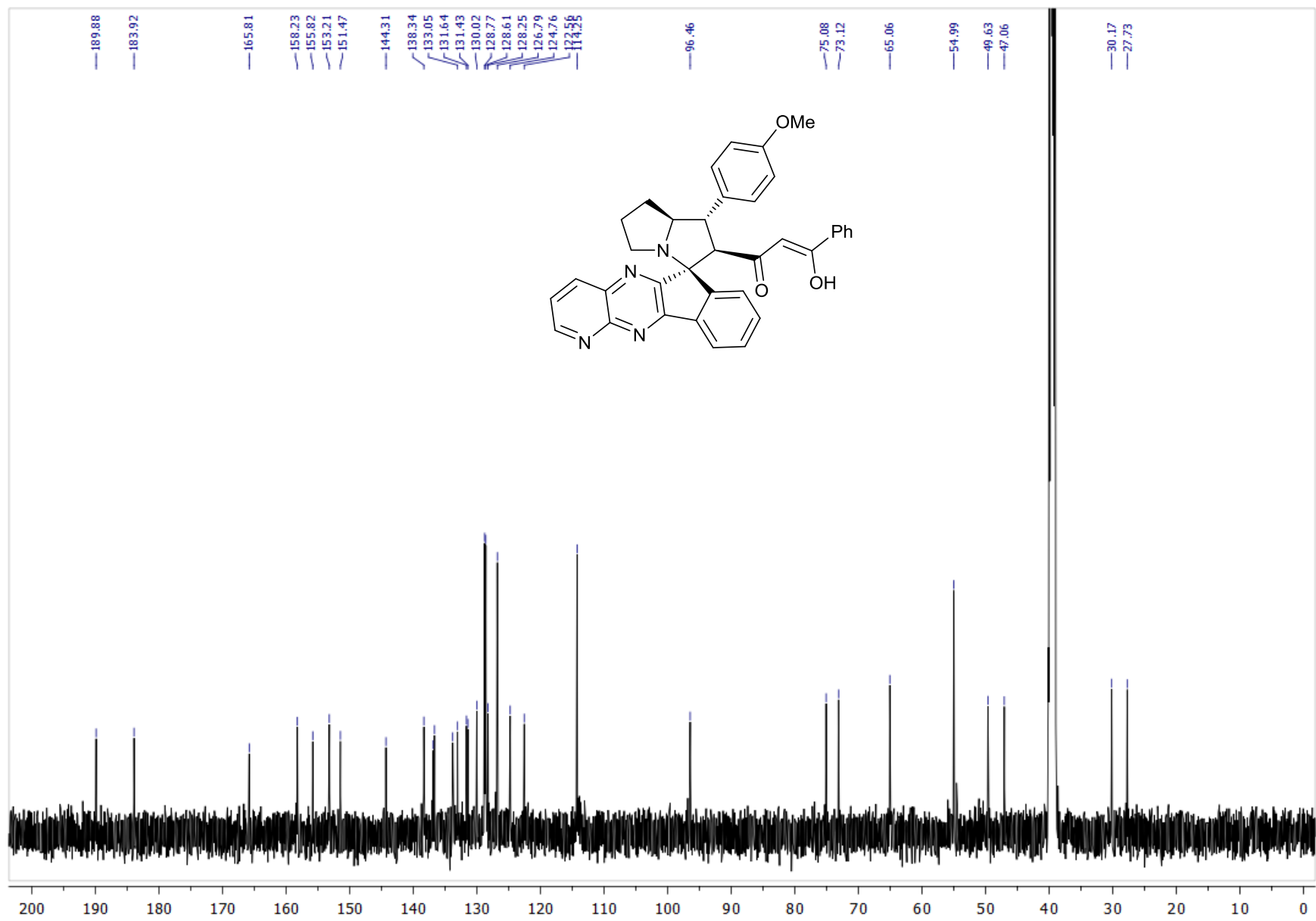
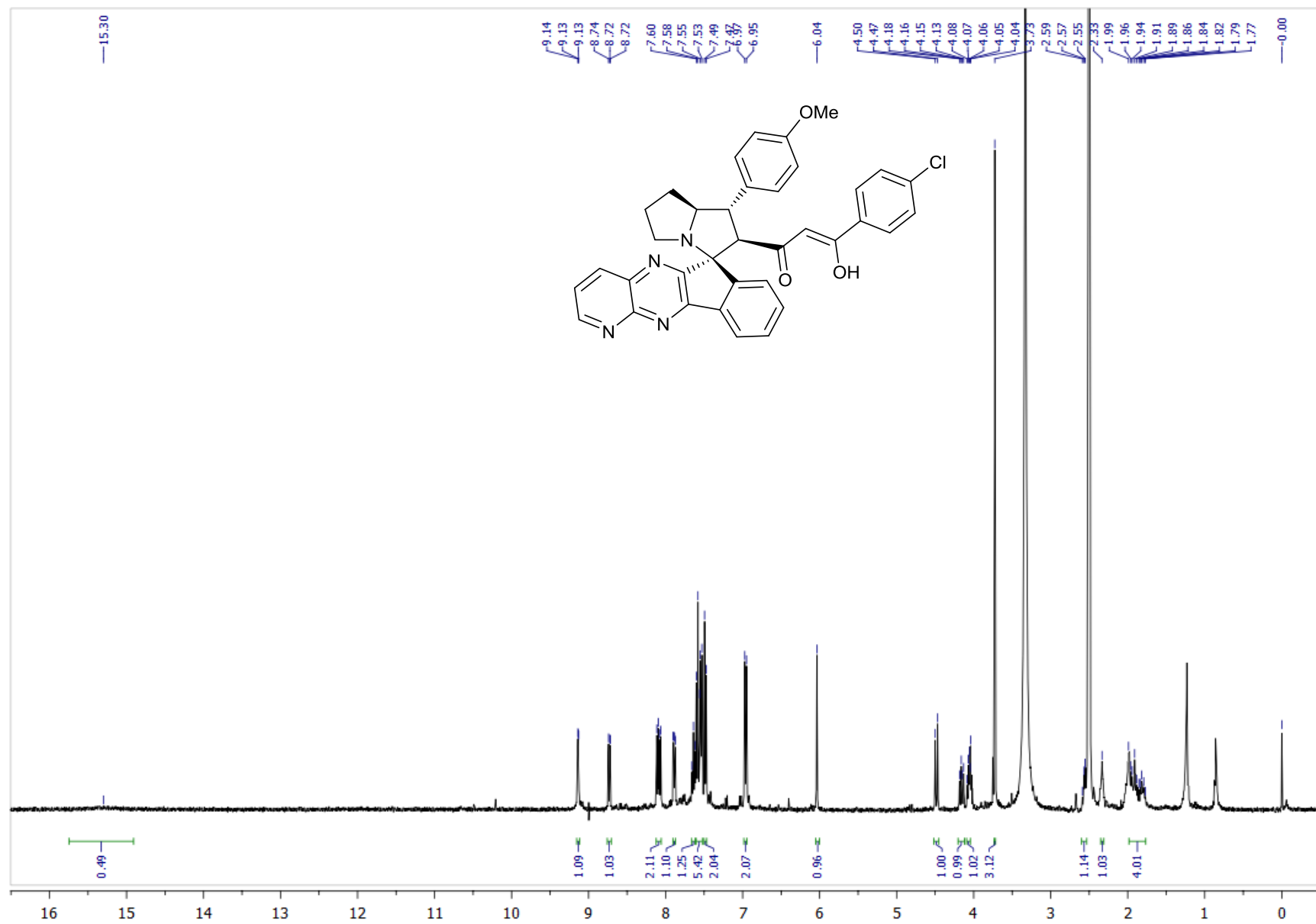


Figure S42. Copy of <sup>1</sup>H NMR spectrum of **3t** in DMSO-*d*<sub>6</sub>



**Figure S43.** Copy of  $^{13}\text{C}$  NMR spectrum of **3t** in  $\text{DMSO-}d_6$



**Figure S44.** Copy of <sup>1</sup>H NMR spectrum of **3u** in DMSO-*d*<sub>6</sub>

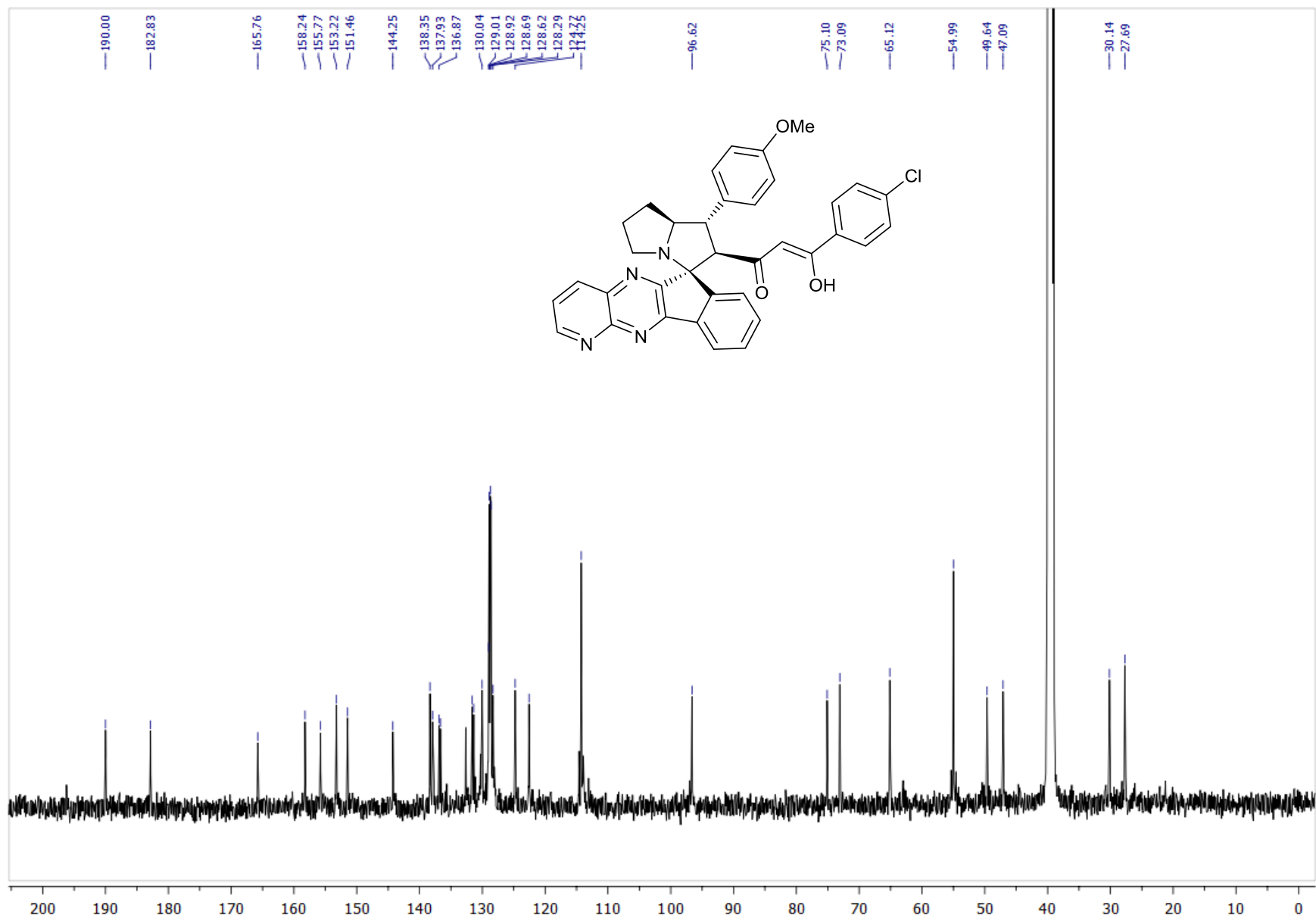
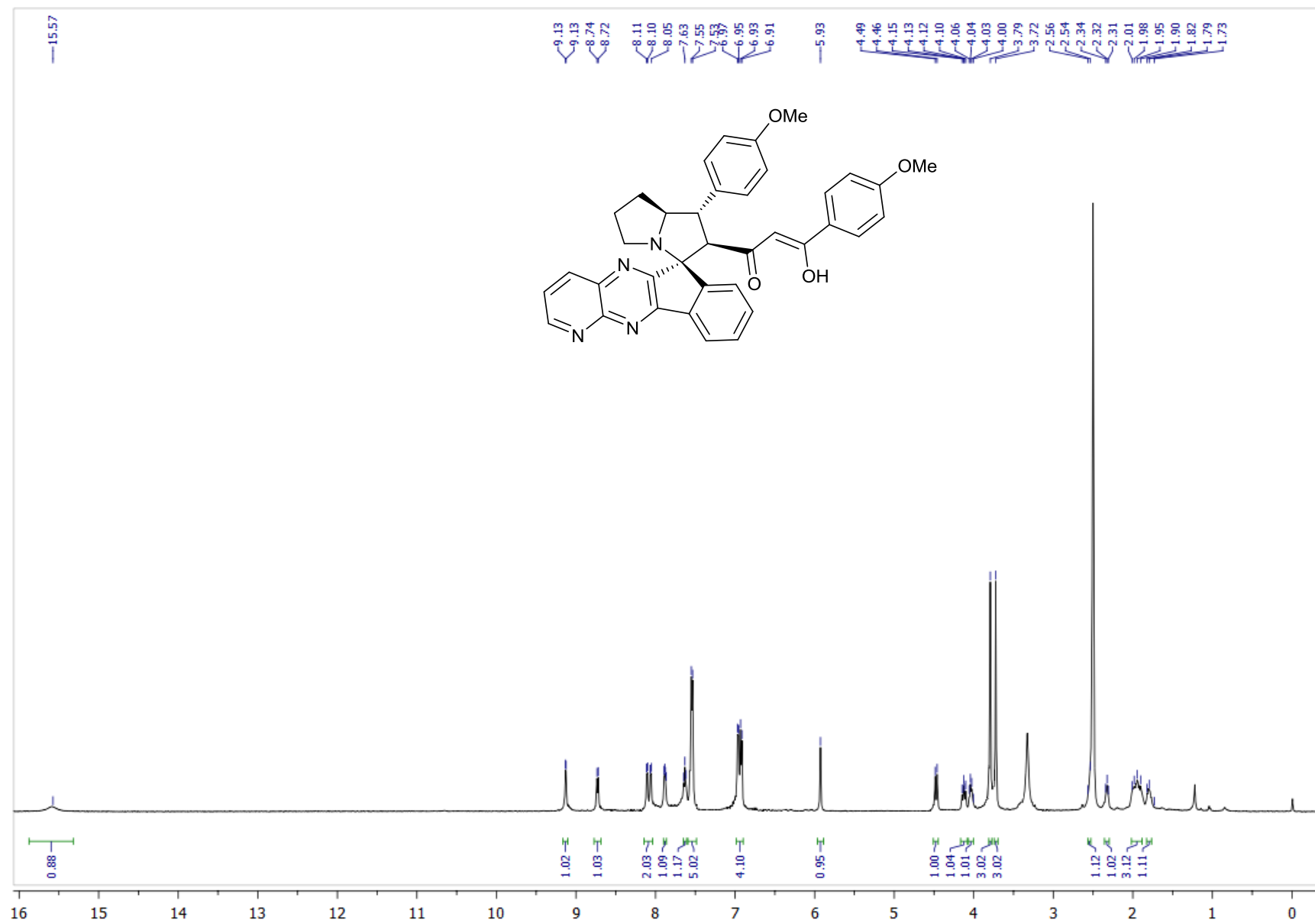


Figure S45. Copy of  $^{13}\text{C}$  NMR spectrum of **3u** in  $\text{DMSO-}d_6$



**Figure S46.** Copy of <sup>1</sup>H NMR spectrum of 3v in DMSO-*d*<sub>6</sub>

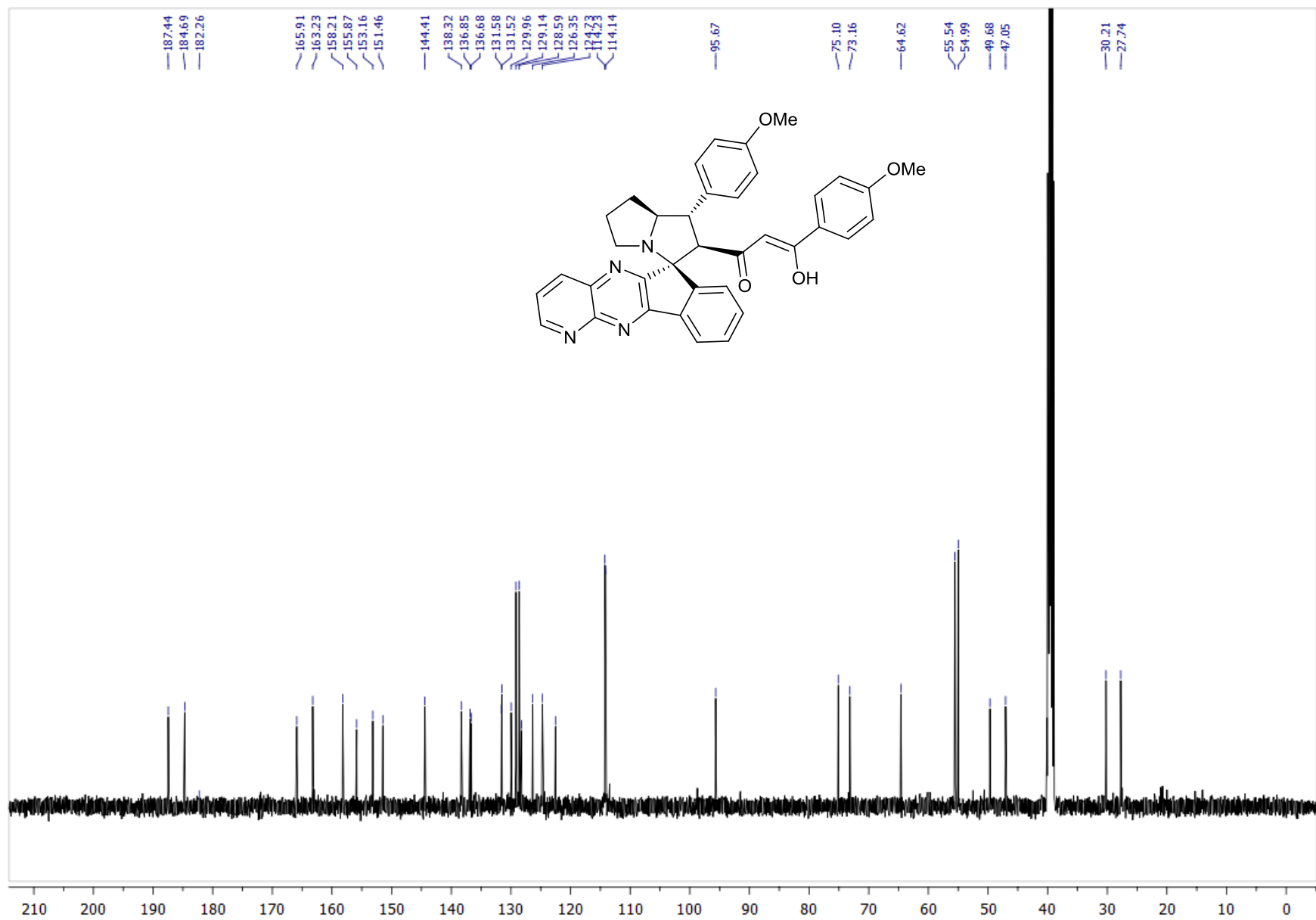
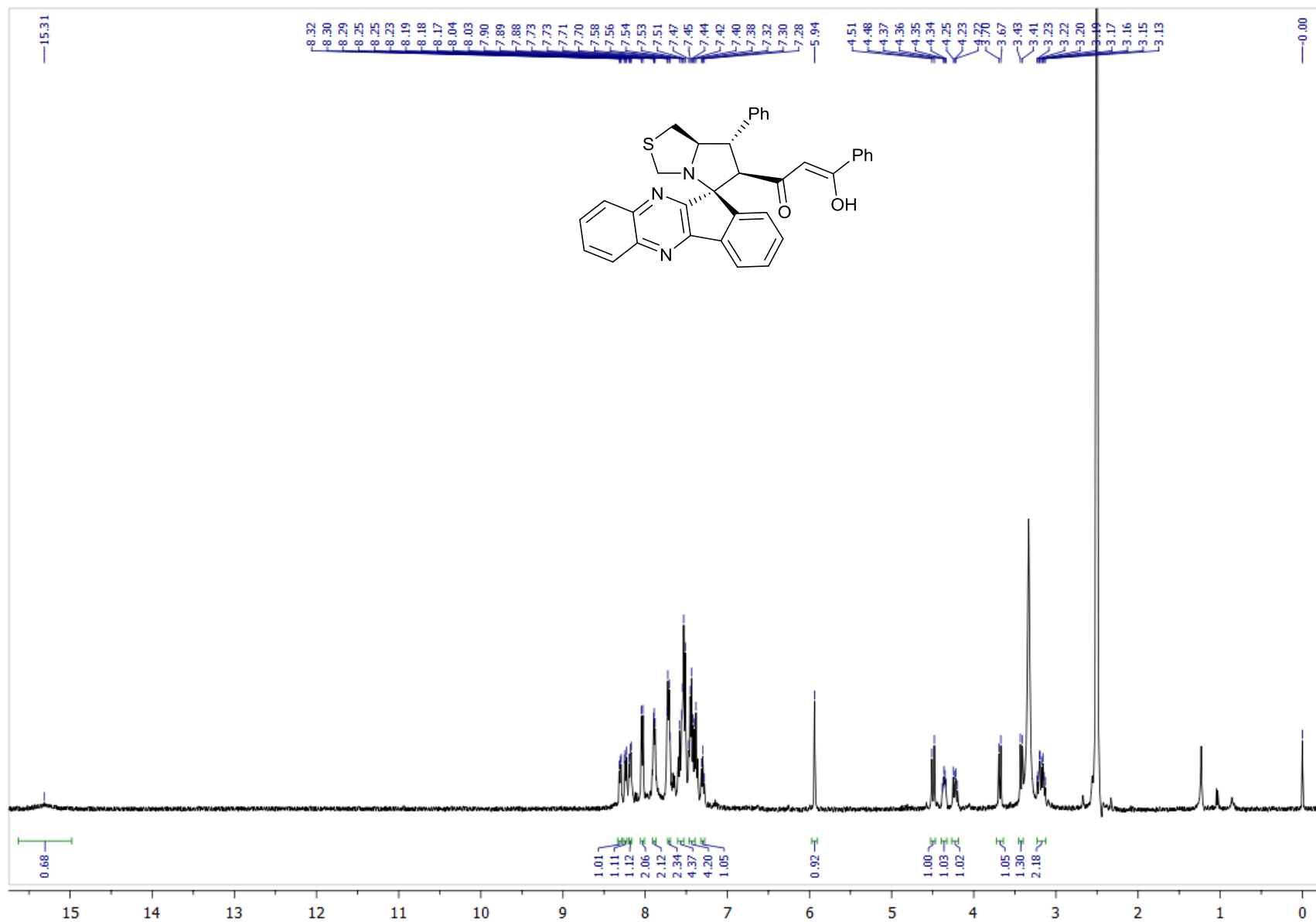


Figure S47. Copy of  $^{13}\text{C}$  NMR spectrum of **3v** in  $\text{DMSO-}d_6$





**Figure S48.** Copy of  $^1\text{H}$  NMR spectrum of **4a** in DMSO- $d_6$

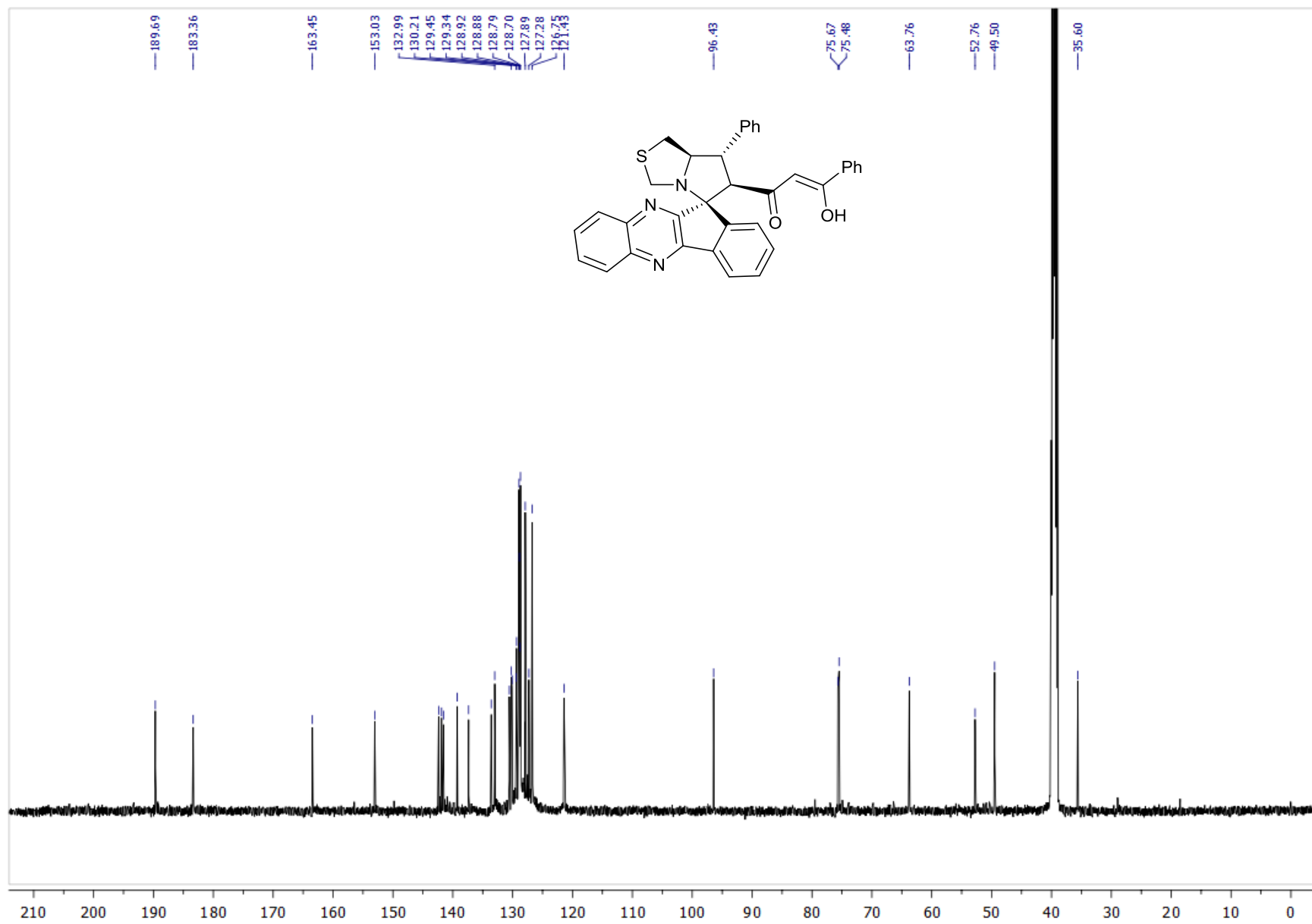
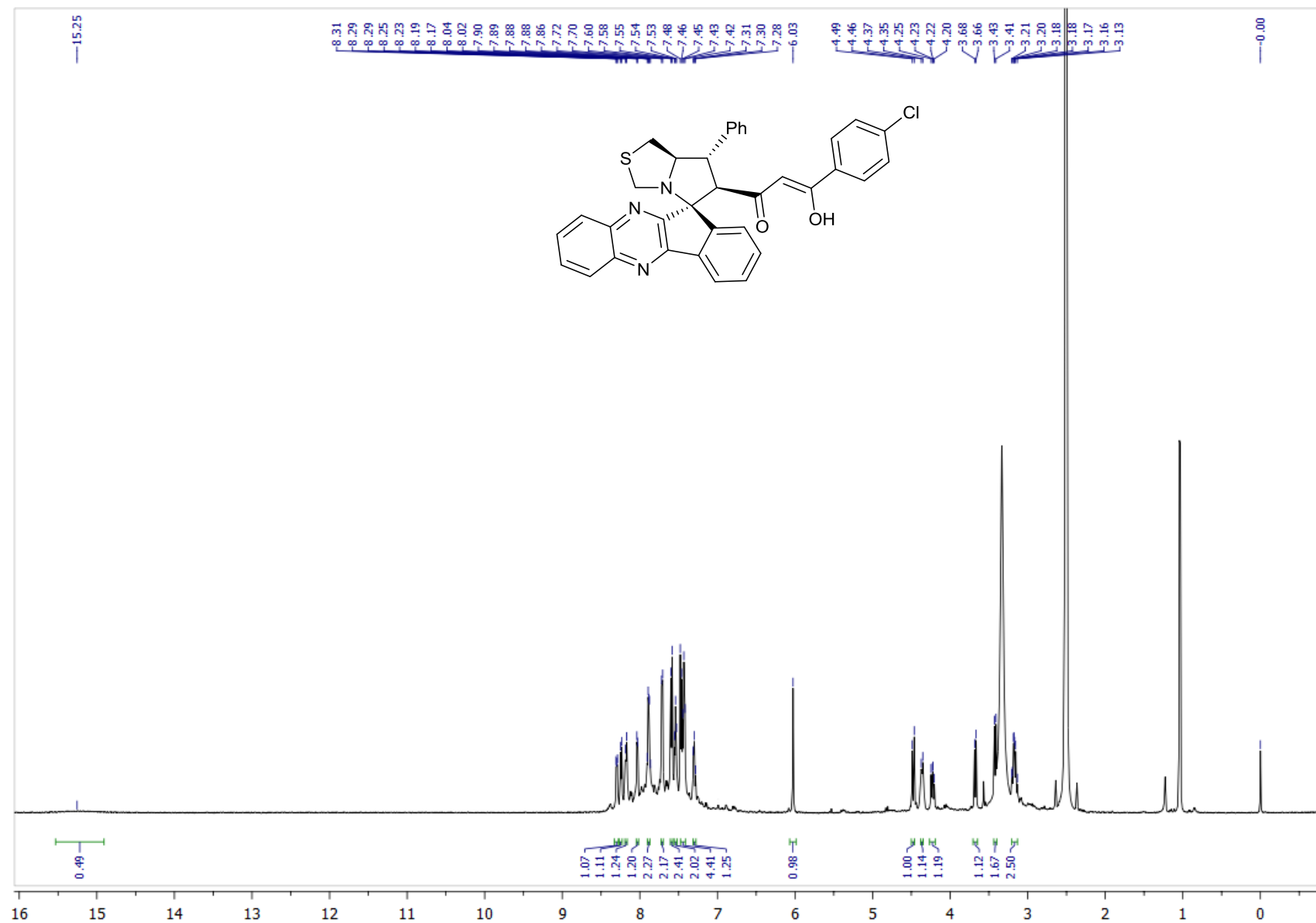


Figure S49. Copy of  $^{13}\text{C}$  NMR spectrum of **4a** in  $\text{DMSO-}d_6$



**Figure S50.** Copy of <sup>1</sup>H NMR spectrum of **4b** in DMSO-*d*<sub>6</sub>

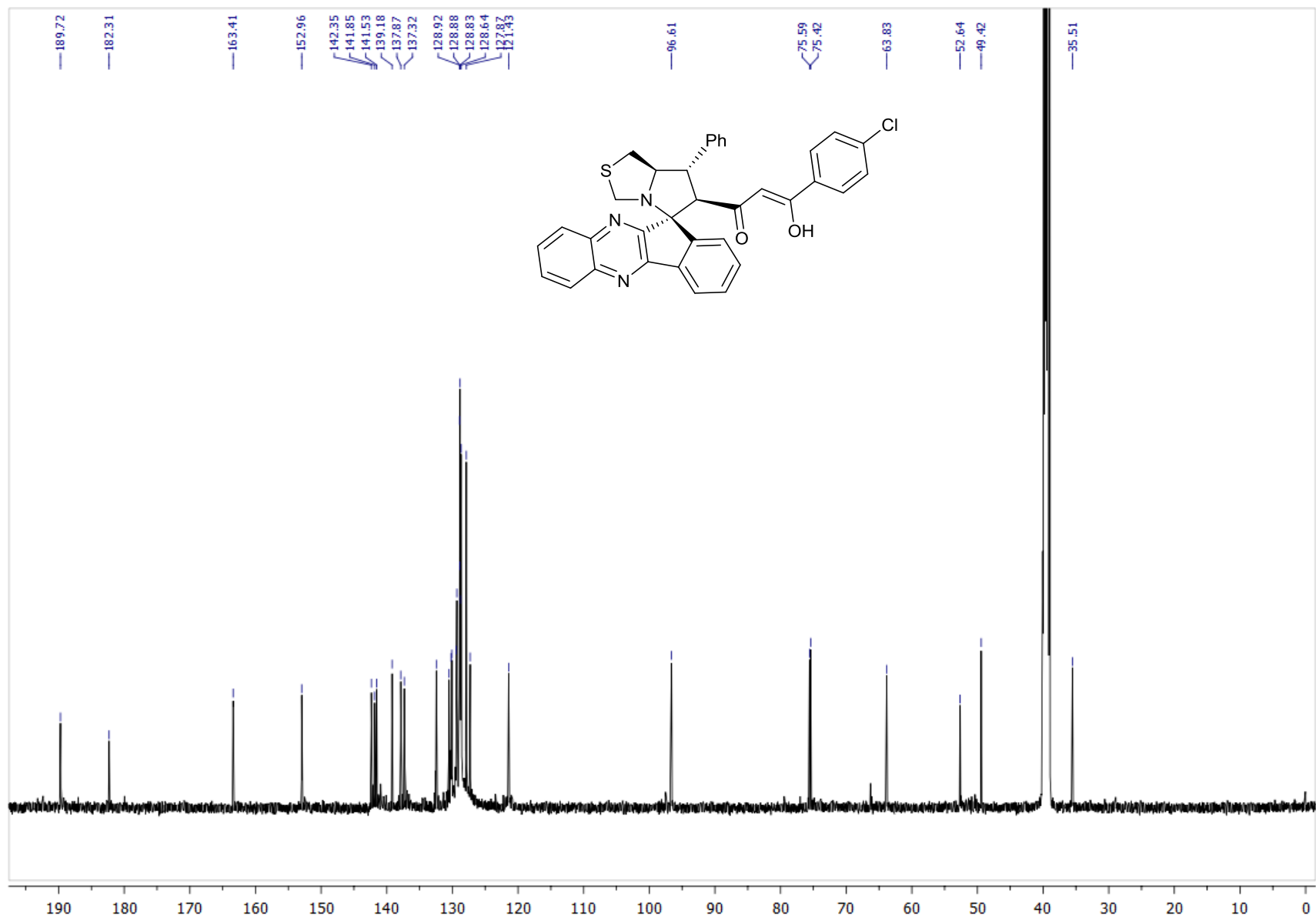
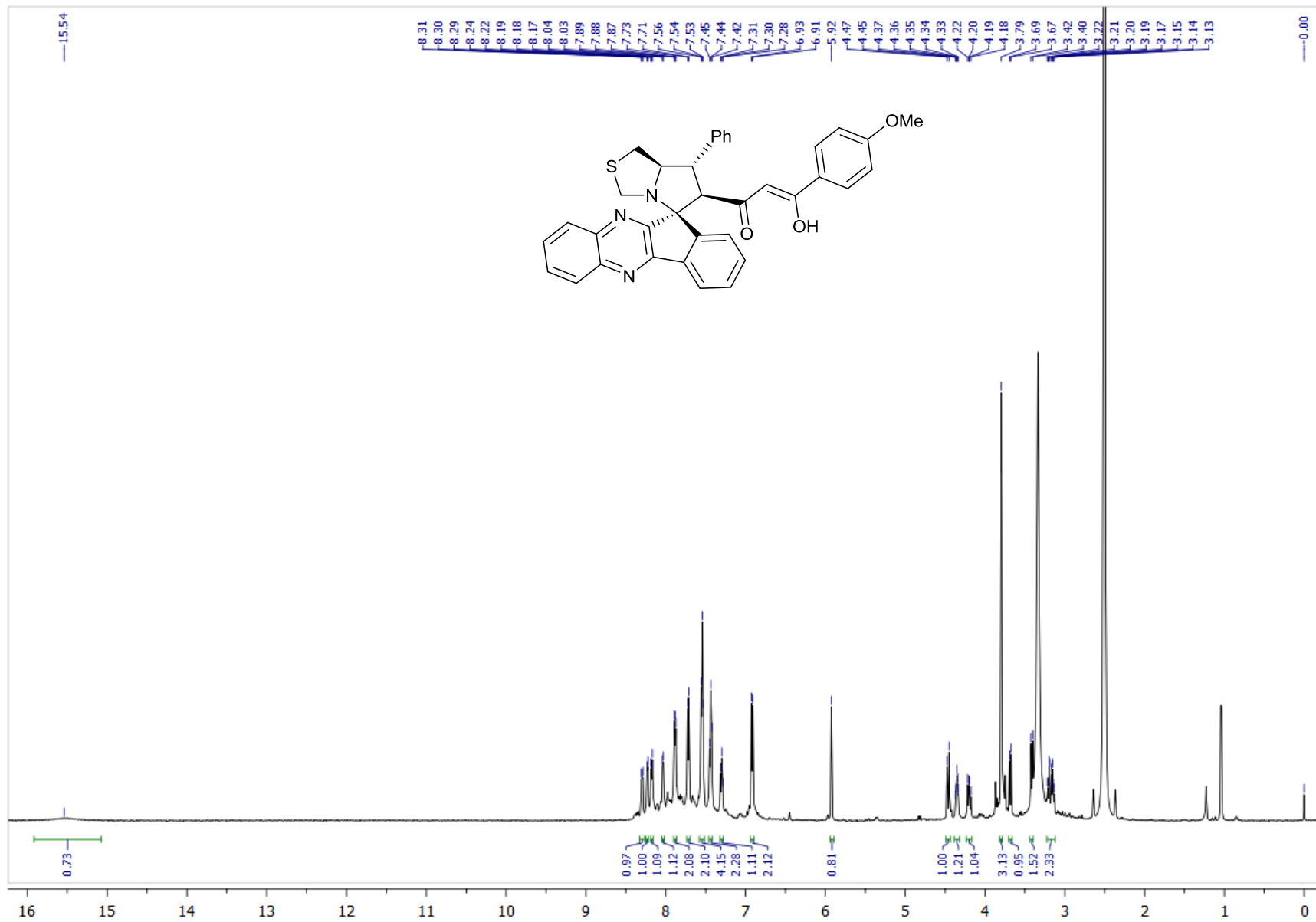


Figure S51. Copy of  $^{13}\text{C}$  NMR spectrum of **4b** in  $\text{DMSO-}d_6$



**Figure S52.** Copy of  $^1\text{H}$  NMR spectrum of **4c** in DMSO- $d_6$

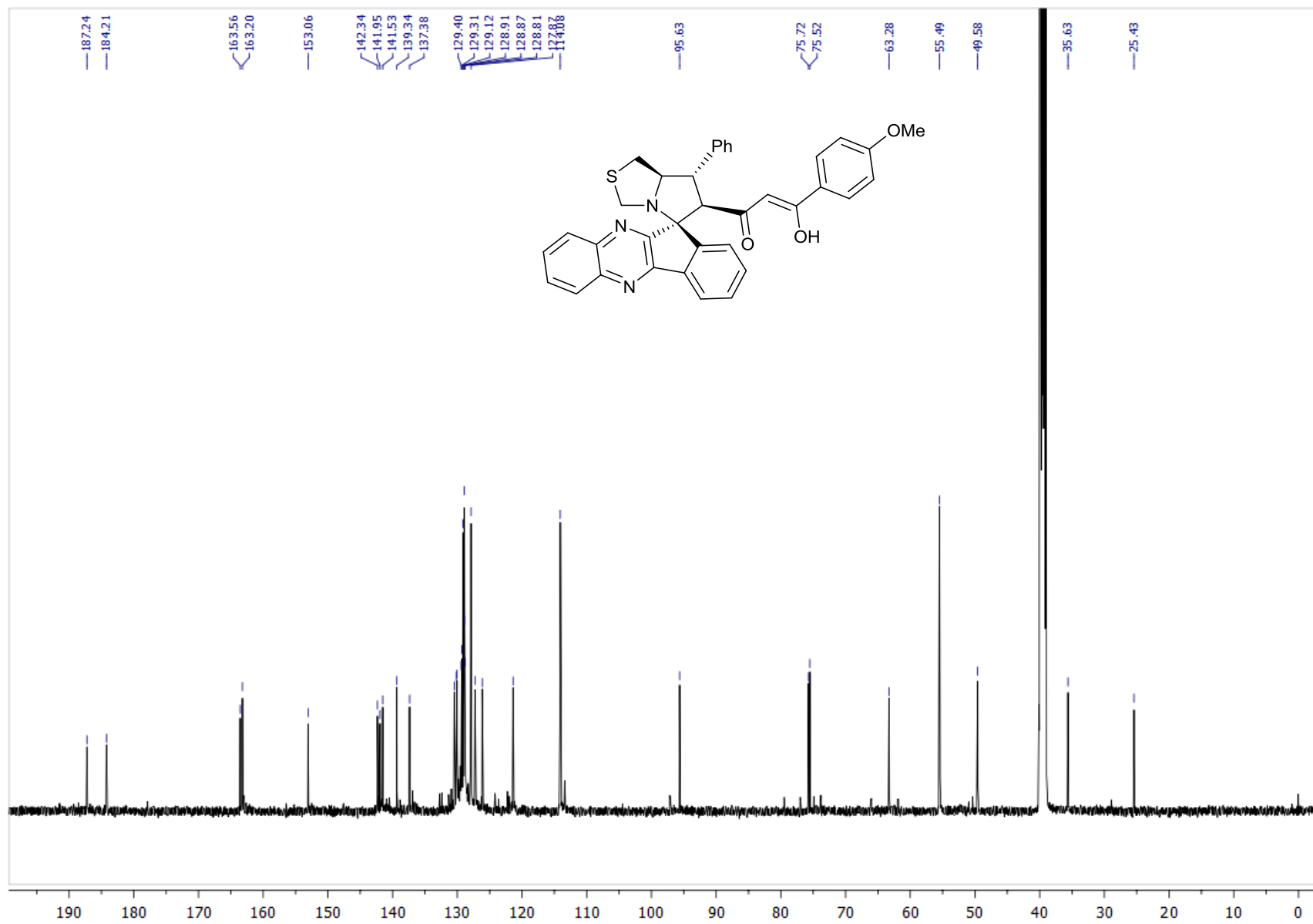


Figure S53. Copy of  $^{13}\text{C}$  NMR spectrum of **4c** in  $\text{DMSO-}d_6$

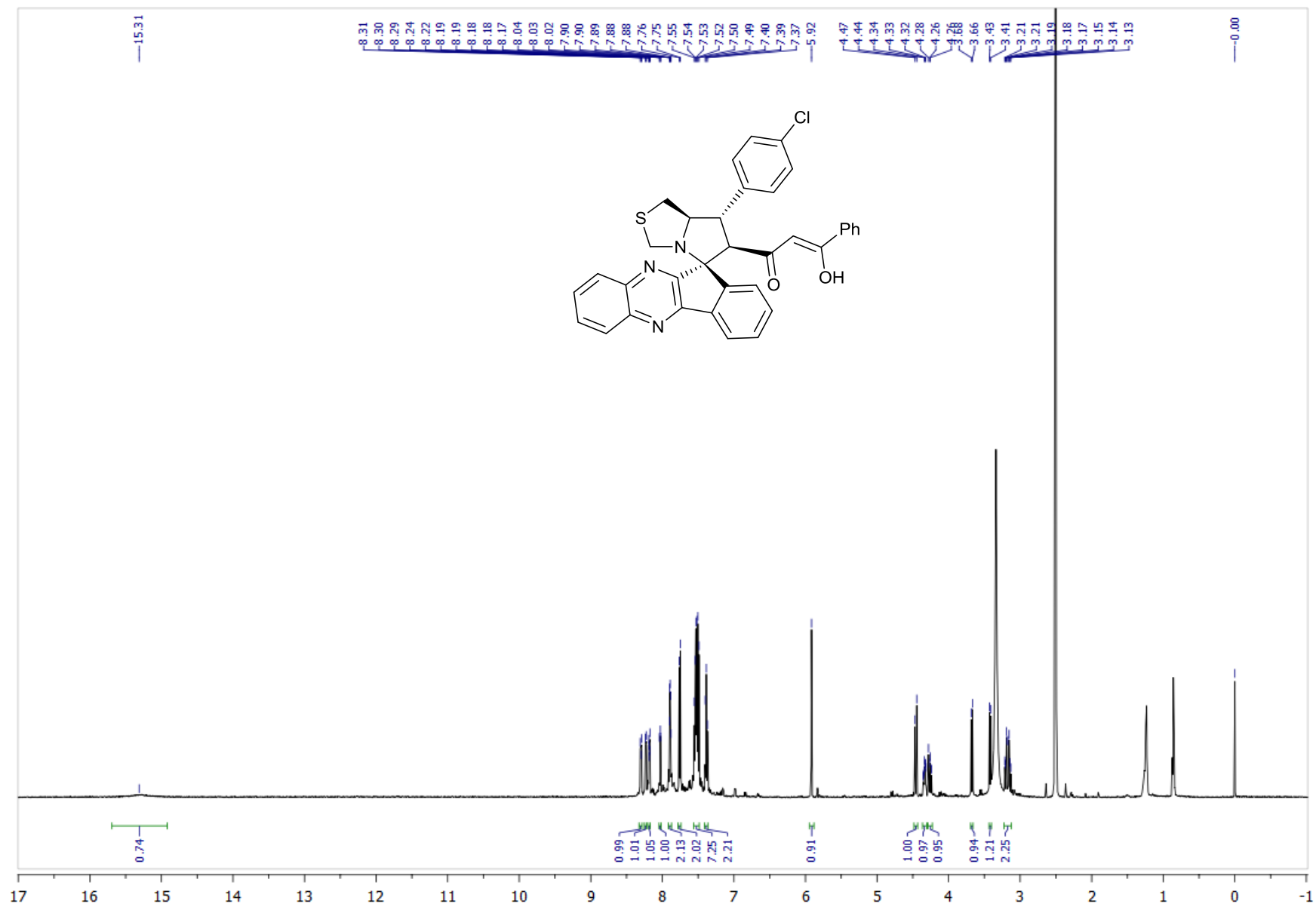


Figure S54. Copy of  $^1\text{H}$  NMR spectrum of **4d** in  $\text{DMSO-}d_6$

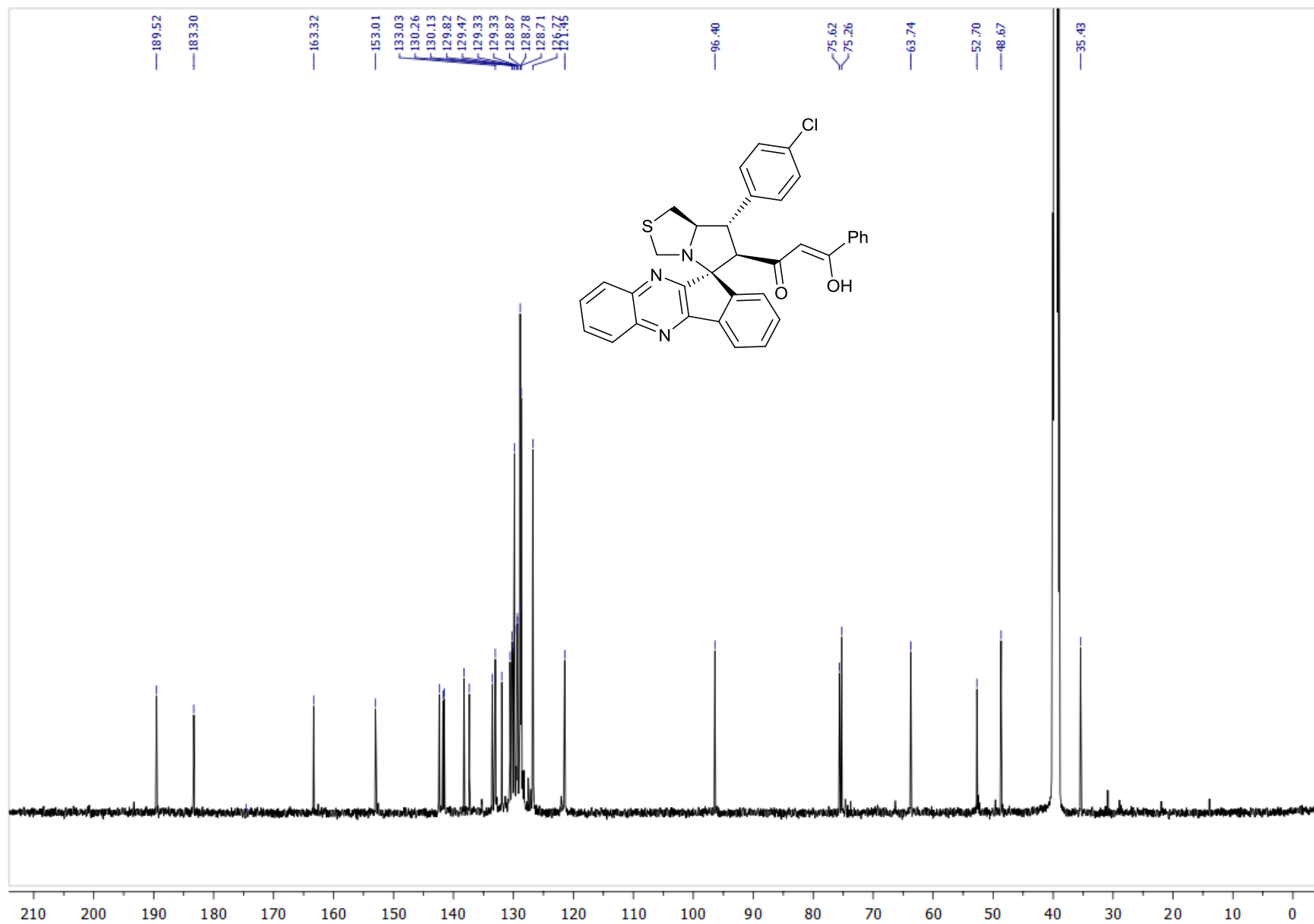


Figure S55. Copy of  $^{13}\text{C}$  NMR spectrum of **4d** in  $\text{DMSO-}d_6$



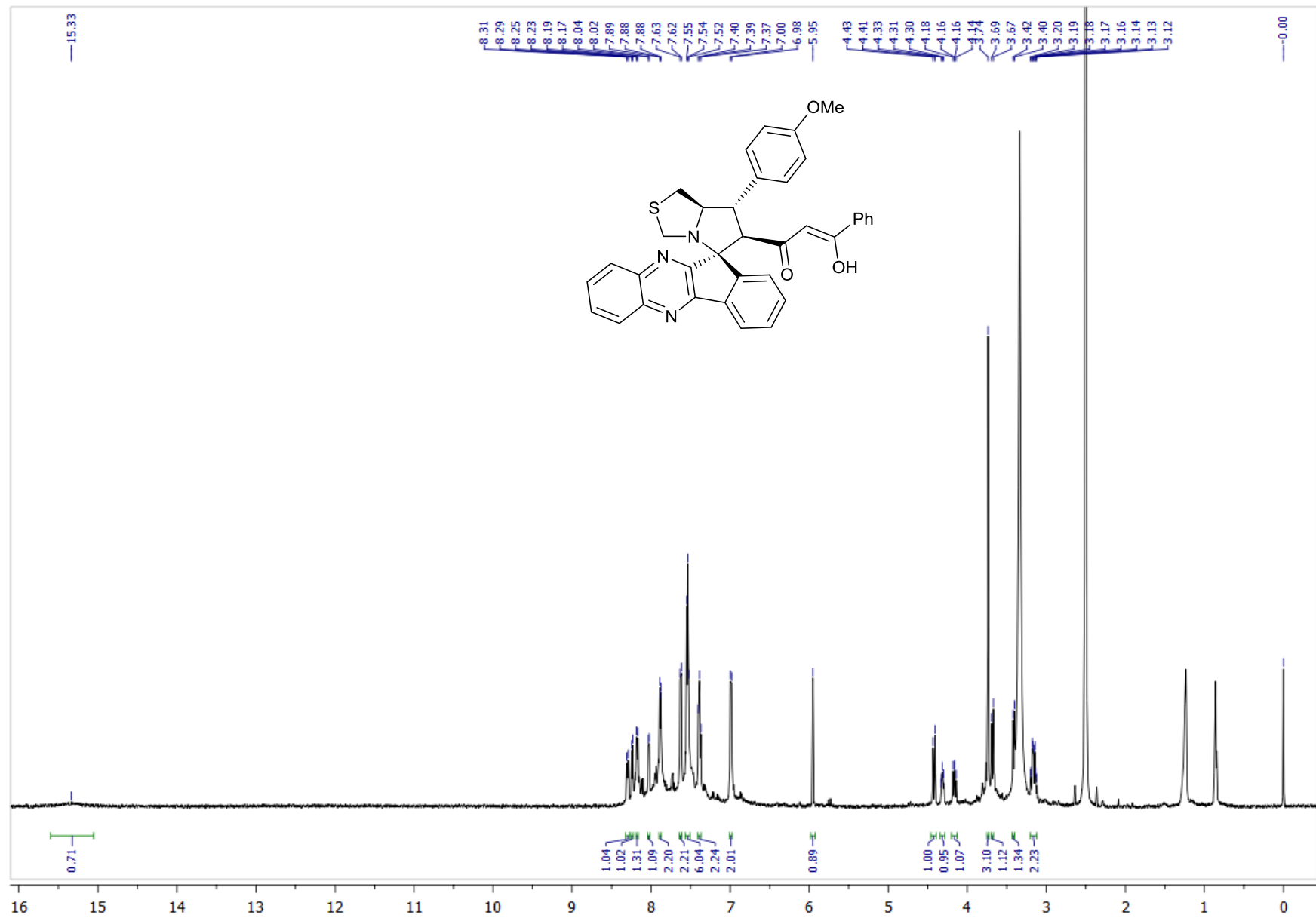


Figure S56. Copy of  $^1\text{H}$  NMR spectrum of **4e** in  $\text{DMSO-}d_6$

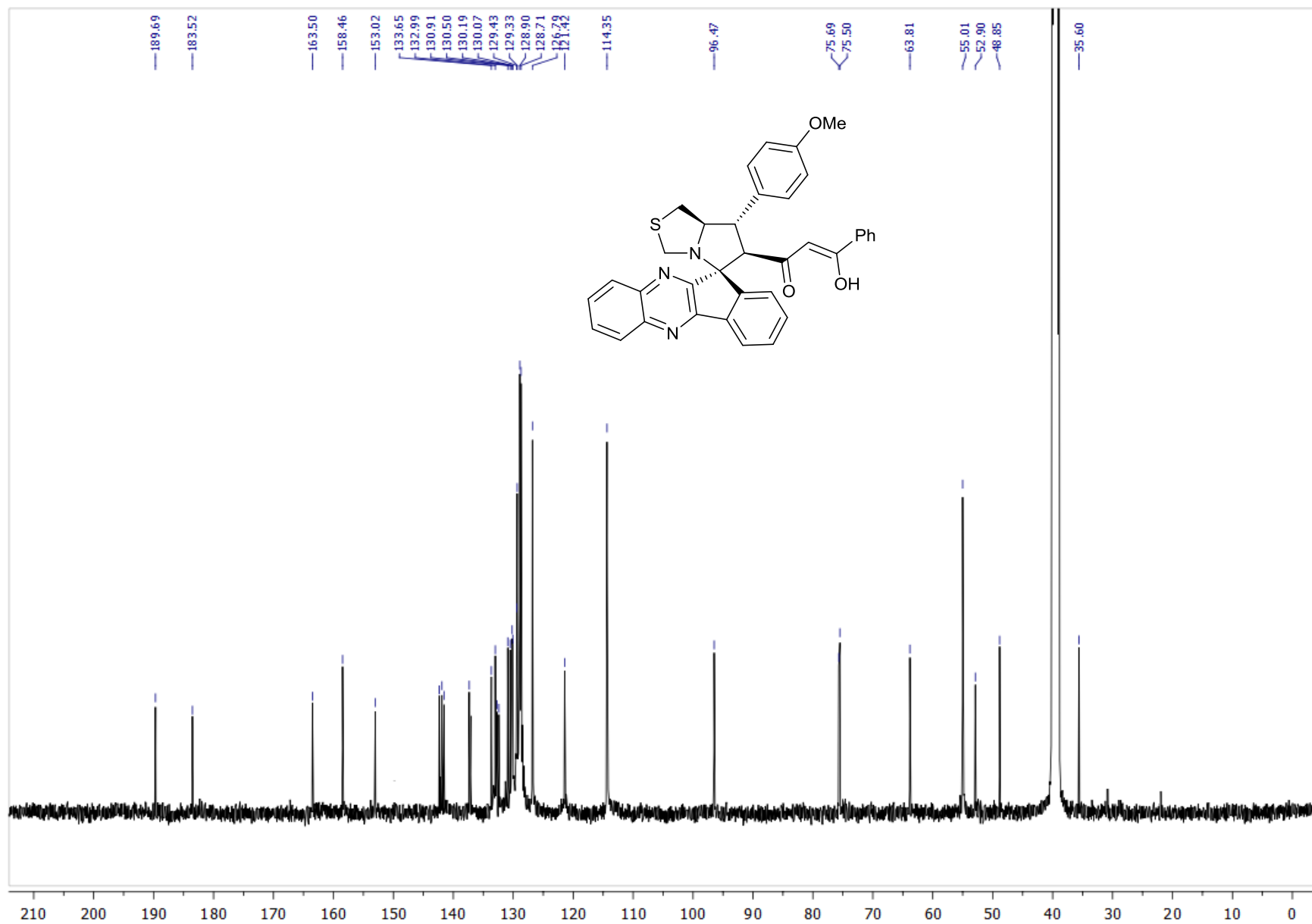


Figure S57. Copy of  $^{13}\text{C}$  NMR spectrum of **4e** in  $\text{DMSO-}d_6$

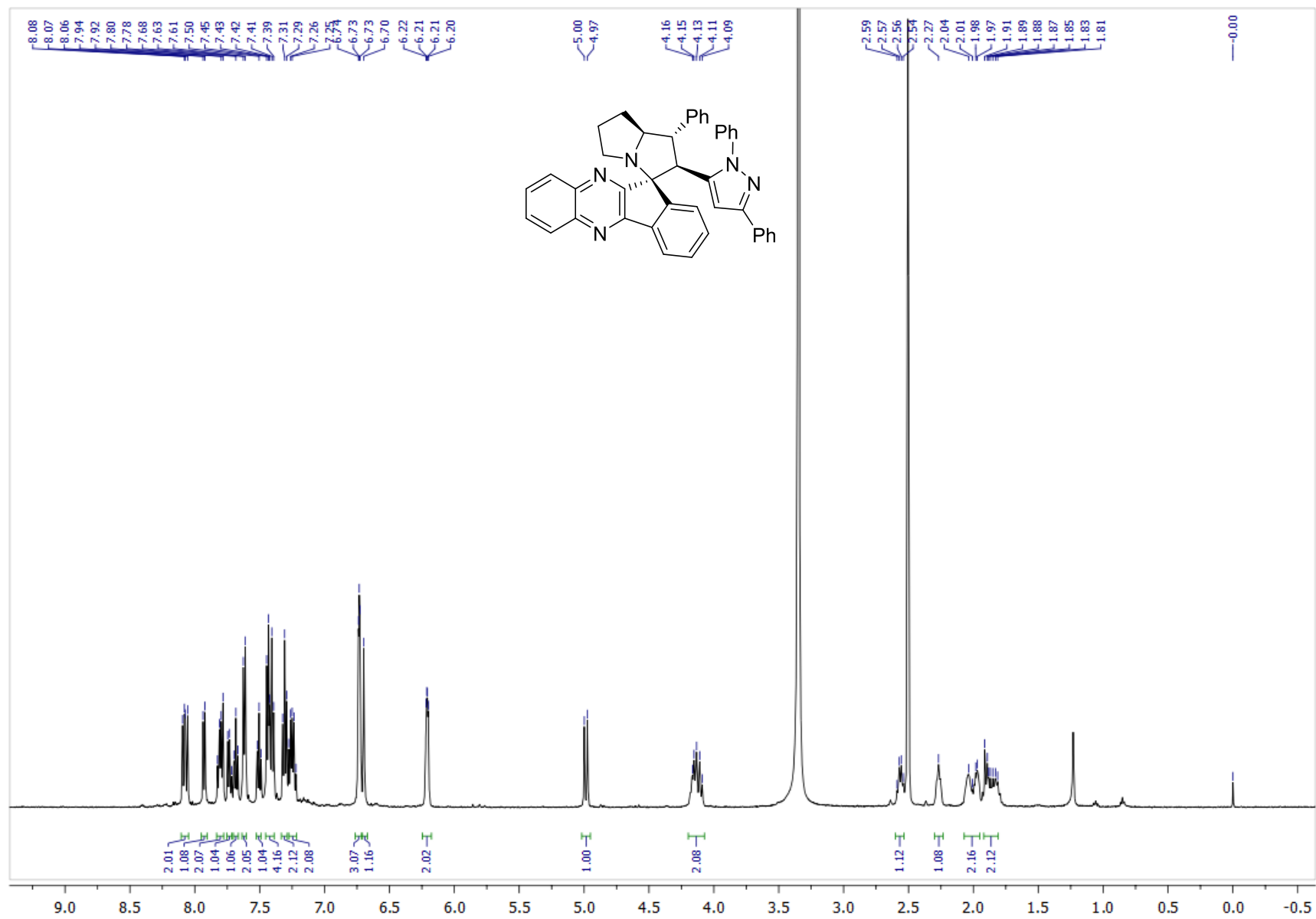


Figure S58. Copy of <sup>1</sup>H NMR spectrum of **5a** in DMSO-*d*<sub>6</sub>

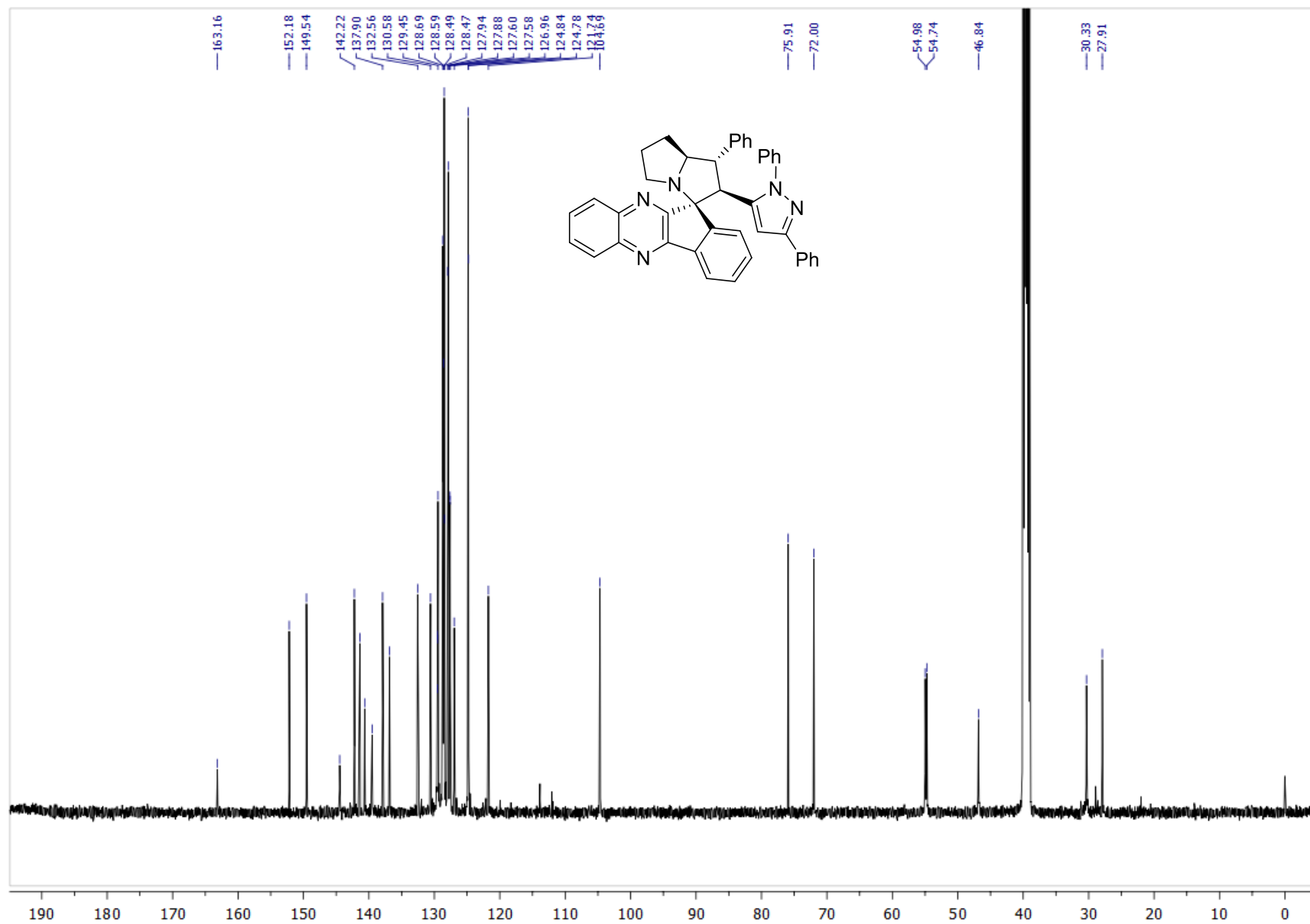
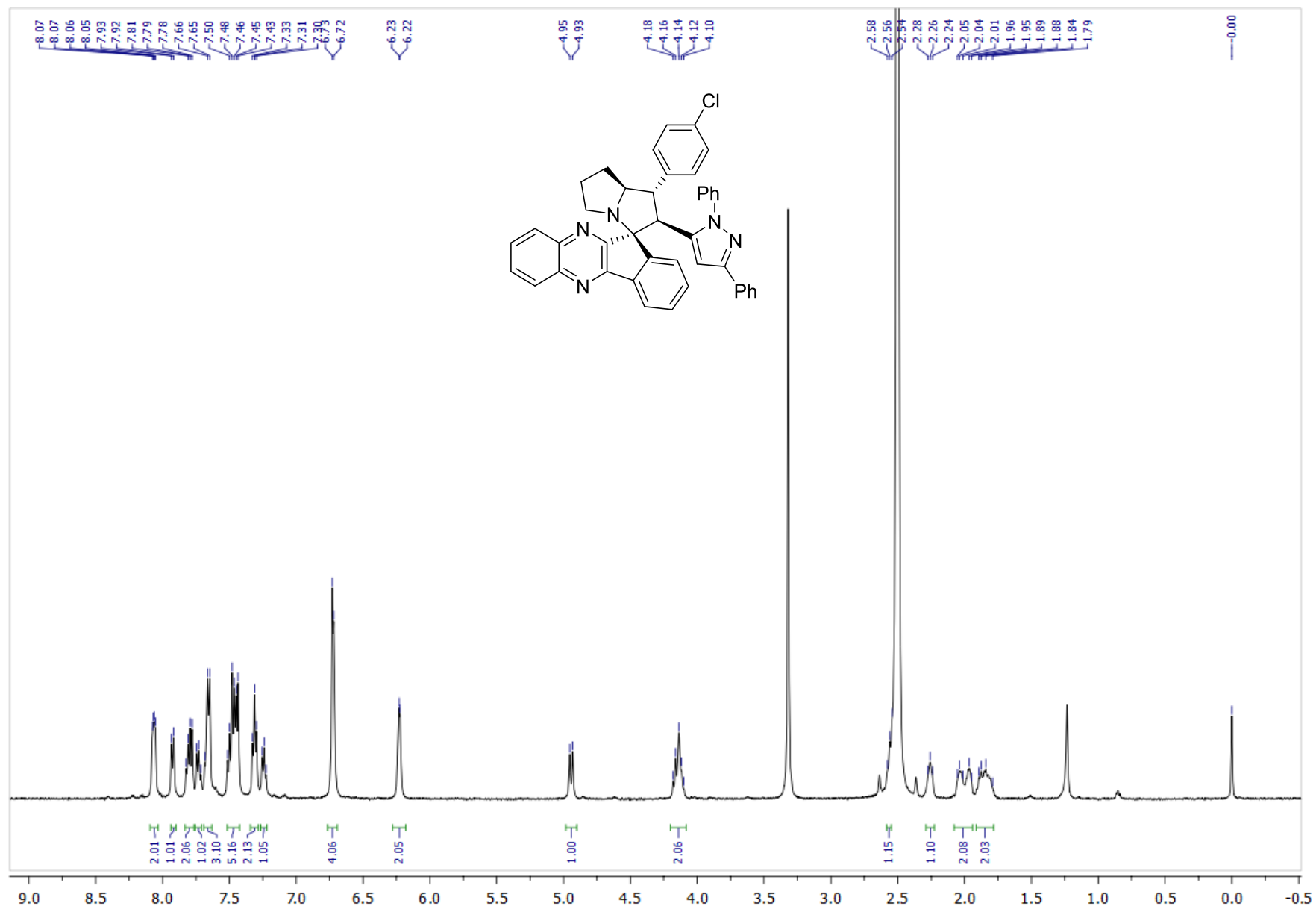


Figure S59. Copy of  $^{13}\text{C}$  NMR spectrum of **5a** in  $\text{DMSO-}d_6$



**Figure S60.** Copy of  $^1\text{H}$  NMR spectrum of **5b** in  $\text{DMSO-}d_6$

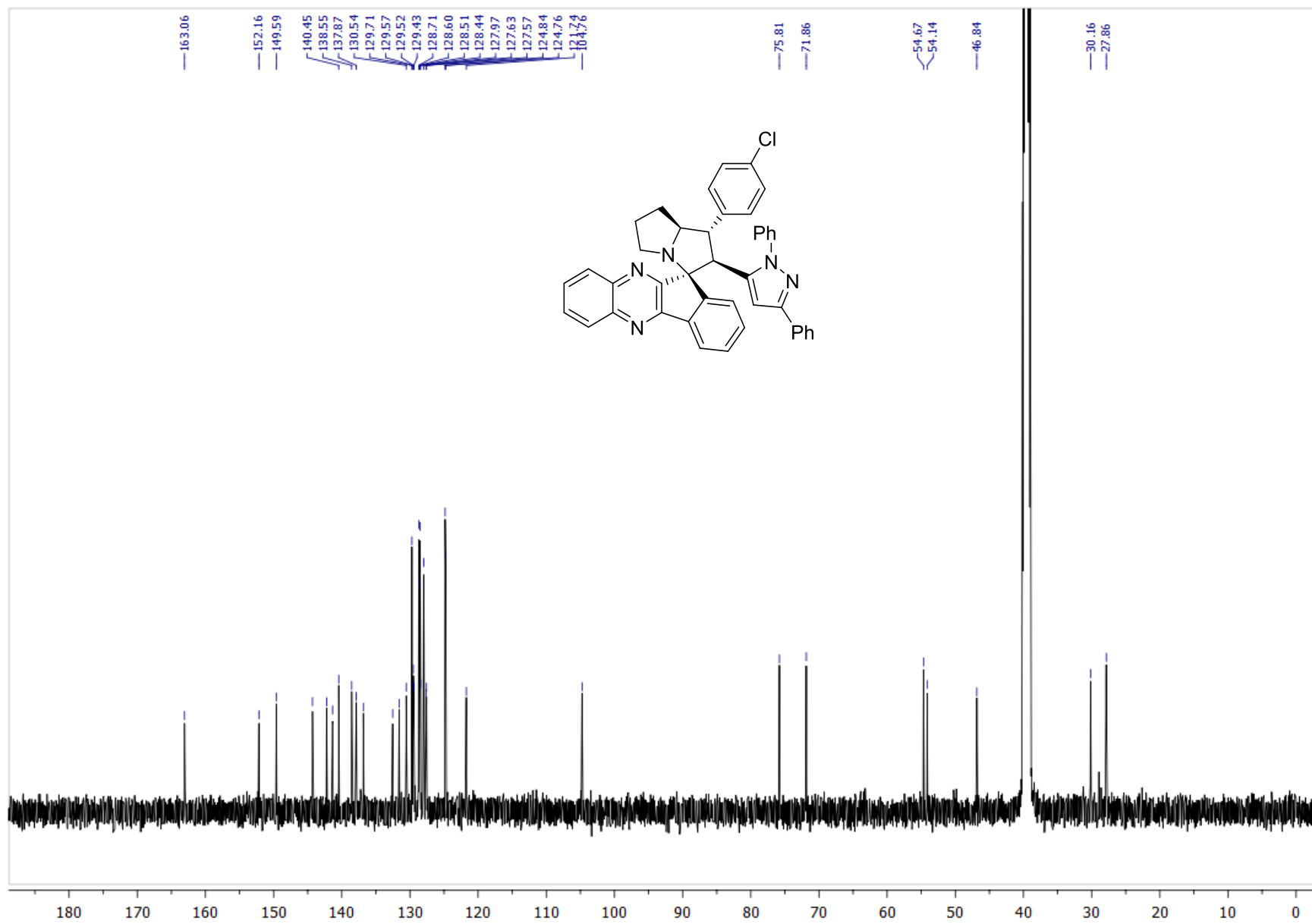


Figure S61. Copy of  $^{13}\text{C}$  NMR spectrum of **5b** in  $\text{DMSO-}d_6$

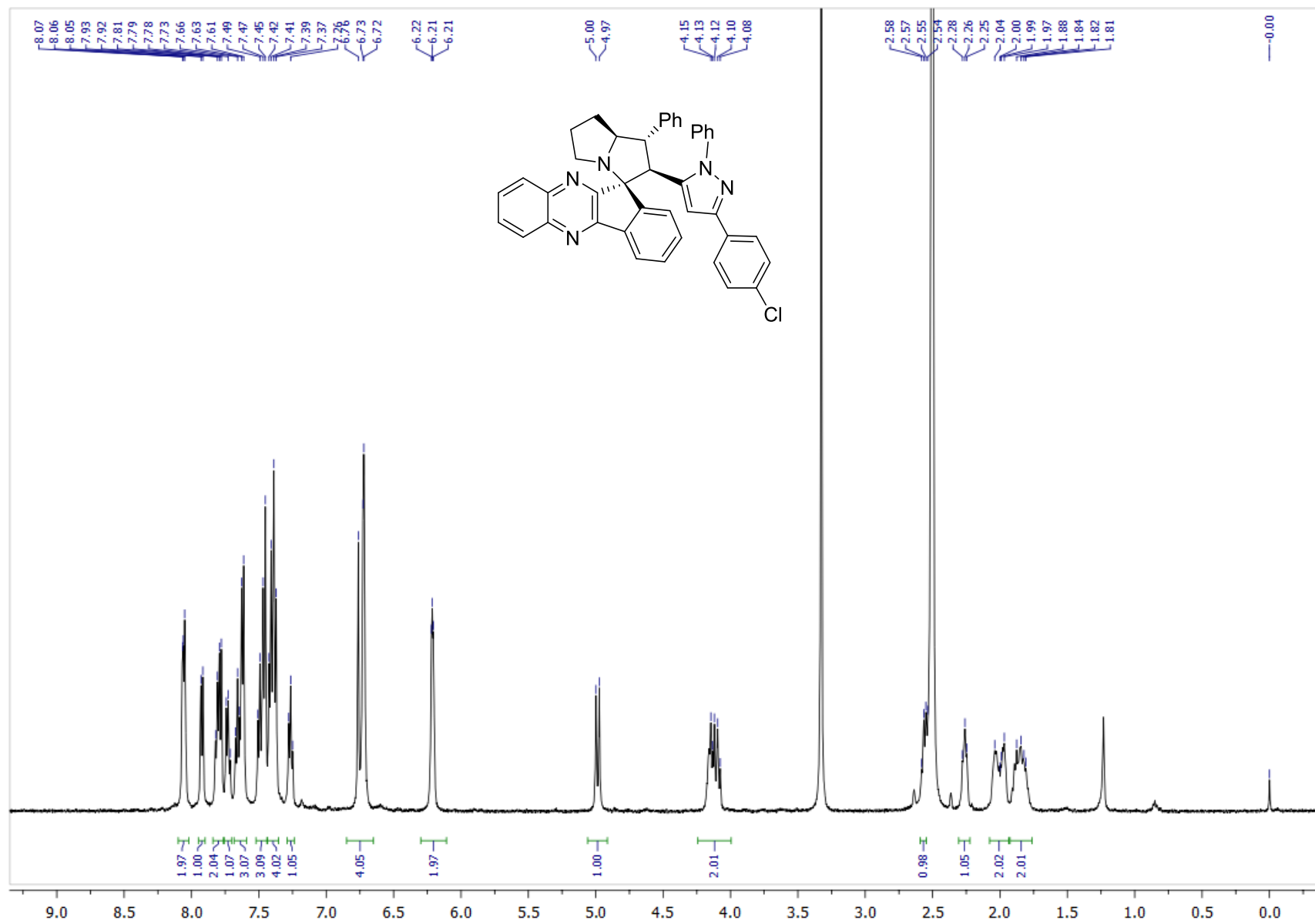


Figure S62. Copy of <sup>1</sup>H NMR spectrum of **5c** in DMSO-*d*<sub>6</sub>

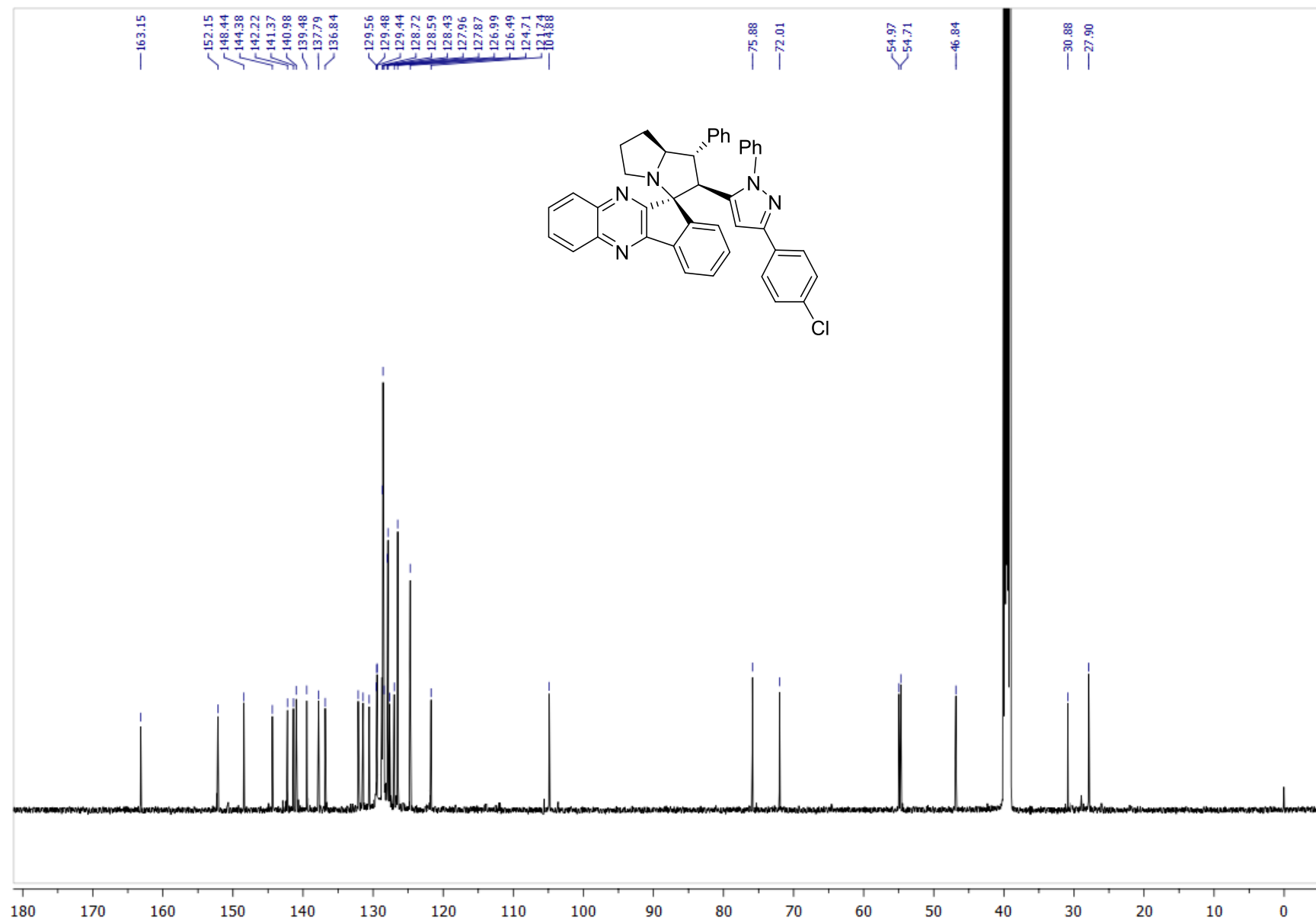
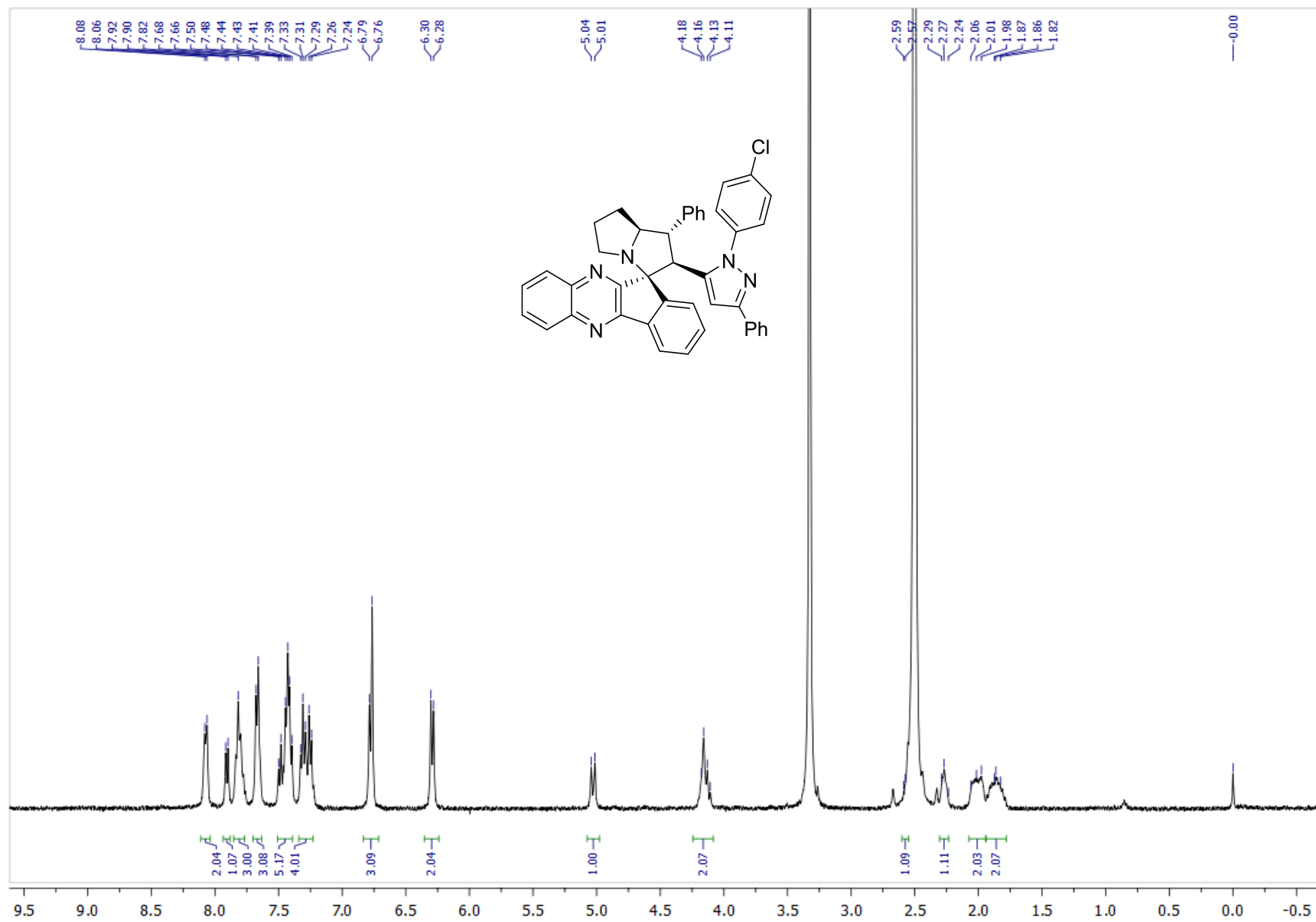


Figure S63. Copy of  $^{13}\text{C}$  NMR spectrum of **5c** in  $\text{DMSO-}d_6$





**Figure S64.** Copy of  $^1\text{H}$  NMR spectrum of **5d** in  $\text{DMSO-}d_6$

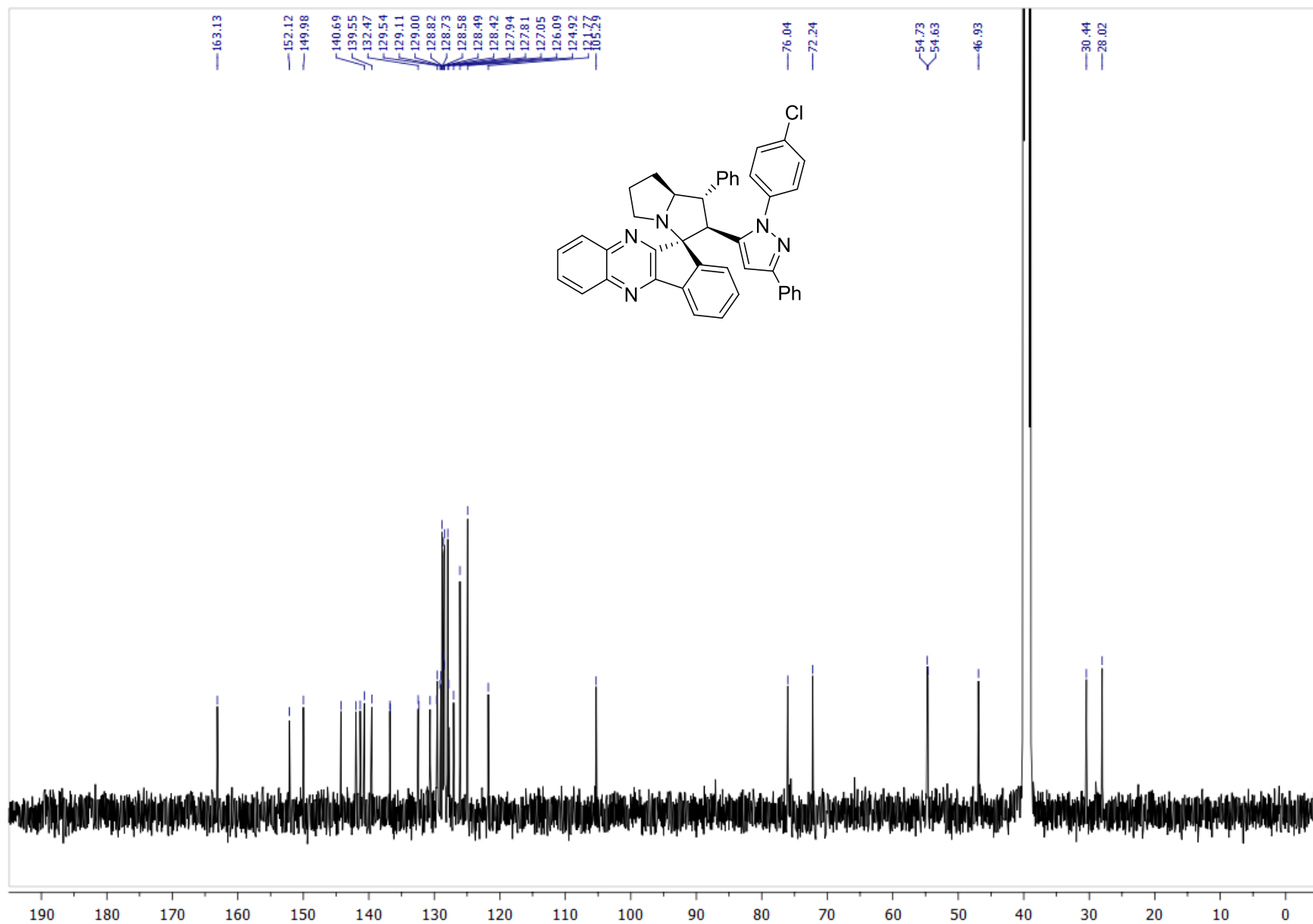


Figure S65. Copy of  $^{13}\text{C}$  NMR spectrum of **5d** in  $\text{DMSO-}d_6$

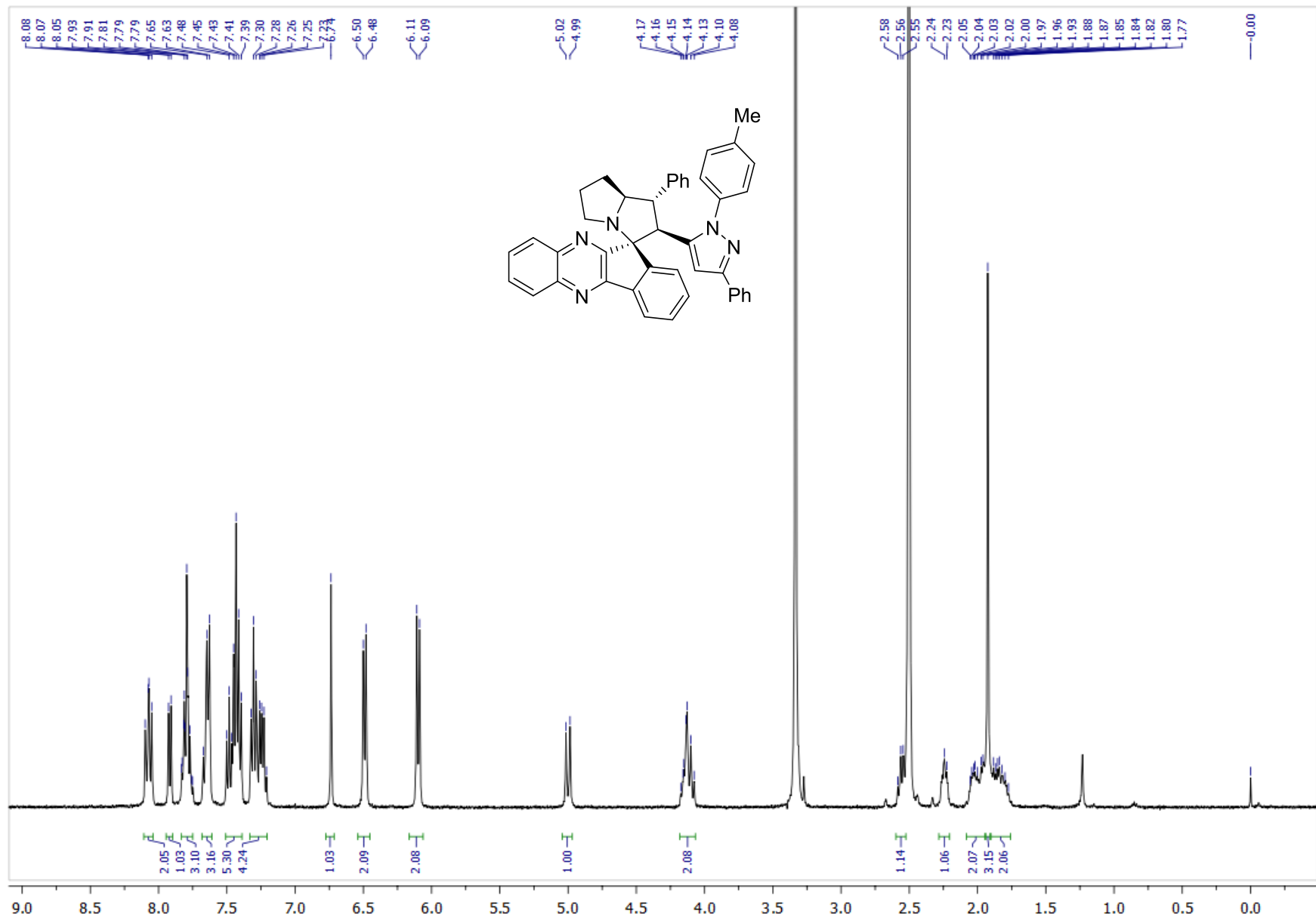


Figure S66. Copy of  $^1\text{H}$  NMR spectrum of **5e** in  $\text{DMSO-}d_6$

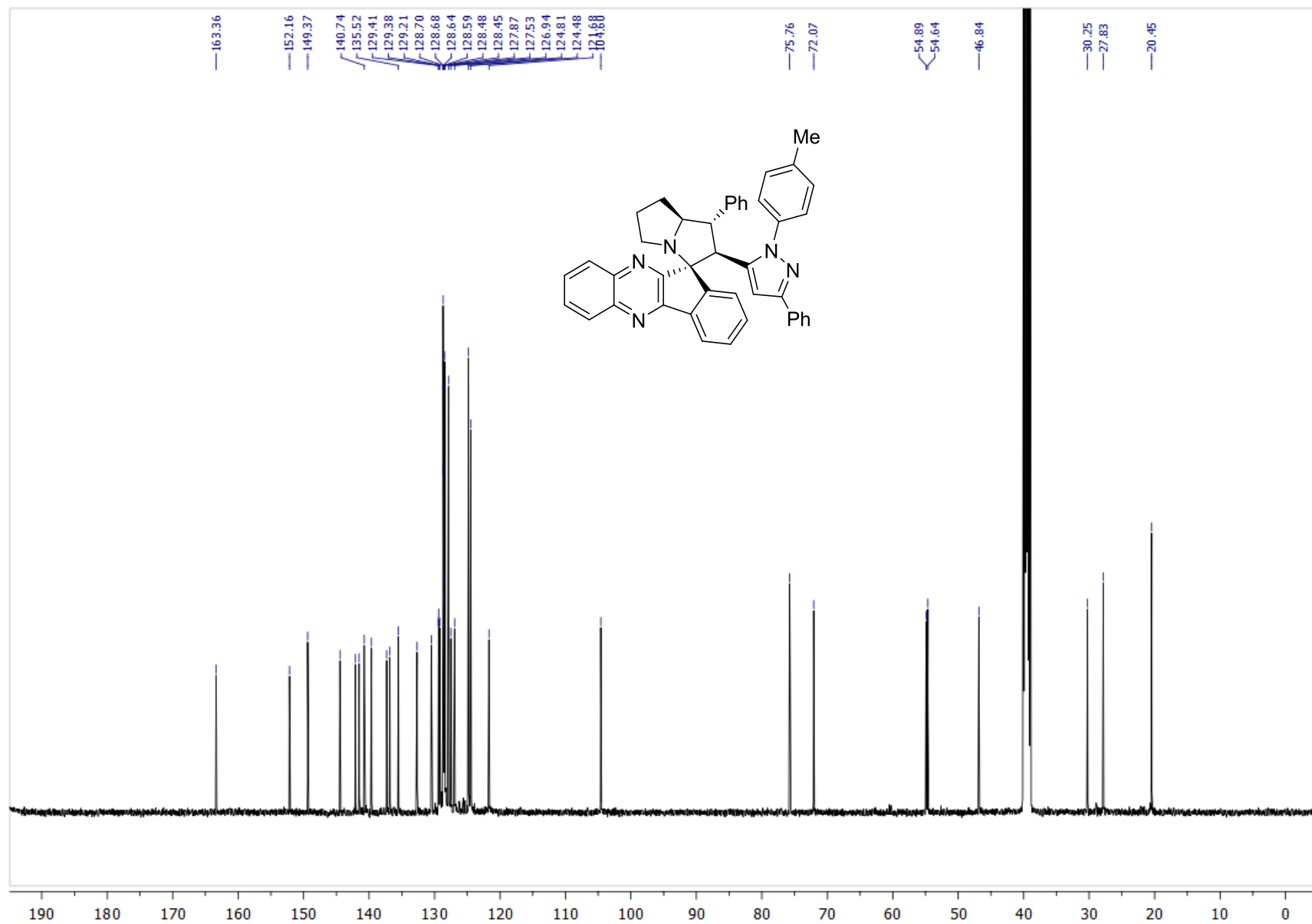


Figure S67. Copy of  $^{13}\text{C}$  NMR spectrum of **5e** in  $\text{DMSO-}d_6$

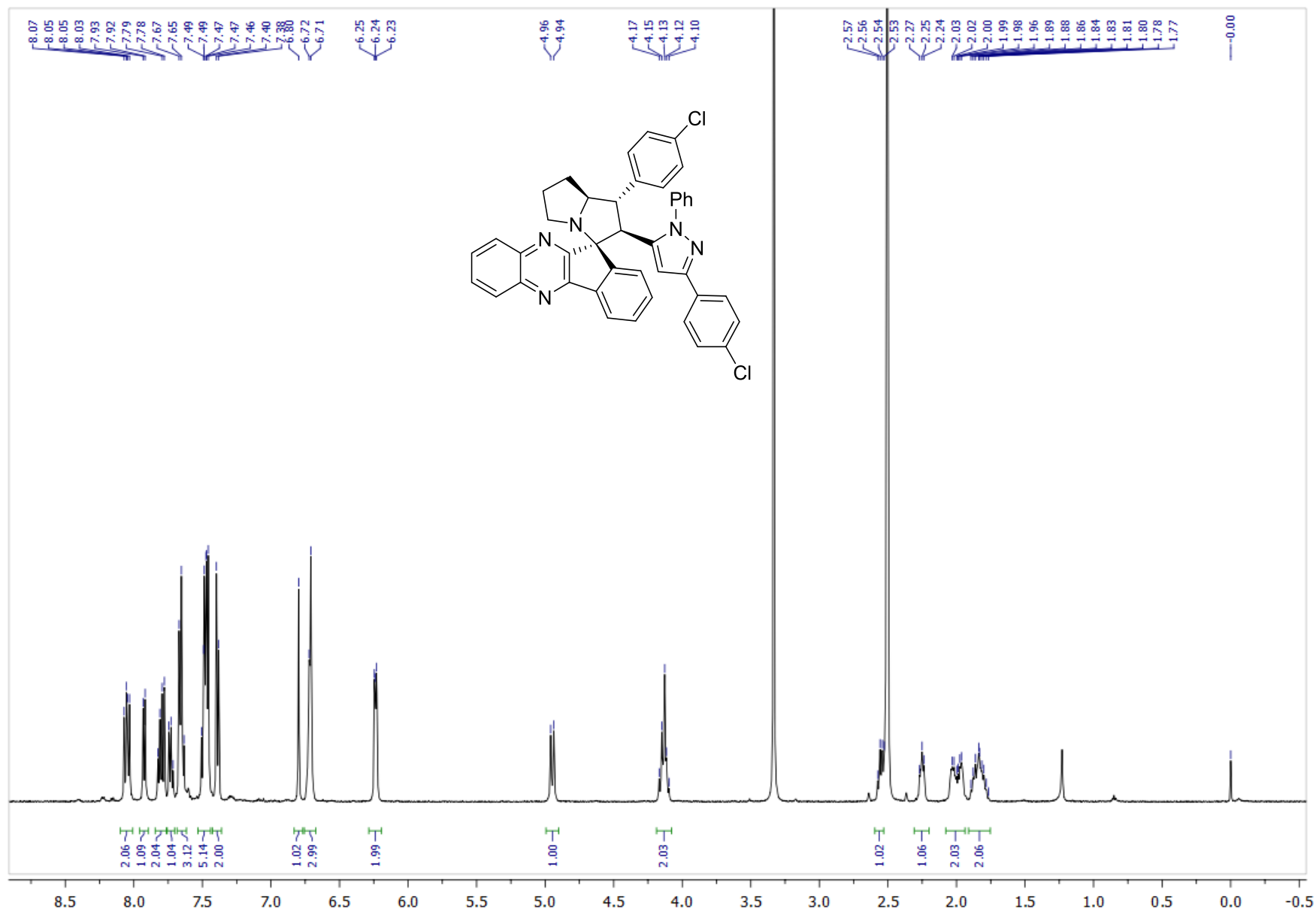


Figure S68. Copy of  $^1\text{H}$  NMR spectrum of **5f** in  $\text{DMSO}-d_6$

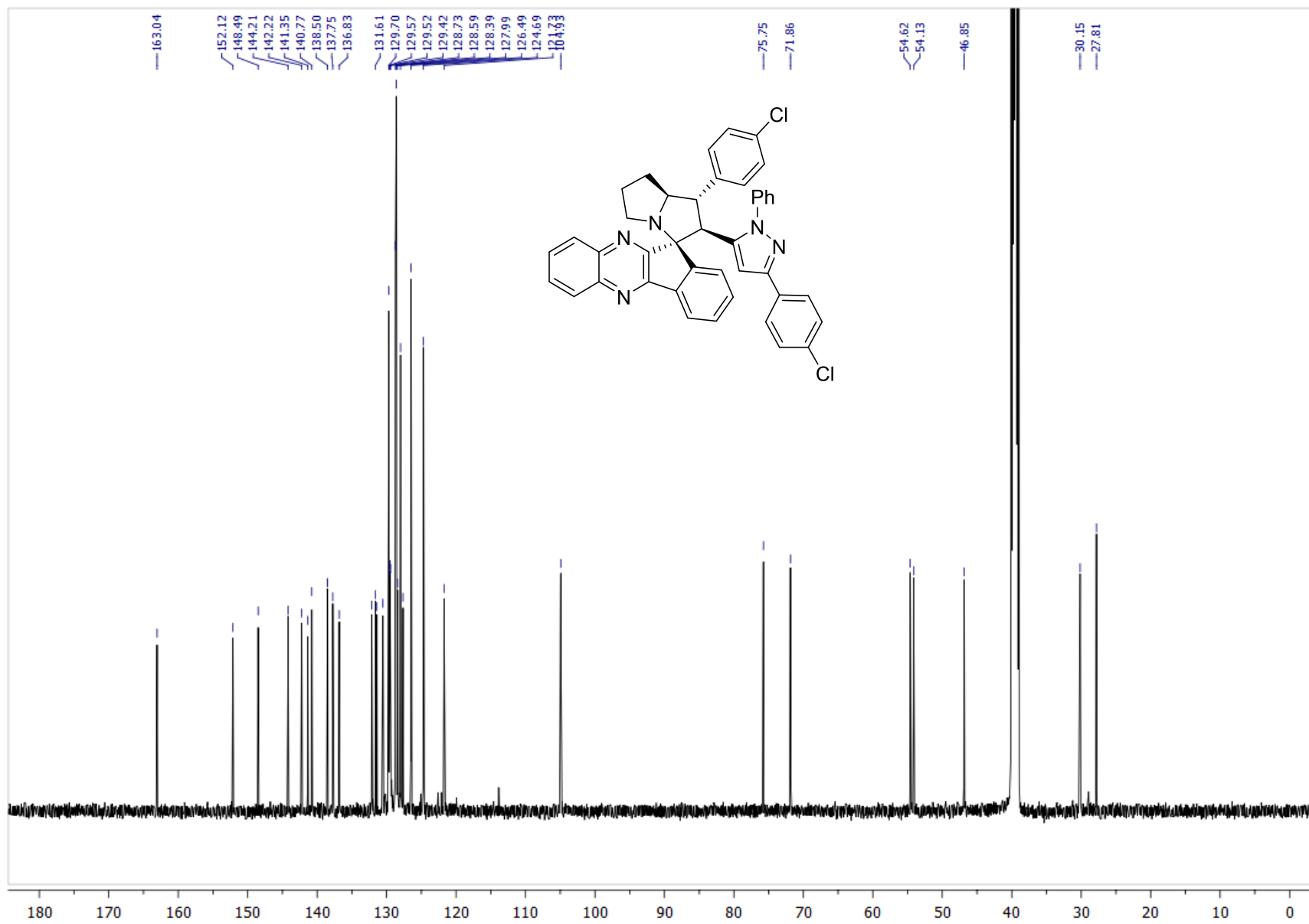
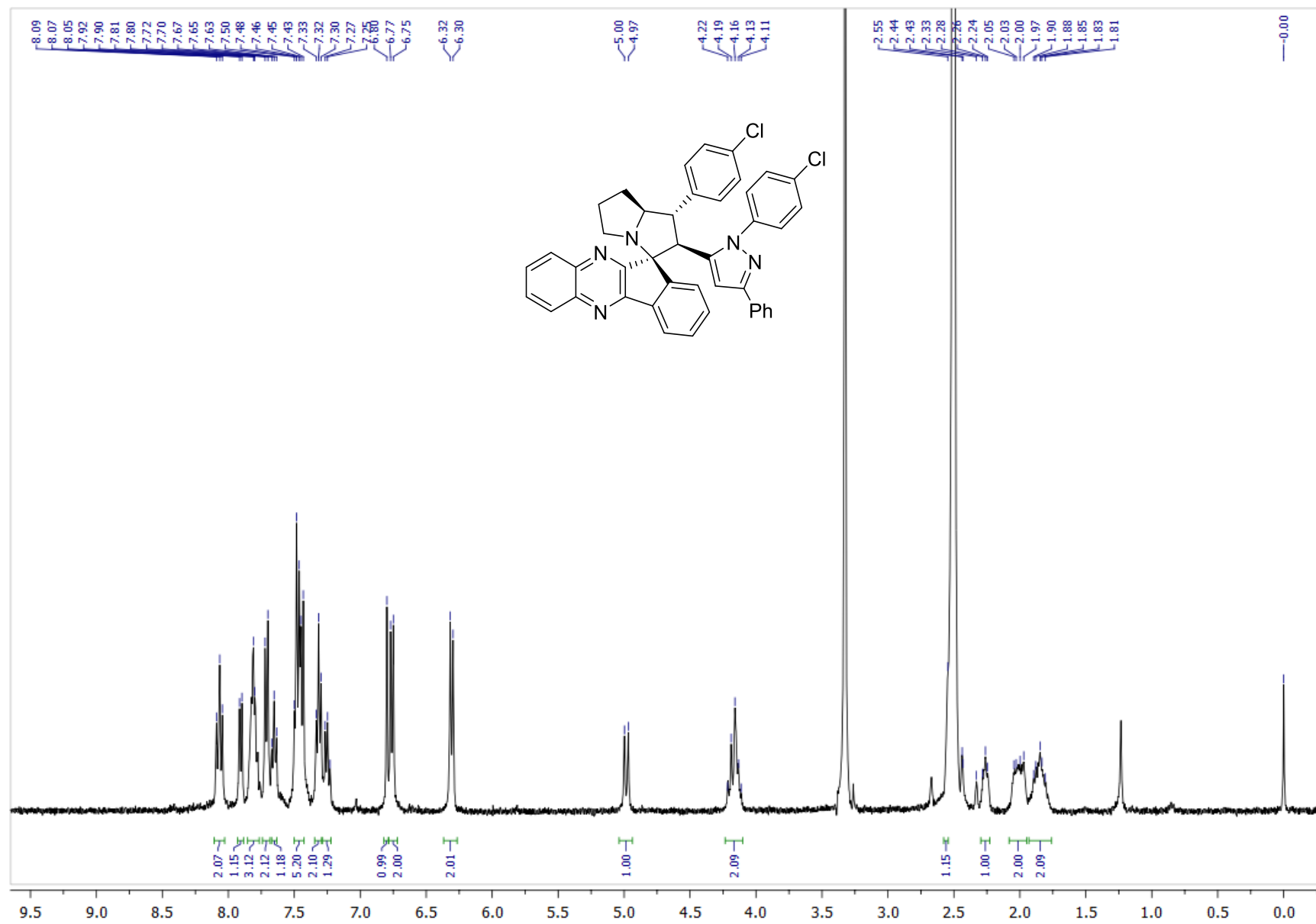


Figure S69. Copy of  $^{13}\text{C}$  NMR spectrum of **5f** in  $\text{DMSO-}d_6$



**Figure S70.** Copy of  $^1\text{H}$  NMR spectrum of **5g** in  $\text{DMSO-}d_6$

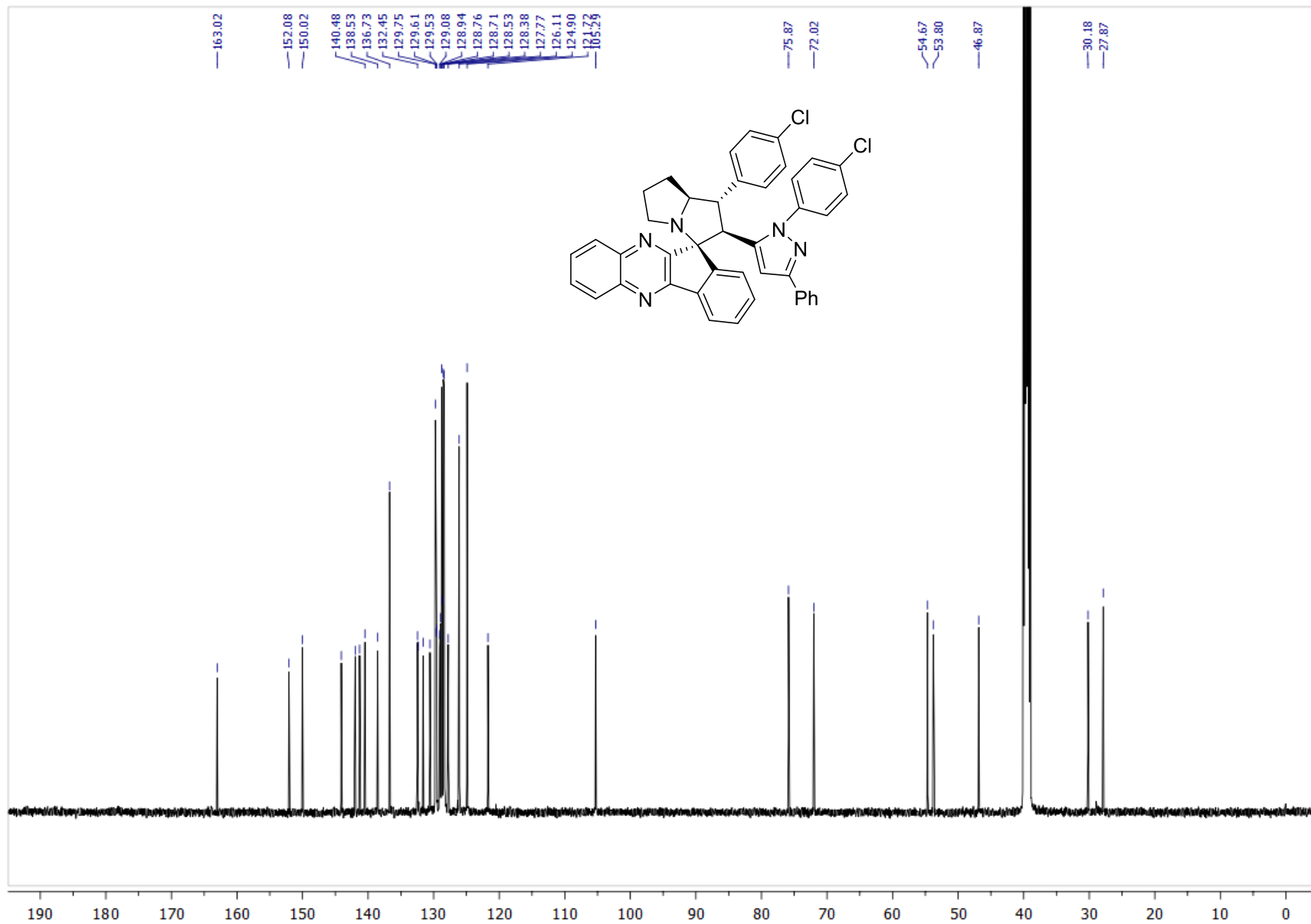
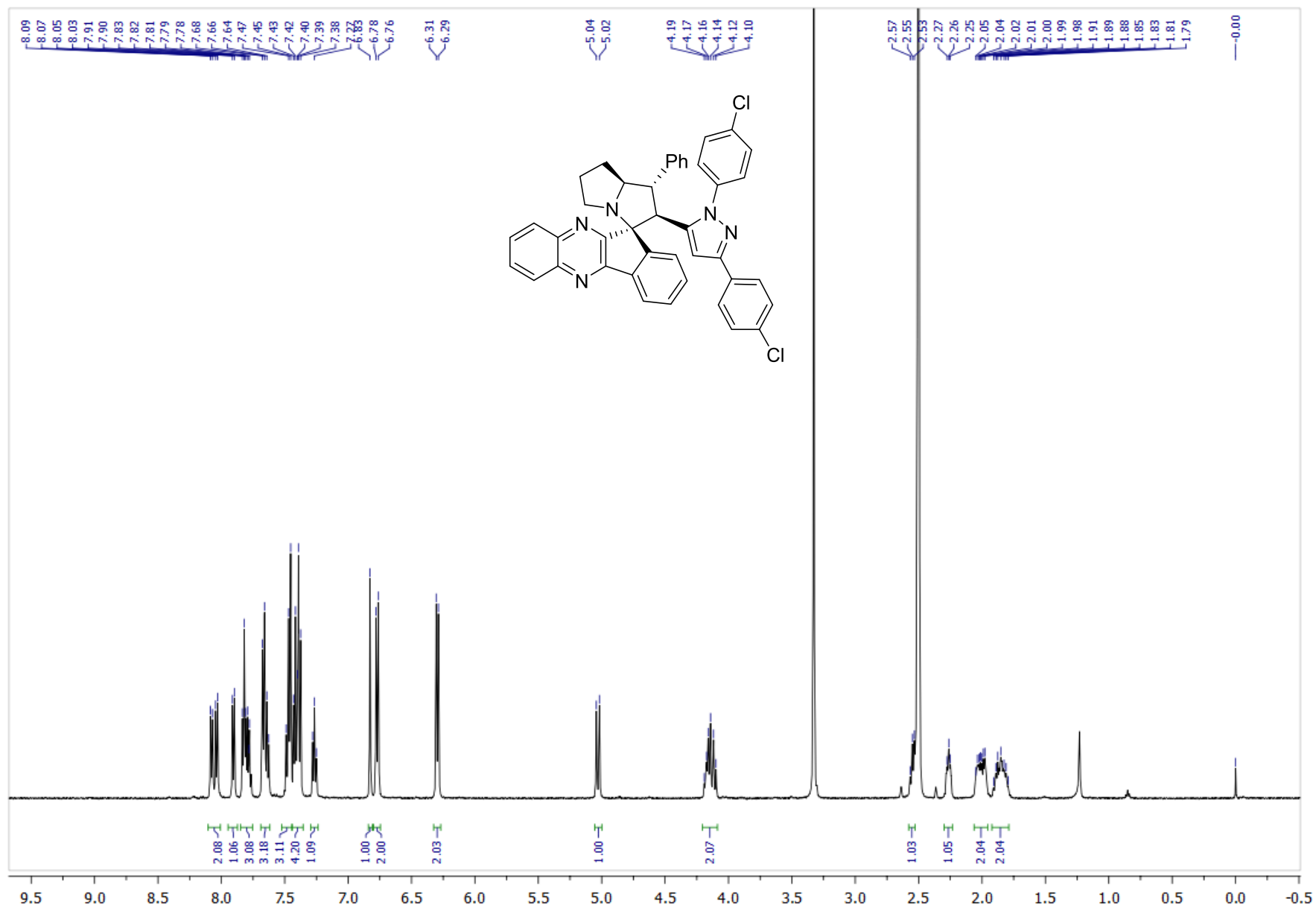


Figure S71. Copy of  $^{13}\text{C}$  NMR spectrum of **5g** in  $\text{DMSO-}d_6$





**Figure S72.** Copy of  $^1\text{H}$  NMR spectrum of **5h** in  $\text{DMSO}-d_6$

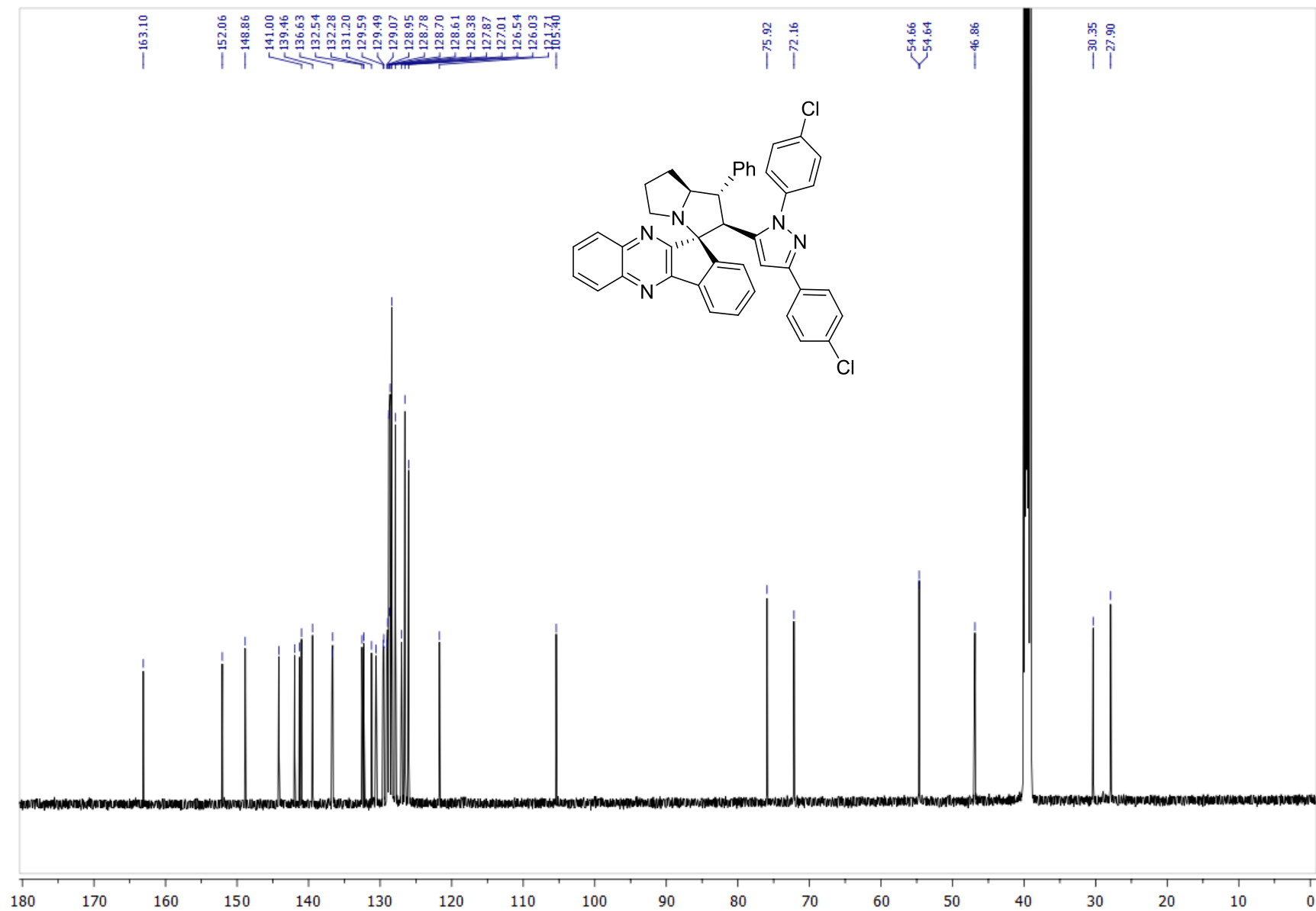


Figure S73. Copy of  $^{13}\text{C}$  NMR spectrum of **5h** in  $\text{DMSO-}d_6$

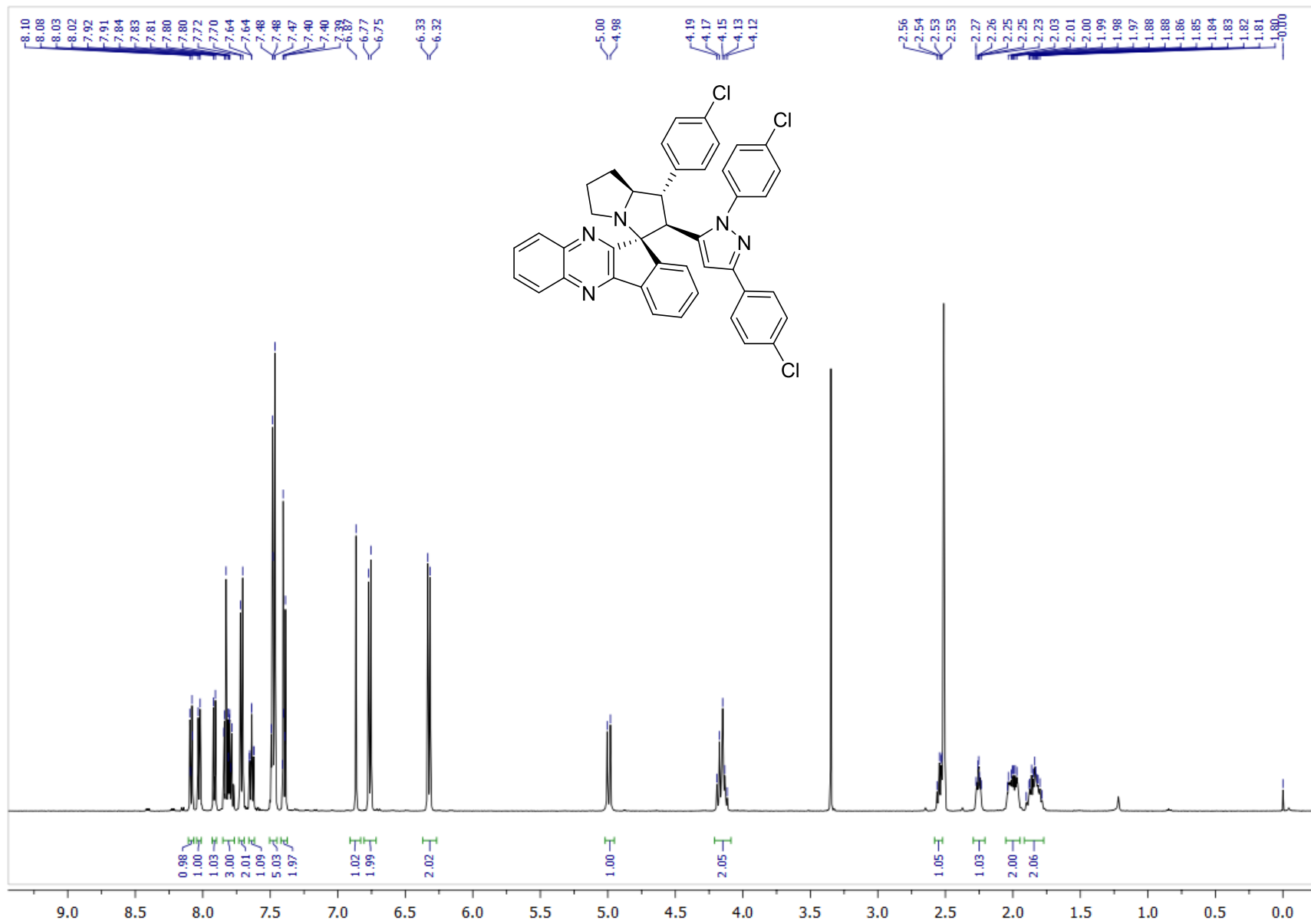
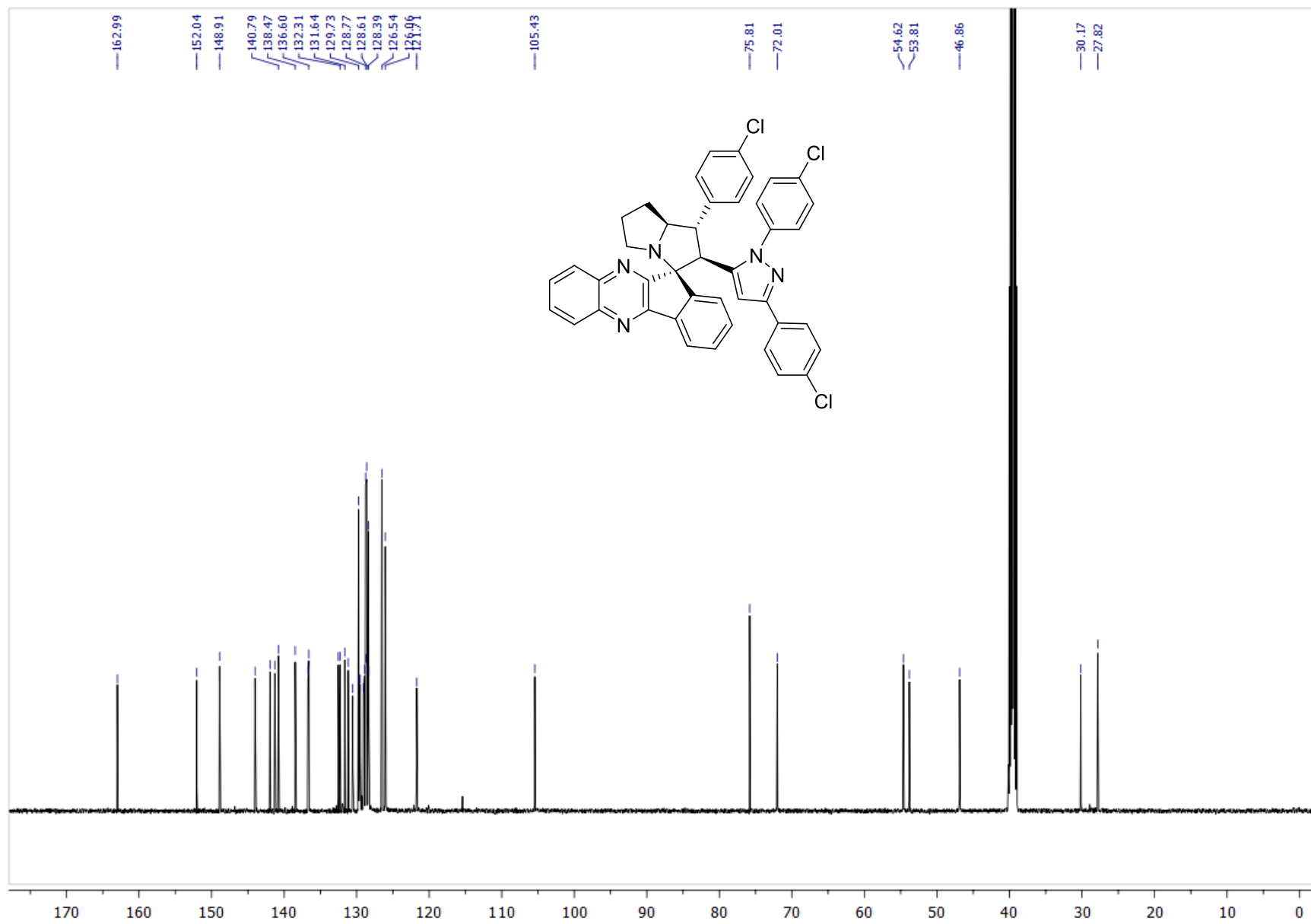


Figure S74. Copy of  $^1\text{H}$  NMR spectrum of **5i** in  $\text{DMSO-}d_6$



**Figure S75.** Copy of  $^{13}\text{C}$  NMR spectrum of **5i** in  $\text{DMSO-}d_6$

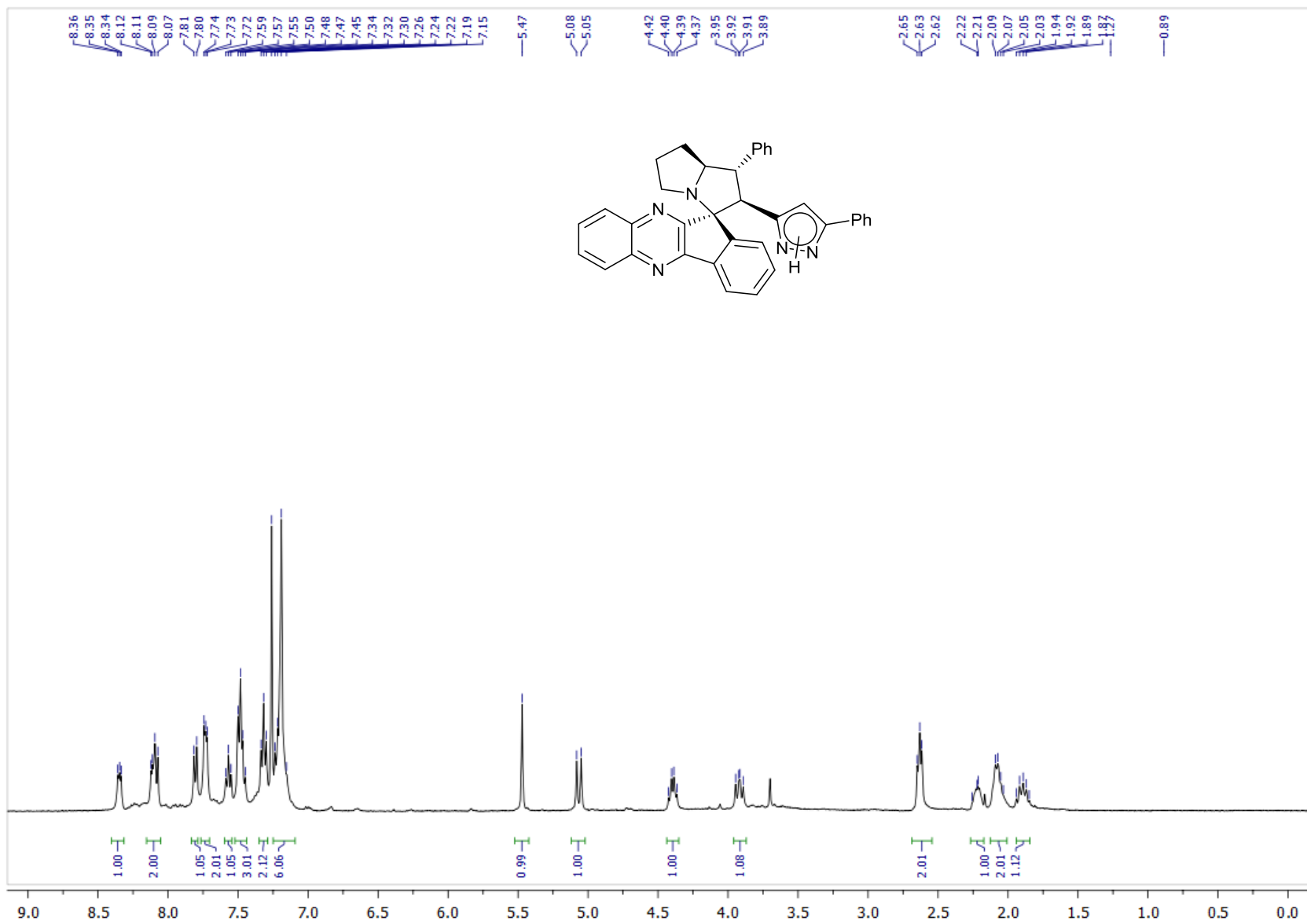
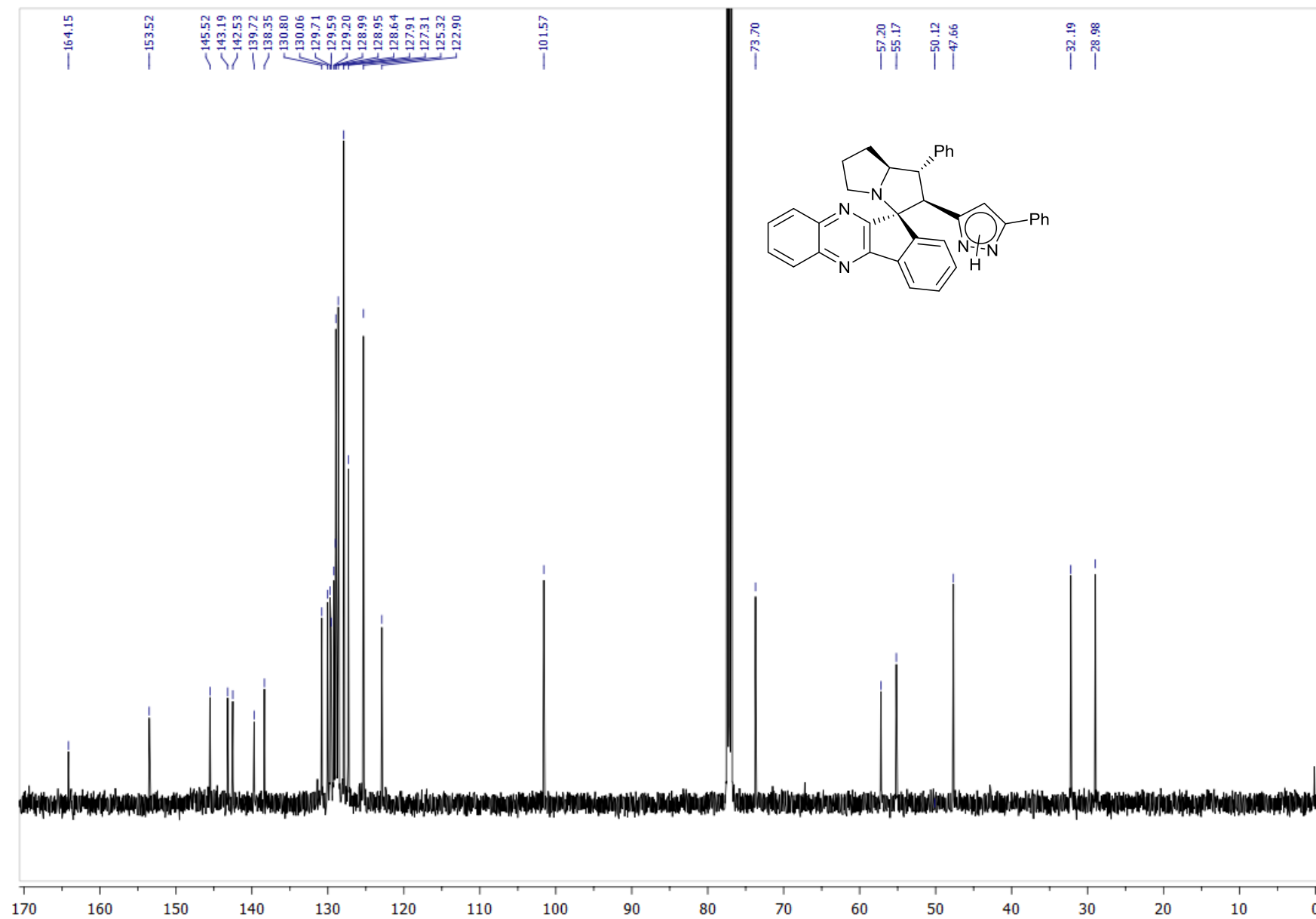


Figure S76. Copy of  $^1\text{H}$  NMR spectrum of **6a** in  $\text{CDCl}_3$



**Figure S77.** Copy of  $^{13}\text{C}$  NMR spectrum of of **6a** in  $\text{CDCl}_3$

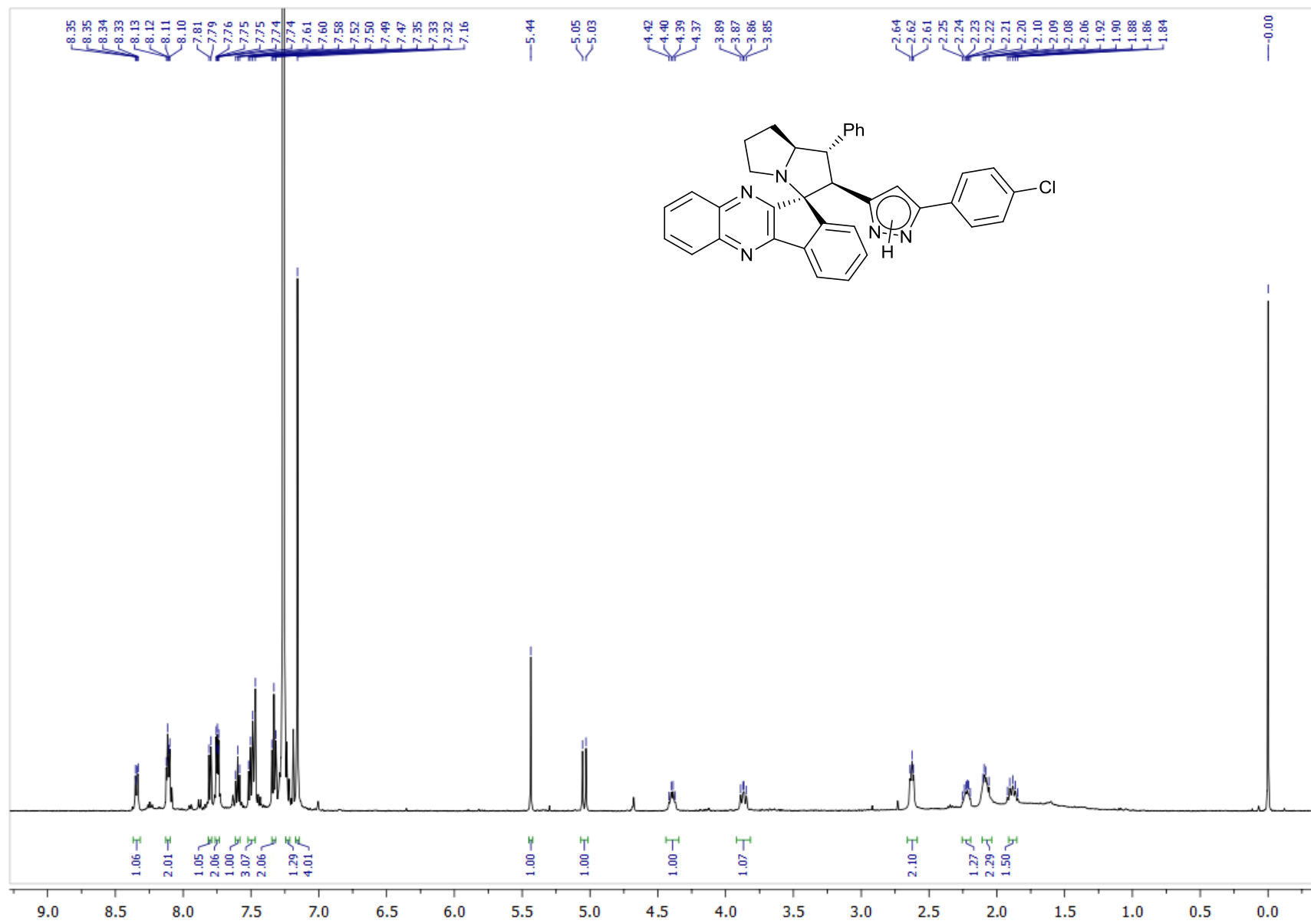


Figure S78. Copy of  $^1\text{H}$  NMR spectrum of **6b** in  $\text{CDCl}_3$

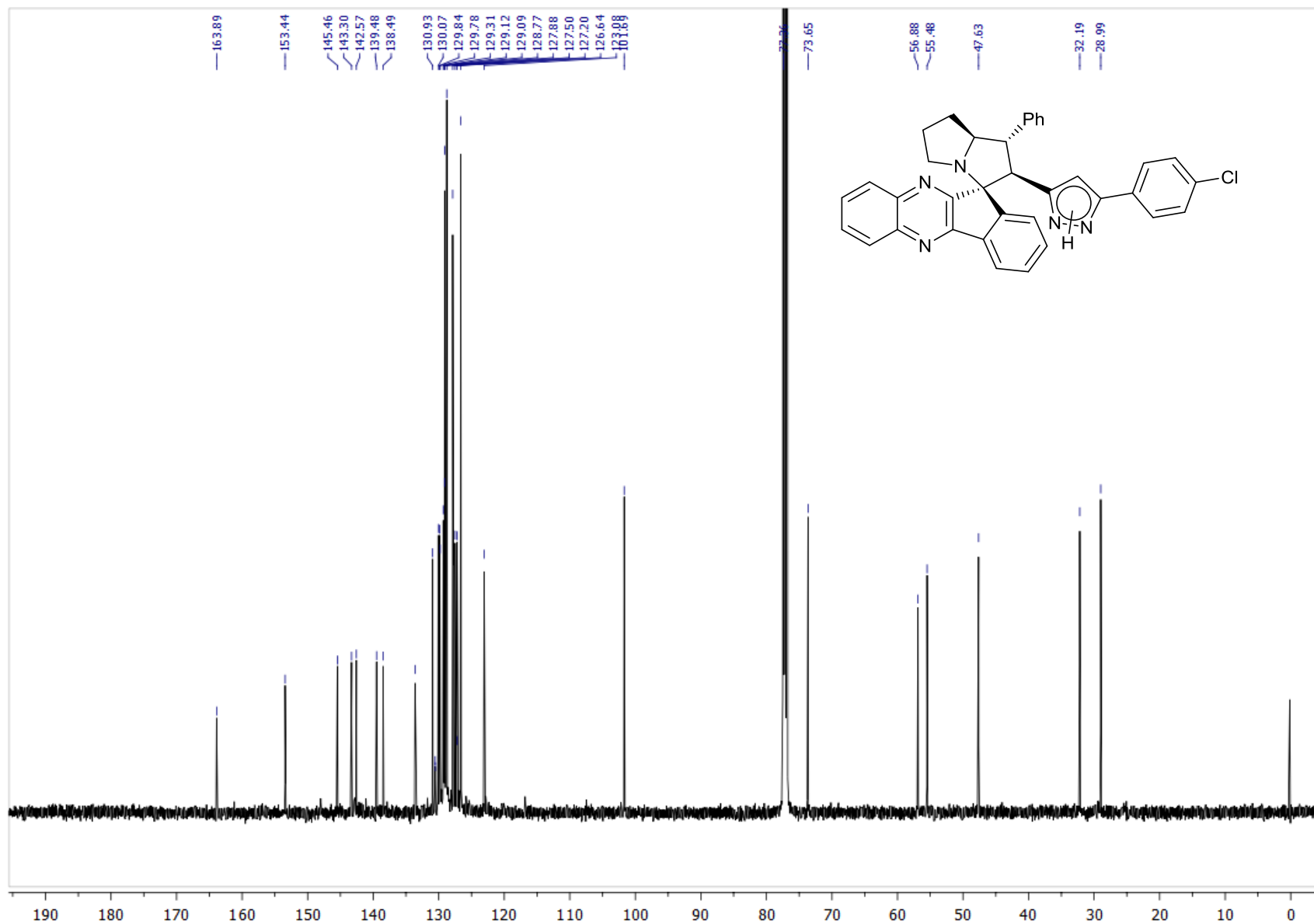


Figure S79. Copy of  $^{13}\text{C}$  NMR spectrum of **6b** in  $\text{CDCl}_3$



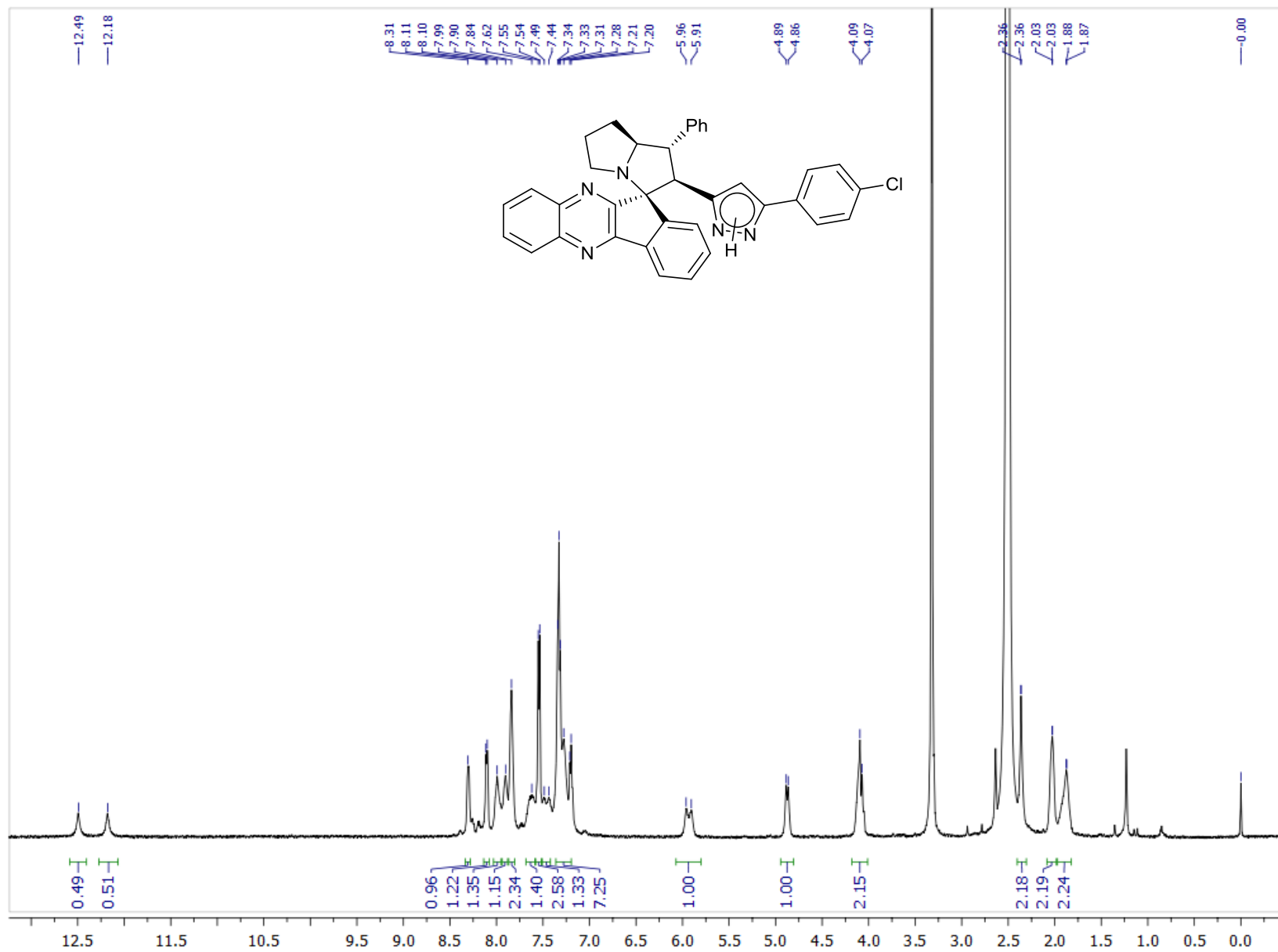


Figure S80. Copy of  $^1\text{H}$  NMR spectrum of the tautomers **6b** and **6'b** in  $\text{DMSO-}d_6$

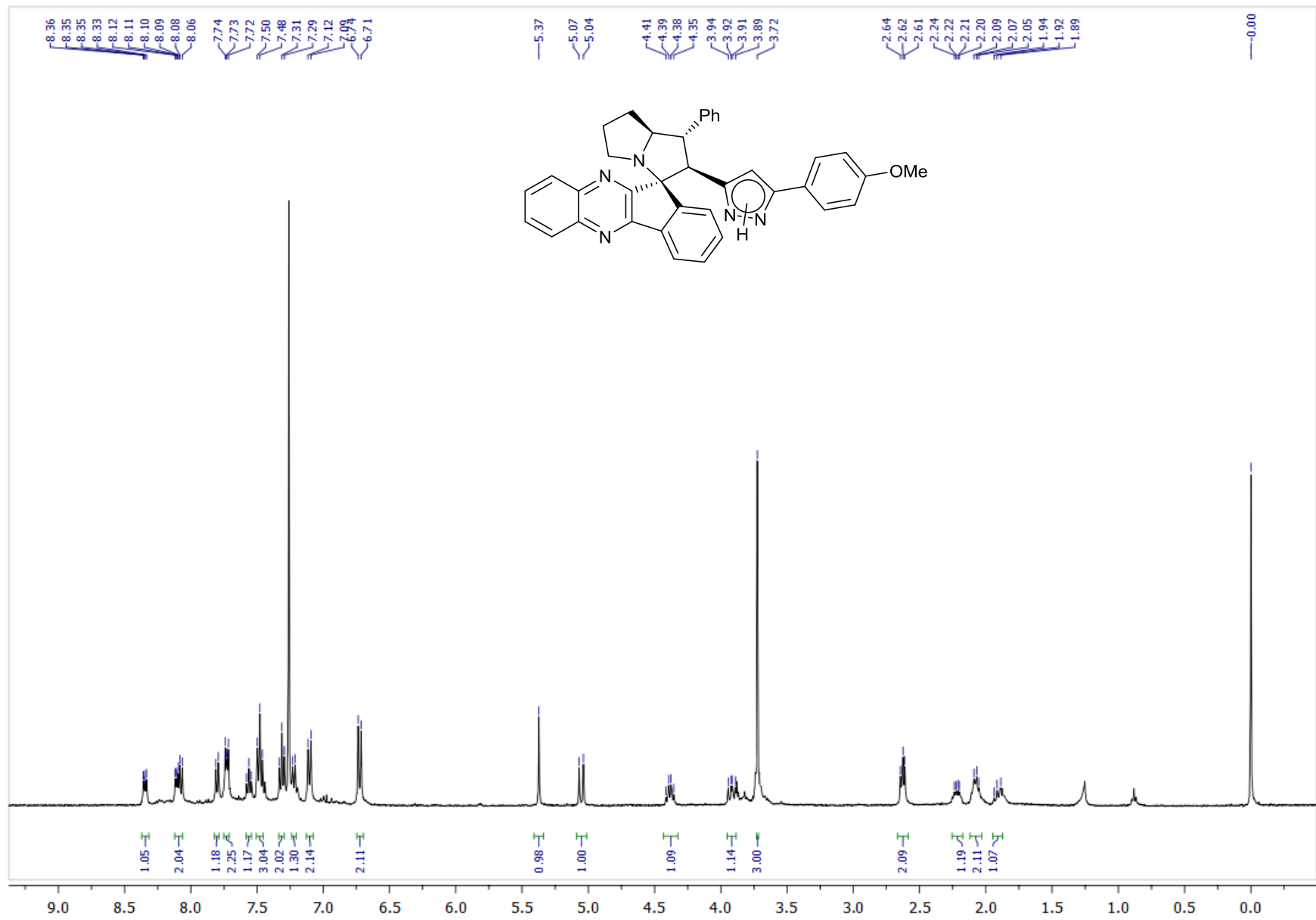


Figure S81. Copy of  $^1\text{H}$  NMR spectrum of **6c** in  $\text{CDCl}_3$

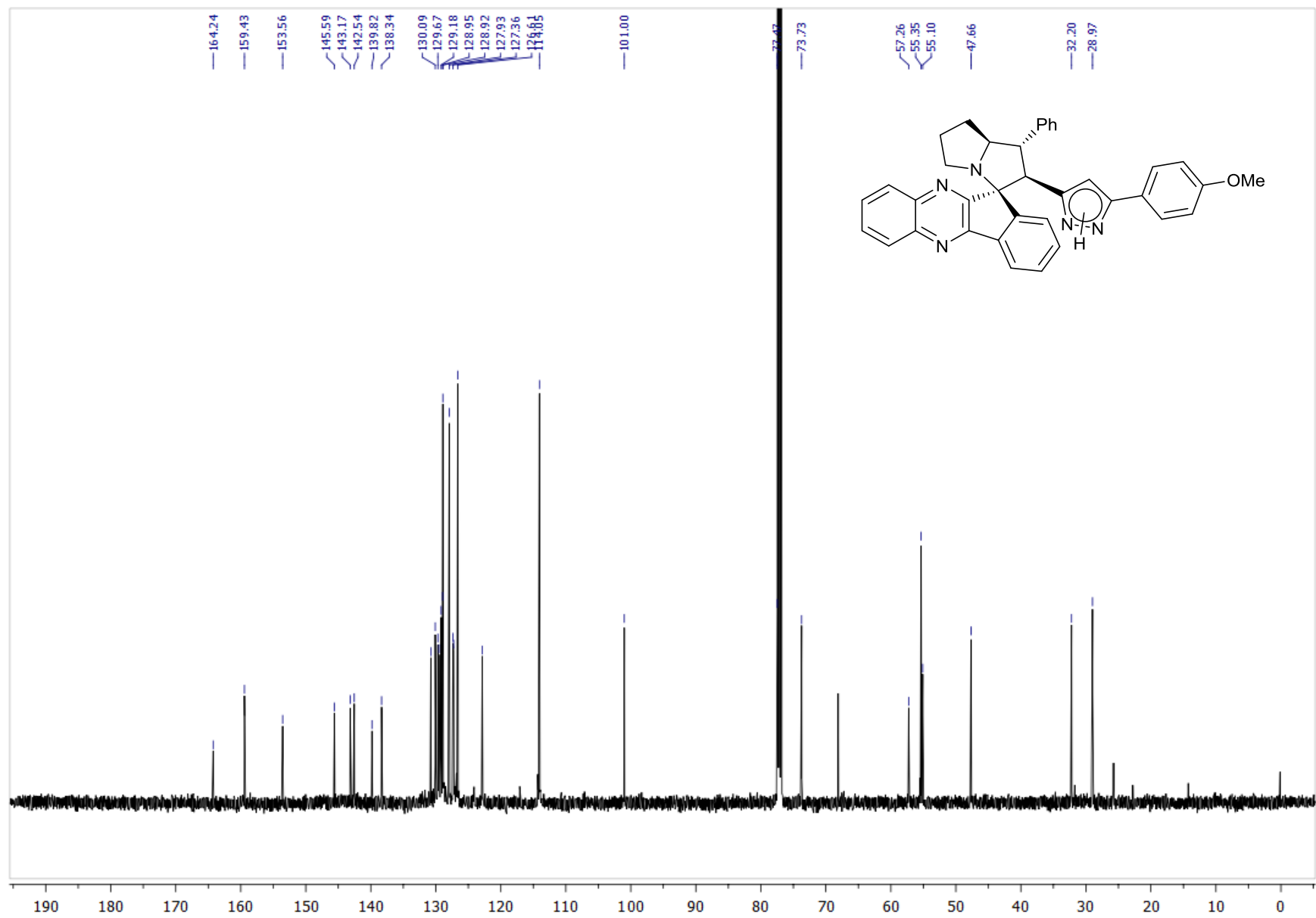


Figure S82. Copy of  $^{13}\text{C}$  NMR spectrum of **6c** in  $\text{CDCl}_3$

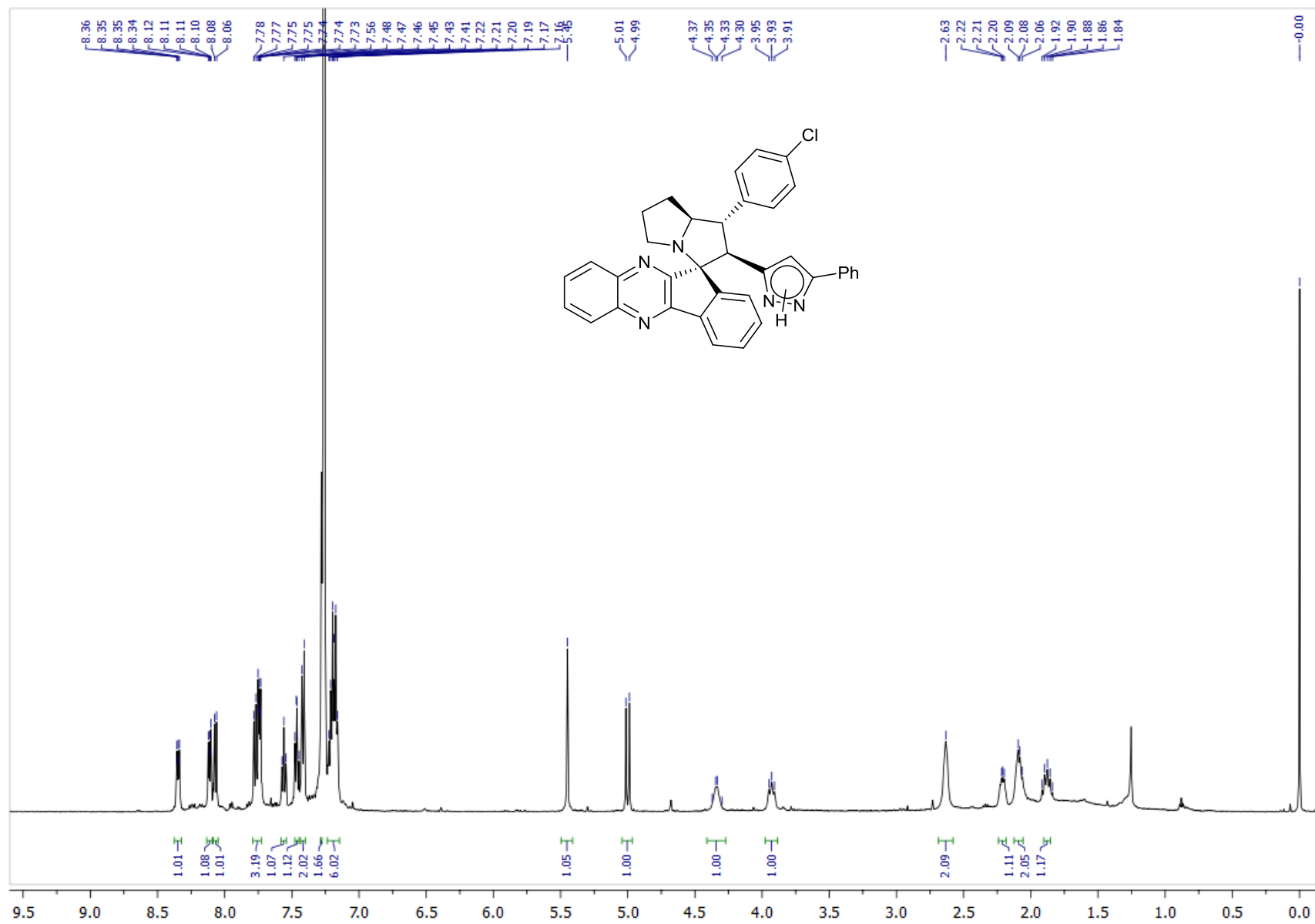


Figure S83. Copy of  $^1\text{H}$  NMR spectrum of **6d** in  $\text{CDCl}_3$

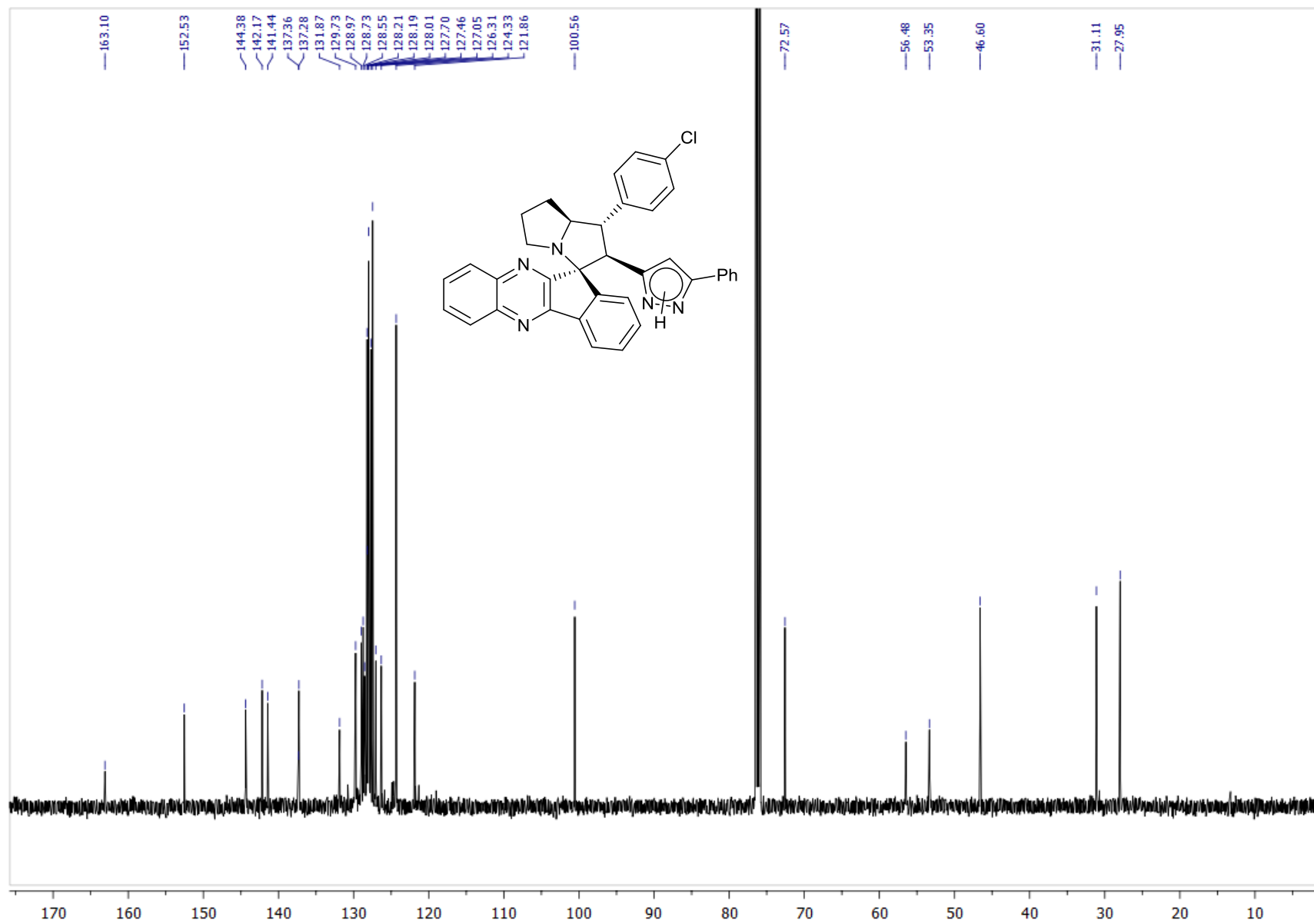


Figure S84. Copy of  $^{13}\text{C}$  NMR spectrum of **6d** in  $\text{CDCl}_3$

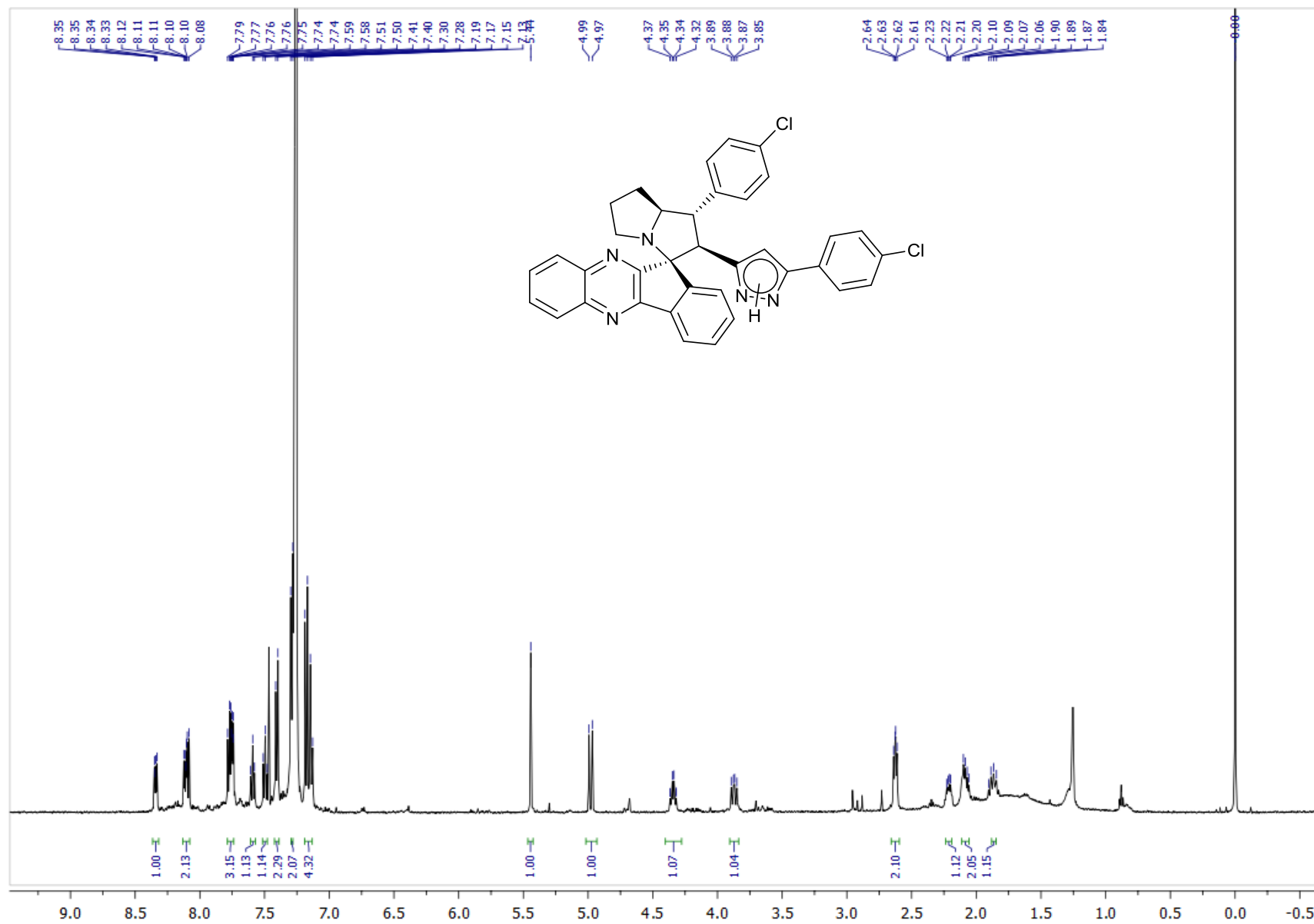


Figure S85. Copy of <sup>1</sup>H NMR spectrum of **6e** in CDCl<sub>3</sub>

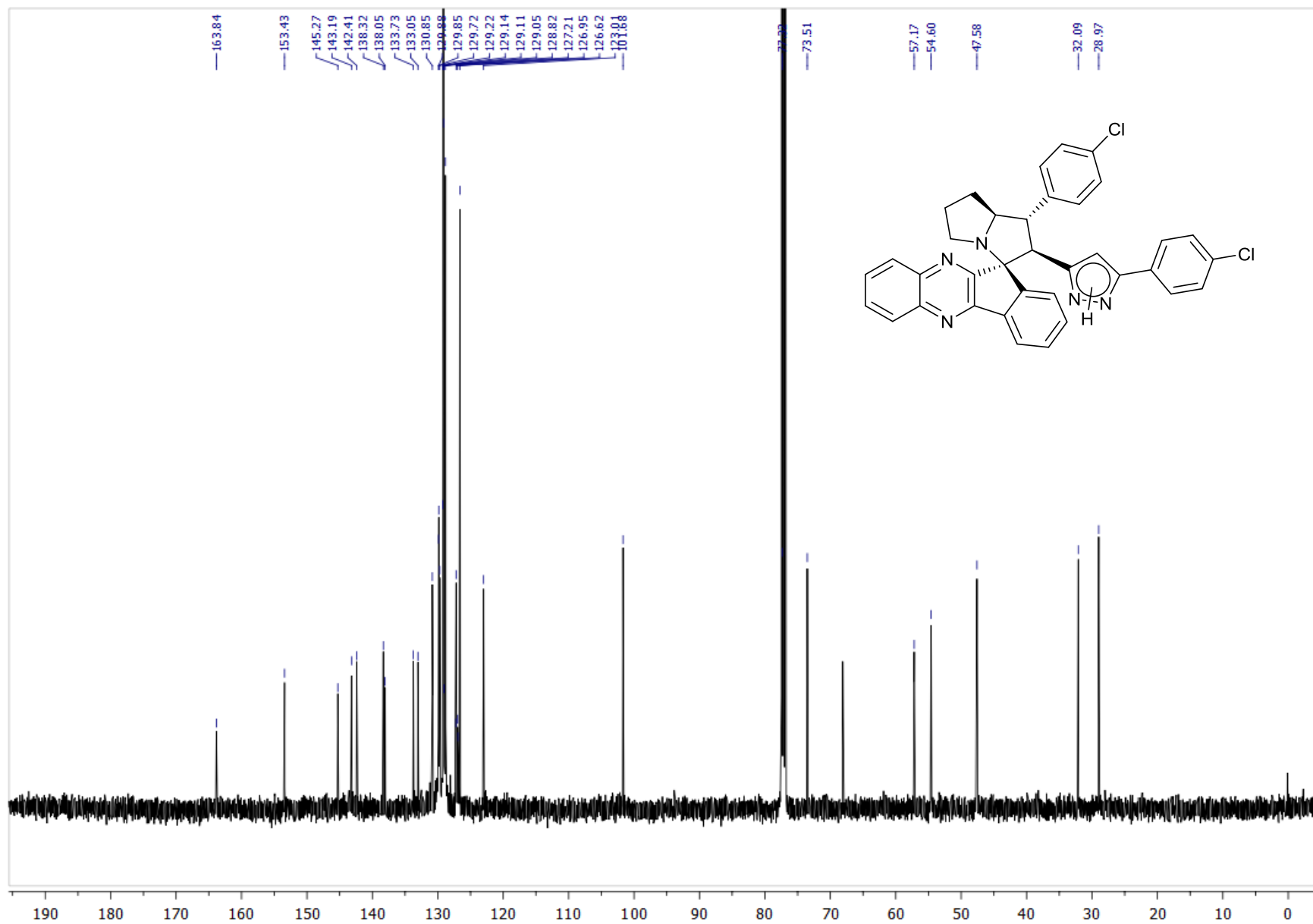


Figure S86. Copy of  $^{13}\text{C}$  NMR spectrum of **6e** in  $\text{CDCl}_3$

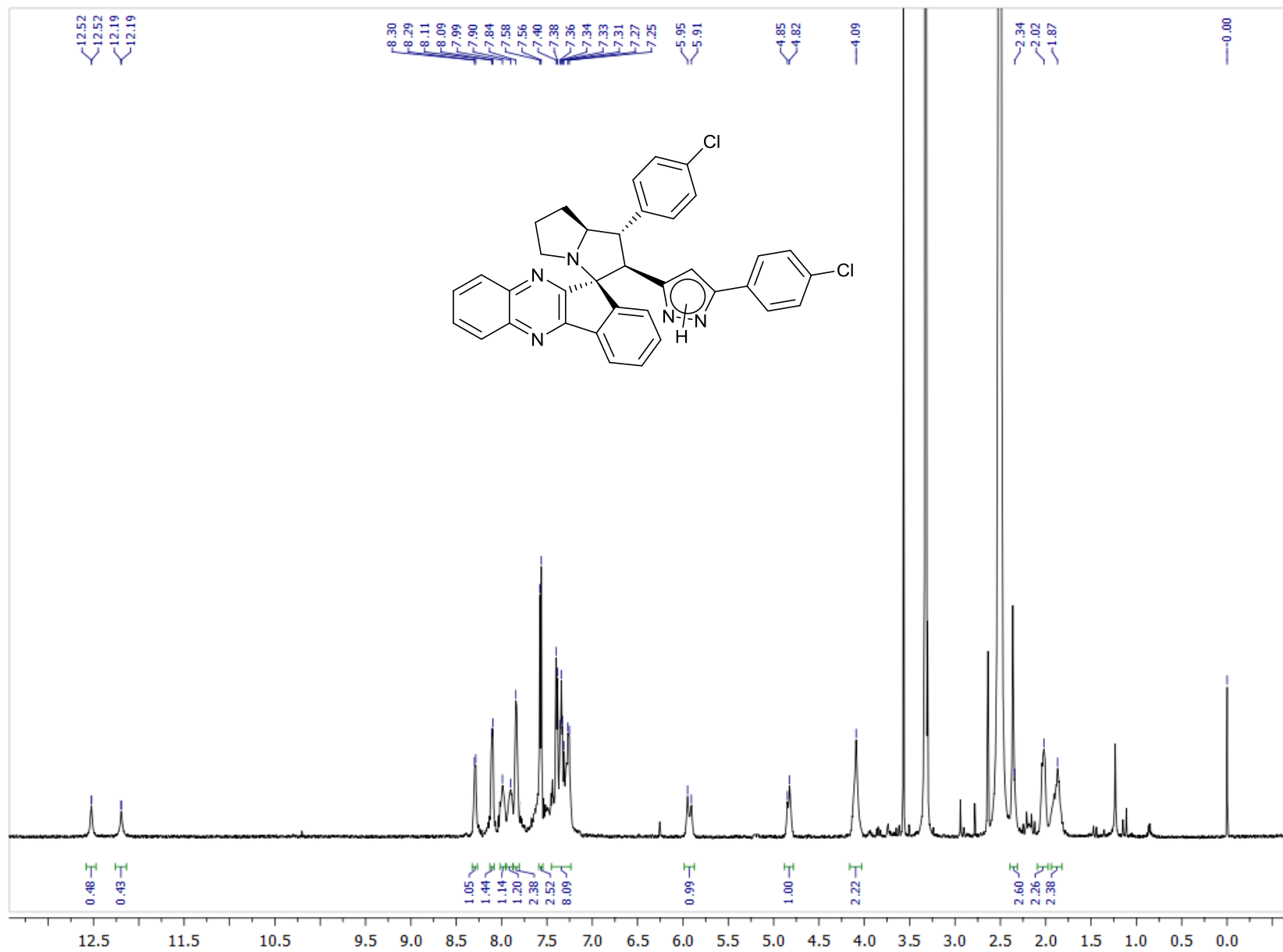


Figure S87. Copy of <sup>1</sup>H NMR spectrum of the tautomers **6e** and **6'e** in DMSO-*d*<sub>6</sub>



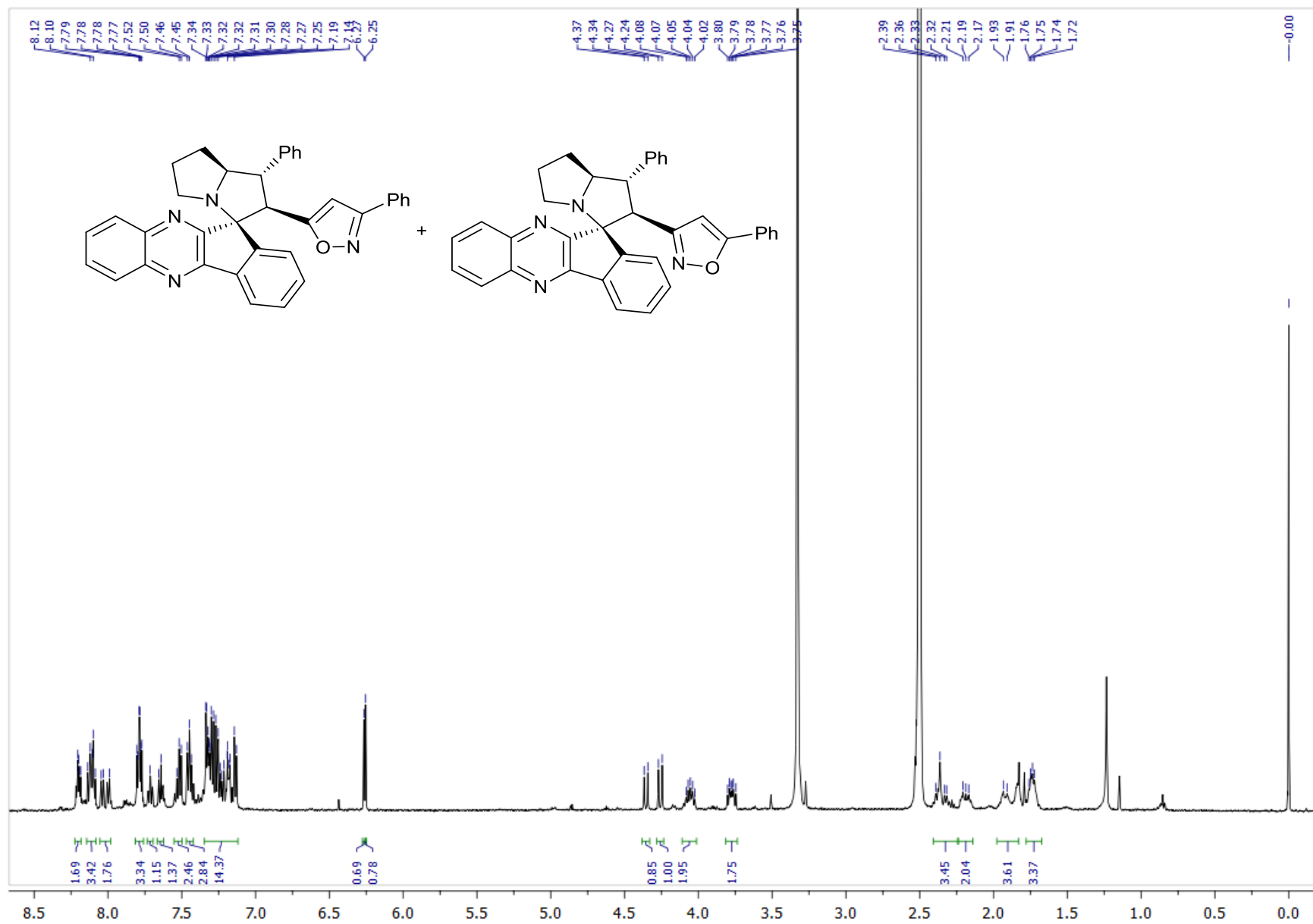


Figure S88. Copy of <sup>1</sup>H NMR spectrum of mixture of **7a** and **7'a** in CDCl<sub>3</sub>

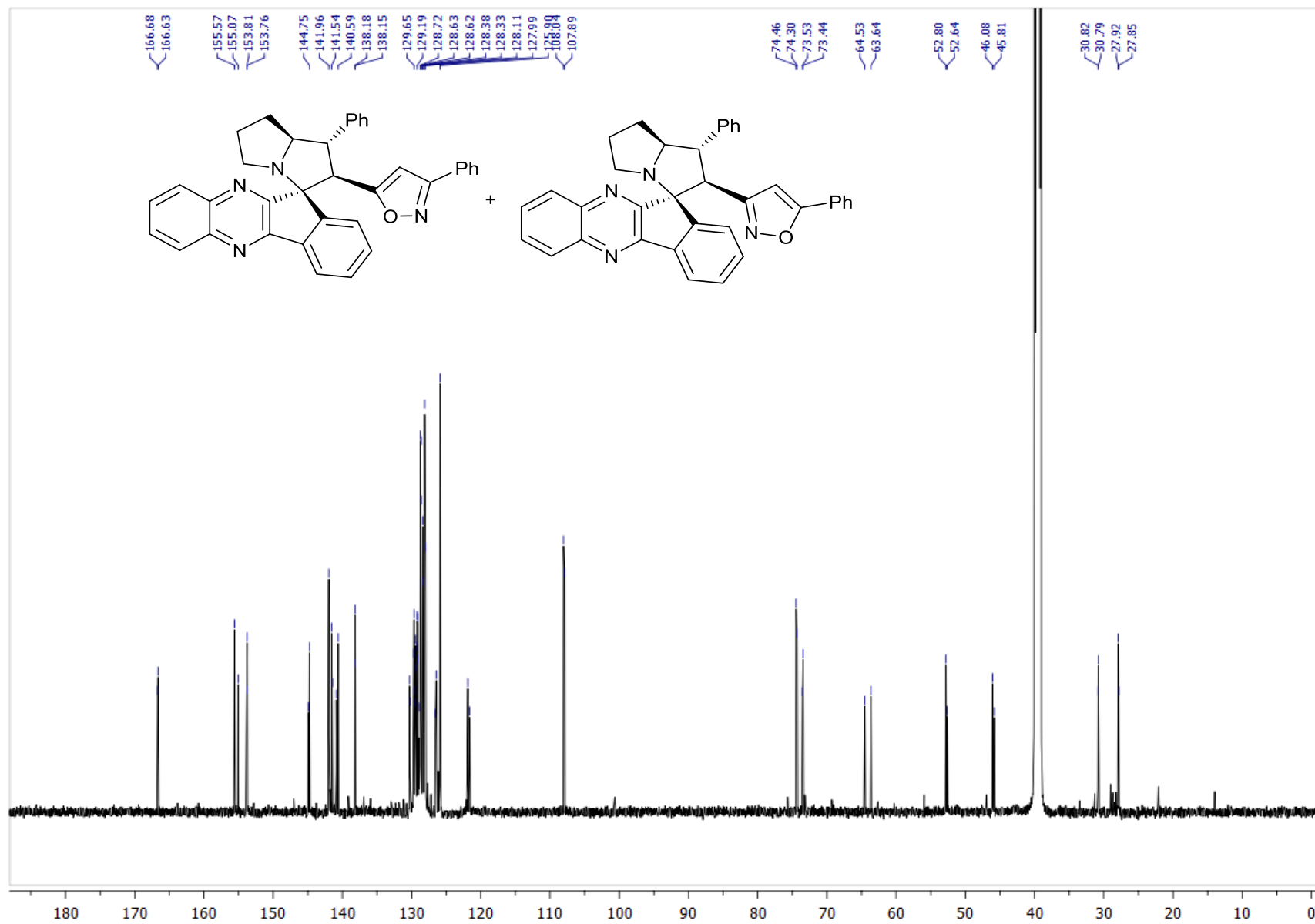


Figure S86. Copy of  $^{13}\text{C}$  NMR spectrum of mixture of **7a** and **7'a** in  $\text{CDCl}_3$

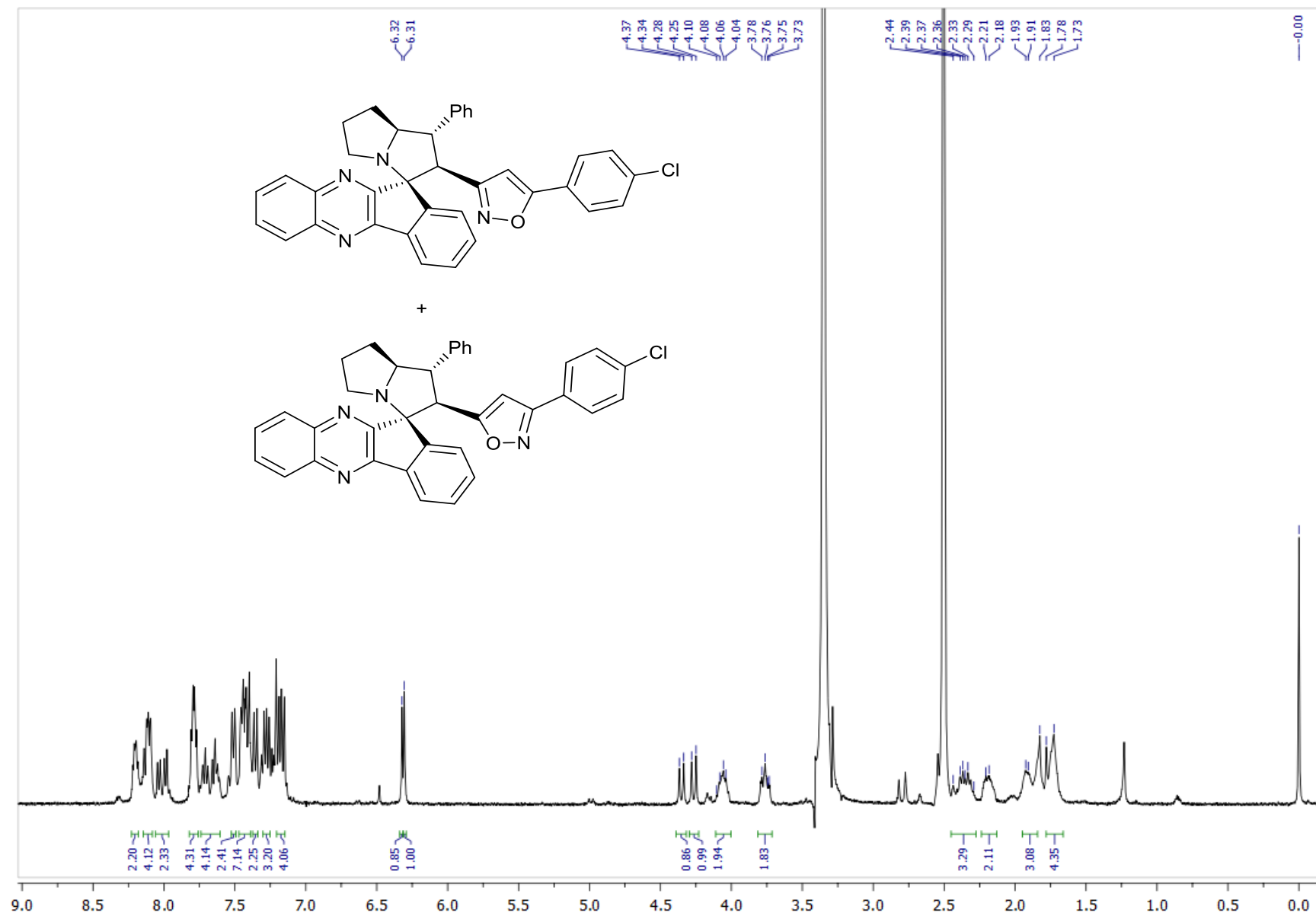


Figure S90. Copy of <sup>1</sup>H NMR spectrum of mixture of **7b** and **7'b** in CDCl<sub>3</sub>

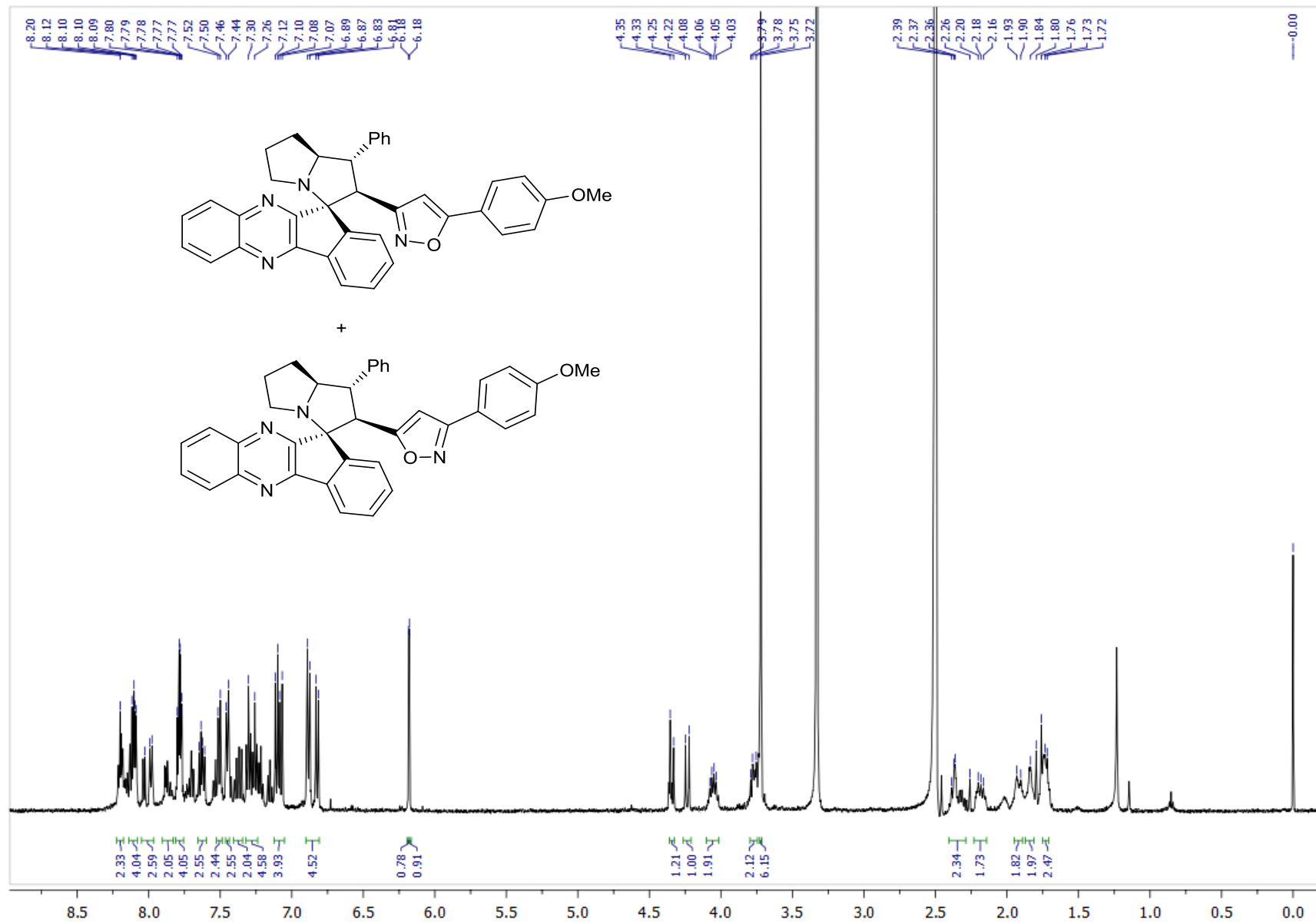


Figure S91. Copy of <sup>1</sup>H NMR spectrum of mixture of **7c** and **7'c** in CDCl<sub>3</sub>