

Supplementary Data:

Identifying opportunities for late-stage C-H alkylation with *in silico* reaction screening and high-throughput experimentation

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1 NMR spectra

¹H NMR (600 MHz, CDCl₃)

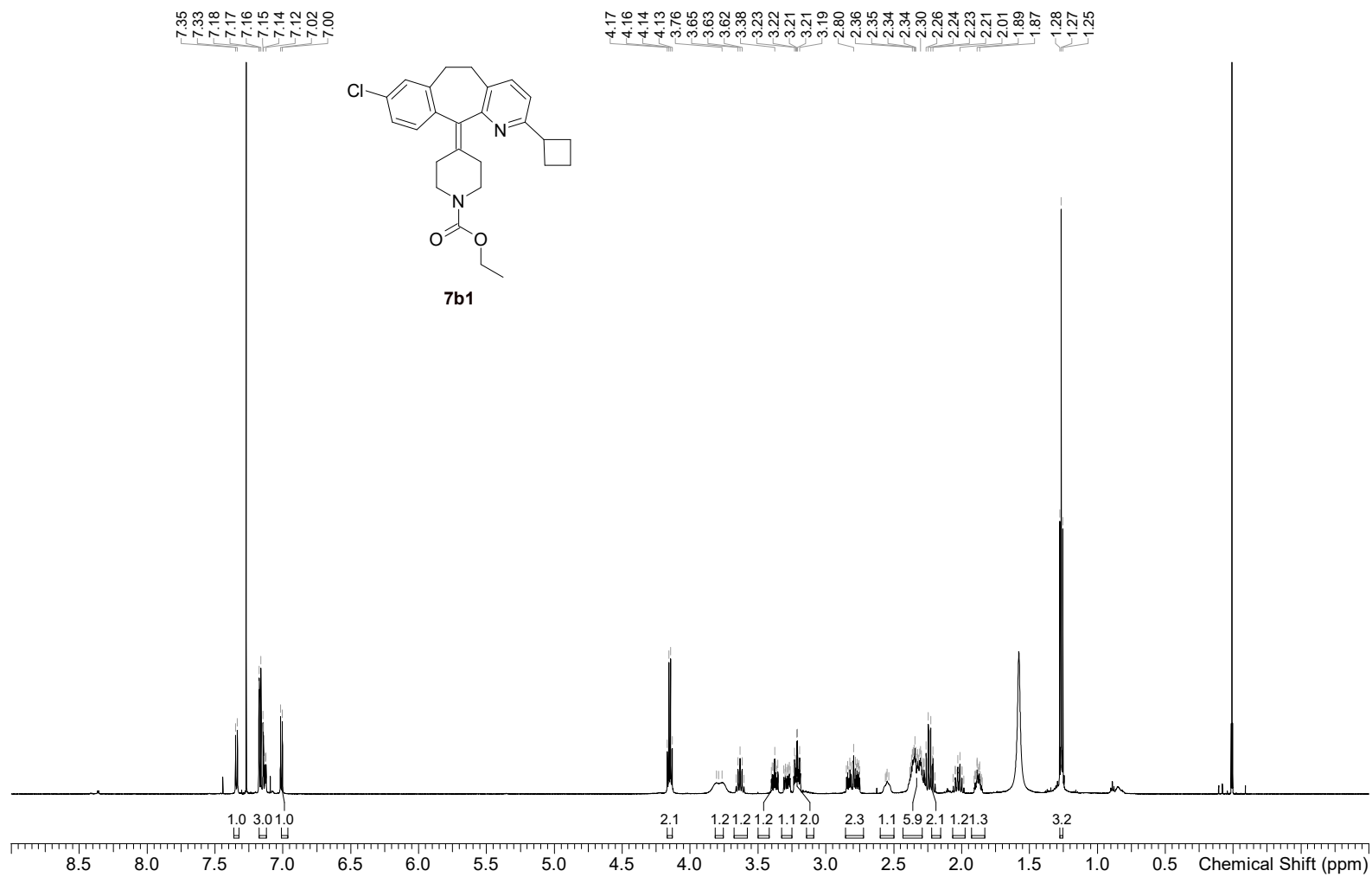


Figure 1: **7b1**, ¹H-NMR spectrum.

^{13}C NMR (151 MHz, CDCl_3)

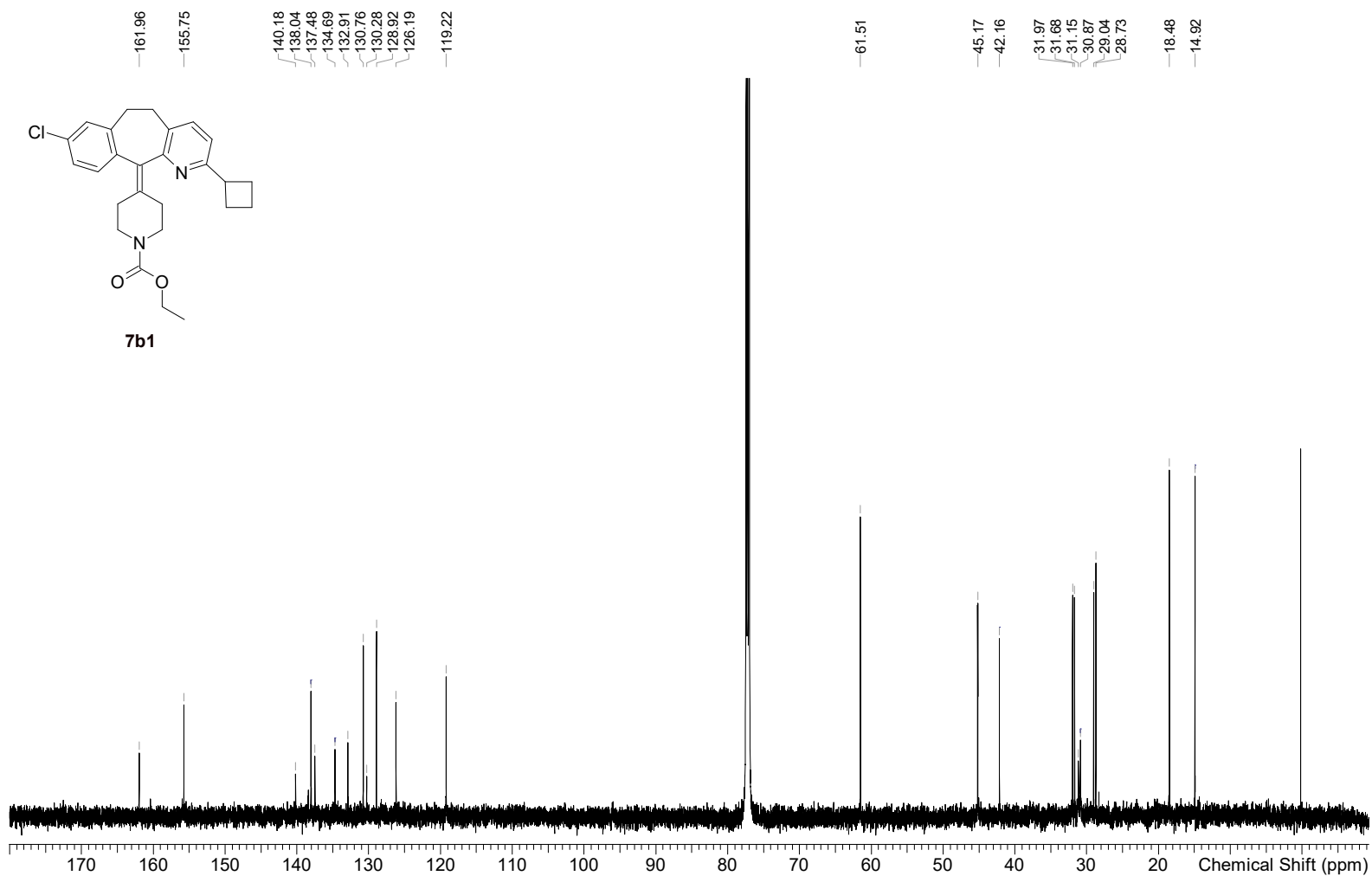


Figure 2: **7b1**, ^{13}C -NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

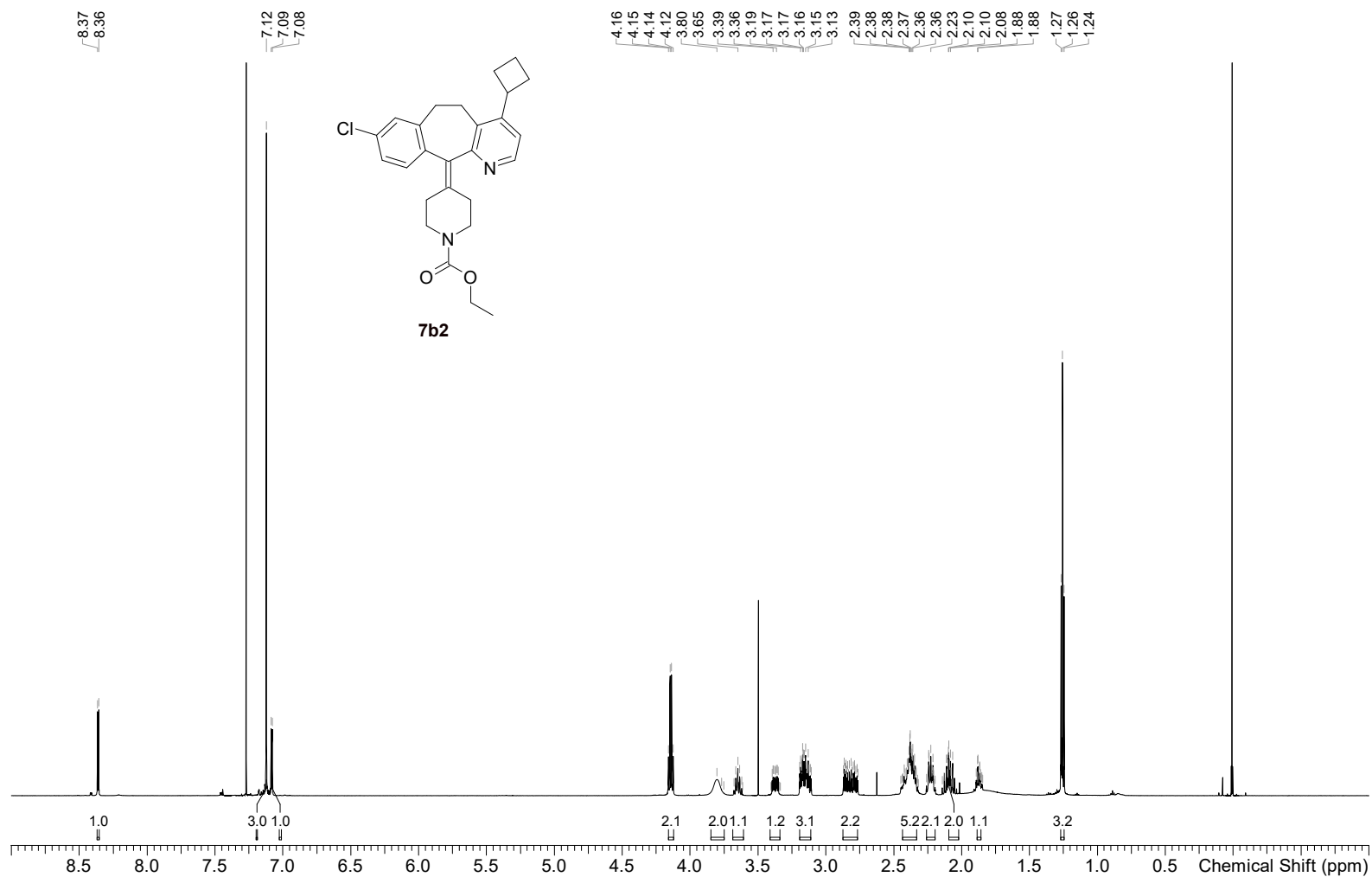


Figure 3: **7b2**, ¹H-NMR spectrum.

^{13}C NMR (151 MHz, CDCl_3)

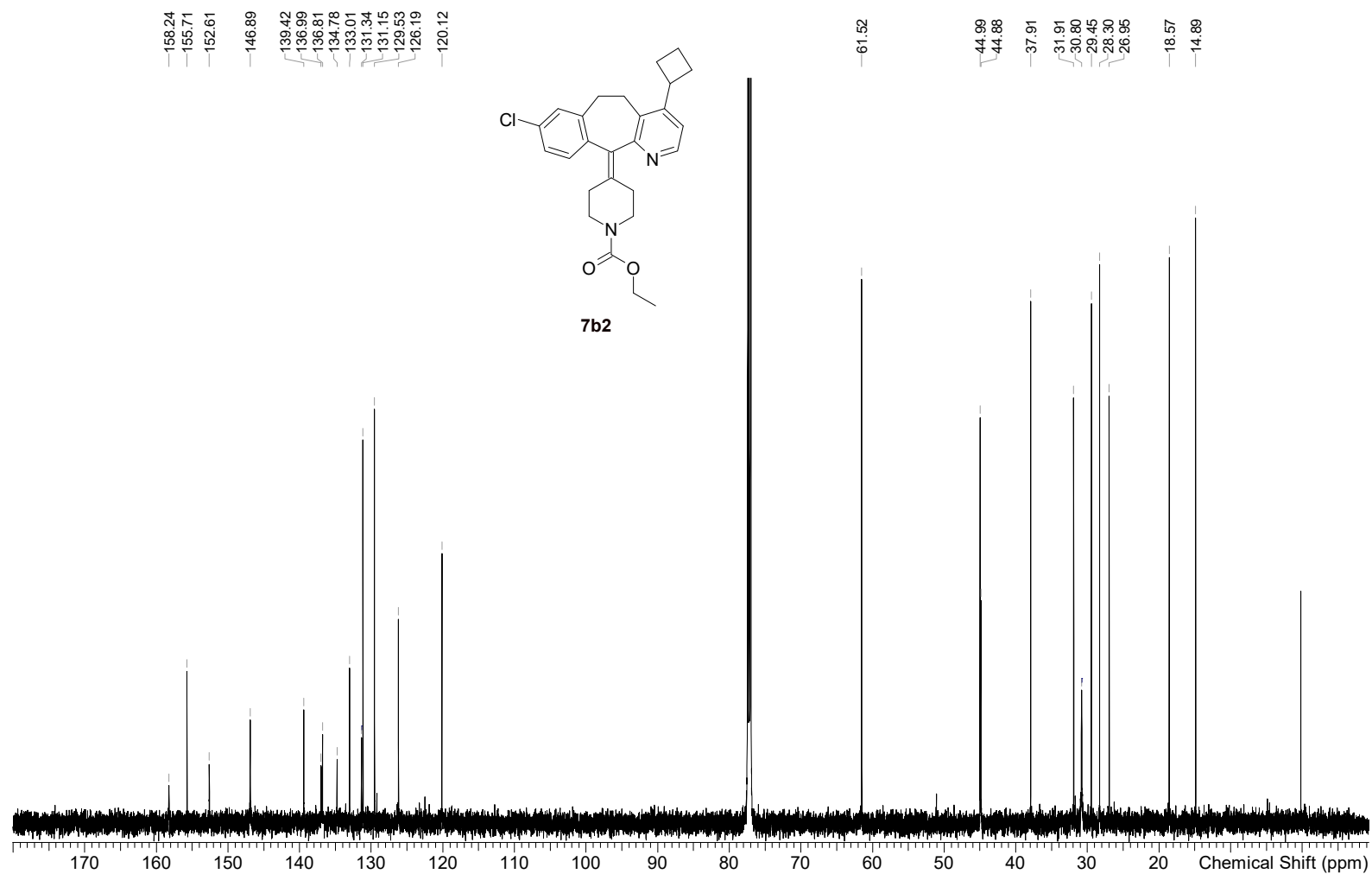


Figure 4: **7b2**, ^{13}C -NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

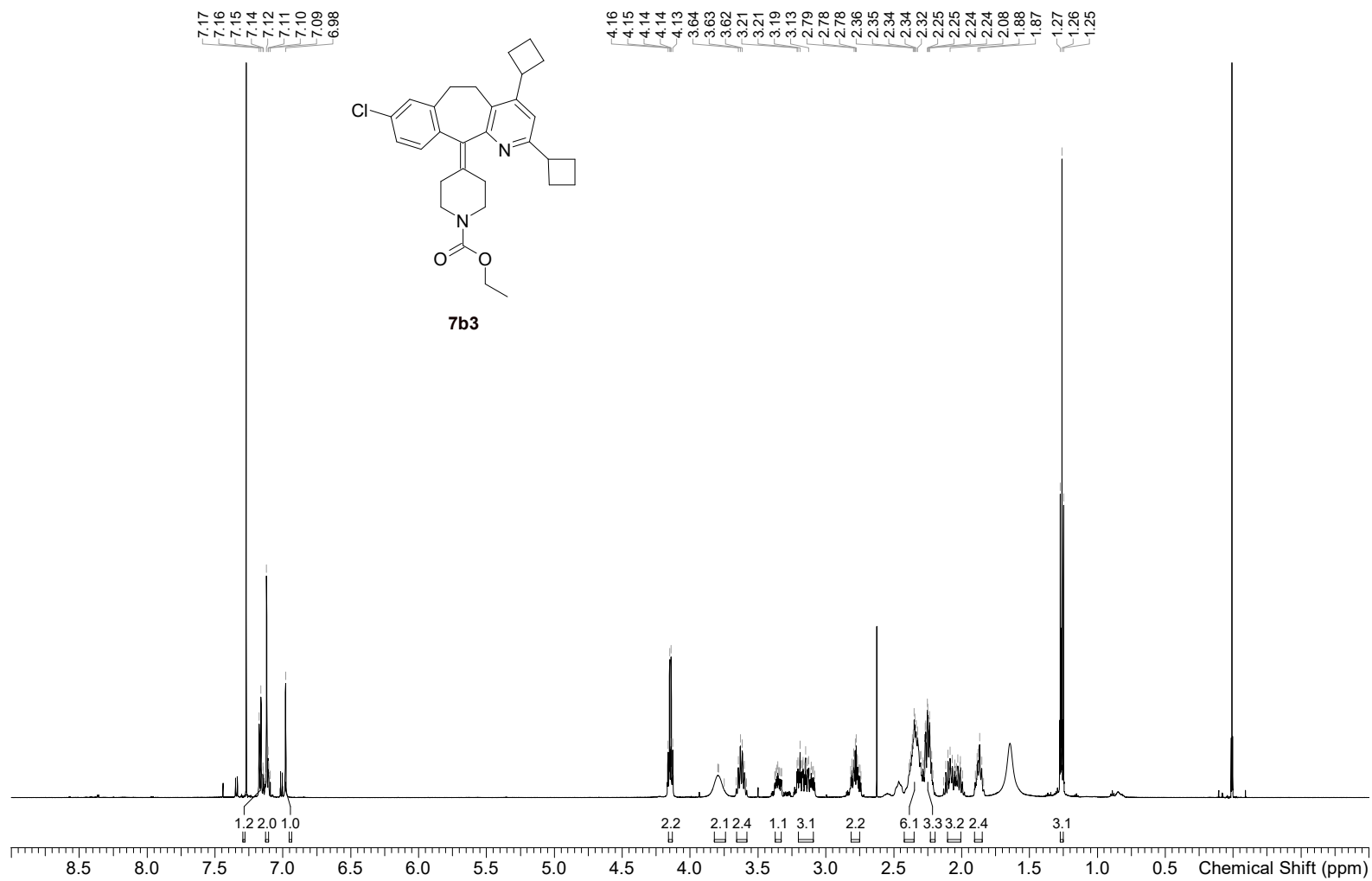


Figure 5: **7b3**, ¹H-NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

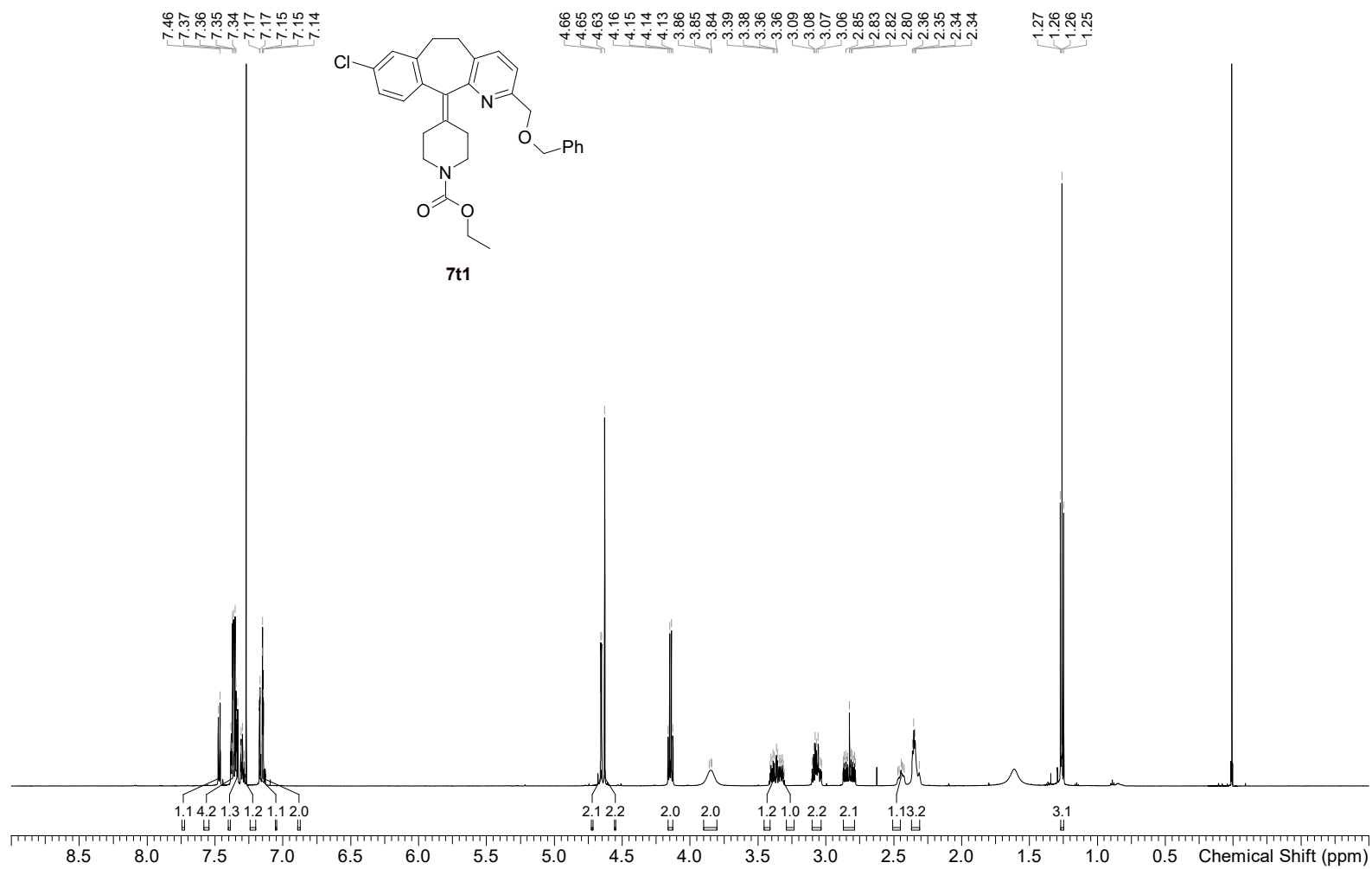


Figure 6: **7t1**, ¹H-NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

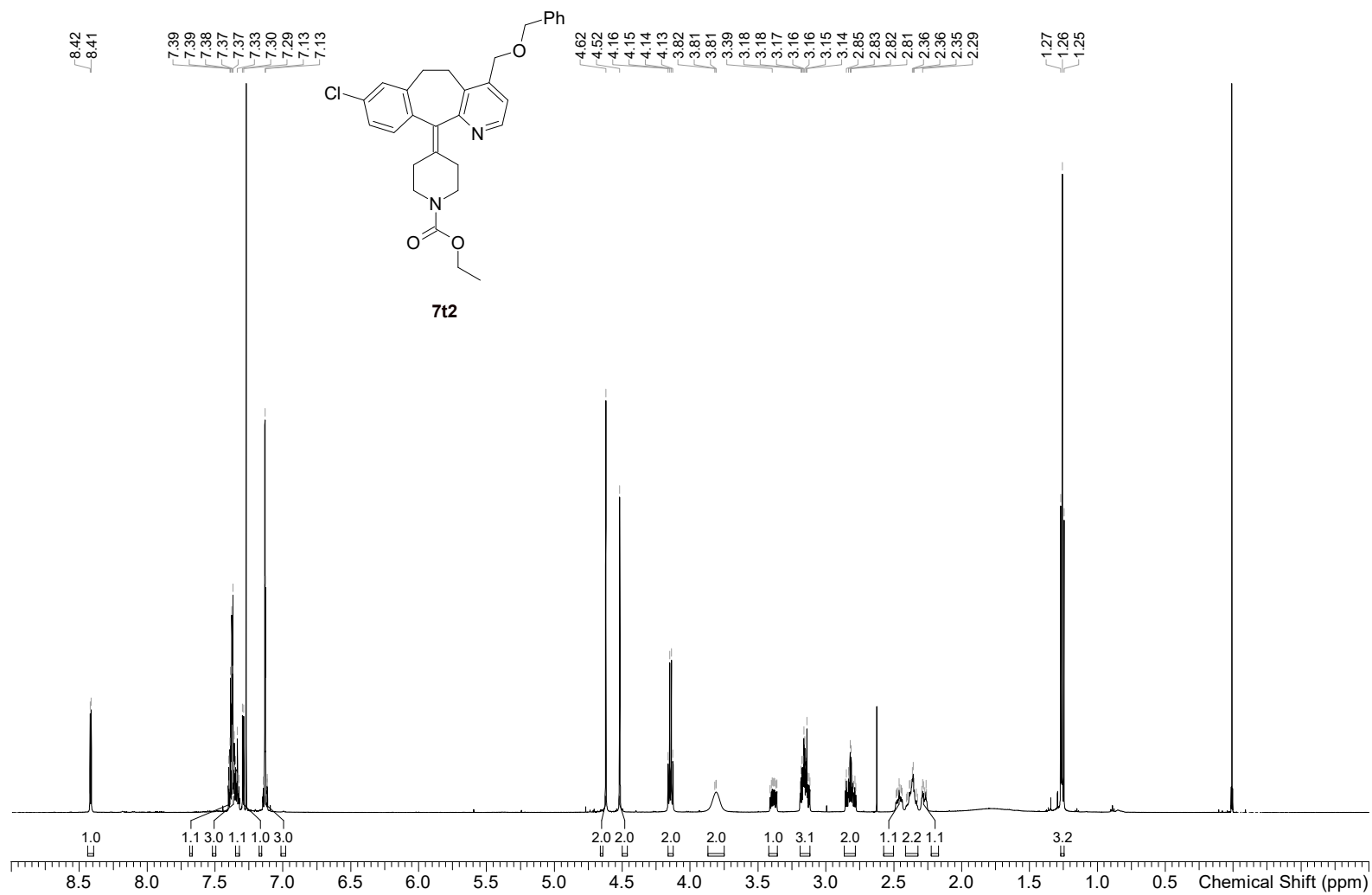


Figure 7: **7t2**, ^1H -NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

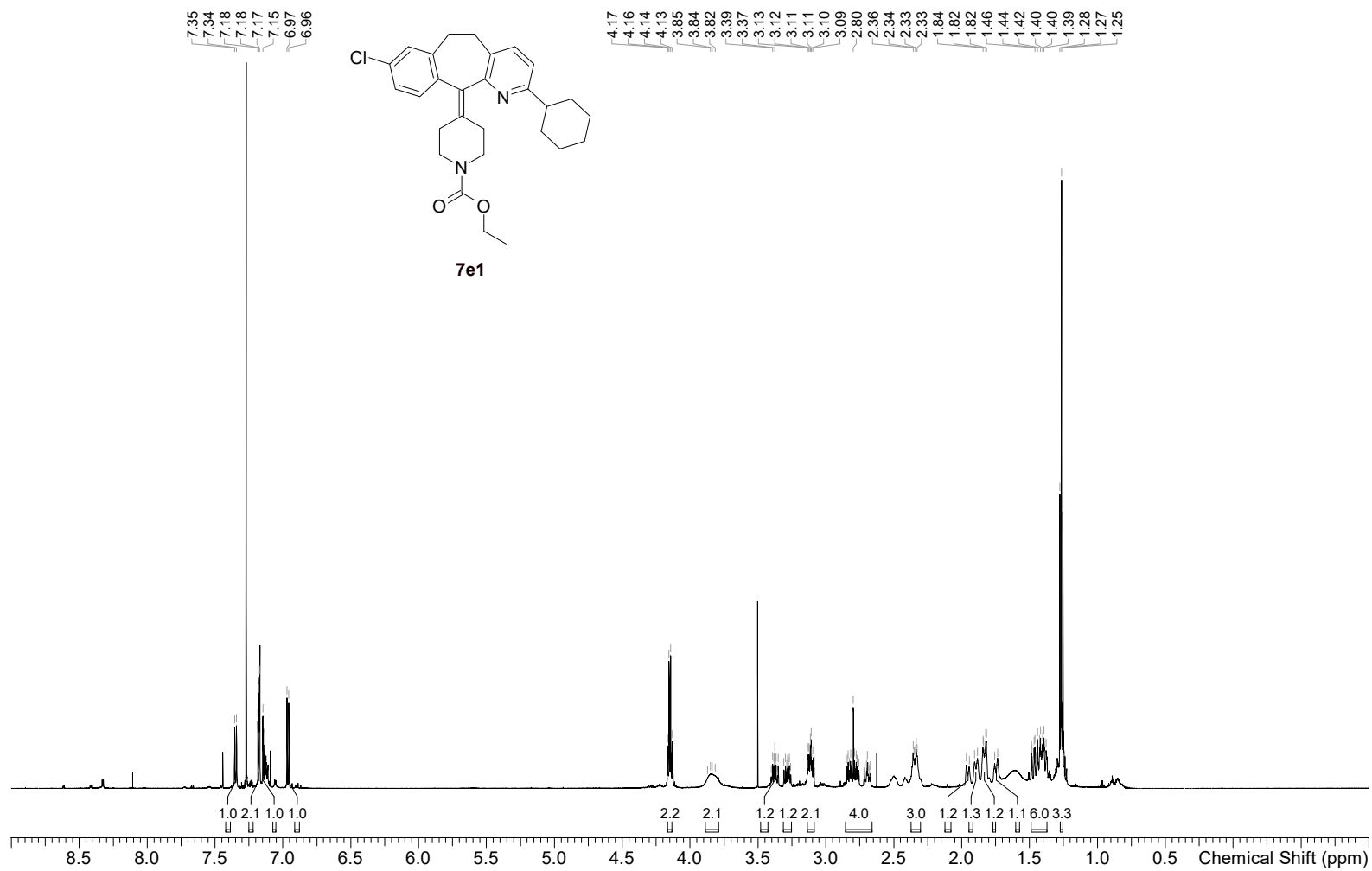


Figure 8: **7e1**, ¹H-NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

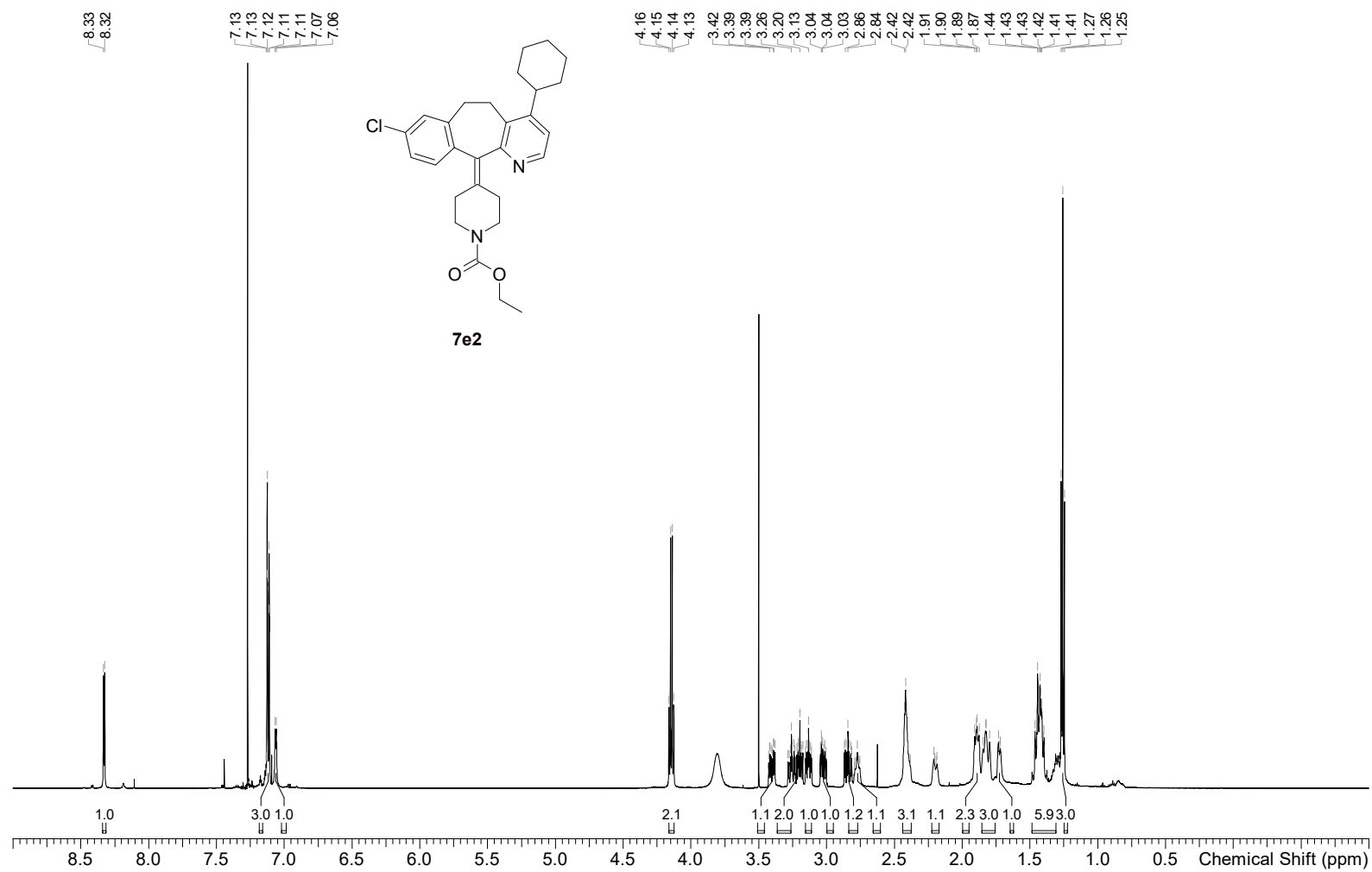


Figure 9: **7e2**, ¹H-NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

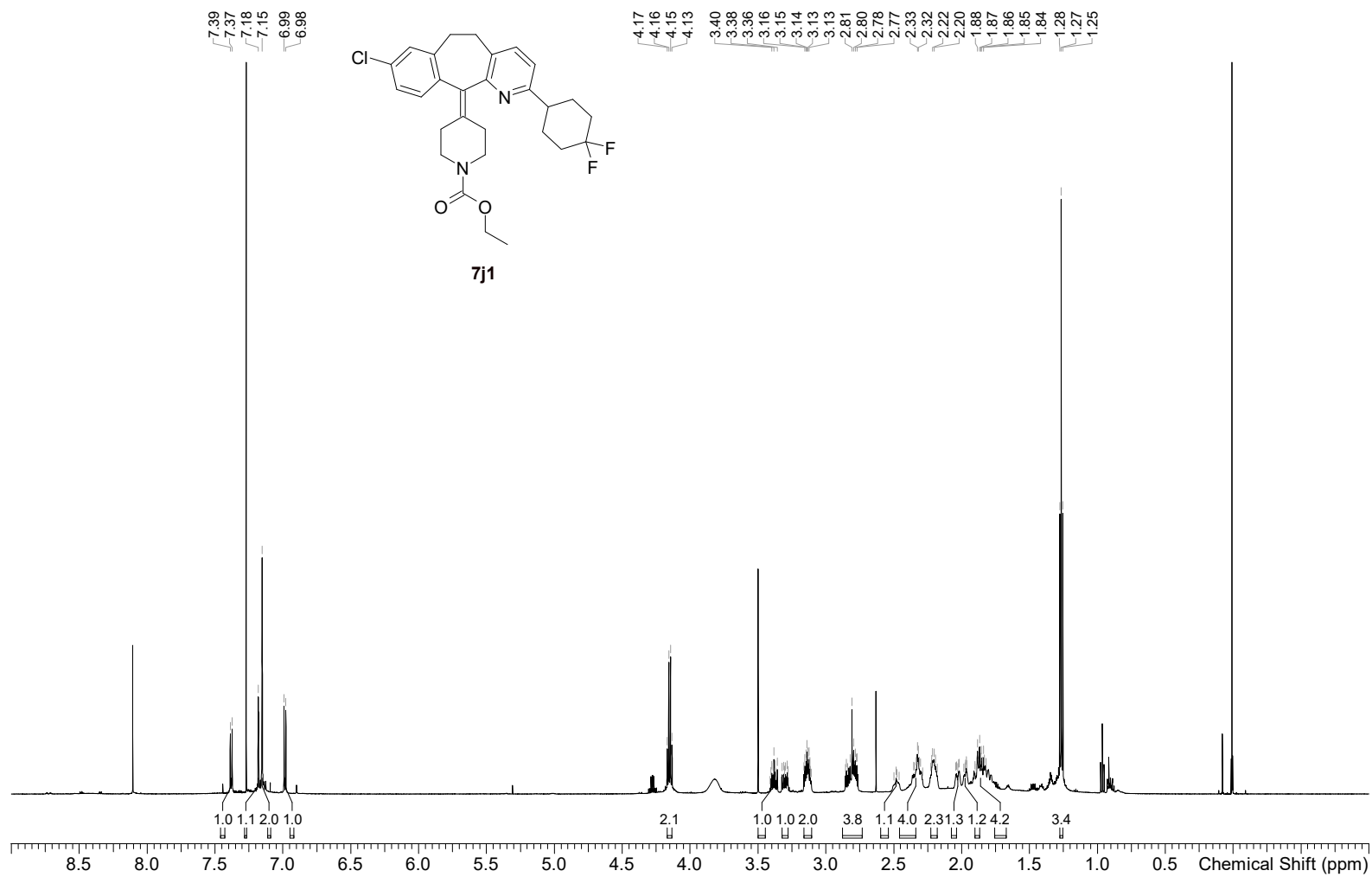


Figure 10: **7j1**, ¹H-NMR spectrum.

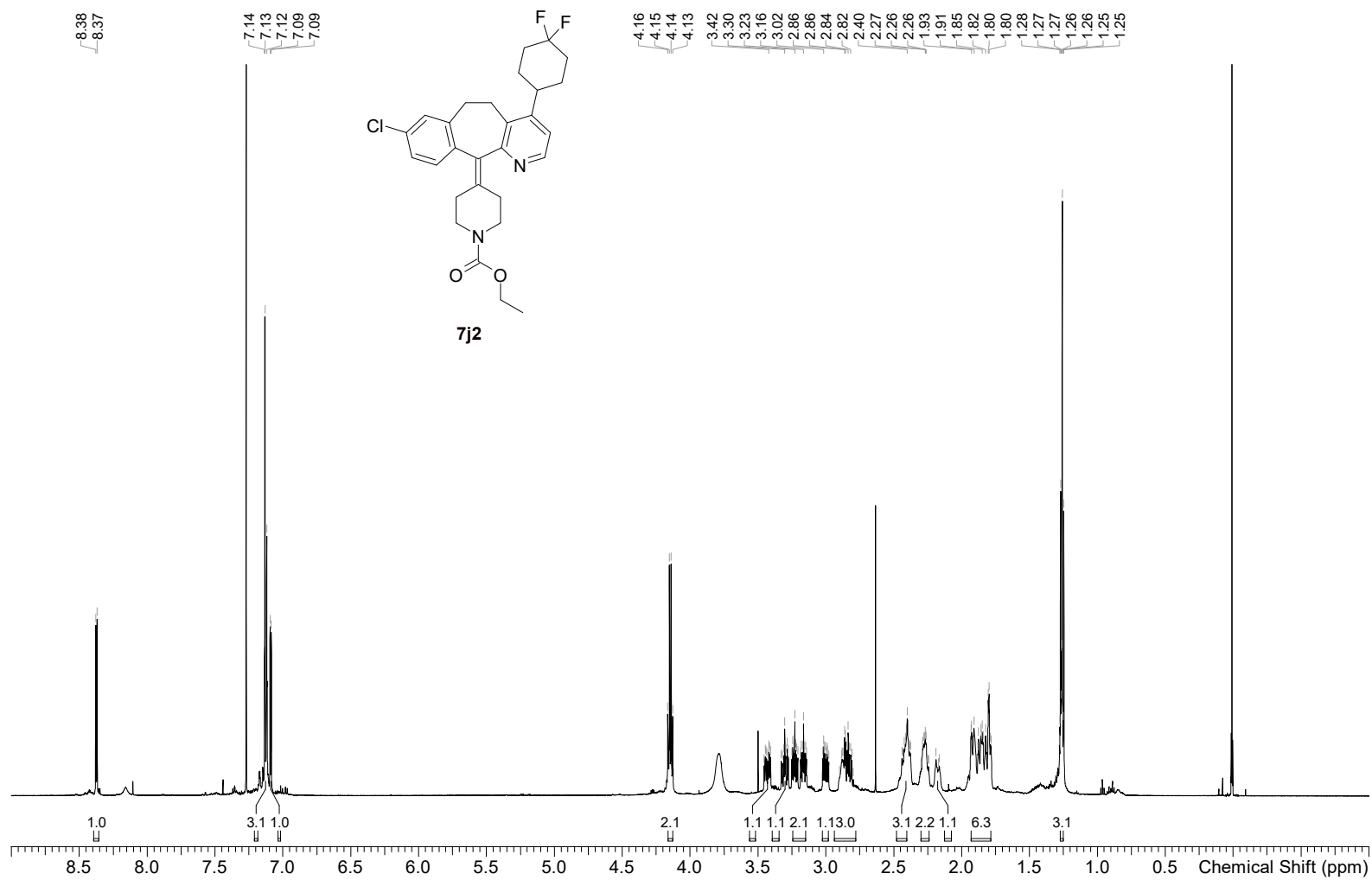


Figure 11: **7j2**, ^1H -NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

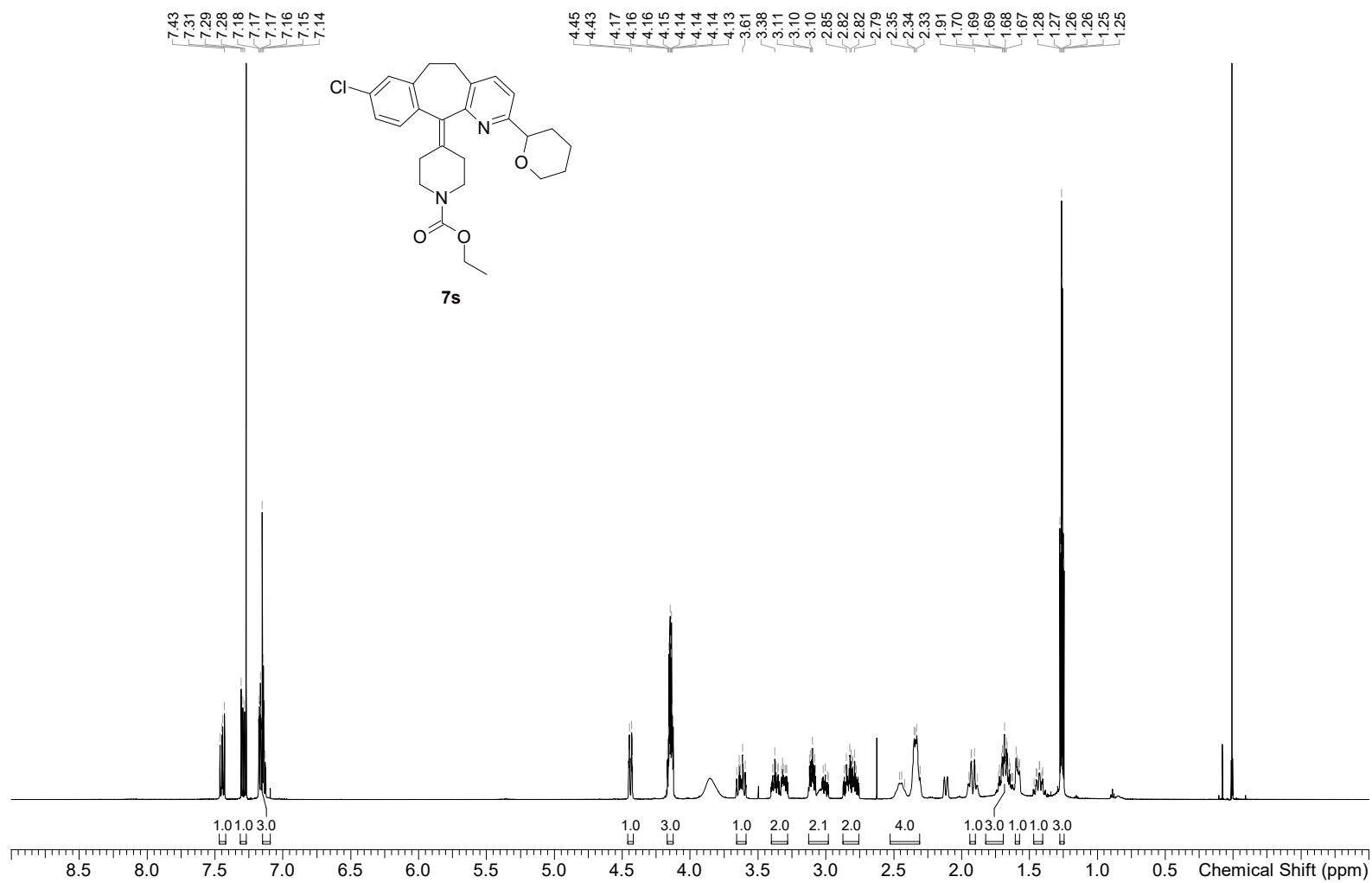


Figure 12: **7s**, ^1H -NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

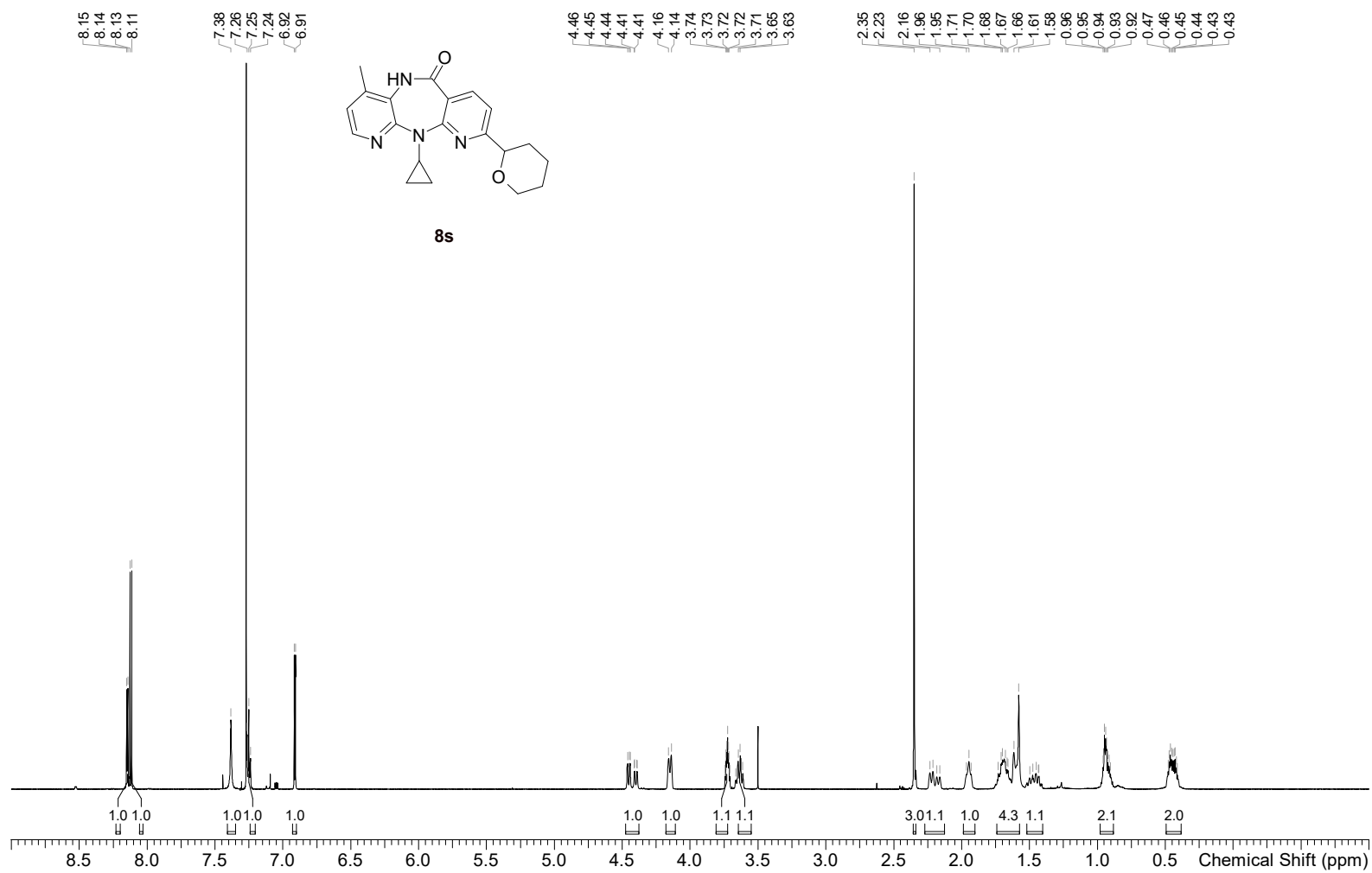


Figure 13: **8s**, ¹H-NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

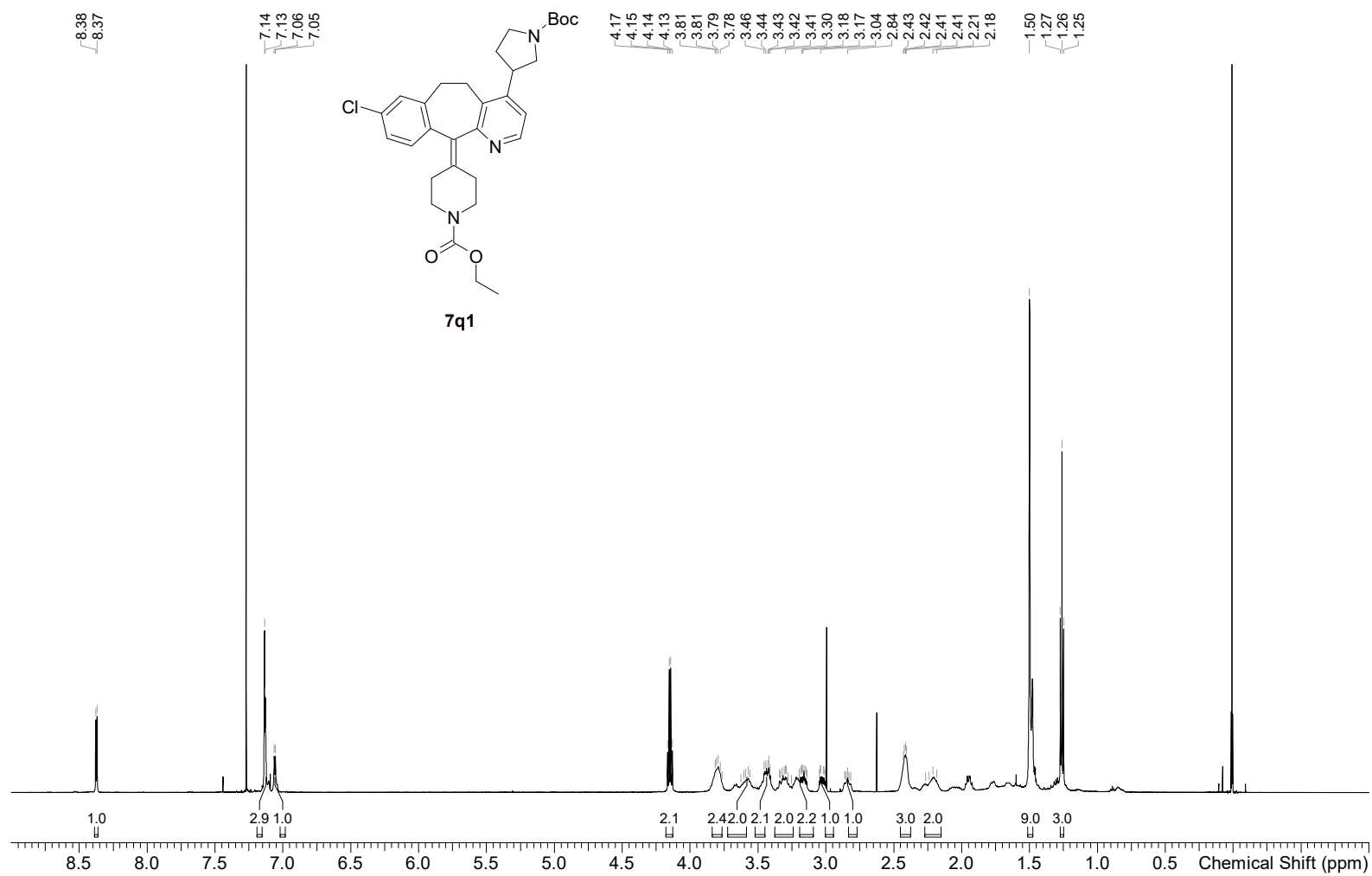


Figure 14: **7q1**, ¹H-NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

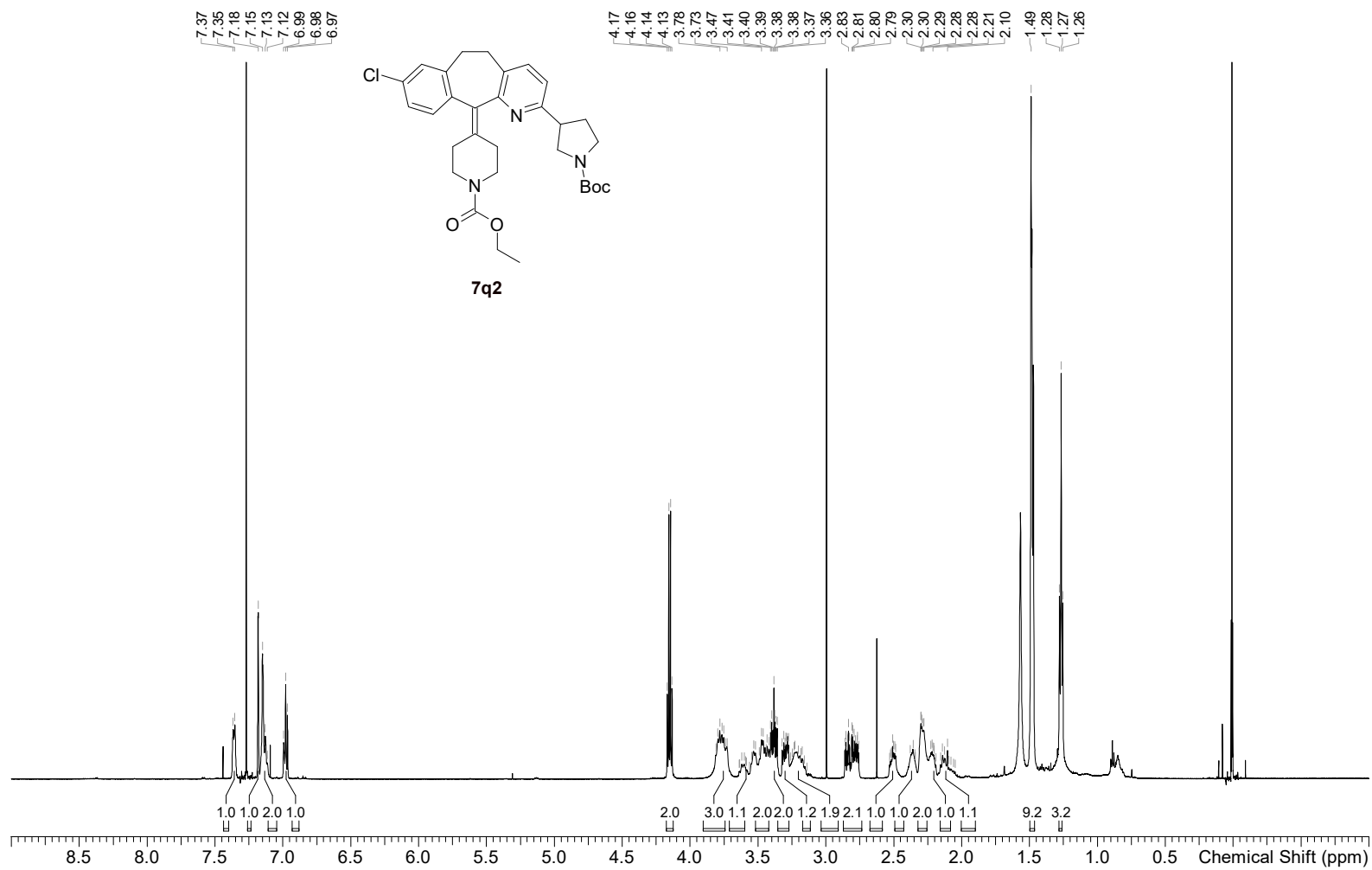


Figure 15: **7q2**, ¹H-NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

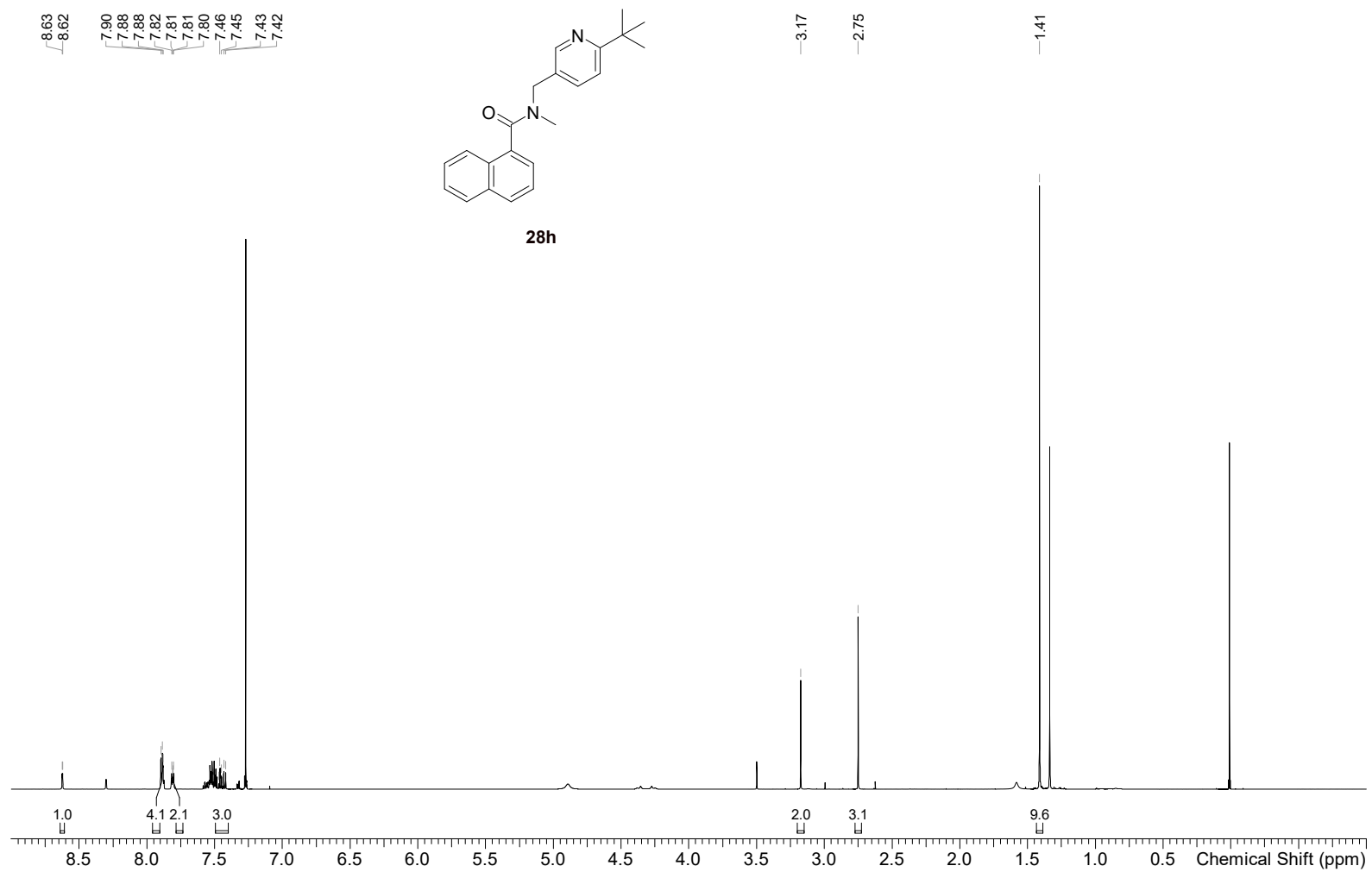


Figure 16: **28h**, ^1H -NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

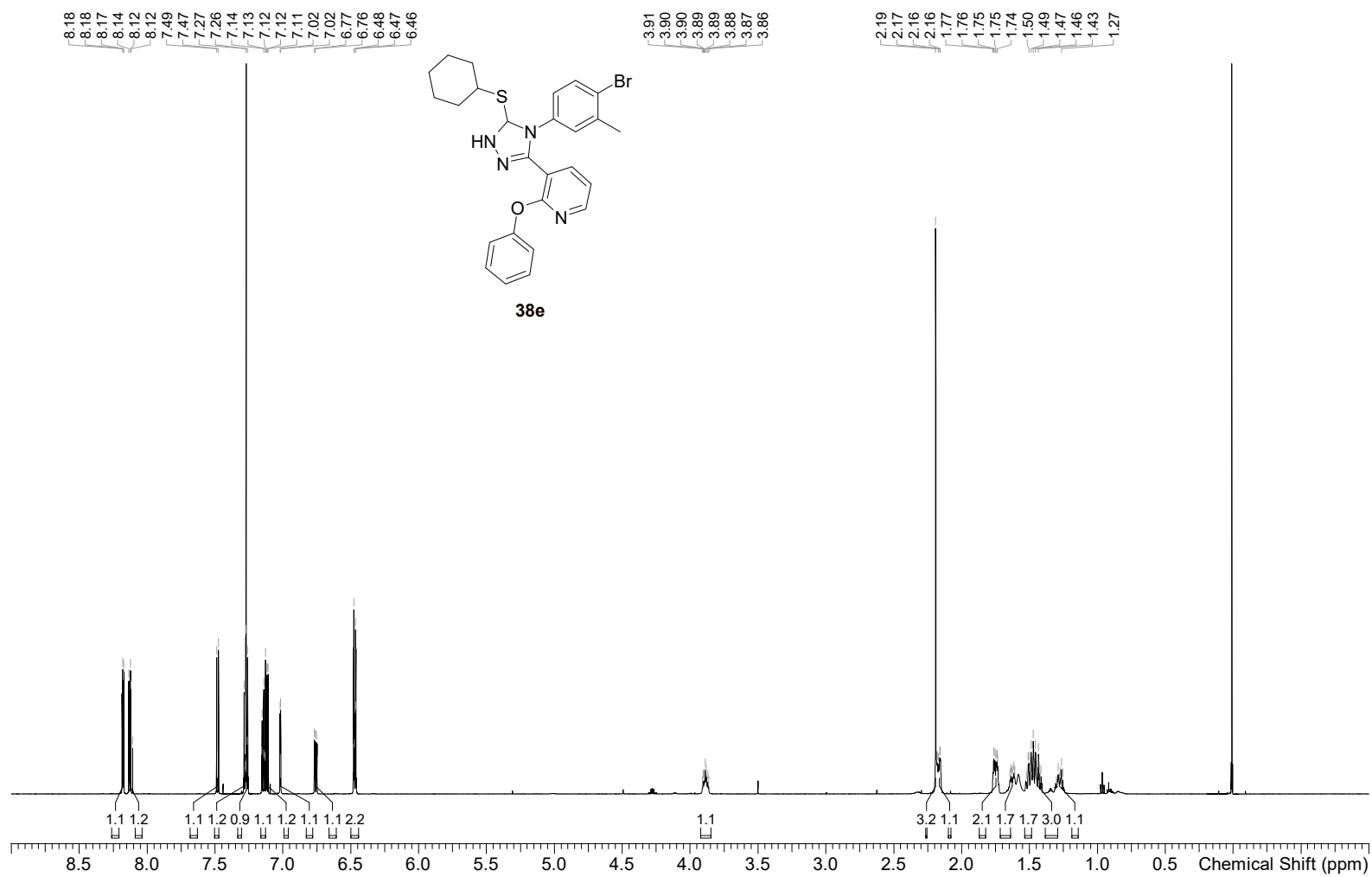


Figure 17: **38e**, ^1H -NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

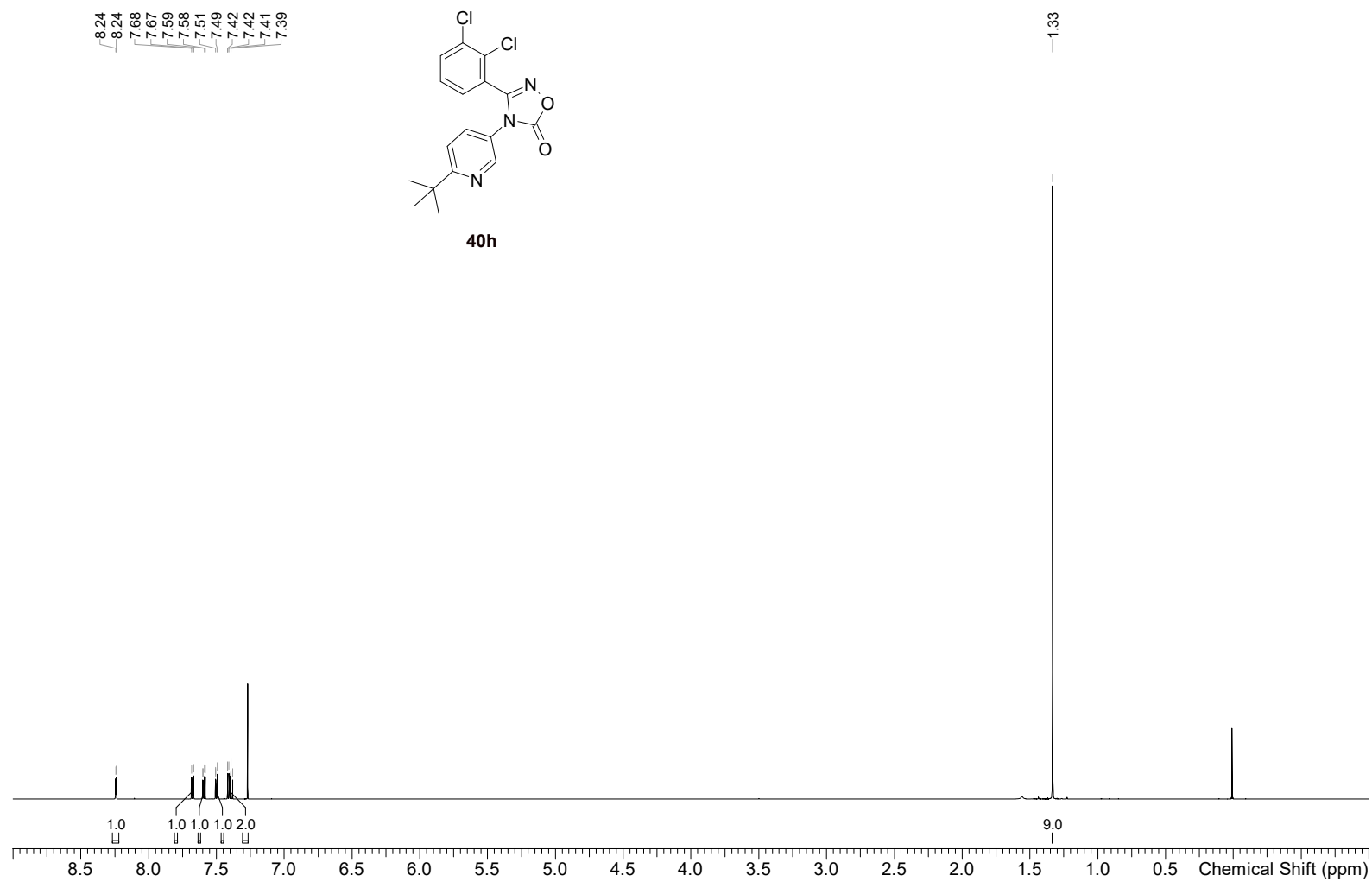


Figure 18: **40h**, ^1H -NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

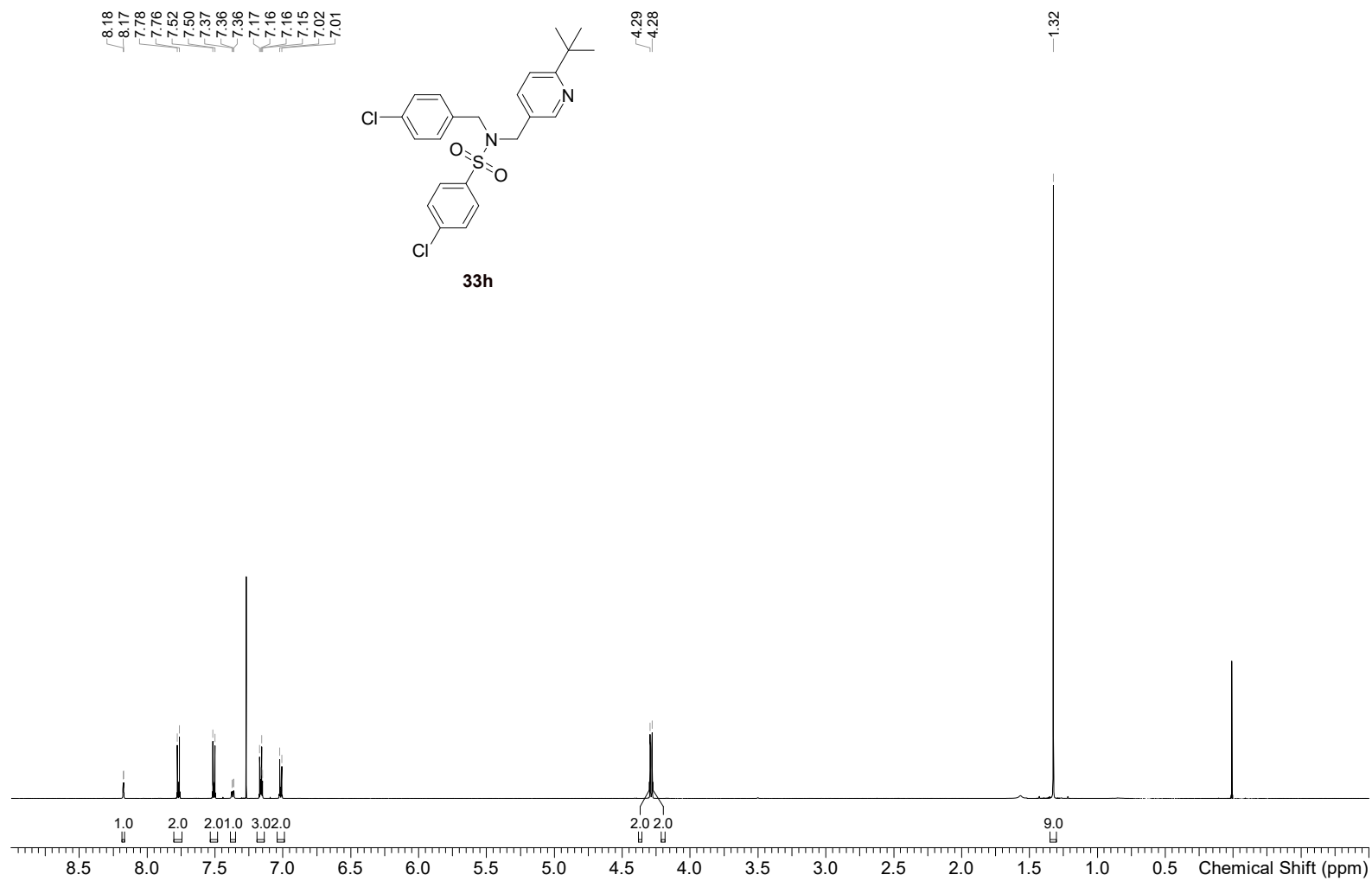


Figure 19: **33h**, ^1H -NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

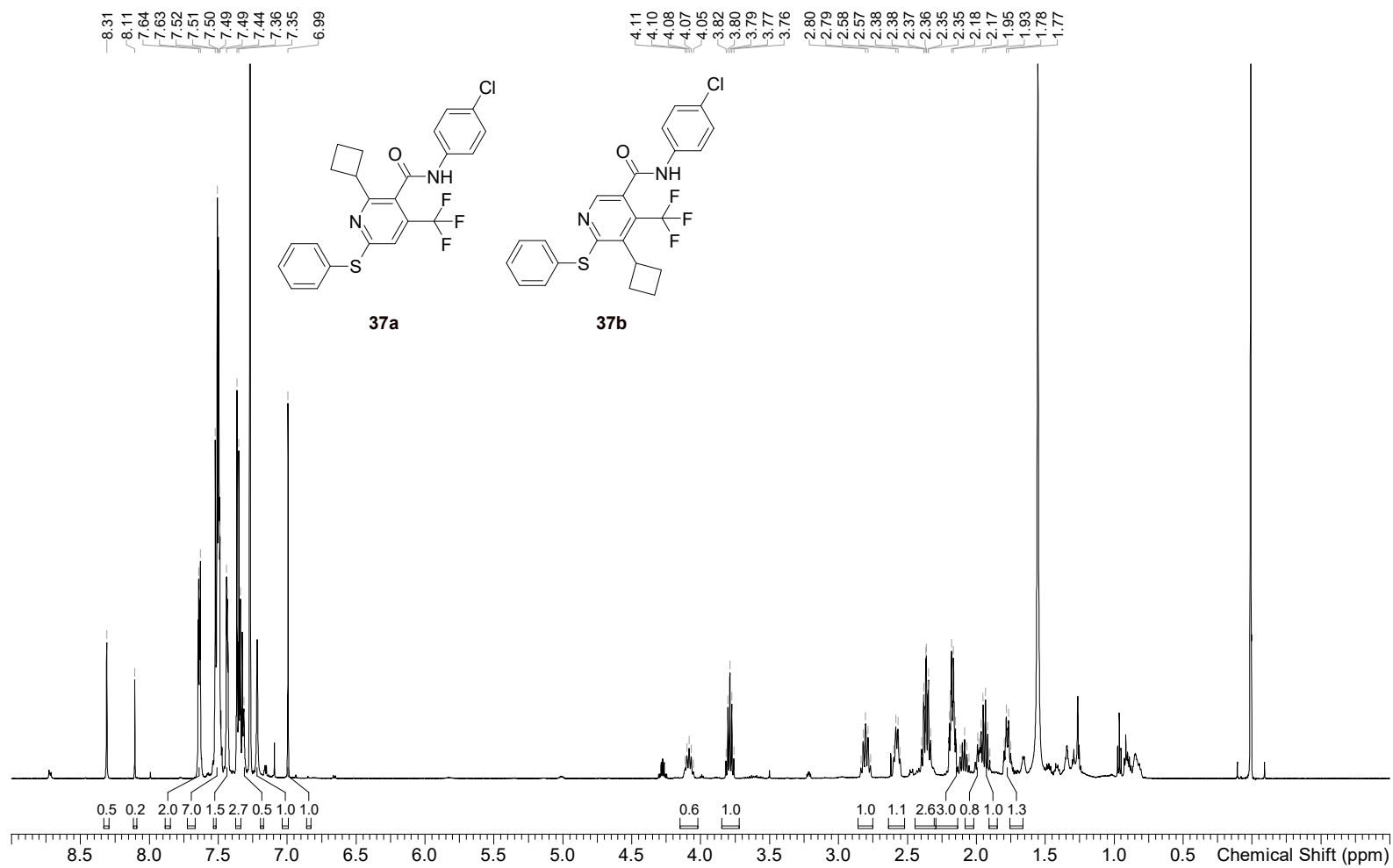


Figure 20: **37b1** & **37b2**, ^1H -NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

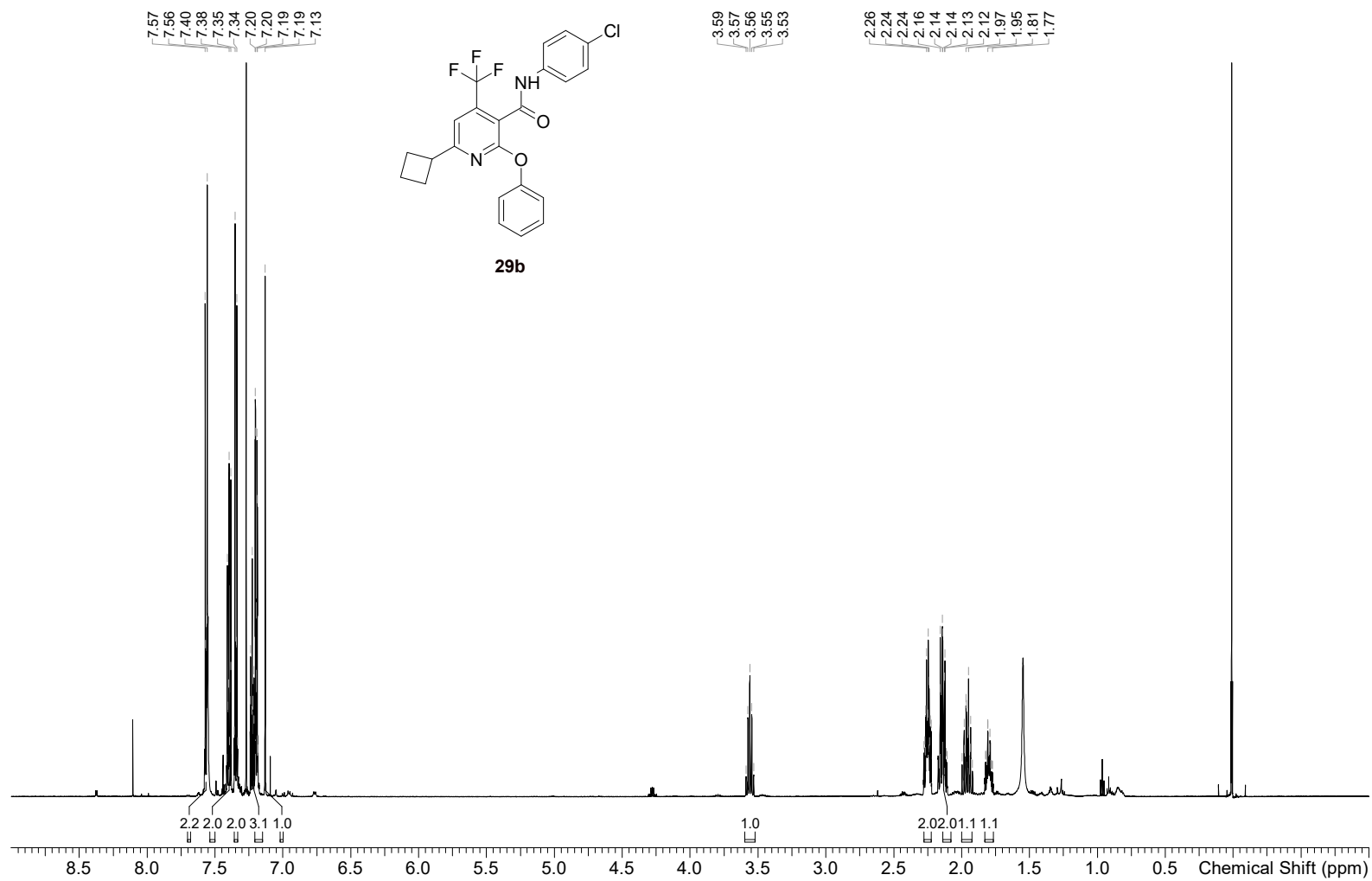


Figure 21: **29b**, ¹H-NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

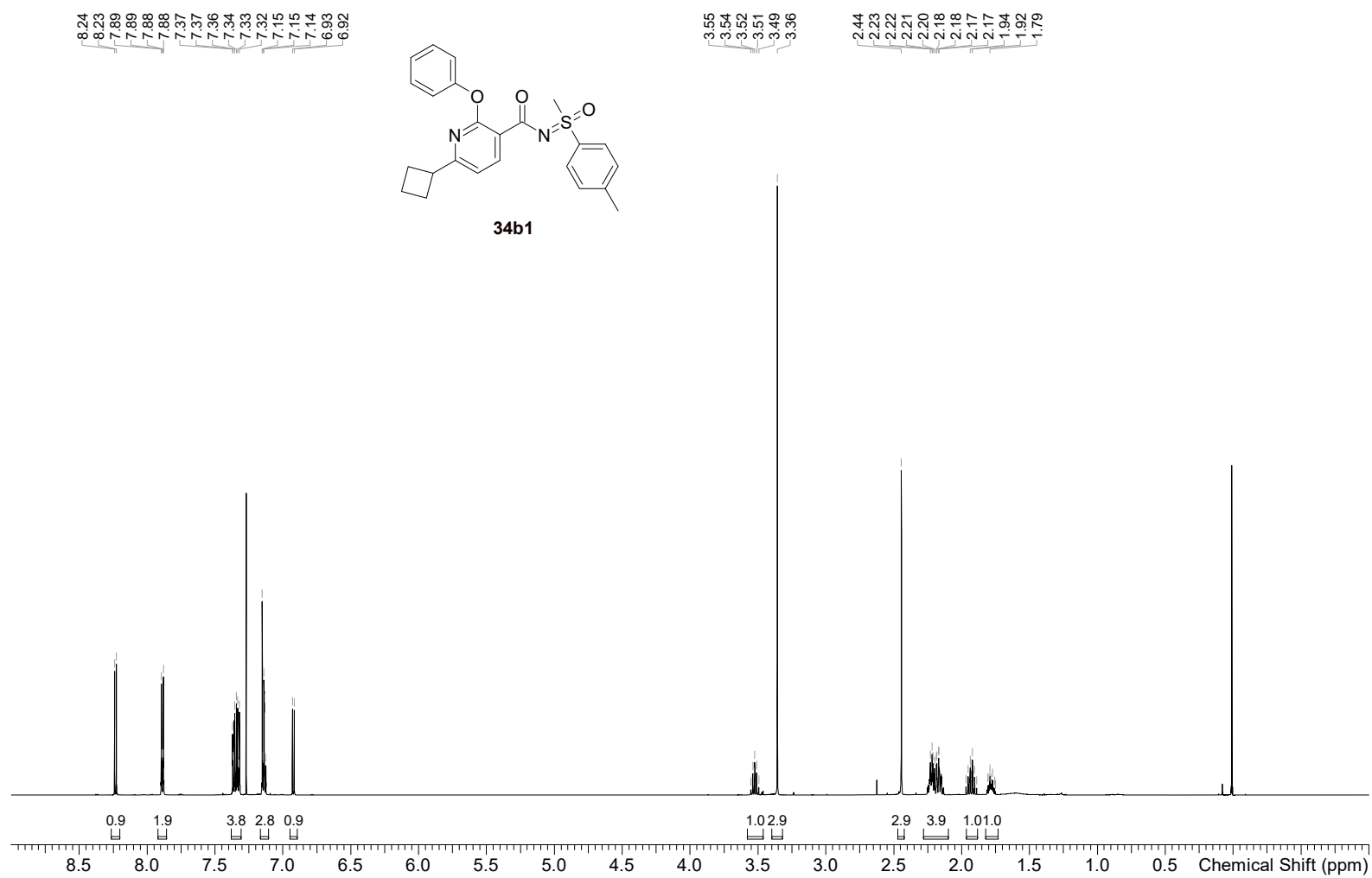


Figure 22: **34b1**, ^1H -NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

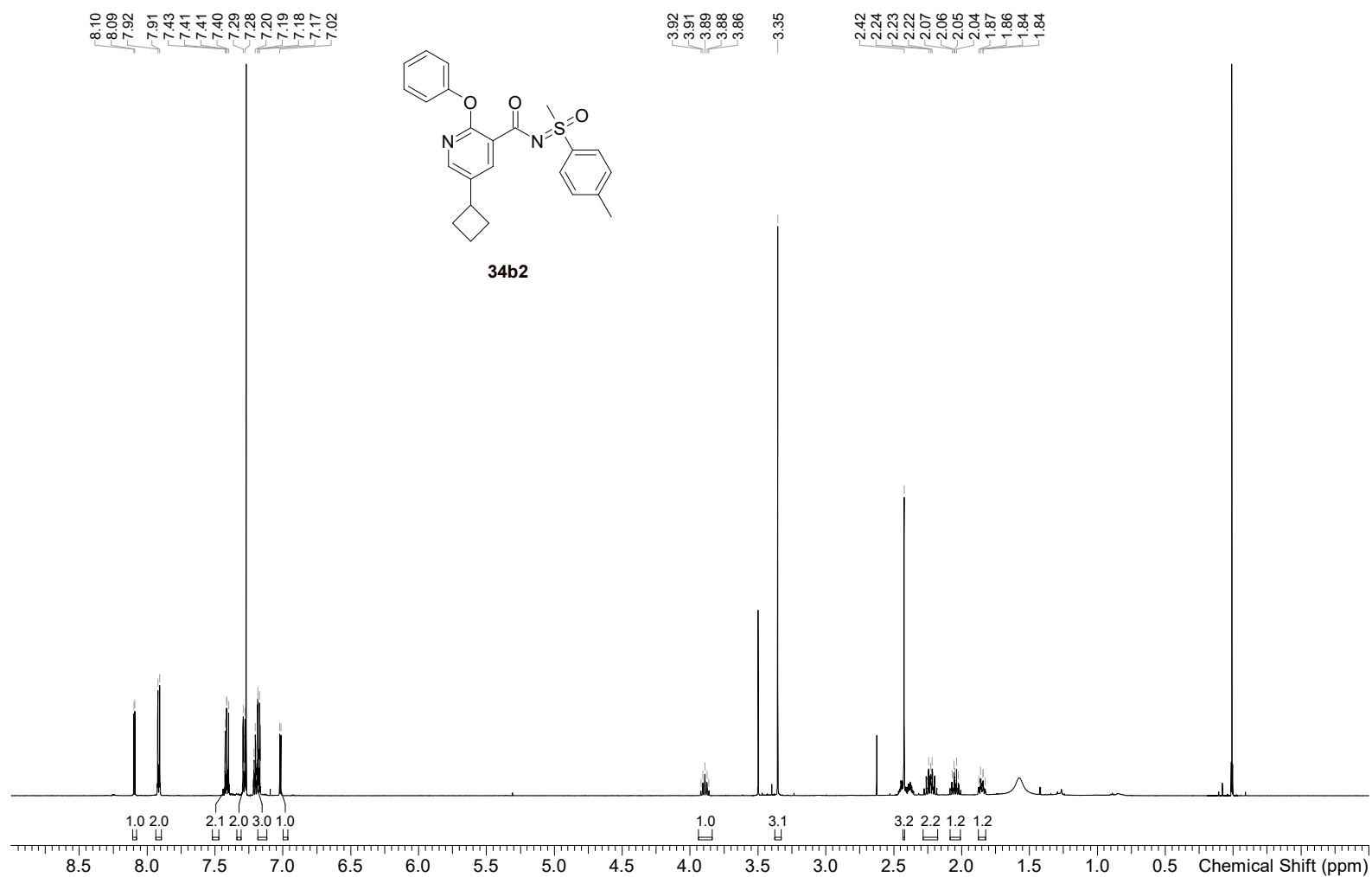


Figure 23: **34b2**, ¹H-NMR spectrum.

¹H NMR (600 MHz, CDCl₃)

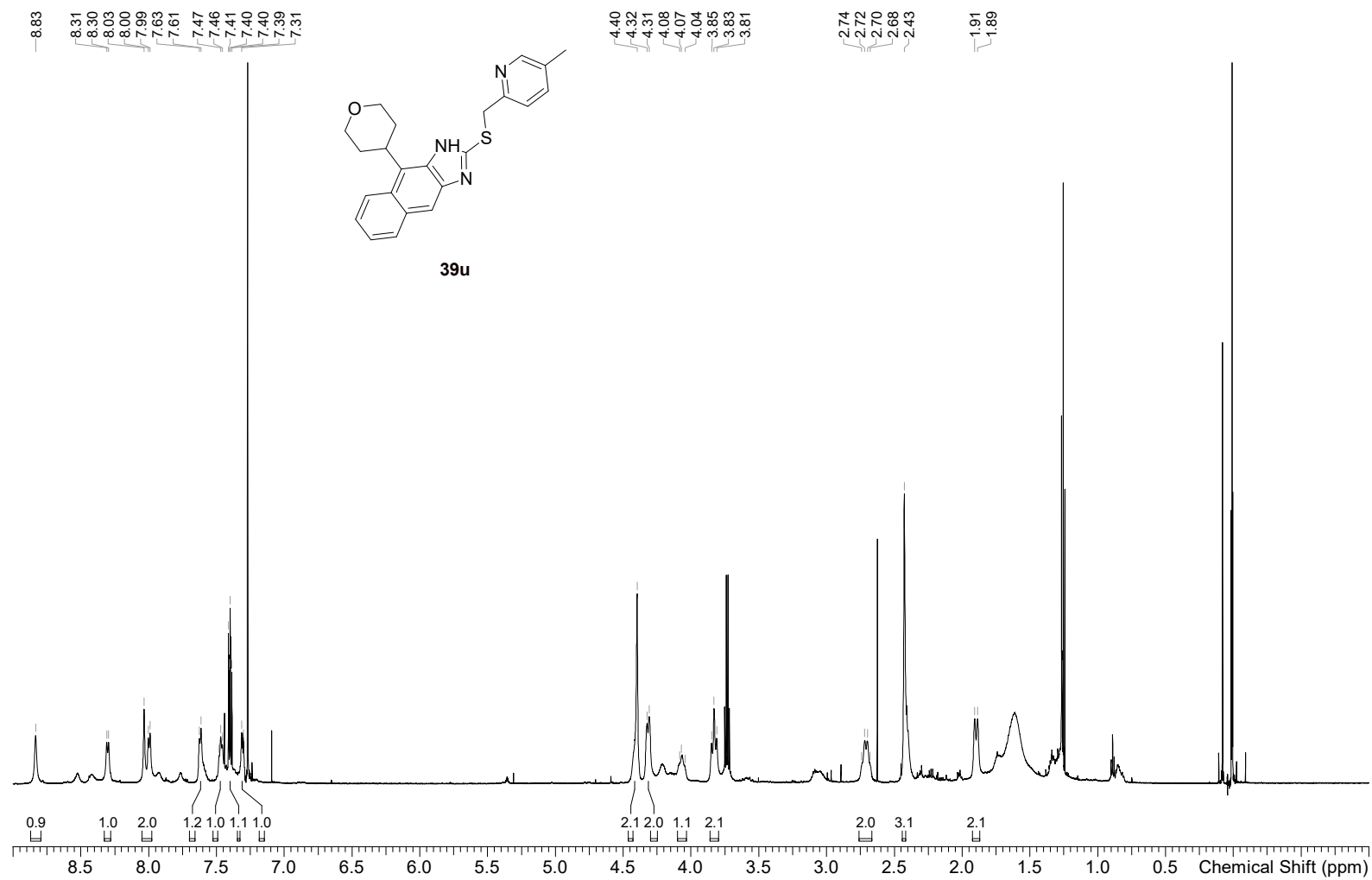


Figure 24: **39u**, ¹H-NMR spectrum.

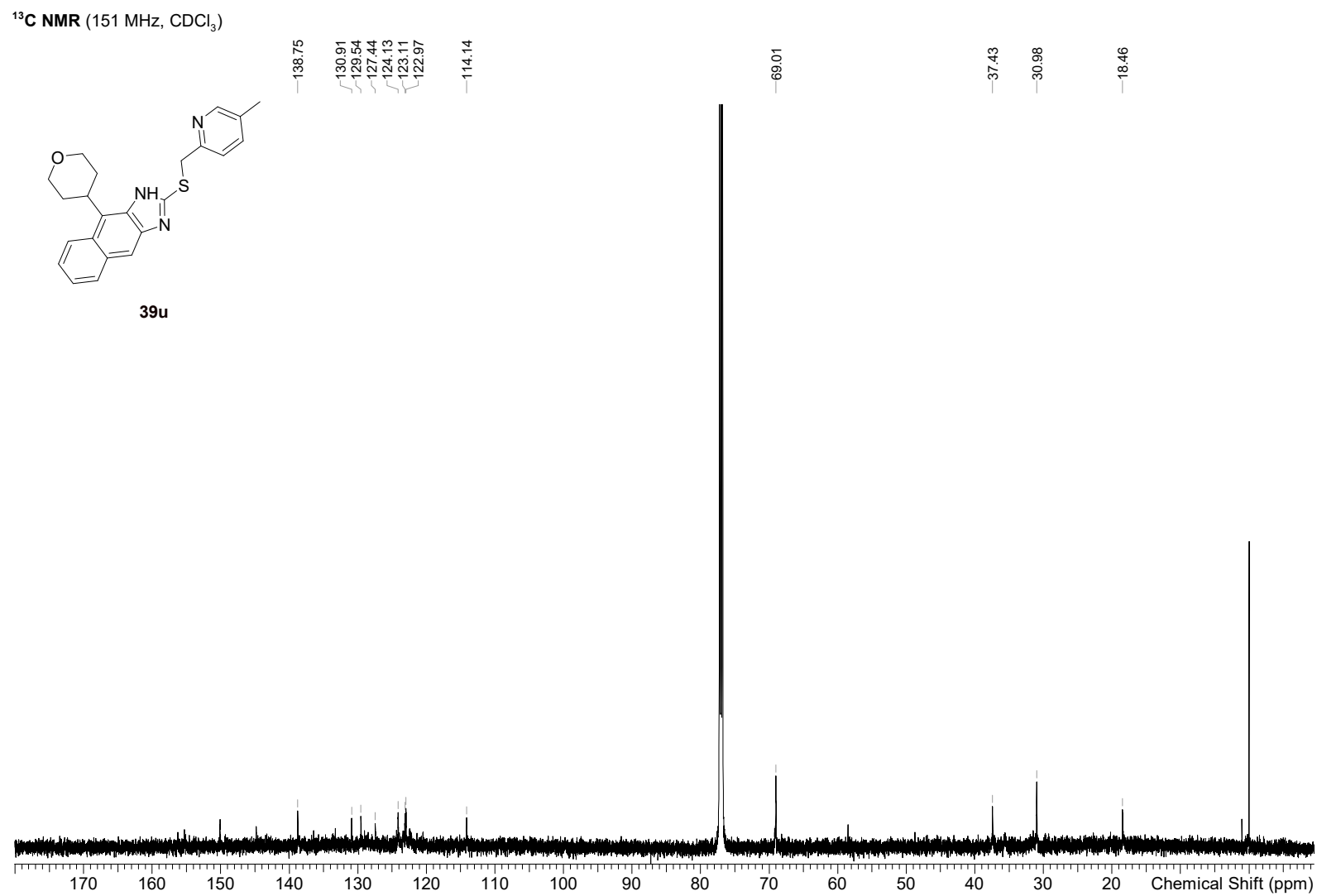


Figure 25: **39u**, ¹³C-NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

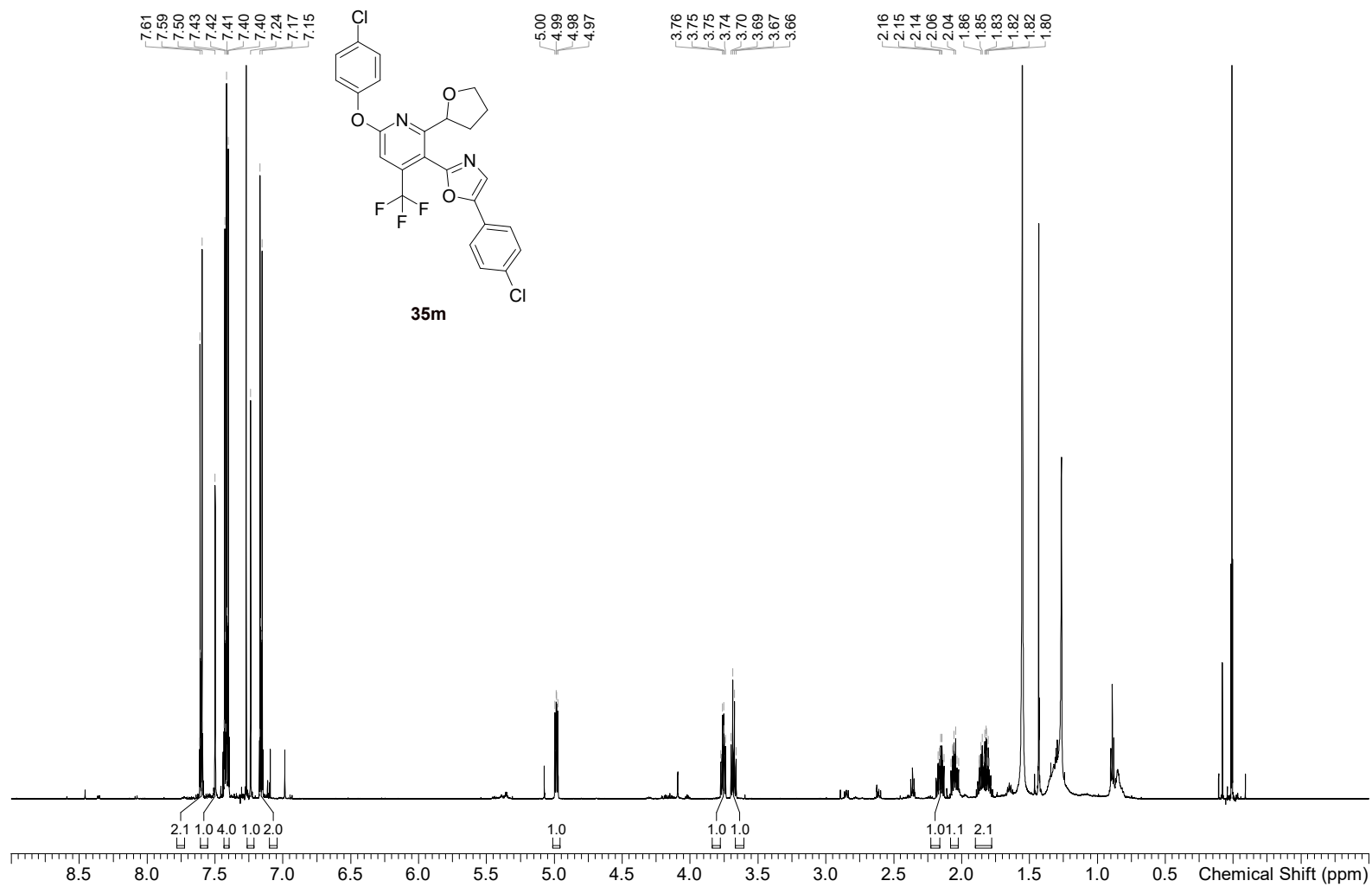


Figure 26: **35m**, ^1H -NMR spectrum.

^{13}C NMR (151 MHz, CDCl_3)

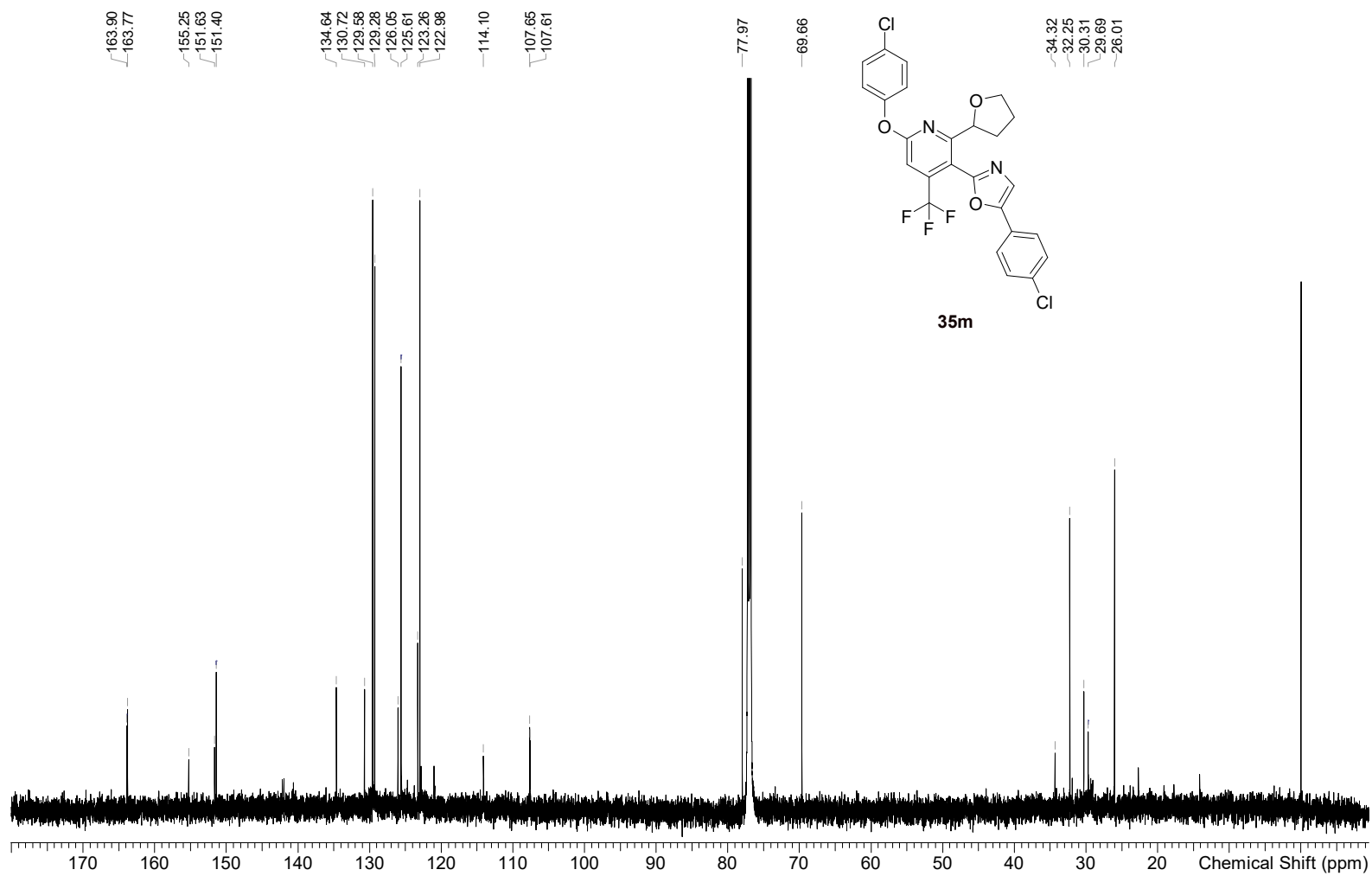


Figure 27: **35m**, ^{13}C -NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

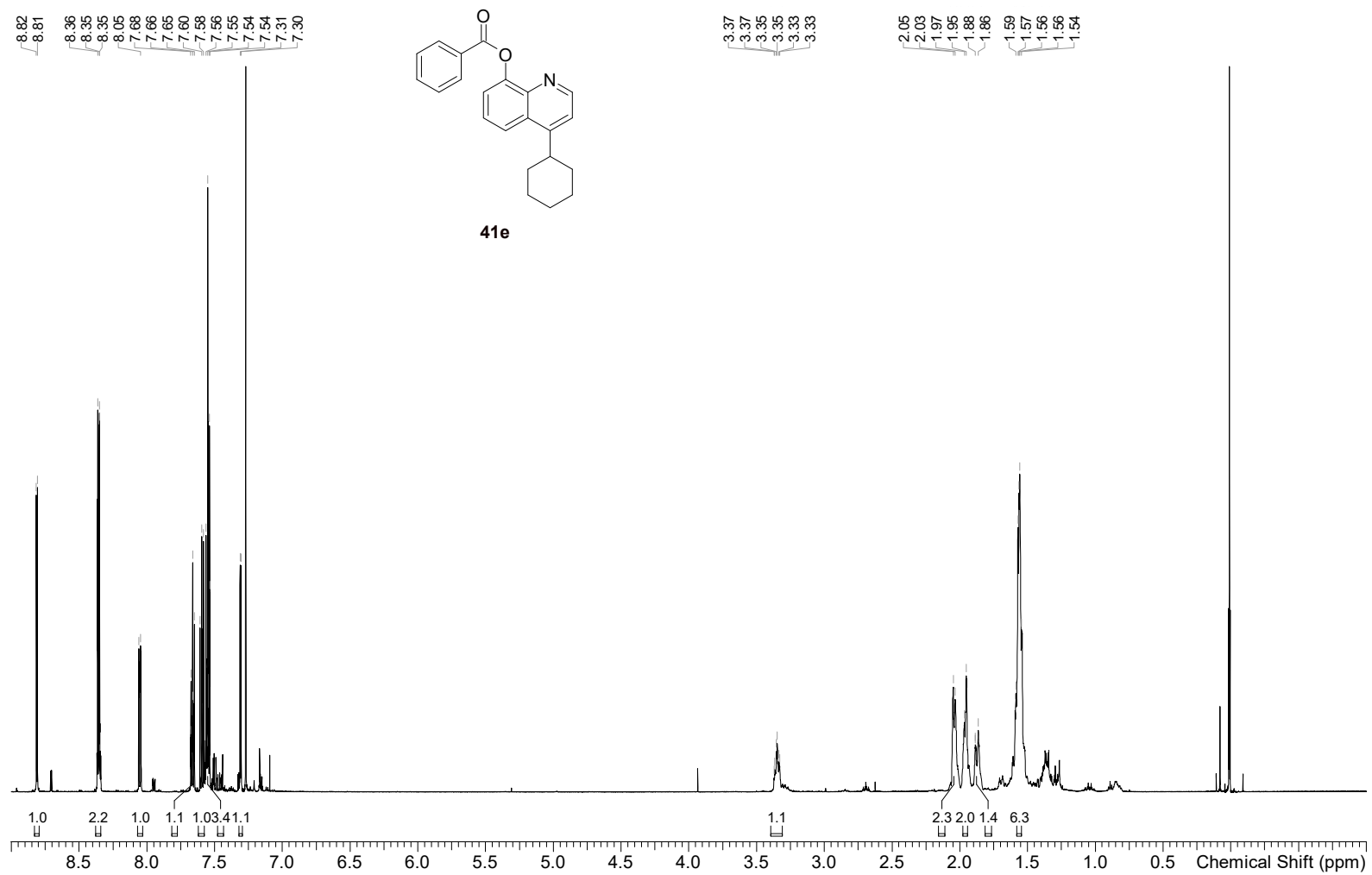


Figure 28: **41e**, ^1H -NMR spectrum.

¹³C NMR (151 MHz, CDCl₃)

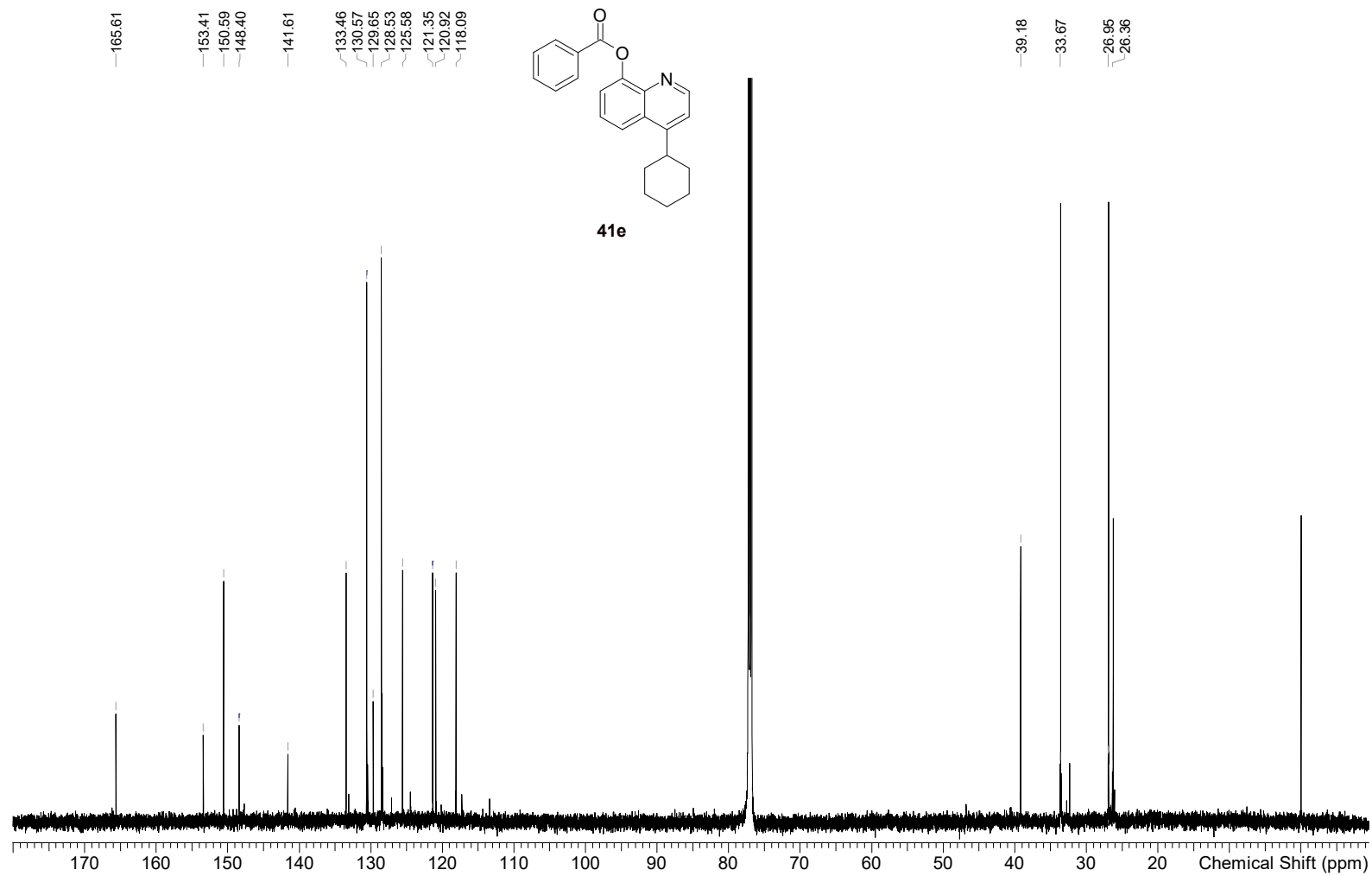


Figure 29: **41e**, ¹³C-NMR spectrum.

^1H NMR (600 MHz, CDCl_3)

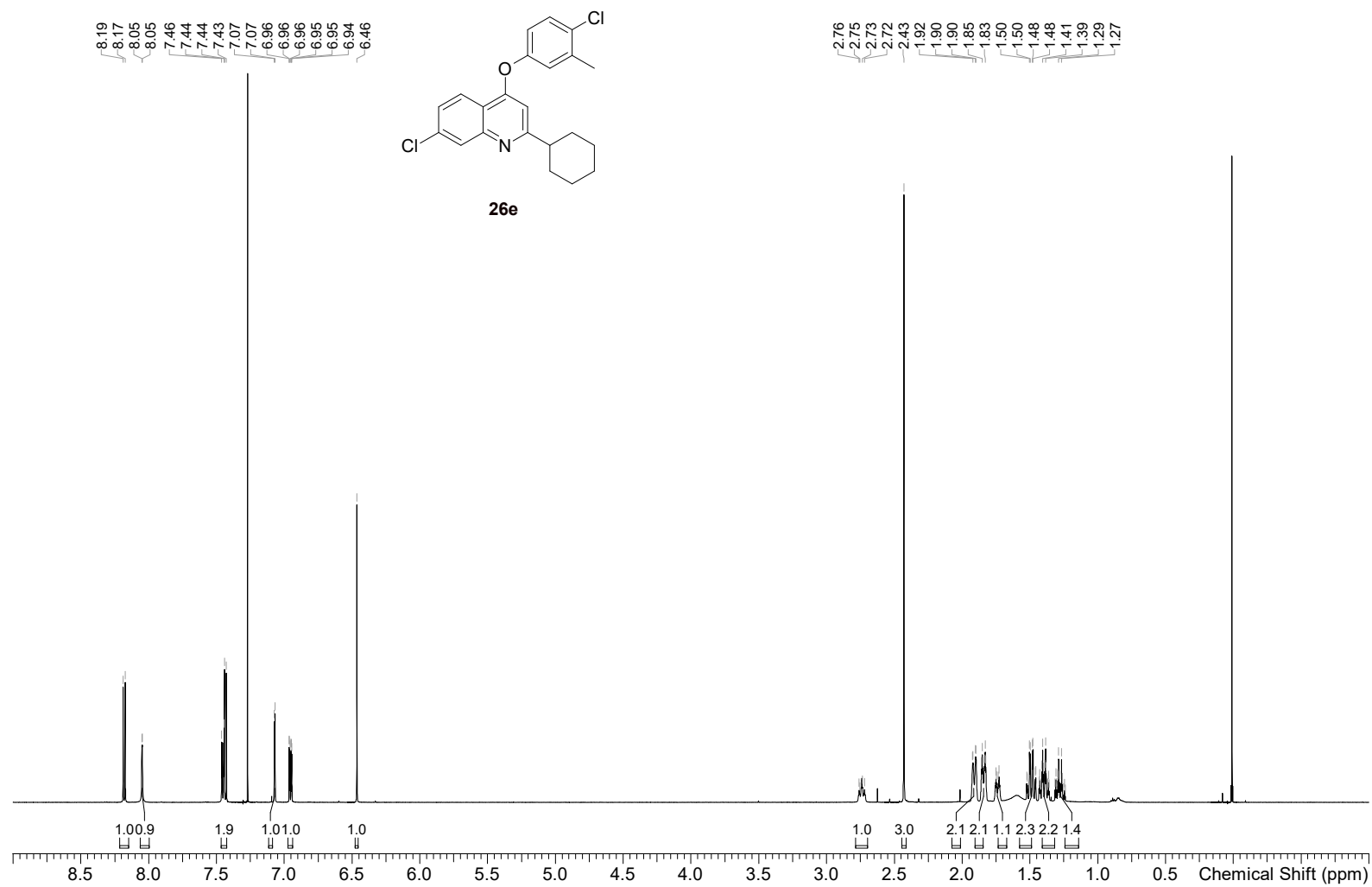


Figure 30: **26e**, ^1H -NMR spectrum.