New Journal of Chemistry

Supporting Information

Atmospheric CO_2 Promoted Synthesis of N-Containing Heterocycles over $B(C_6F_5)_3$ Catalyst

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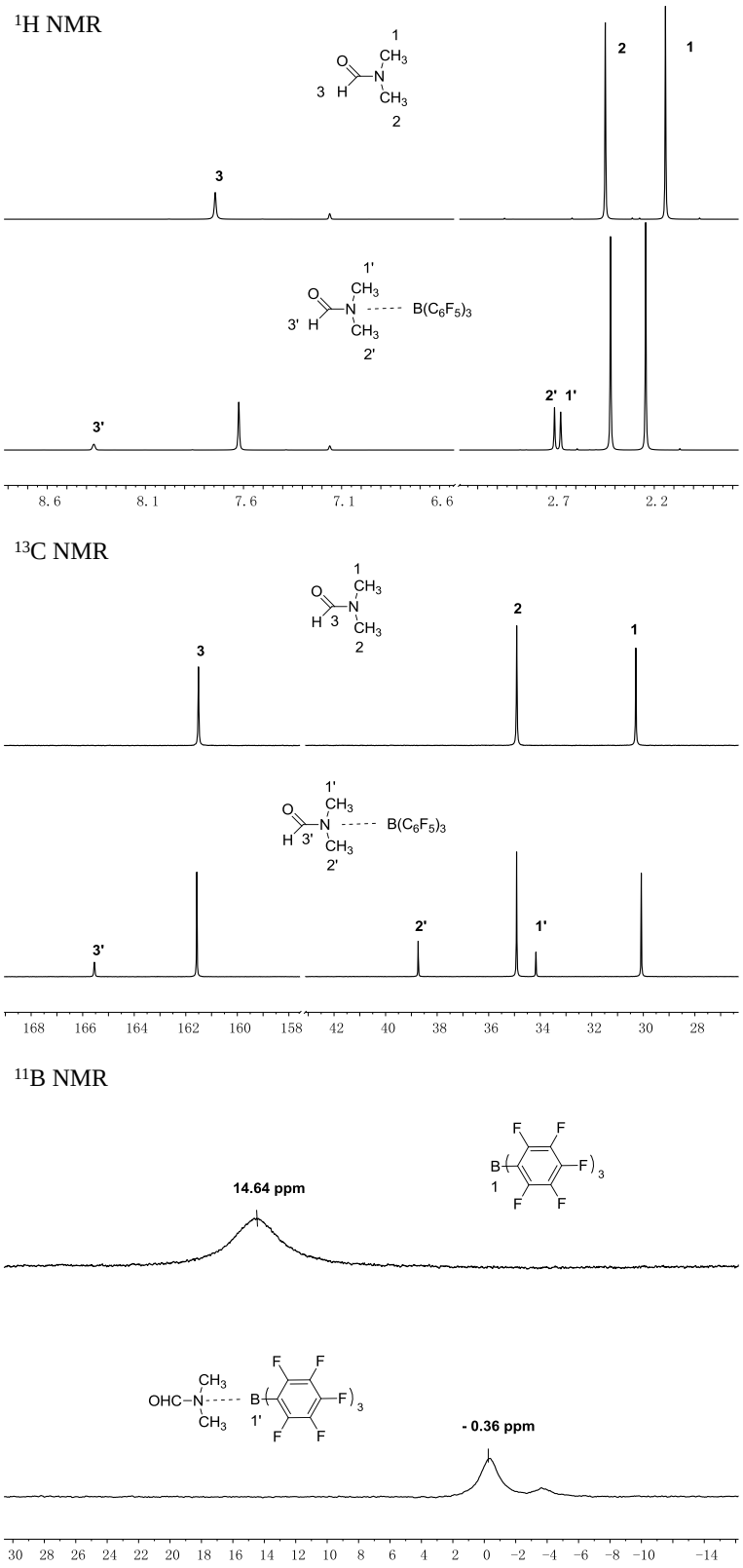
1. **NMR spectrums of N,N-dimethylformamide (DMF) and $B(C_6F_5)_3$, Figure S1**



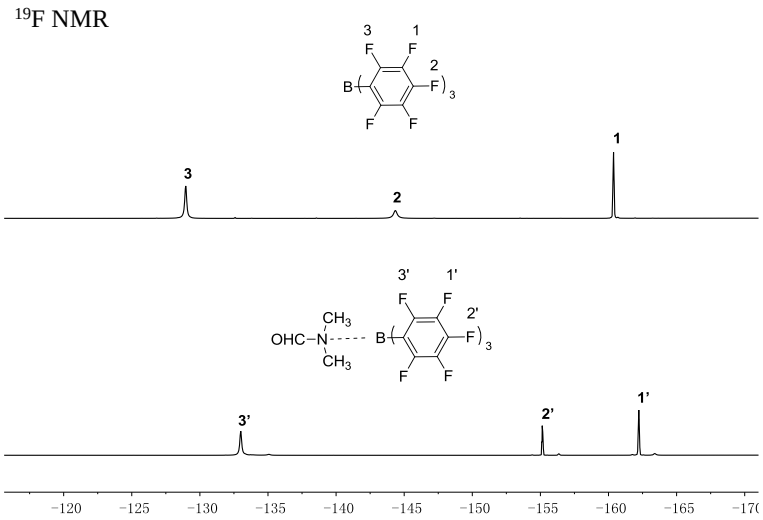
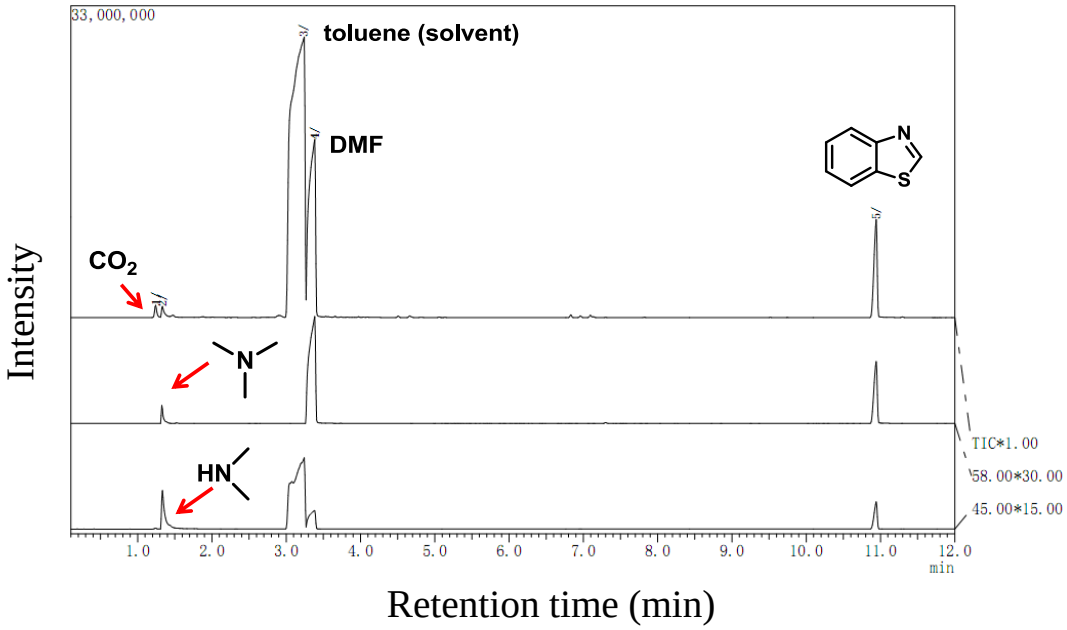


Figure S1. ^{1}H, ^{13}C, ^{11}B and ^{19}F NMR spectrums of N,N-dimethylformamide (DMF) before and after mixing with $B(C_6F_5)_3$, (molar ratio 4:1, 298 K, C_6D_6 for ^{1}H, ^{13}C NMR, $CDCl_3$ for ^{11}B, ^{19}F NMR).

2. GC-MS analysis data



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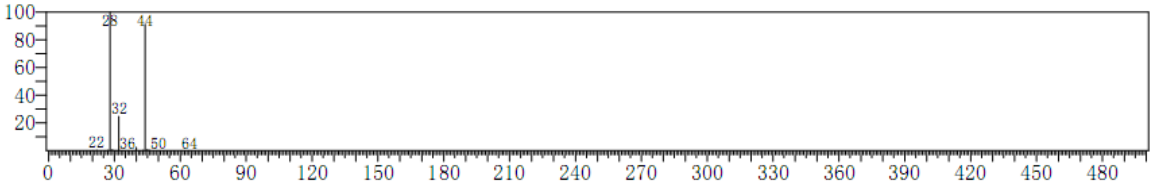

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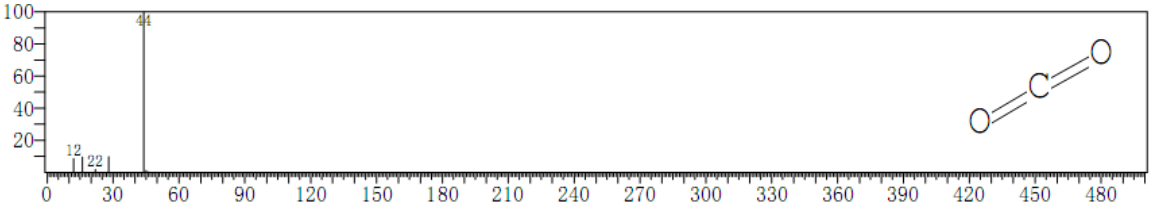

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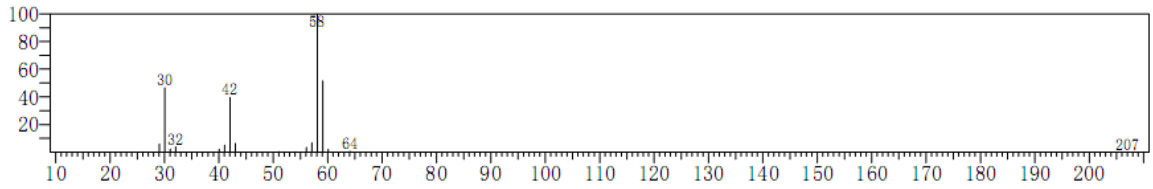

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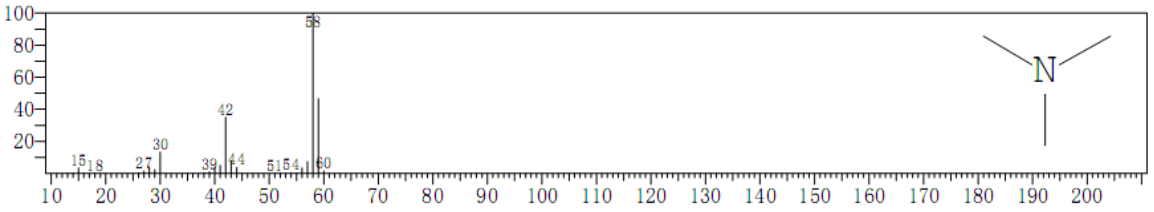

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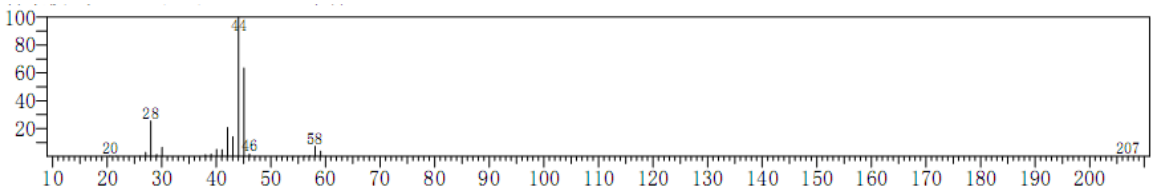

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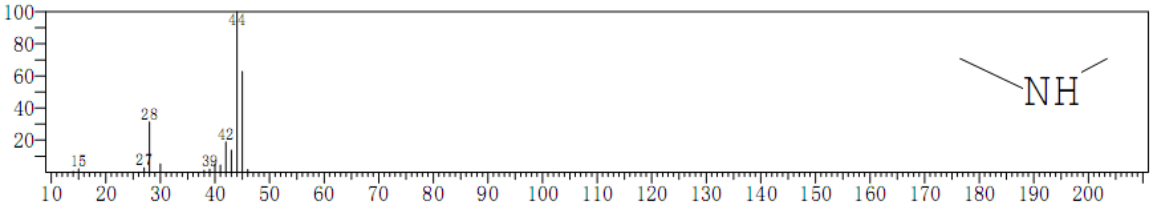

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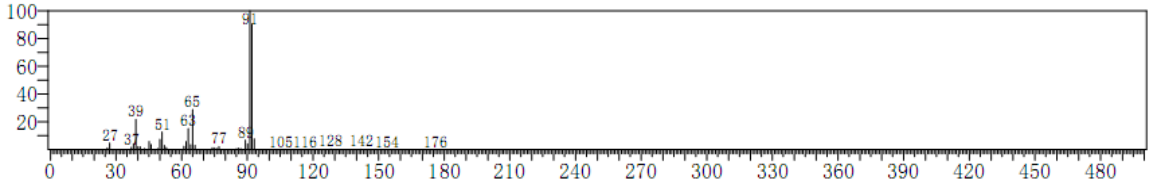

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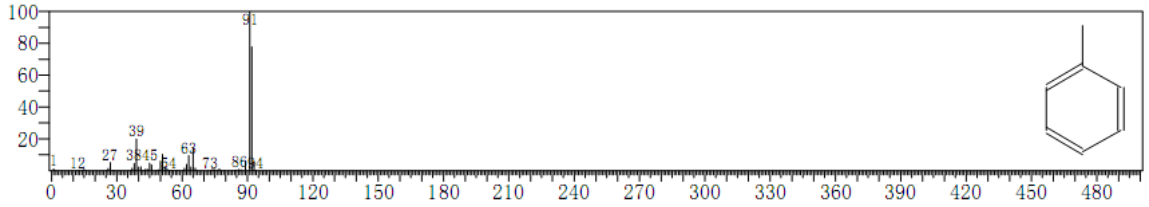

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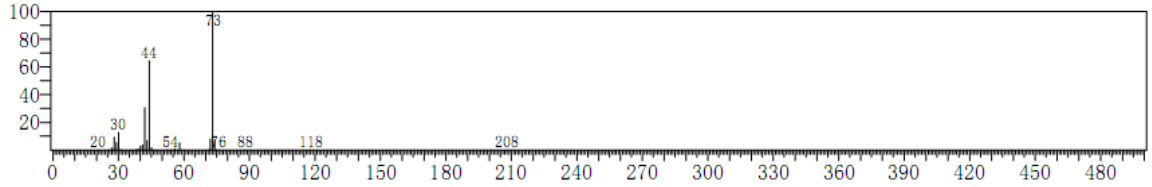

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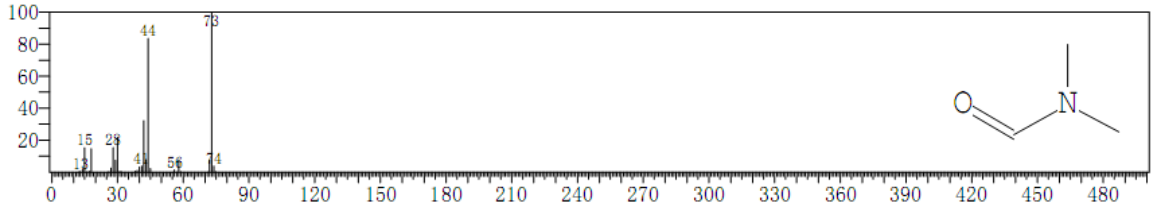

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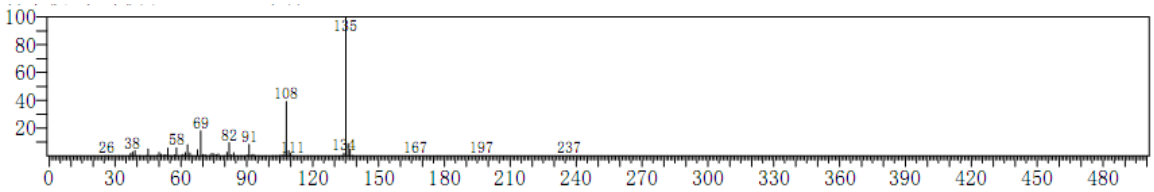

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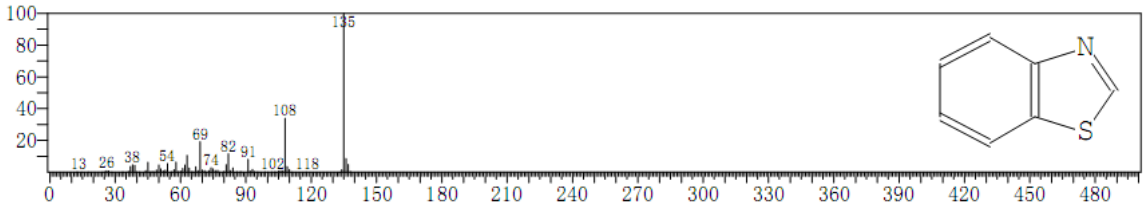

Figure S2. GC-MS spectrum of the reaction solution in toluene. Reaction conditions: 2-aminothiophenol (0.5 mmol), $B(C_6F_5)_3$ (5 mol%), Et_2SiH_2 (2 mmol), DMF (1 mL), CO_2 (0.1 MPa), 120 ^oC, 15 h.

3. ^{1}H and ^{13}C NMR spectra of the products, Figure S3-S33

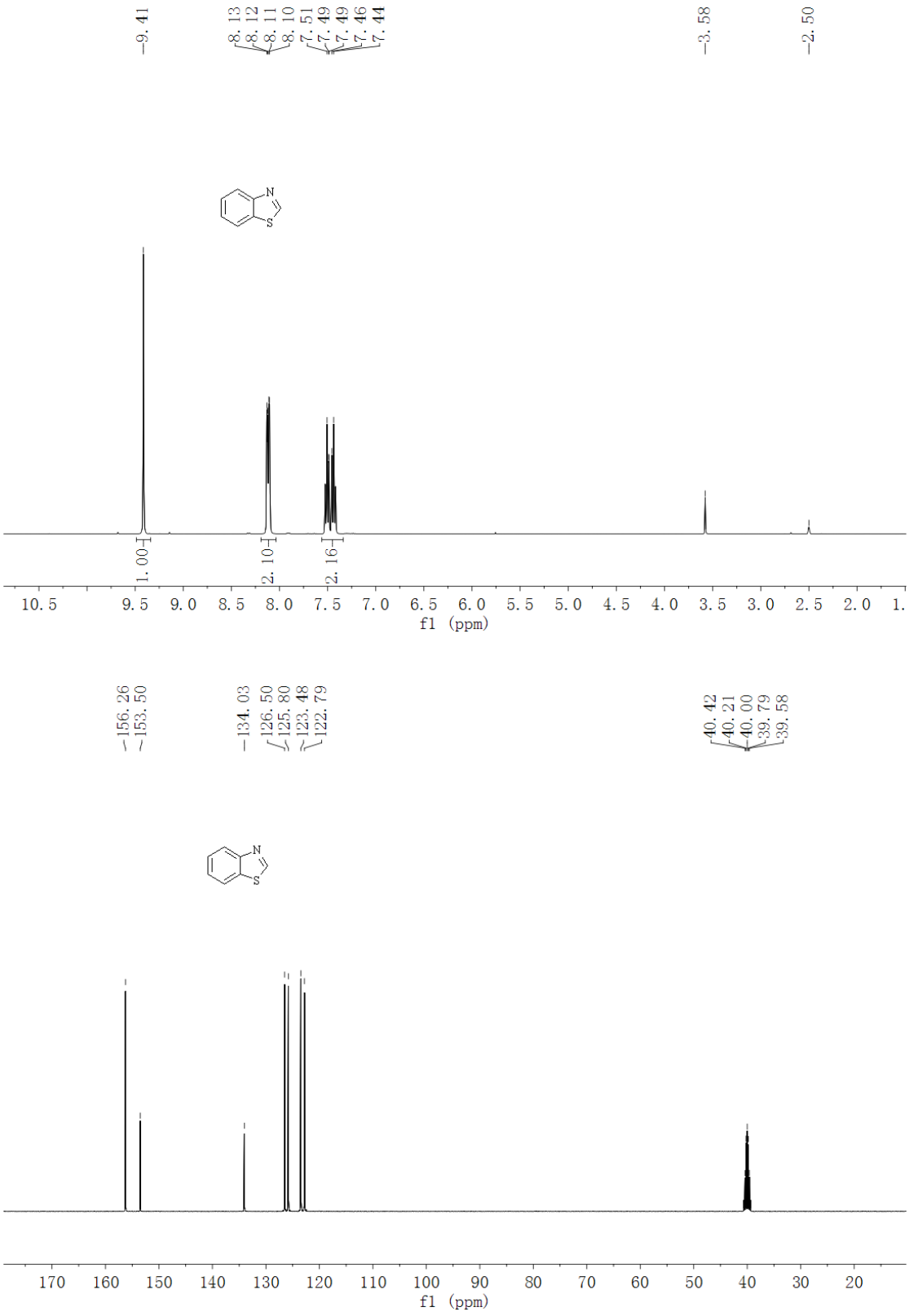

Figure S3. ^{1}H NMR and ^{13}C NMR spectra of benzothiazole (1a)

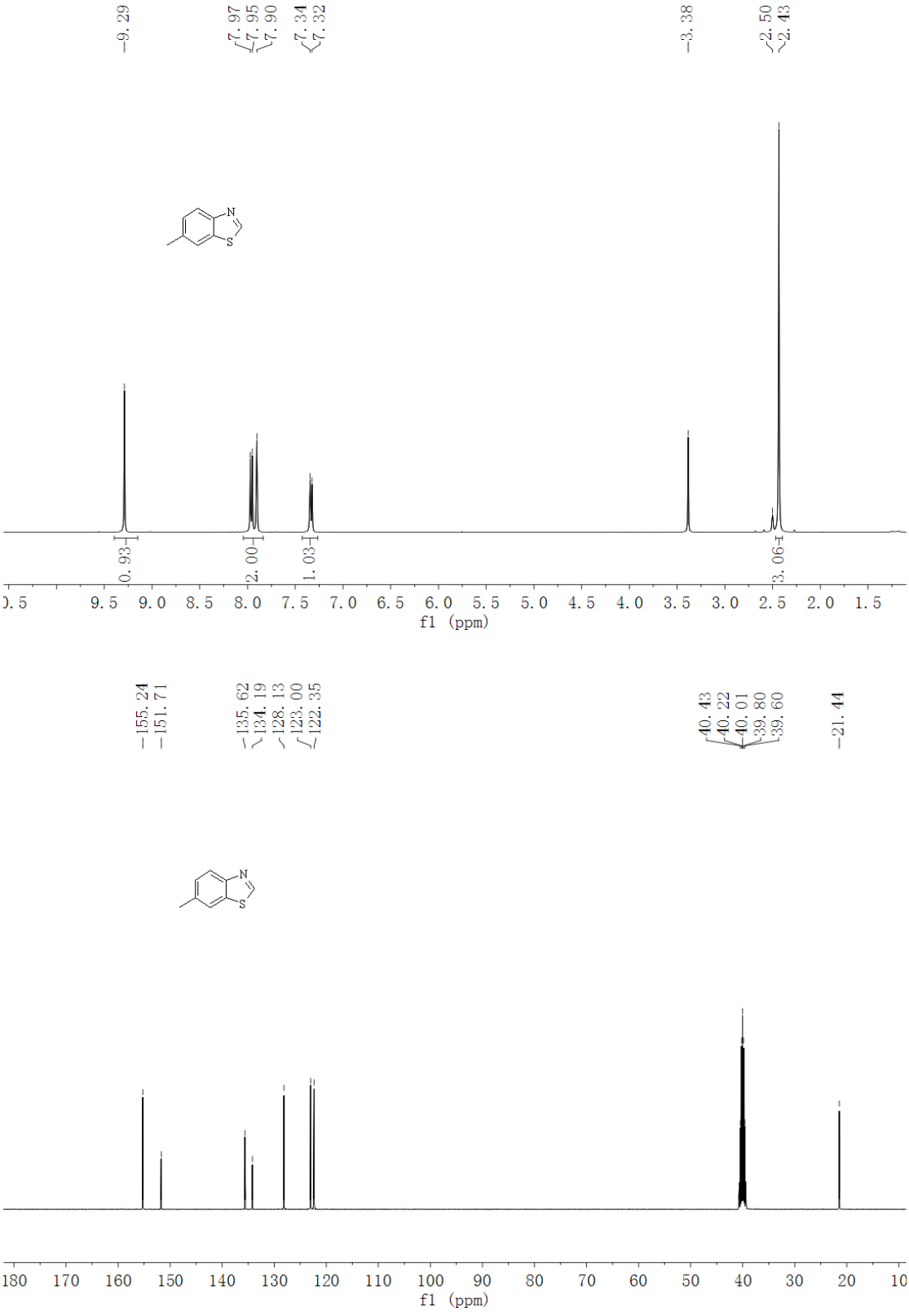

Figure S4. ^{1}H NMR and ^{13}C NMR spectra of 5-methylbenzothiazole (1b)

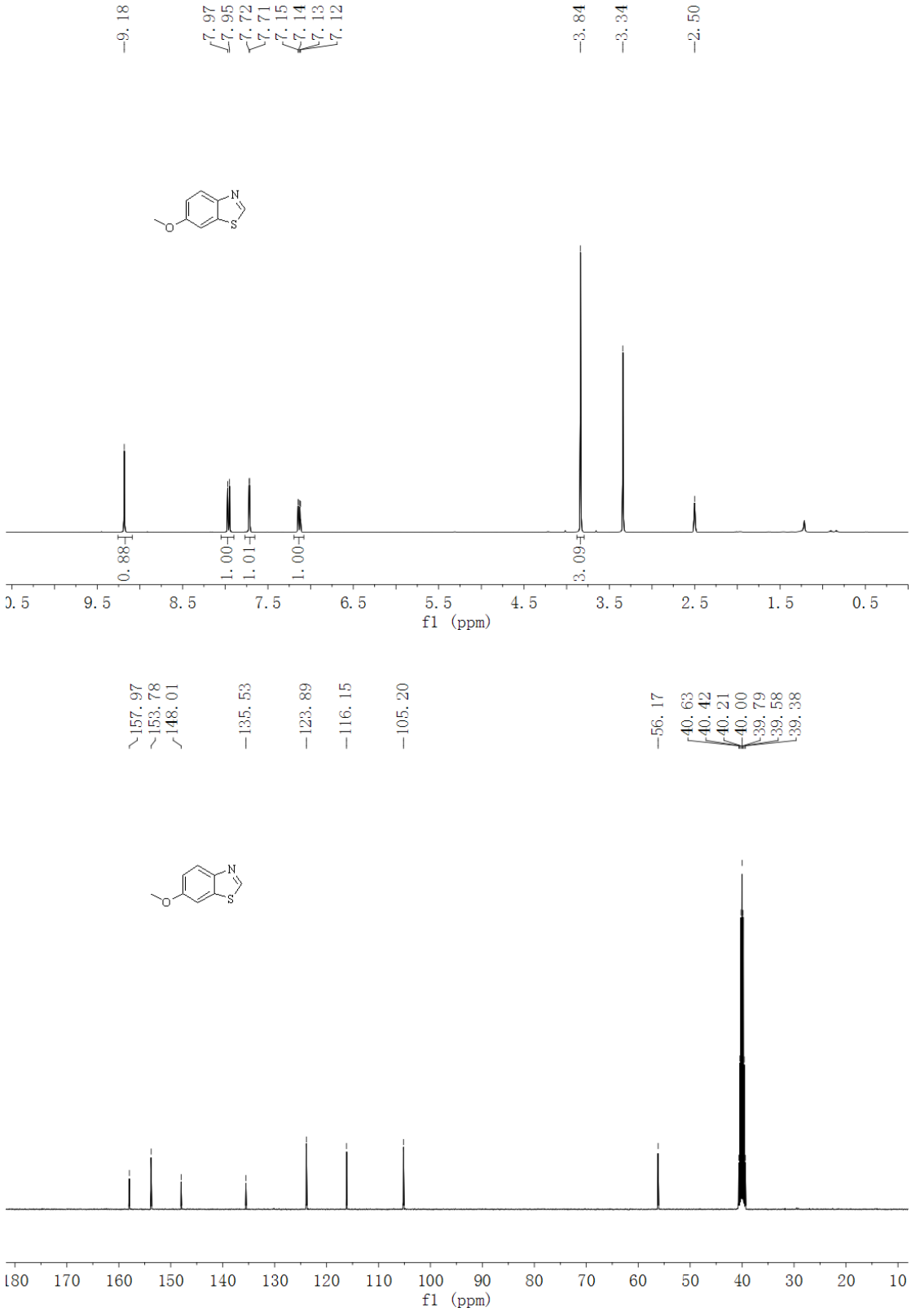

Figure S5. ^{1}H NMR and ^{13}C NMR spectra of 5-methoxybenzothiazole (1c)

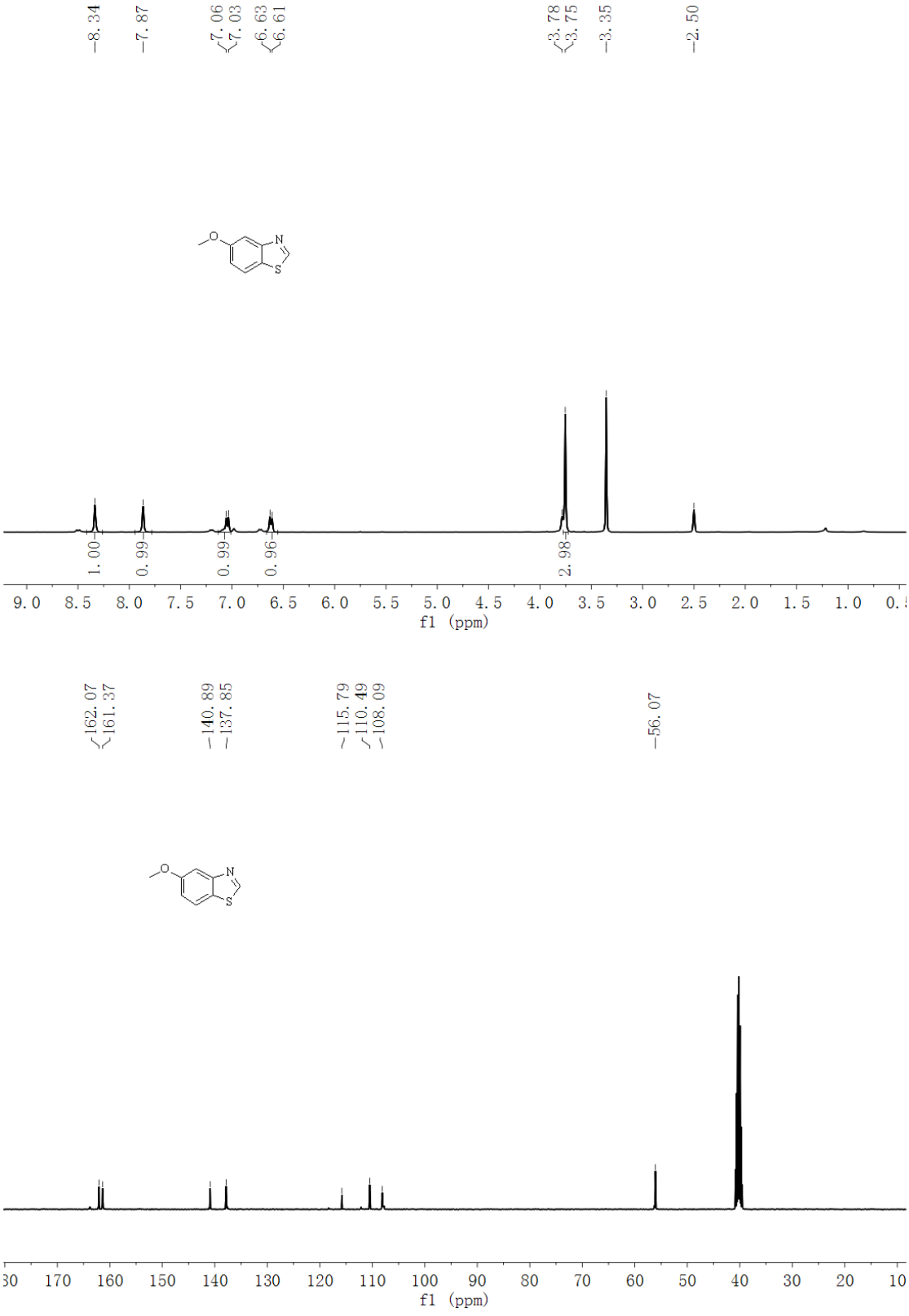

Figure S6. ^{1}H NMR and ^{13}C NMR spectra of 6-methoxybenzothiazole (1d)

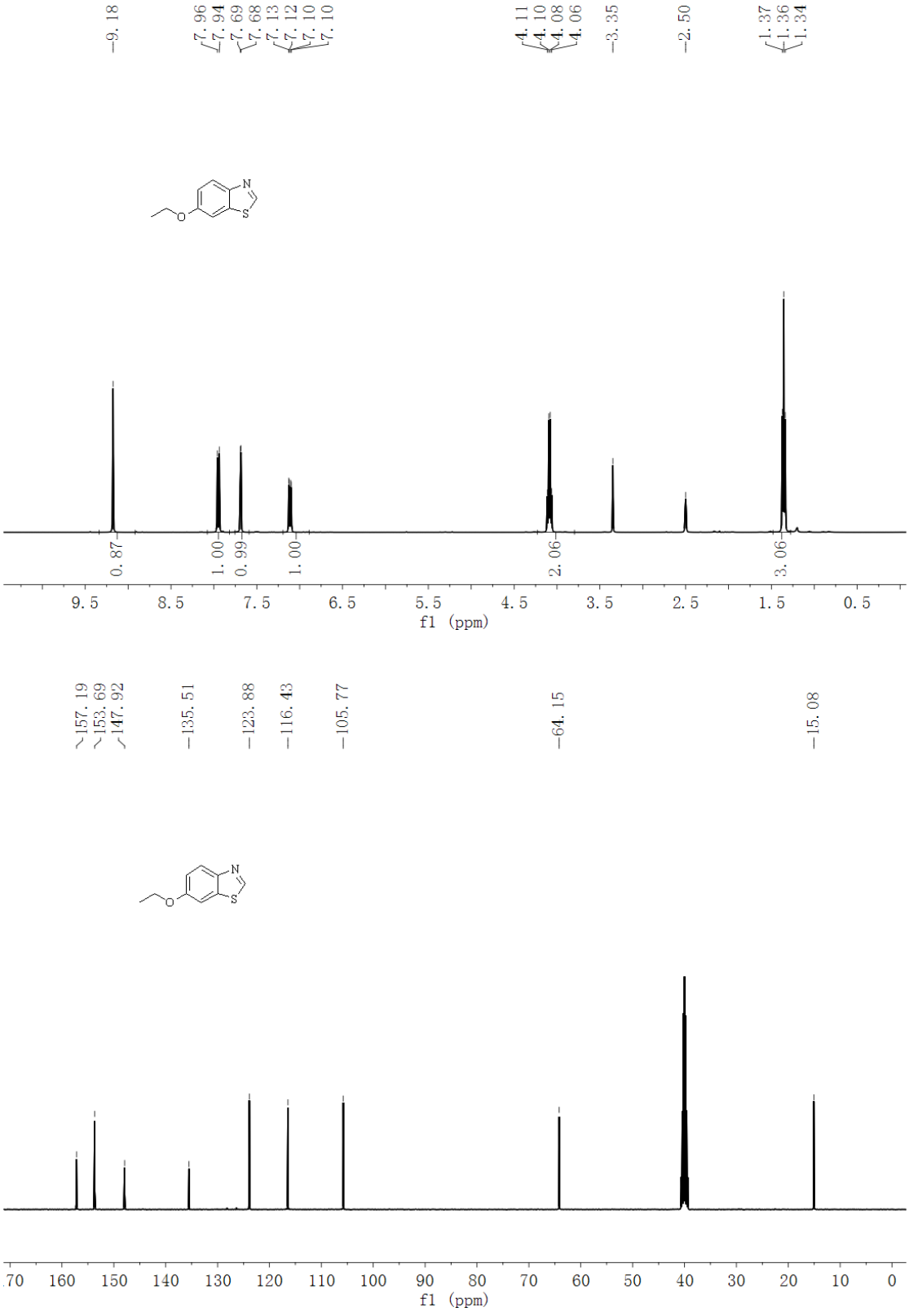

Figure S77. ^{1}H NMR and ^{13}C NMR spectra of 5-ethoxybenzothiazole (1e)

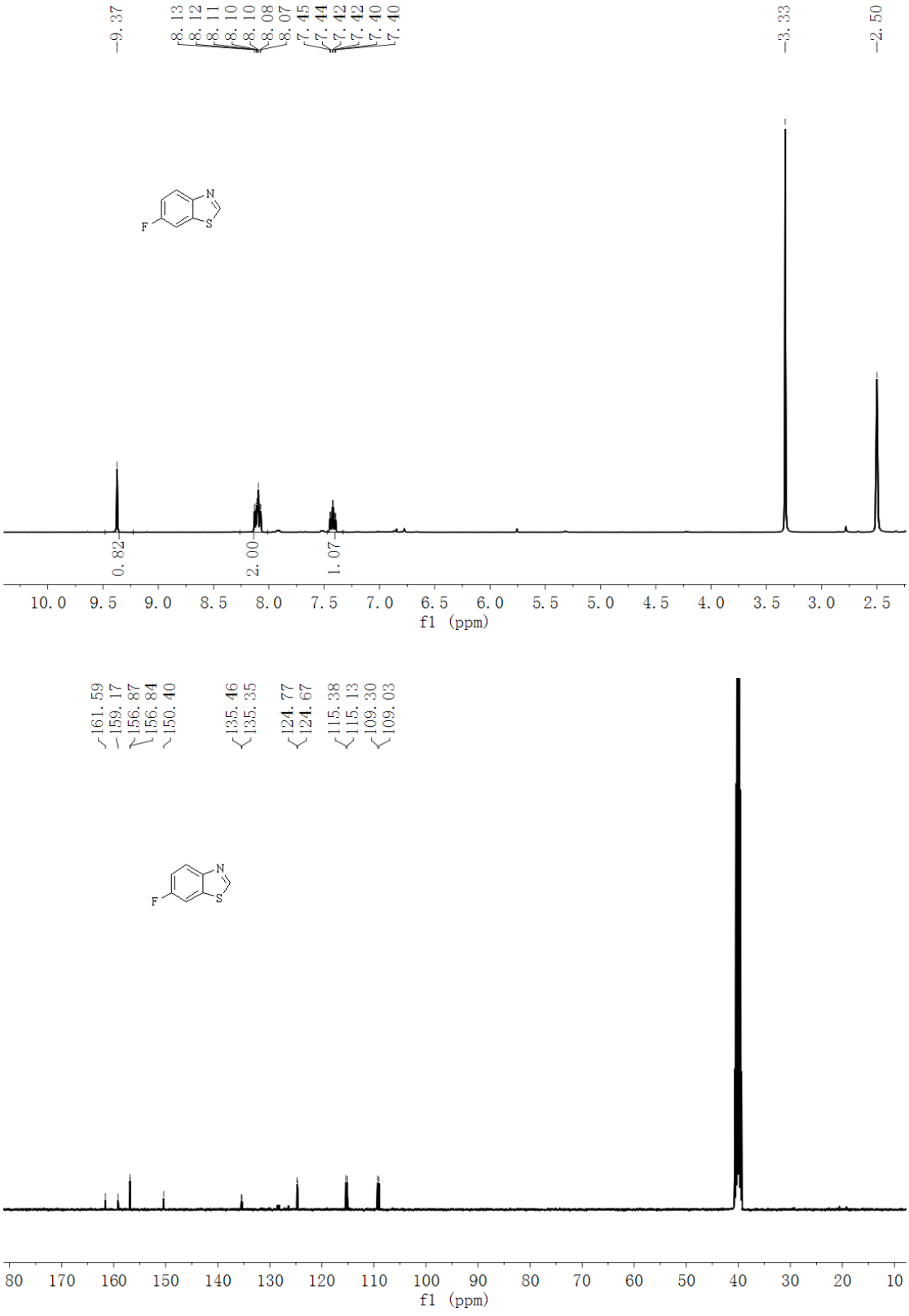

Figure S8. ^{1}H NMR and ^{13}C NMR spectra of 5-fluorobenzothiazole (1f)

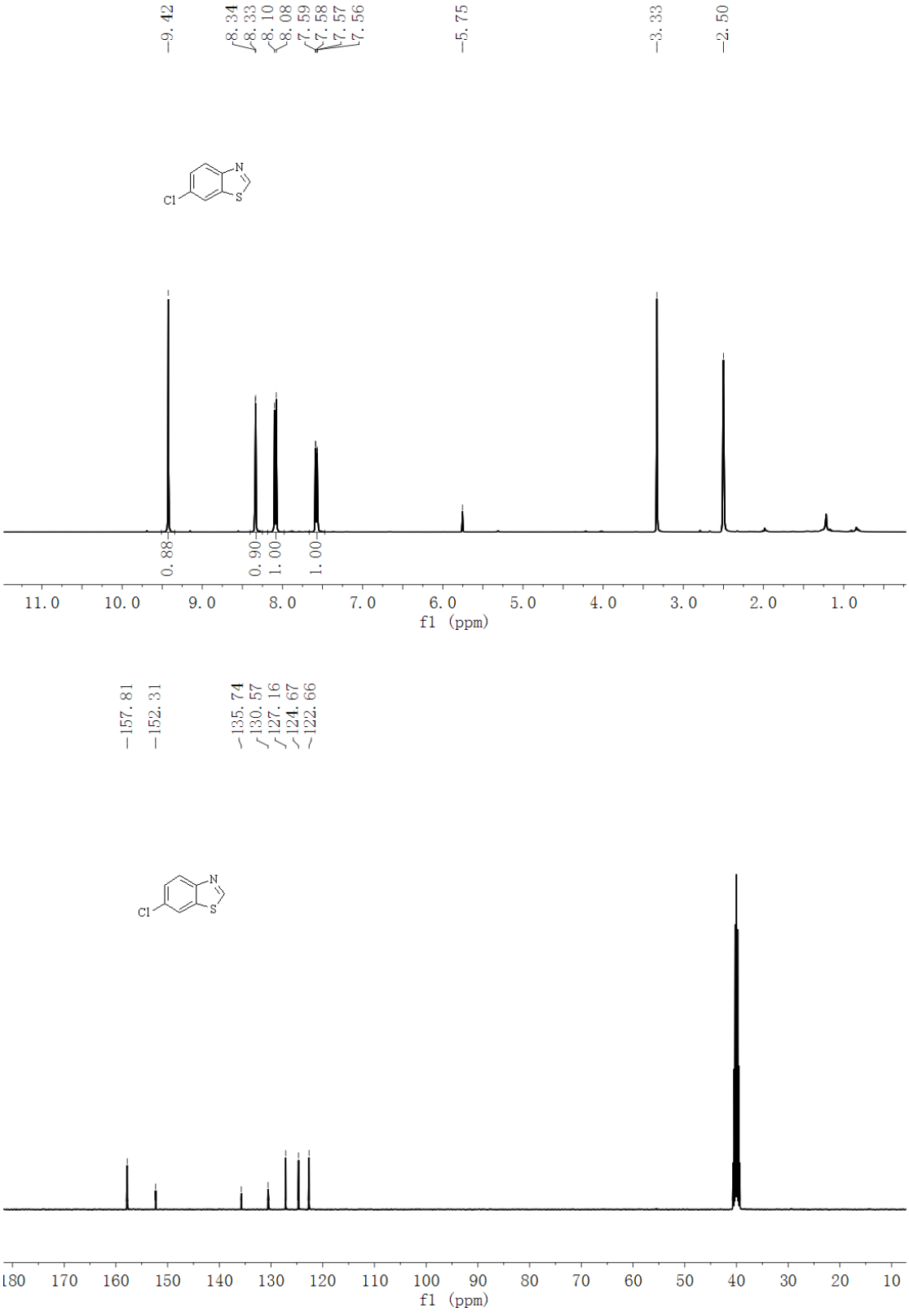

Figure S9. ^{1}H NMR and ^{13}C NMR spectra of 5-chlorobenzothiazole (1g)

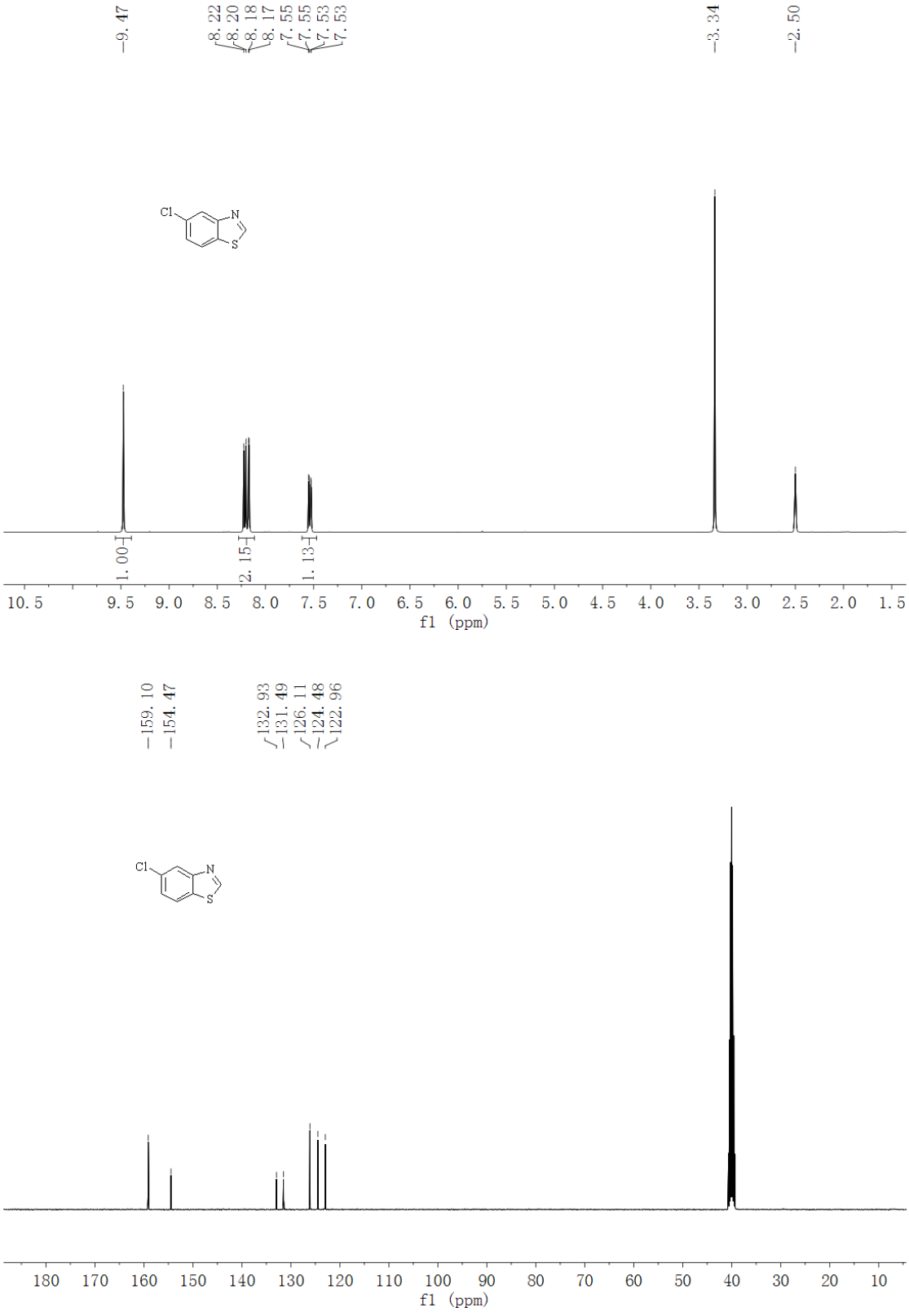

Figure S10. ^{1}H NMR and ^{13}C NMR spectra of 6-chlorobenzothiazole (1h)

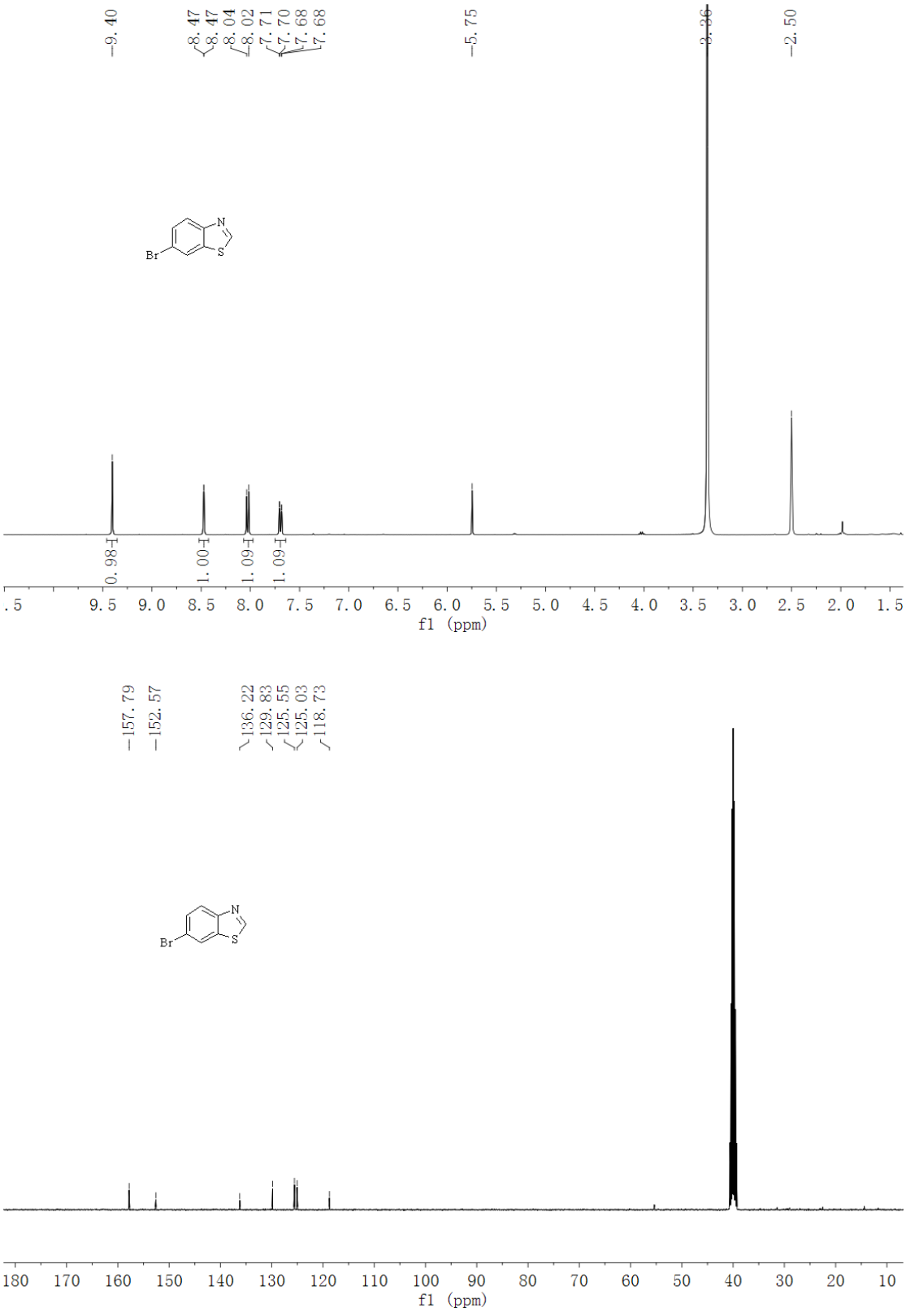

Figure S11. ^{1}H NMR and ^{13}C NMR spectra of 5-bromobenzothiazole (1i)

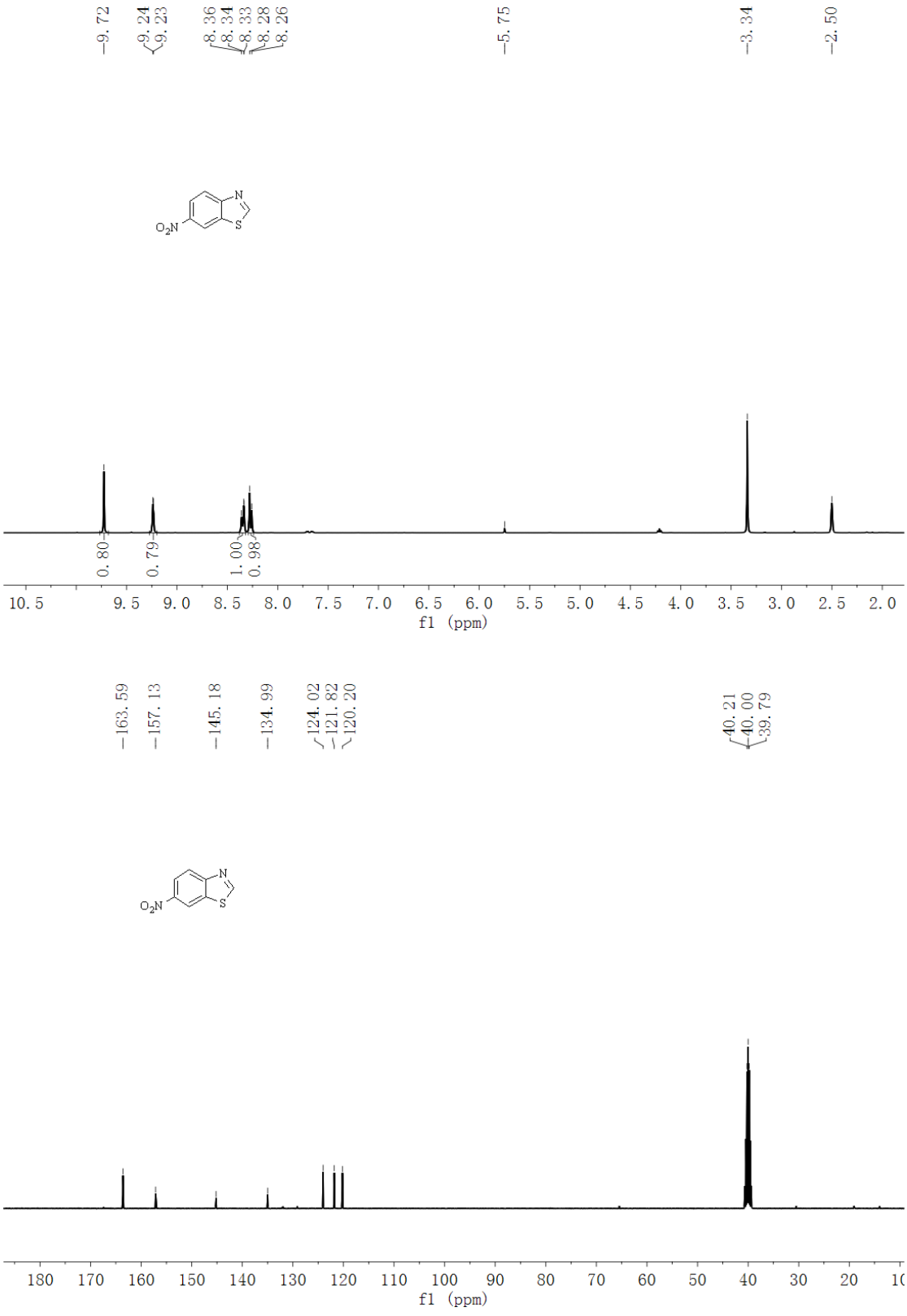

Figure S12. ^{1}H NMR and ^{13}C NMR spectra of 5-nitrobenzothiazole (1j)

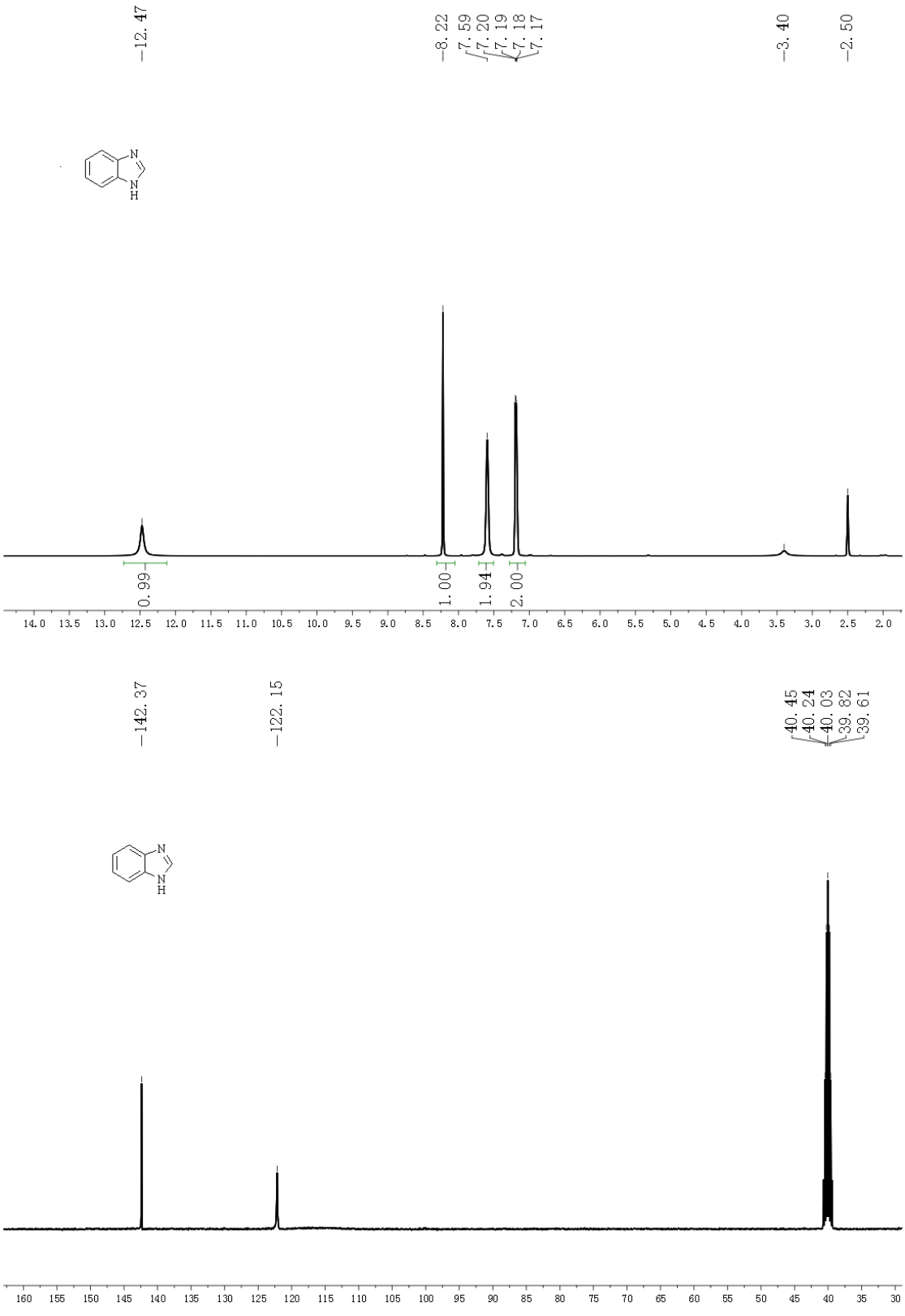

Figure S13. ^{1}H NMR and ^{13}C NMR spectra of benzimidazole (2a)

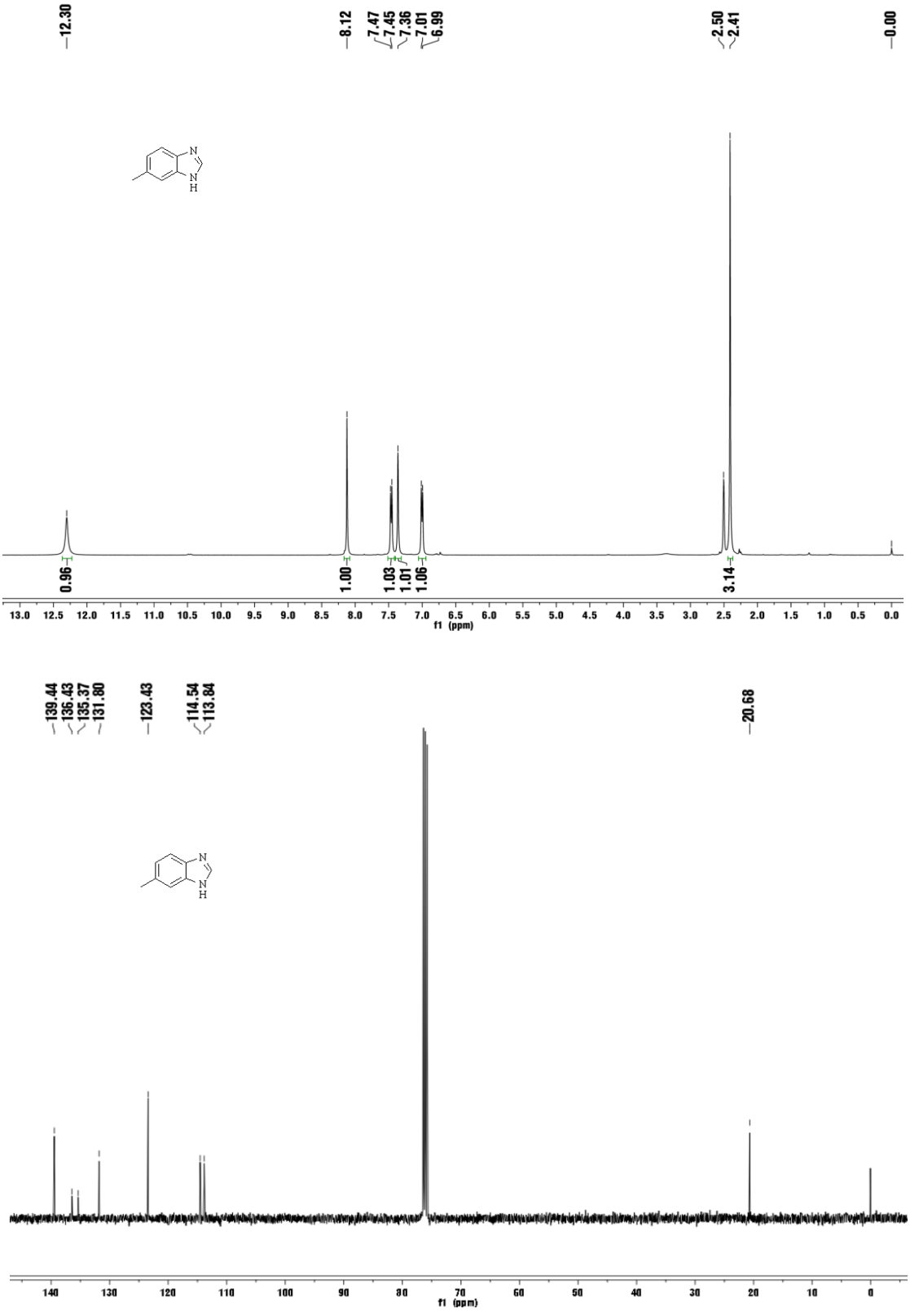

Figure S14. ^{1}H NMR and ^{13}C NMR spectra of 6-methylbenzimidazole (2b)

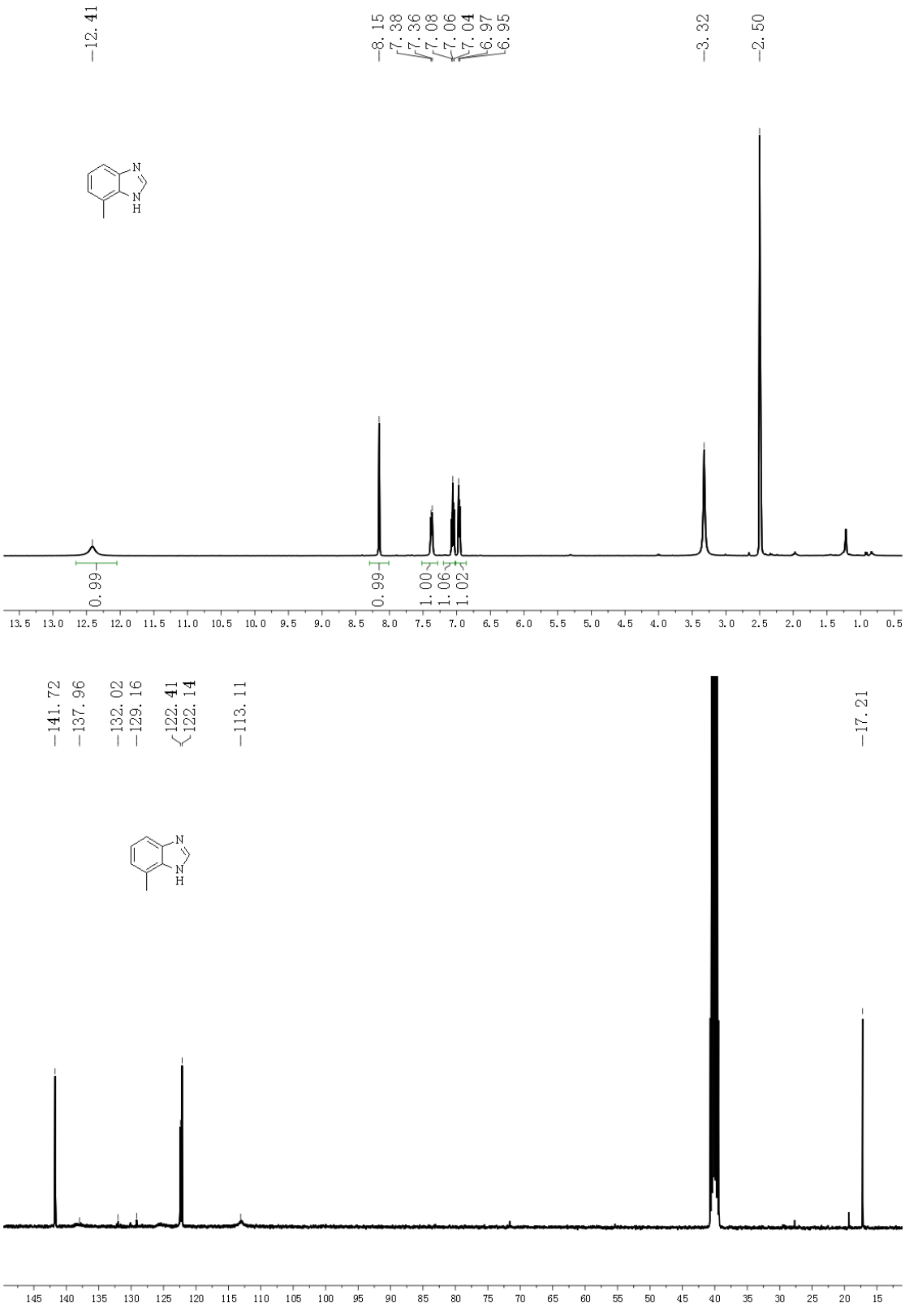

Figure S15. ^{1}H NMR and ^{13}C NMR spectra of 7-methylbenzimidazole (2c)

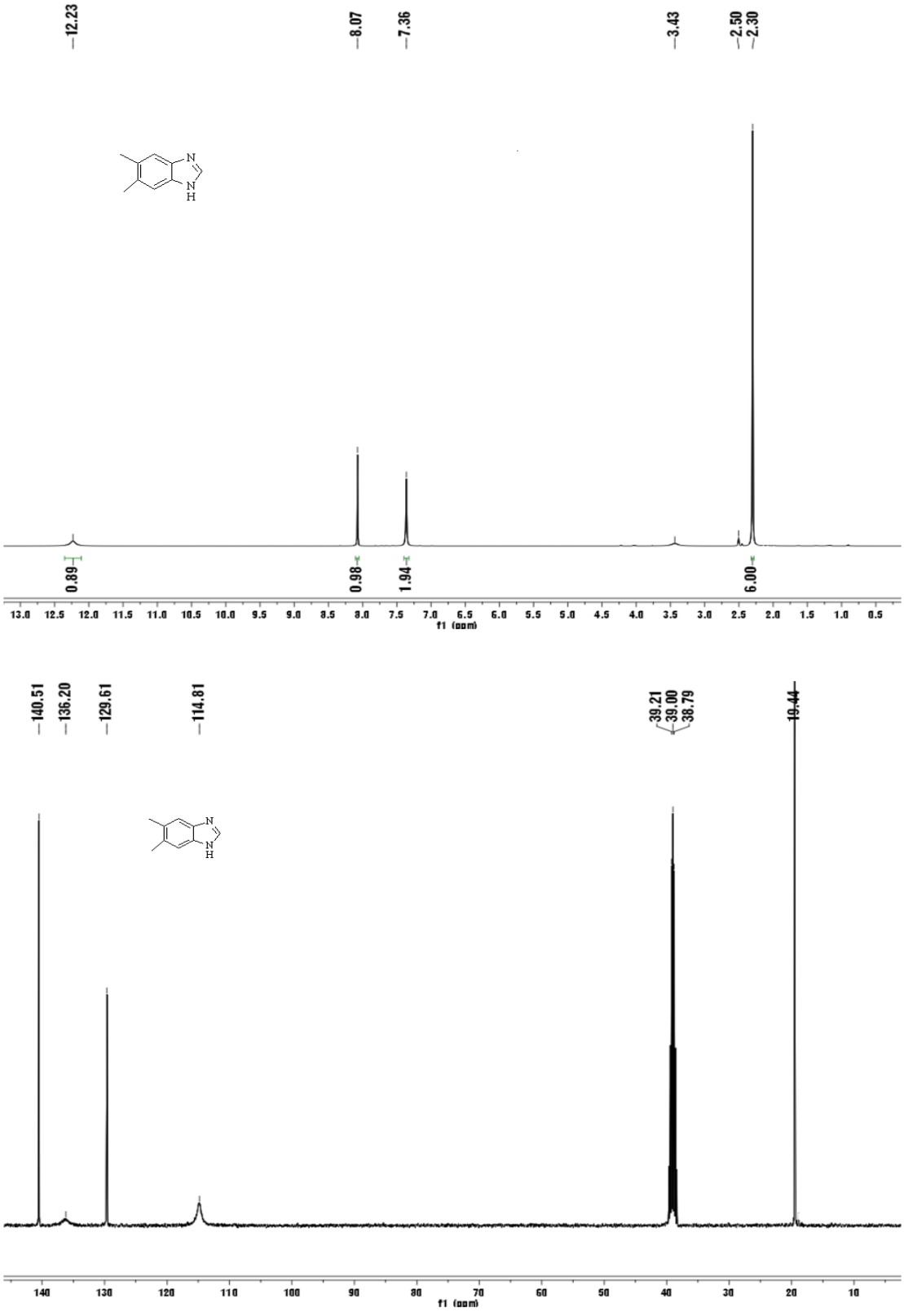

Figure S16. ^{1}H NMR and ^{13}C NMR spectra of 5, 6-dimethylbenzimidazole (2d)

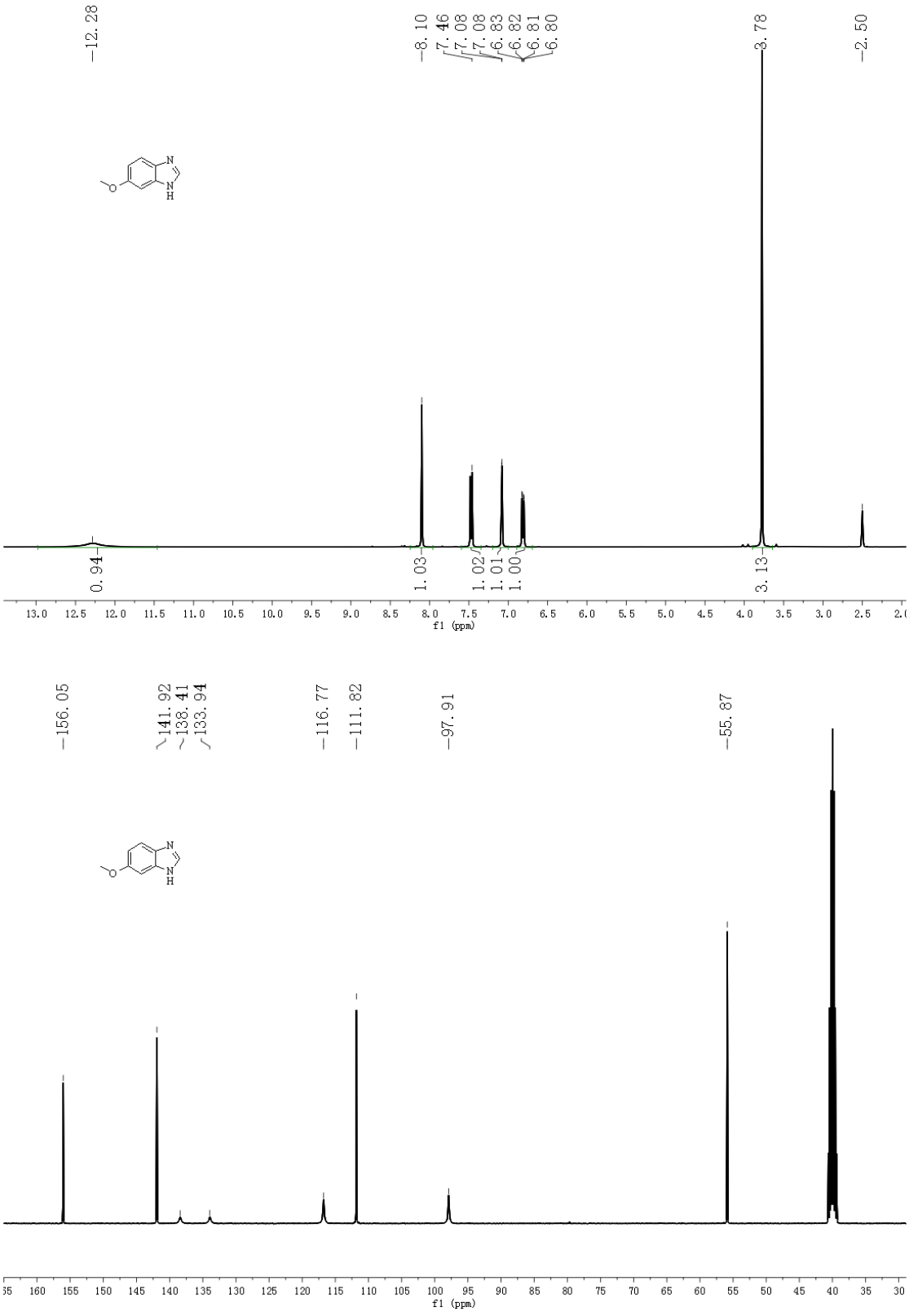

Figure S17. ^{1}H NMR and ^{13}C NMR spectra of 6-methoxybenzimidazole (2e)

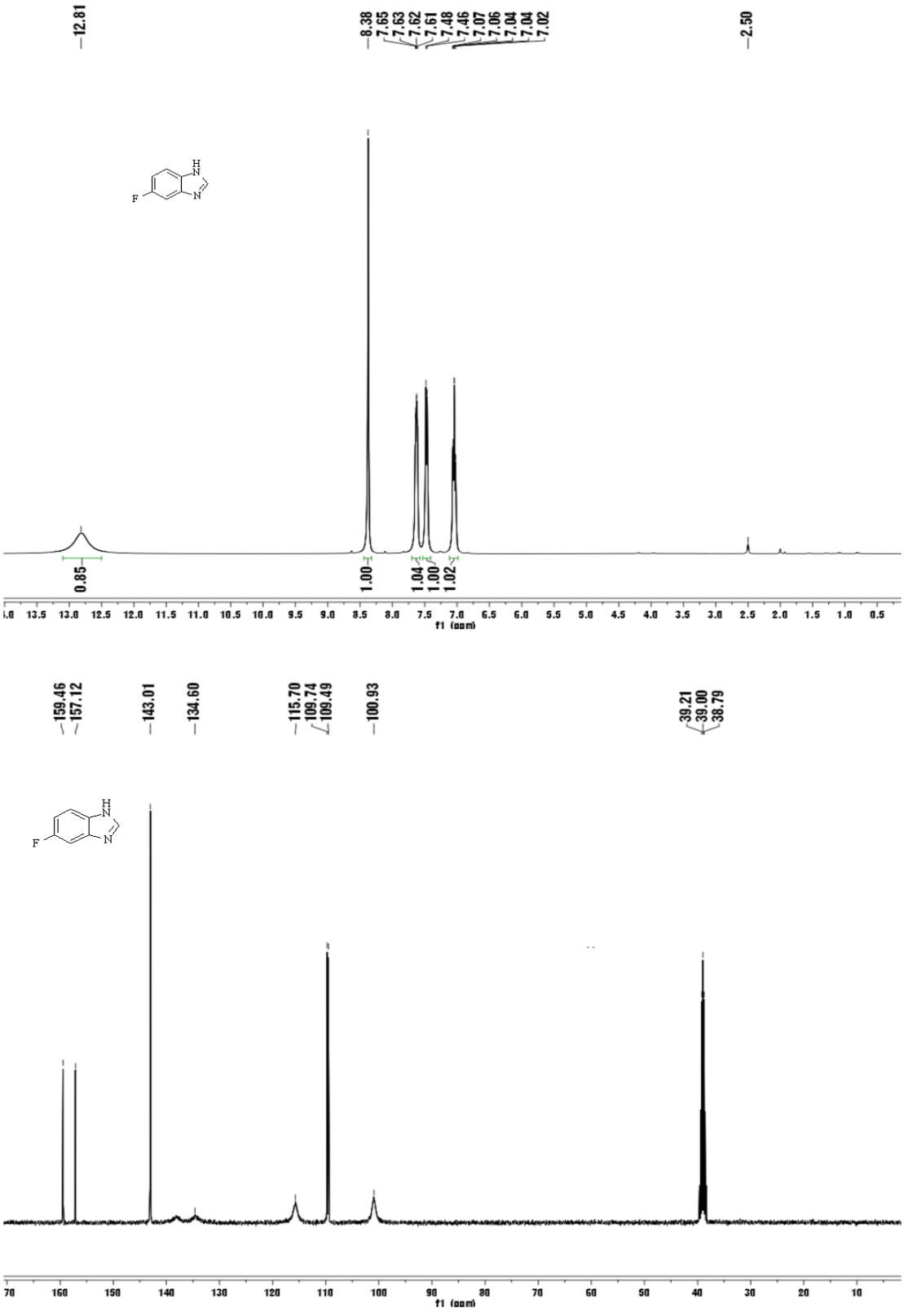

Figure S18. ^{1}H NMR and ^{13}C NMR spectra of 5-fluorobenzimidazole (2f)

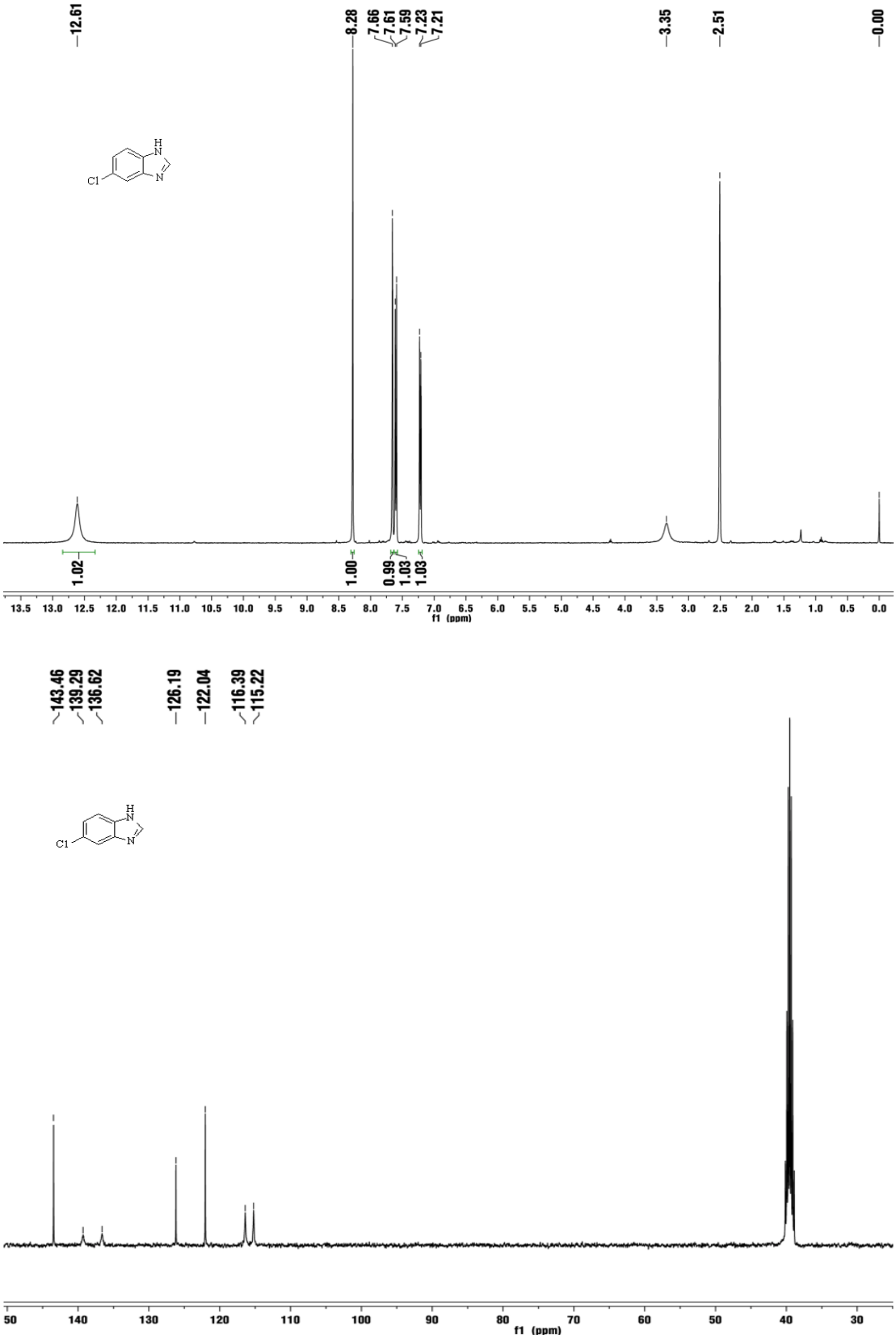

Figure S19. ^{1}H NMR and ^{13}C NMR spectra of 5-chlorobenzimidazole (2g)

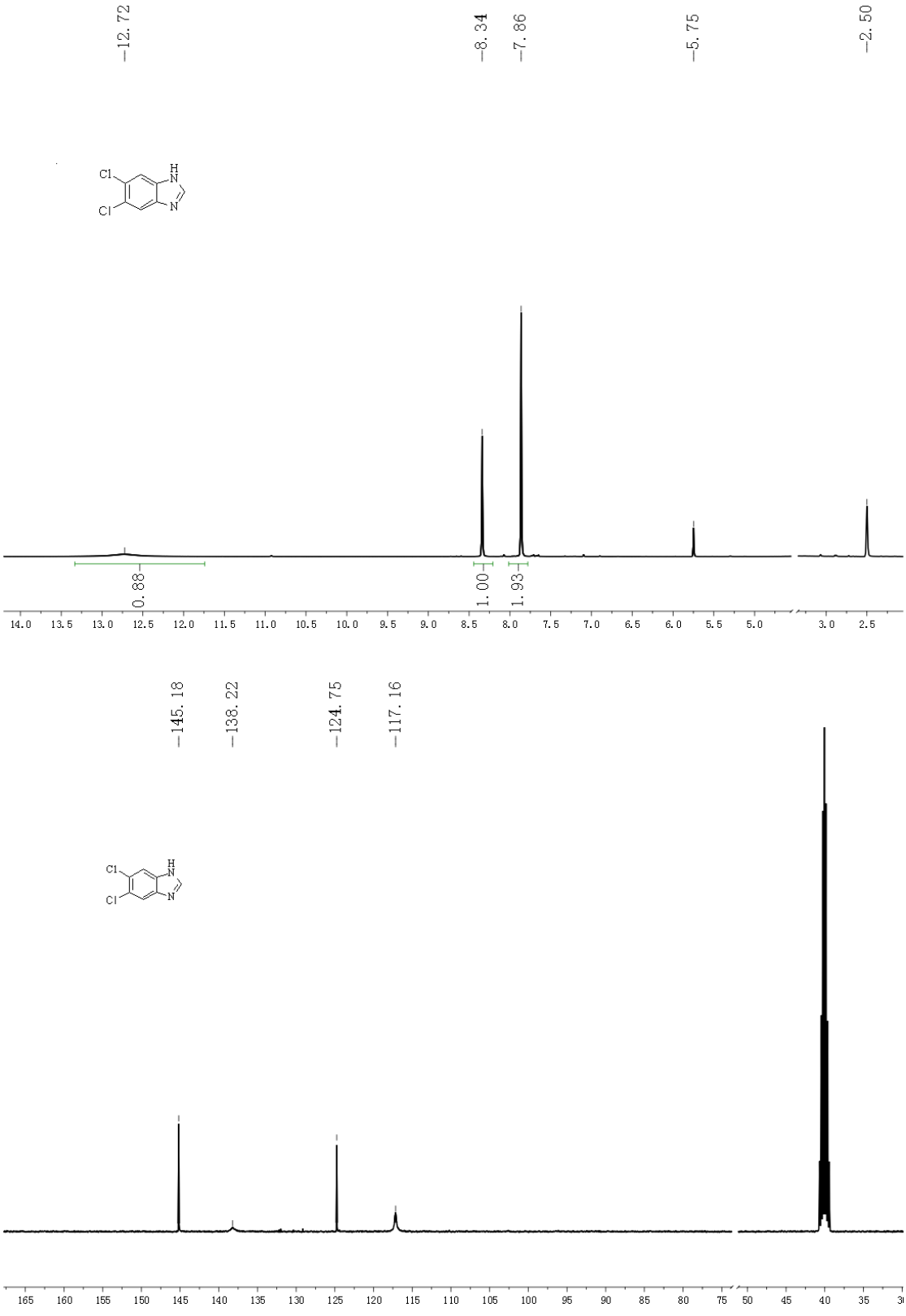

Figure S20. ^{1}H NMR and ^{13}C NMR spectra of 5, 6-dichlorobenzimidazole (2h)

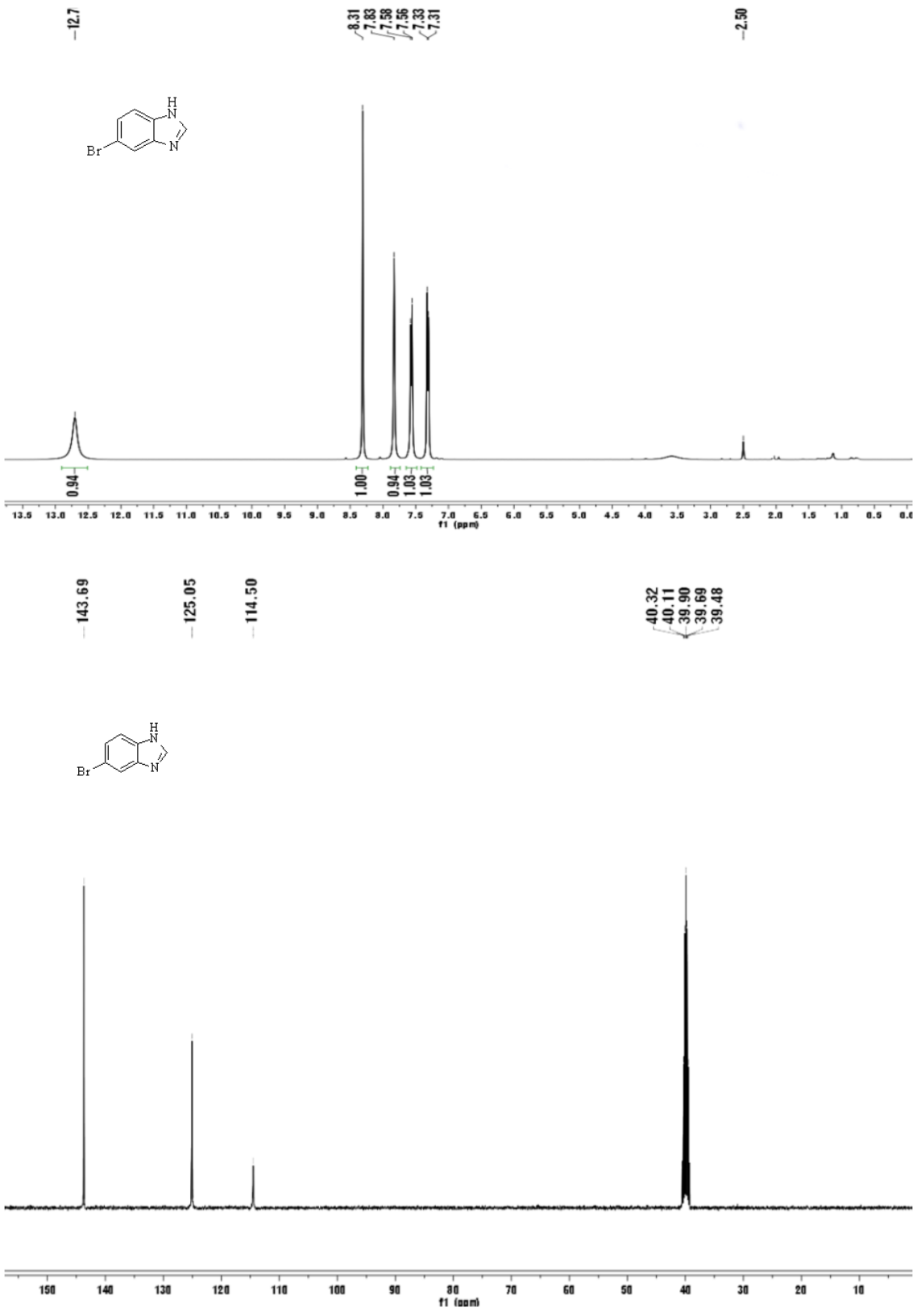

Figure S21. ^{1}H NMR and ^{13}C NMR spectra of 5-bromobenzimidazole (2i)

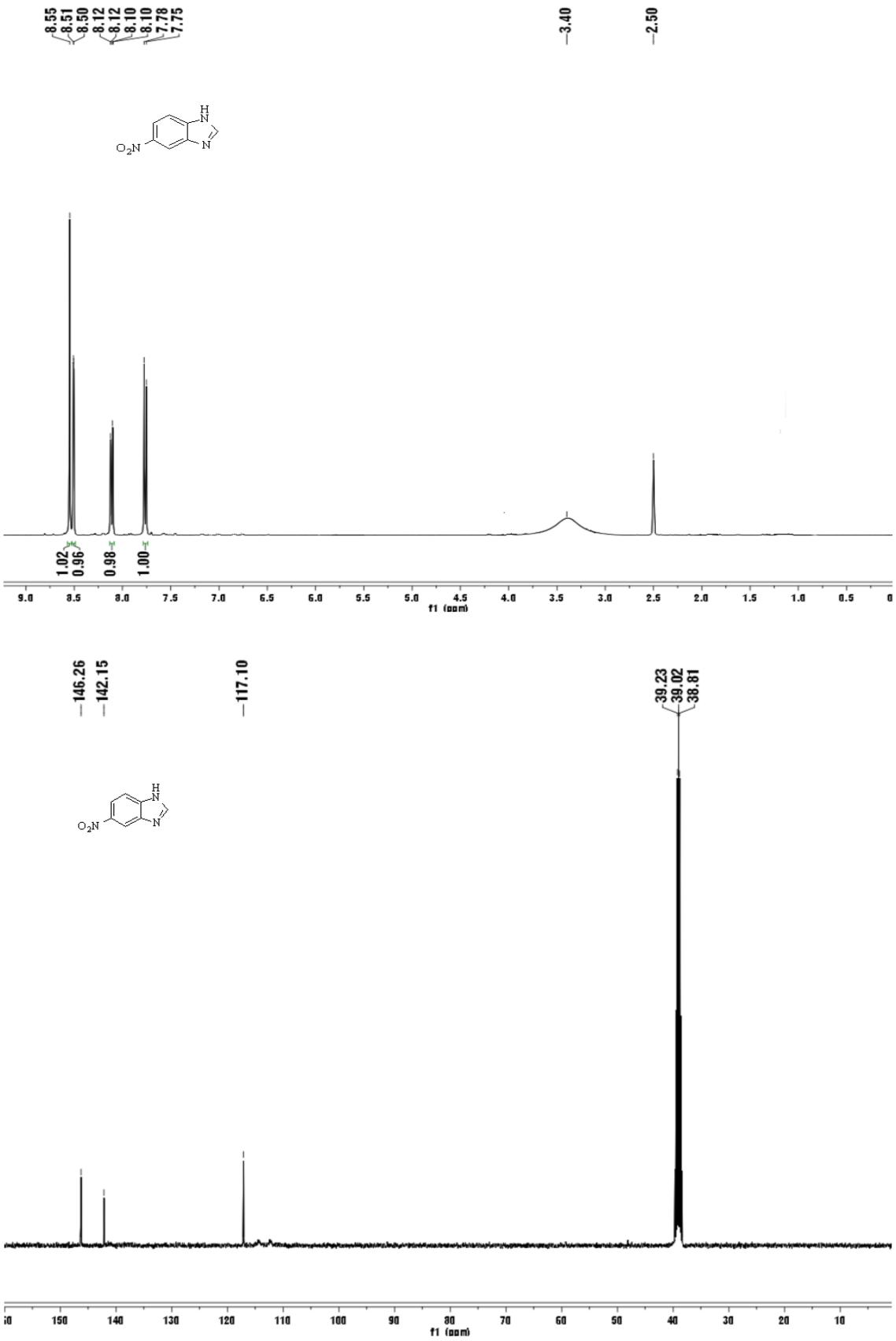

Figure S22. ^{1}H NMR and ^{13}C NMR spectra of 5-nitrobenzimidazole (2j)

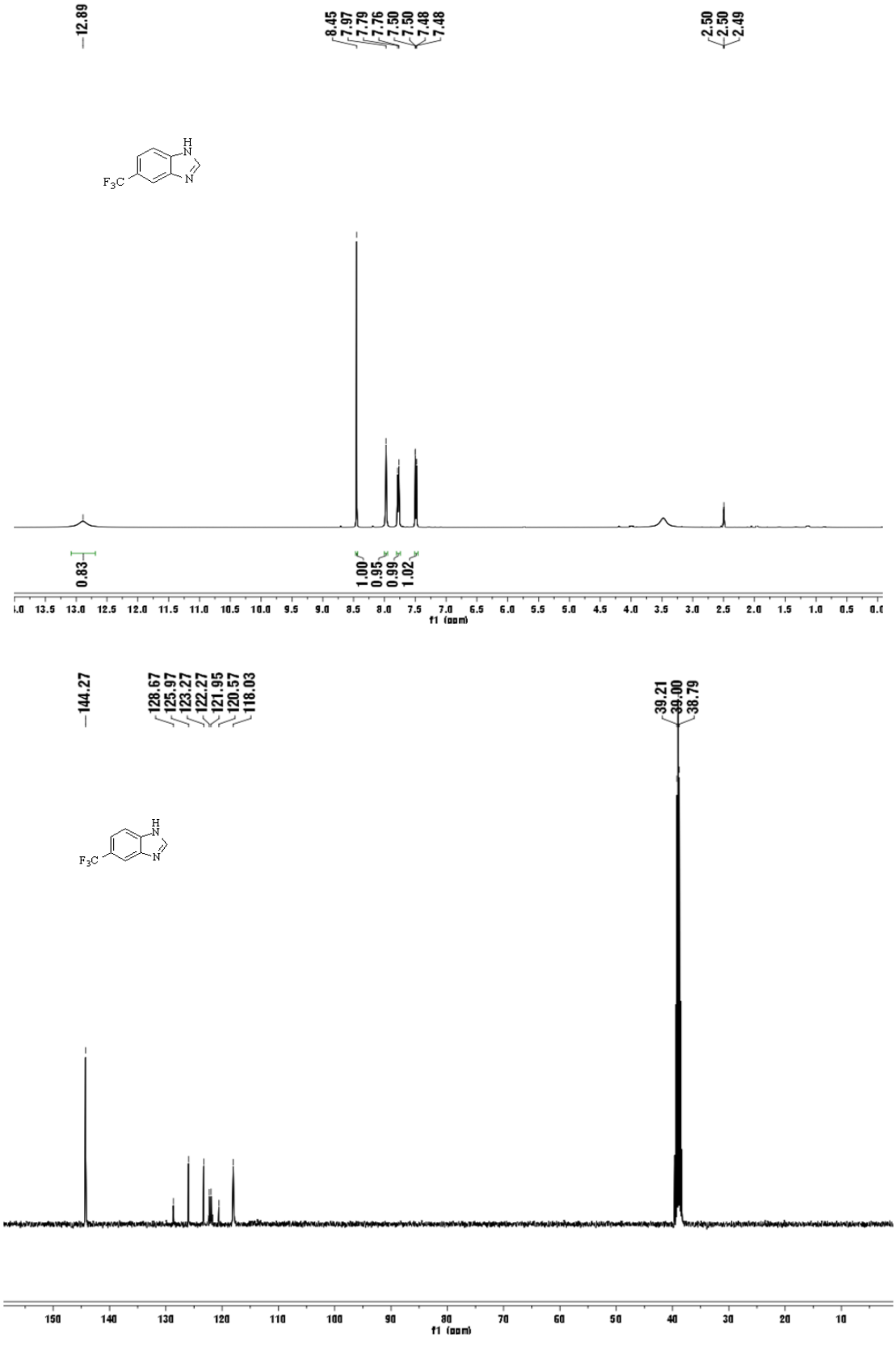

Figure S23. ^{1}H NMR and ^{13}C NMR spectra of 5-trifluoromethylbenzimidazole (2k)

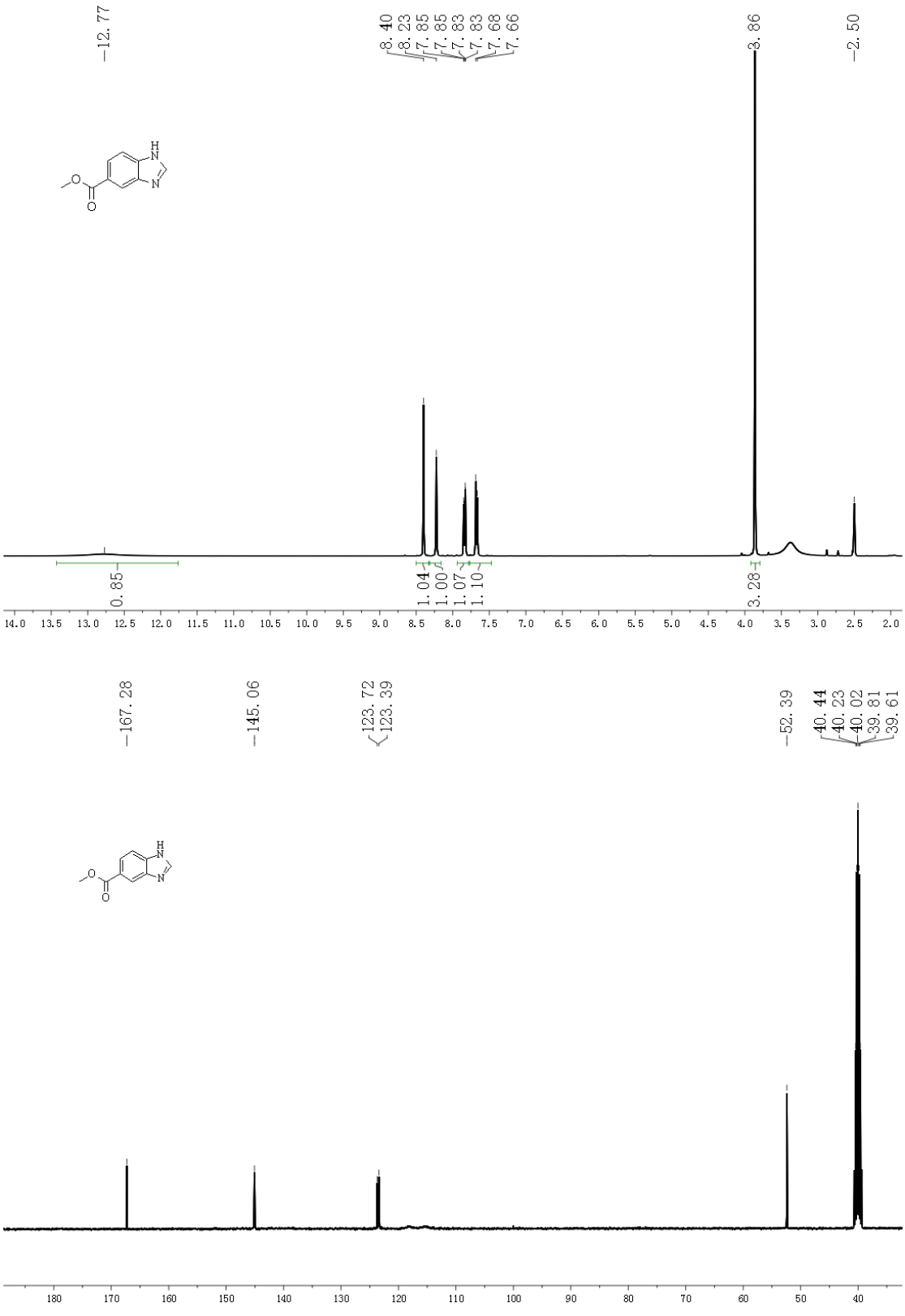

Figure S24. ^{1}H NMR and ^{13}C NMR spectra of methyl benzimidazole-5-carboxylate (2l)

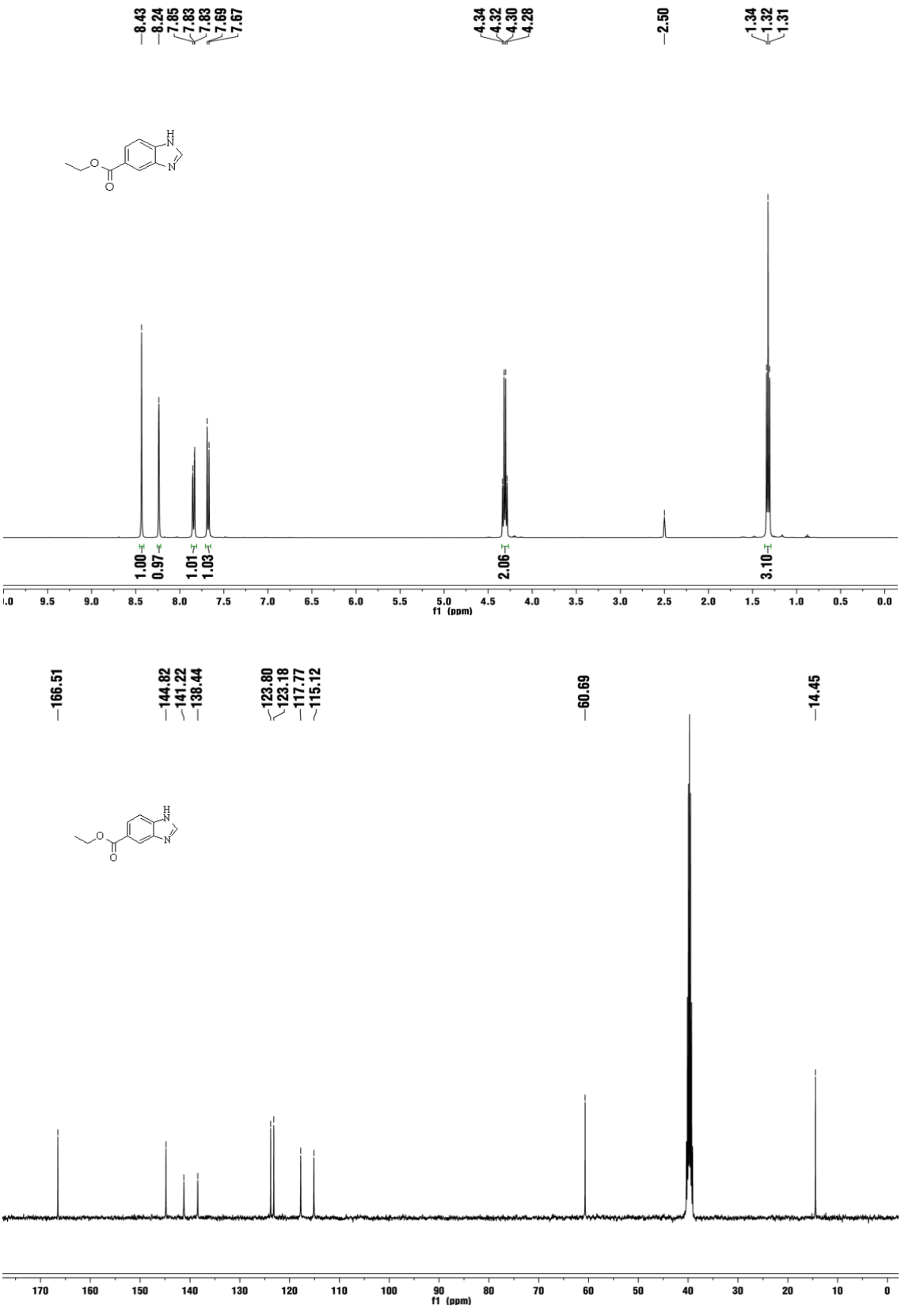

Figure S25. ^{1}H NMR and ^{13}C NMR spectra of etheyl benzimidazole-5-carboxylate (2m)

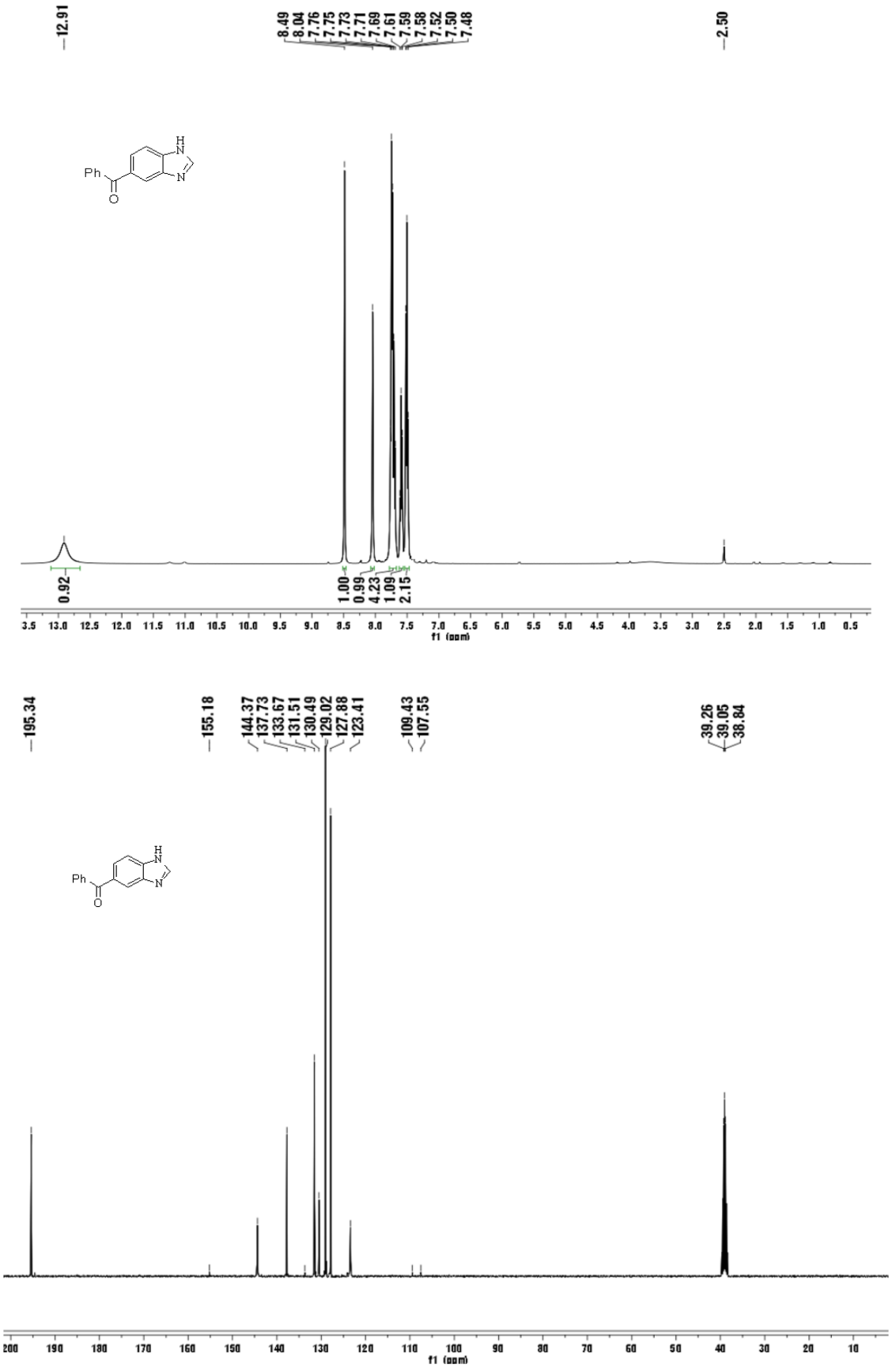

Figure S26. ^{1}H NMR and ^{13}C NMR spectra of 5-benzoylbenzimidazole (2n)

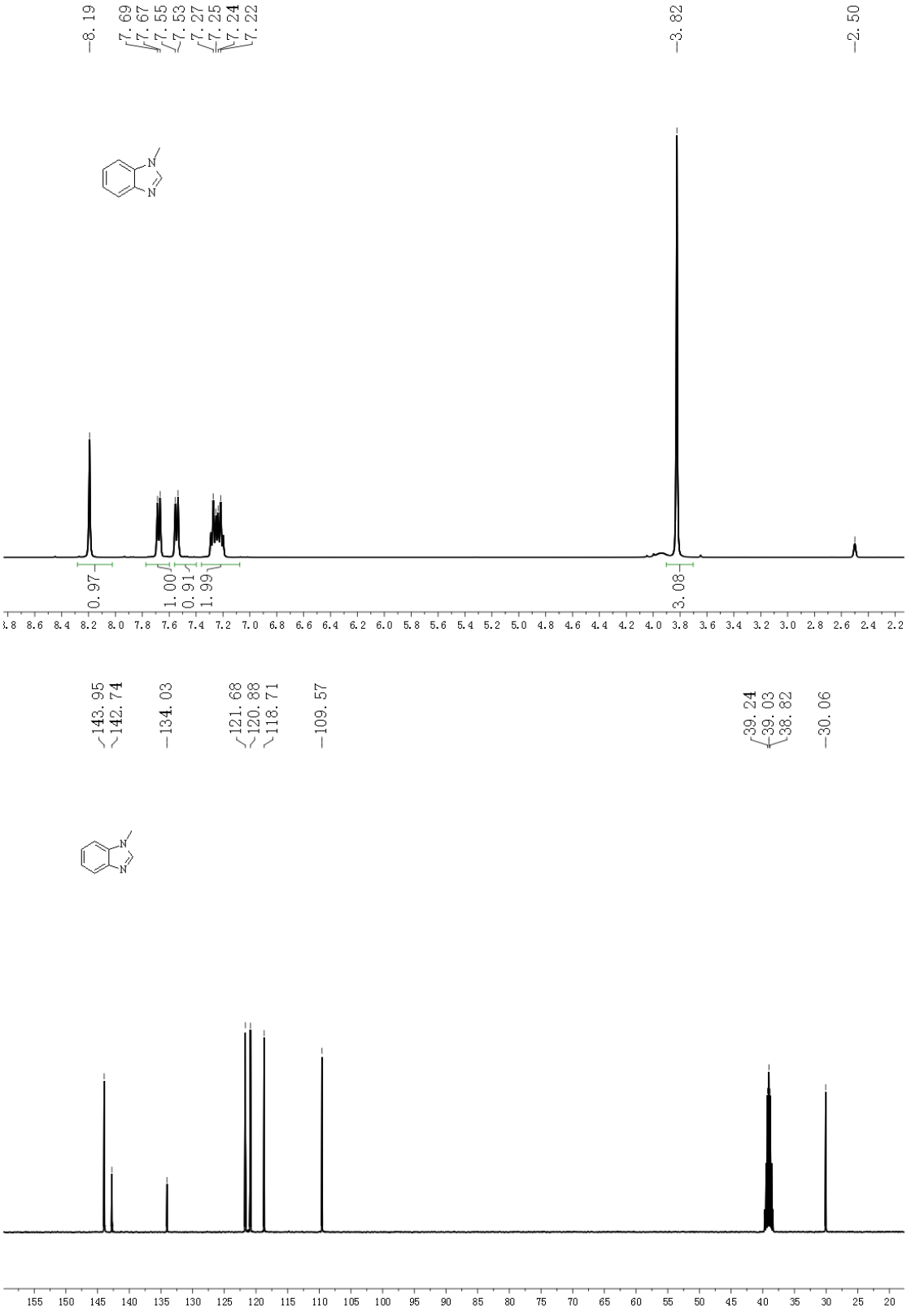

Figure S27. ^{1}H NMR and ^{13}C NMR spectra of N-methylbenzimidazole (2o)

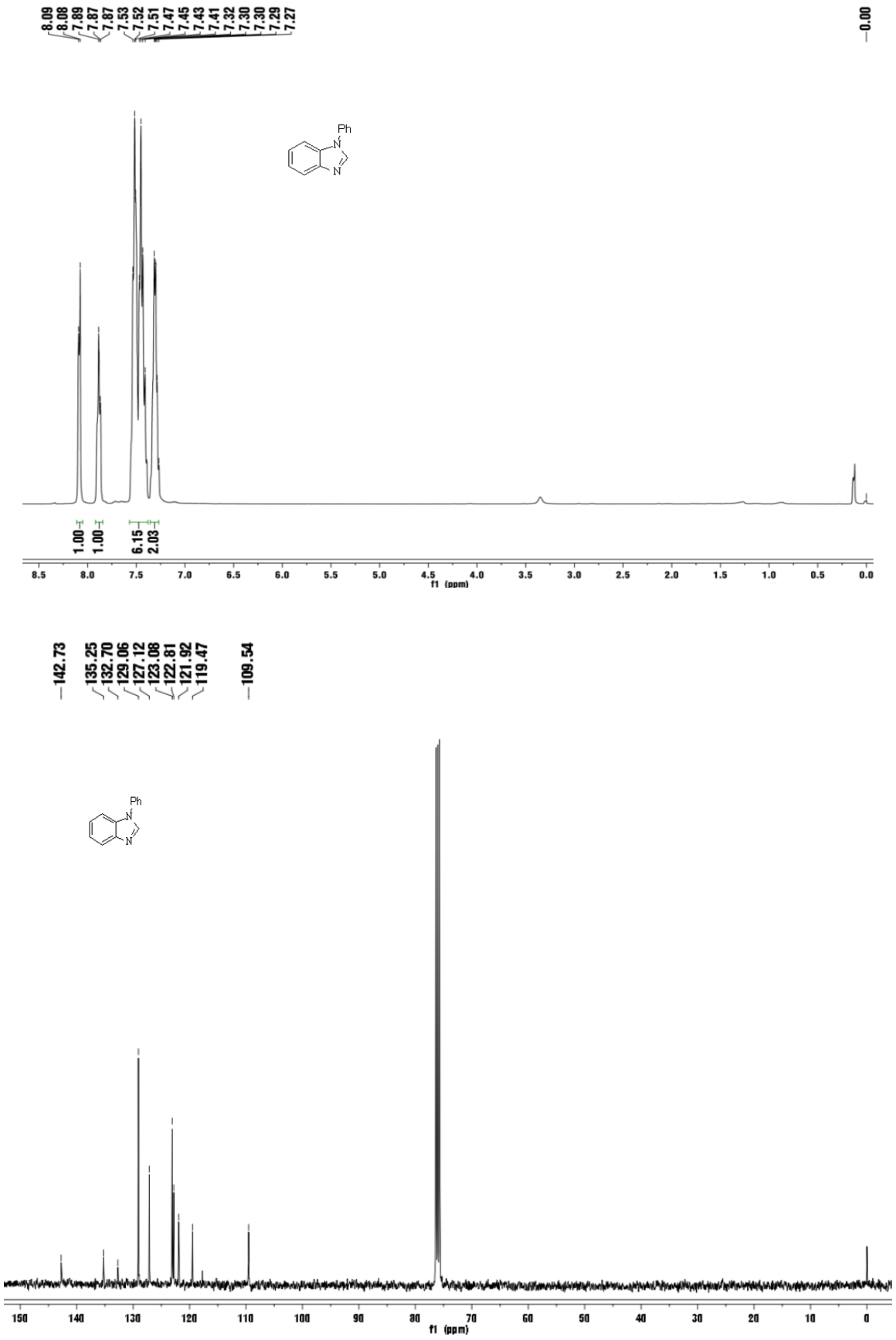

Figure S28. ^{1}H NMR and ^{13}C NMR spectra of N-phenylbenzimidazole (2p)

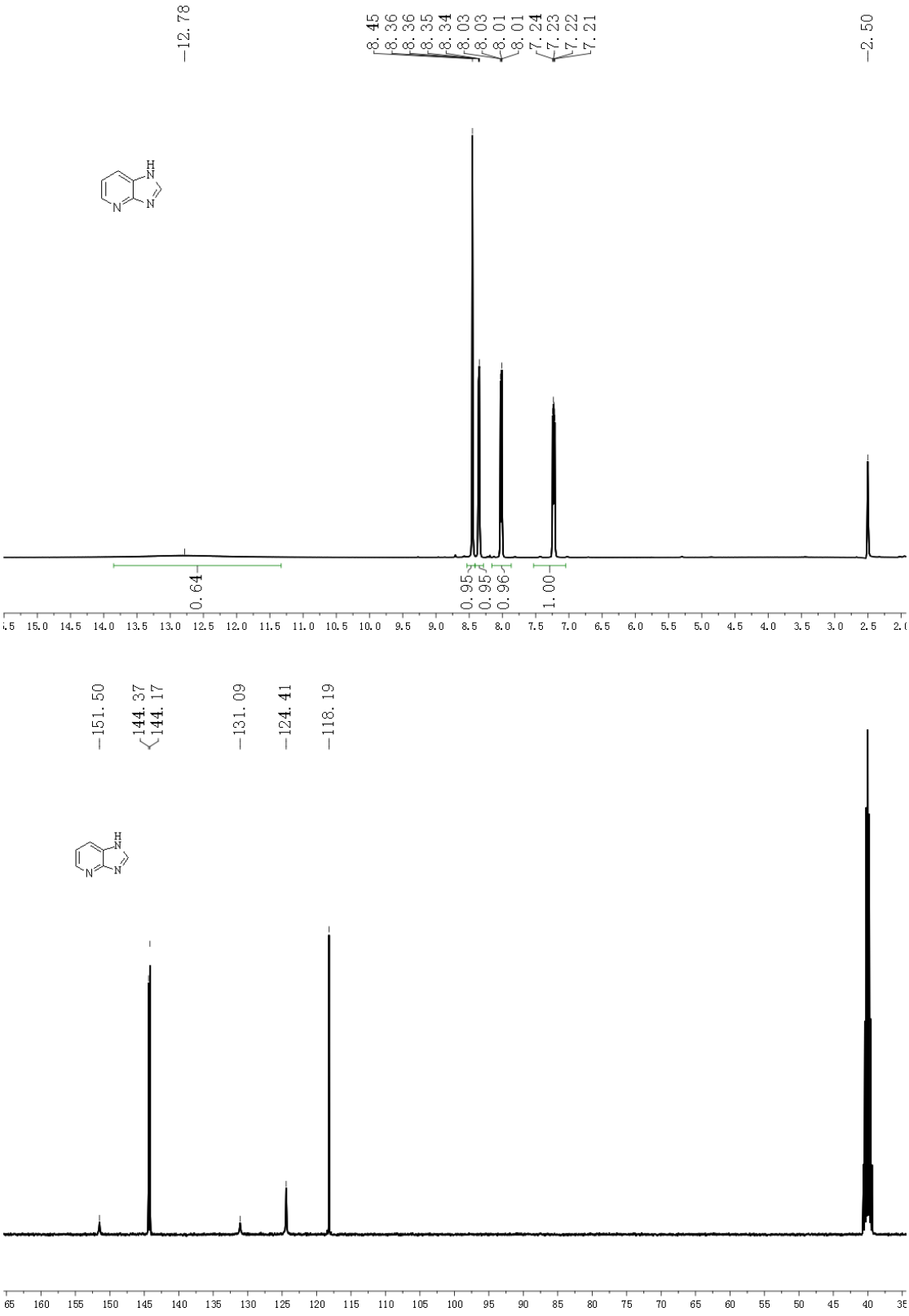

Figure S29. ^{1}H NMR and ^{13}C NMR spectra of 4-azabenzimidazole (2q)

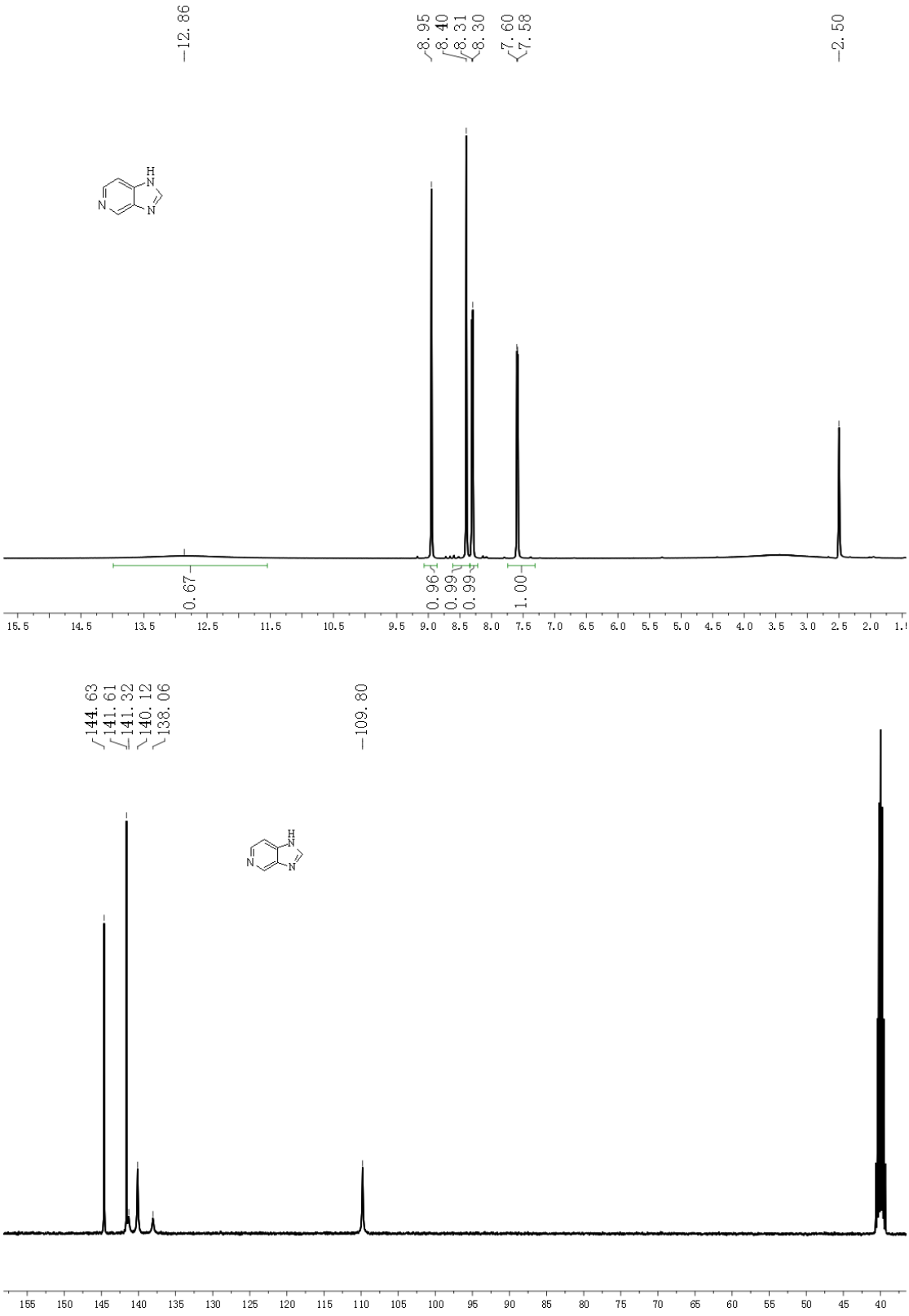

Figure S30. ^{1}H NMR and ^{13}C NMR spectra of 5-azabenzimidazole (2r)

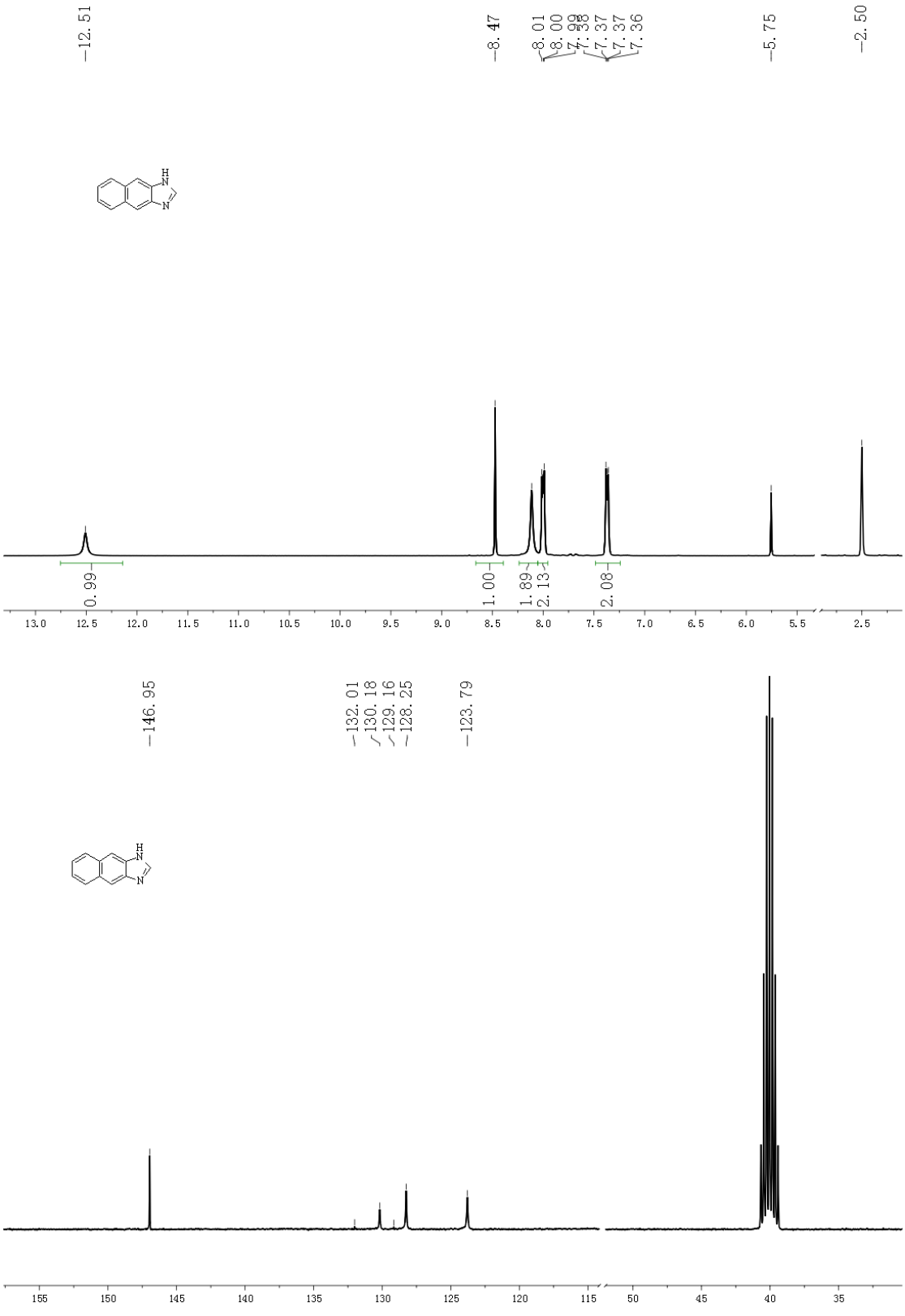

Figure S31. ^{1}H NMR and ^{13}C NMR spectra of 5-azabenzimidazole (2s)

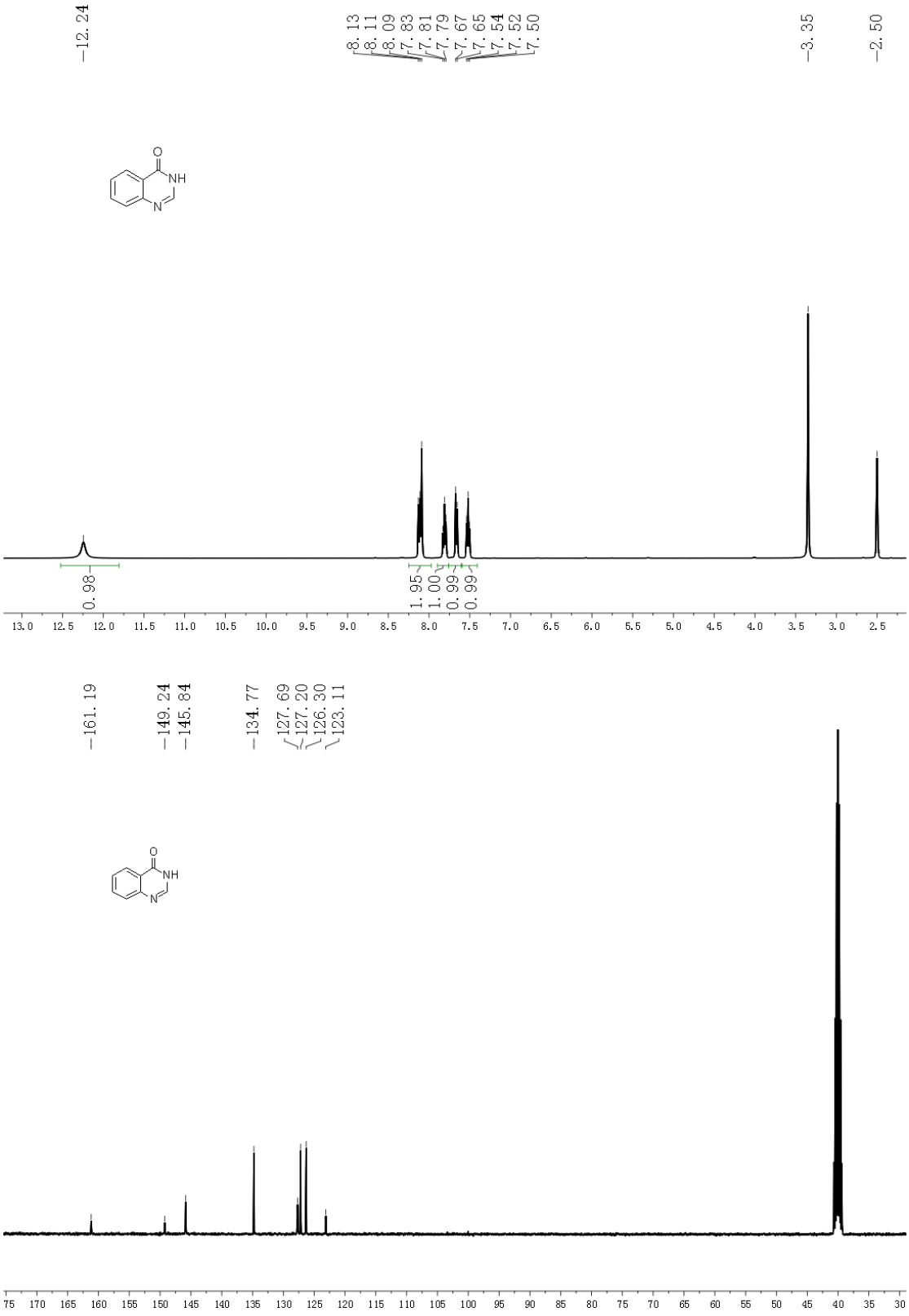

Figure S32. ^{1}H NMR and ^{13}C NMR spectra of quinazolinone benzoxazole (3a)

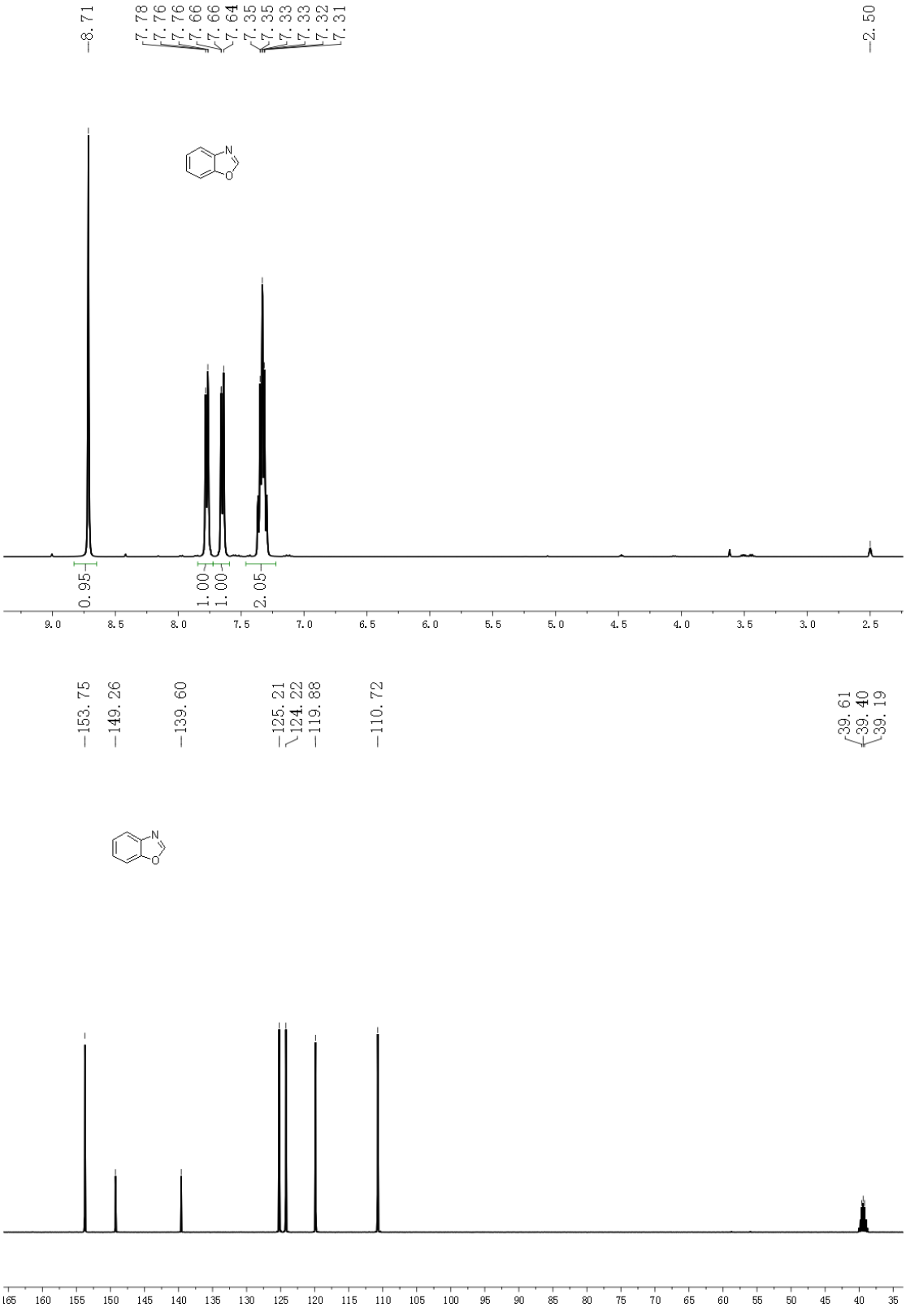

Figure S33. ^{1}H NMR and ^{13}C NMR spectra of benzoxazole (4a)

4. References

[1] S. Tzanopoulou, M. Sagnou, M. Paravatou-Petsotas, E. Gourni, G. Loudos, S. Xanthopoulos, D. Lafkas, H. Kiaris, A. Varvarigou, I. C. Pirmettis, M. Papadopoulos, M. Pelecanou, *J. Med. Chem.* **2010**, *53*, 4633-4641.

[2] M. C. Cui, X. D.Wang, P. R Yu, J. M. Zhang, Z. J. Li, X. J. Zhang, Y. P Yang, M. Ono, H. M.Jia, H. Saji, B. L Liu, *J. Med. Chem.* **2012**, *55*, 9283-9296.

[3] C. A. Mathis, Y. Wang, D. P. Holt, G. F. Huang, M. L. Debnath, W. E. Klunk, *J. Med. Chem.* **2003**, *46*, 2740-2754.

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