Supporting Information

Pd-catalyzed tandem reaction of N-(2-cyanoaryl)benzamides with arylboronic acids: synthesis of quinazolines

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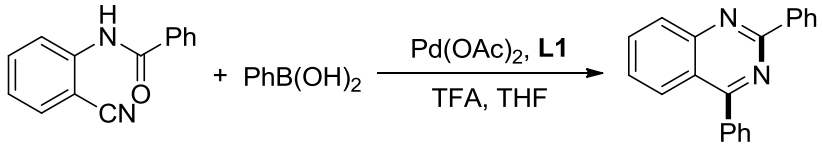
† These authors contributed equally.

1.1. Optimization of Reaction Conditions

Table S1. Conditions Screening for the Synthesis of Quinazoline[a]



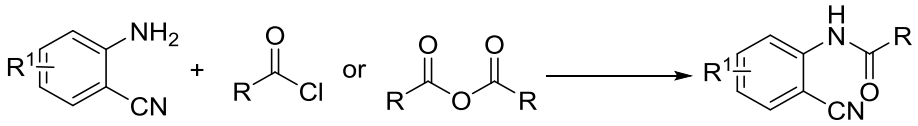
1a **2a** **3a**

entry	TFA (*x* equiv)	temperature (°C)	time (h)	yield (%)[b]
1	0.5	80	24	30
2	1	80	24	52
3	2	80	24	95
4	4	80	24	90
5	2	60	24	78
6	2	100	24	95
7	2	120	24	93
8	2	80	6	47
9	2	80	12	78
10	2	80	36	89

[a]Conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), $Pd(OAc)_2$ (5 mol %), **L1** (10 mol %), TFA (*x* equiv), THF (1 mL), 80 °C, 24 h, air. [b]Isolated yield.

1.2 General Procedure for the Synthesis of *N*-(2-Cyanophenyl)benzamides

N-(2-Cyanophenyl)acetamides were synthesized from 2-aminobenzonitriles and the appropriate acyl chloride or anhydride according to the modified procedure of the literatures.



2-Aminobenzonitriles (8 mmol) and dichloromethane (25 mL) were added to a 100 mL round bottom flask fitted with a rubber septum then the system was charged with nitrogen. The corresponding acyl chloride or anhydride (12 mmol) was slowly added dropwise under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 12-24 h. The reaction mixture was washed with saturated $NaHCO_3$ solution (3 × 20 mL), with brine (2 × 20 mL), dried over anhydrous Na_2SO_4, filtered and evaporated. The residue was purified by flash column chromatography with petroleum ether/ethyl acetate to afford *N*-(2-cyanophenyl) benzamides.

Copies of ^{1}H and ^{13}C NMR Spectra

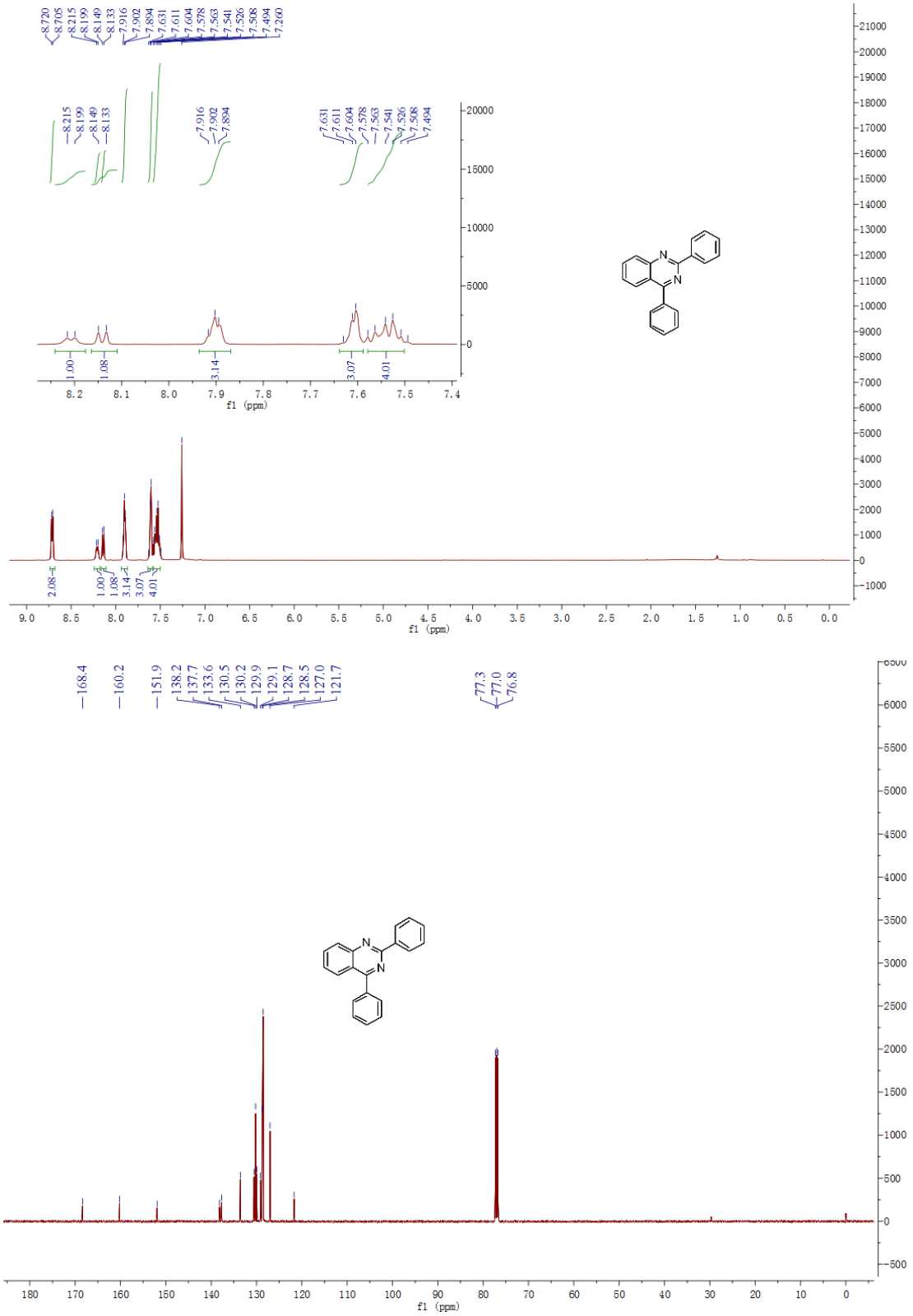


Figure S1. ^{1}H NMR of **3a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3a** (125 MHz, $CDCl_3$).

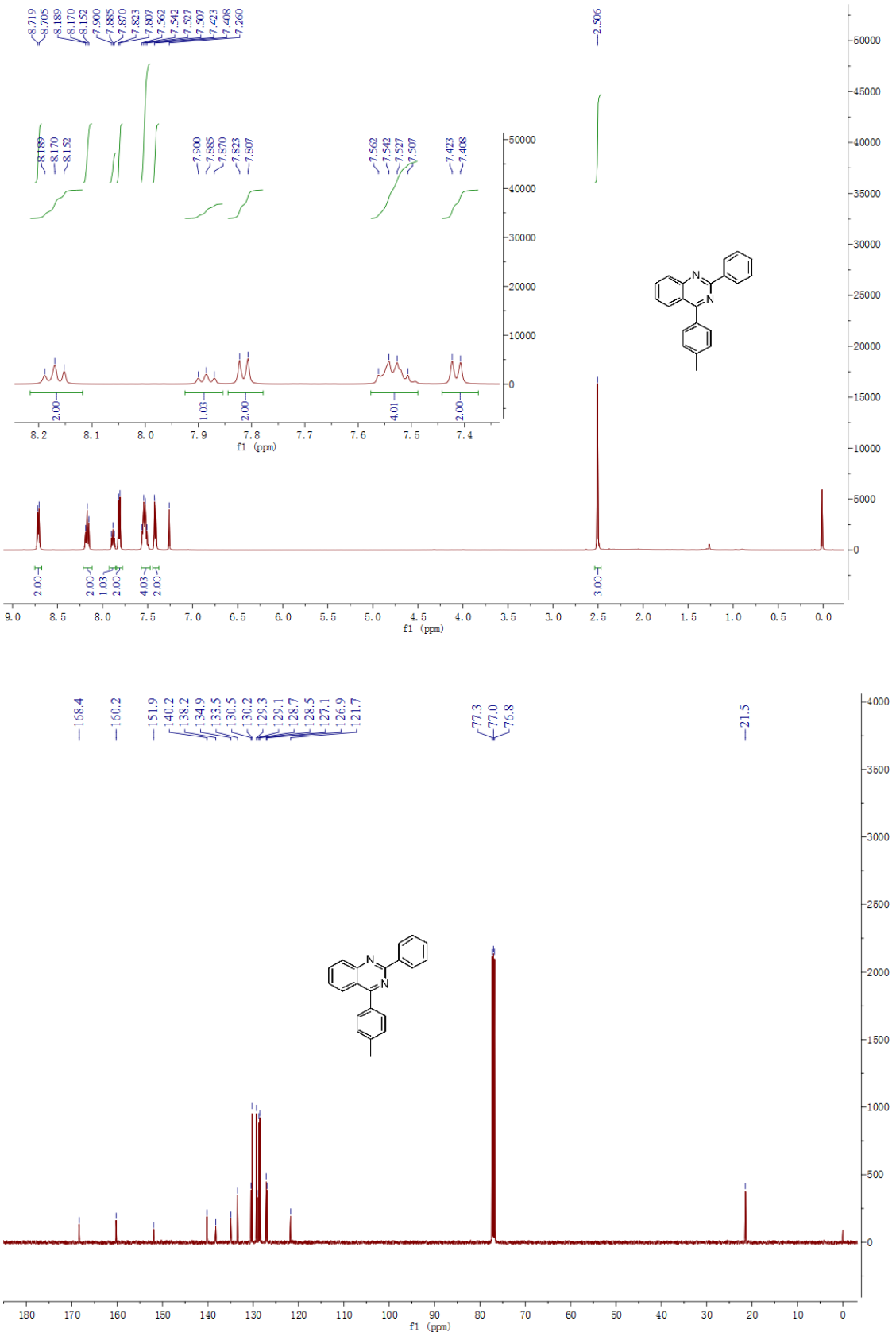


Figure S2. ^{1}H NMR of **3b** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3b** (125 MHz, $CDCl_3$)

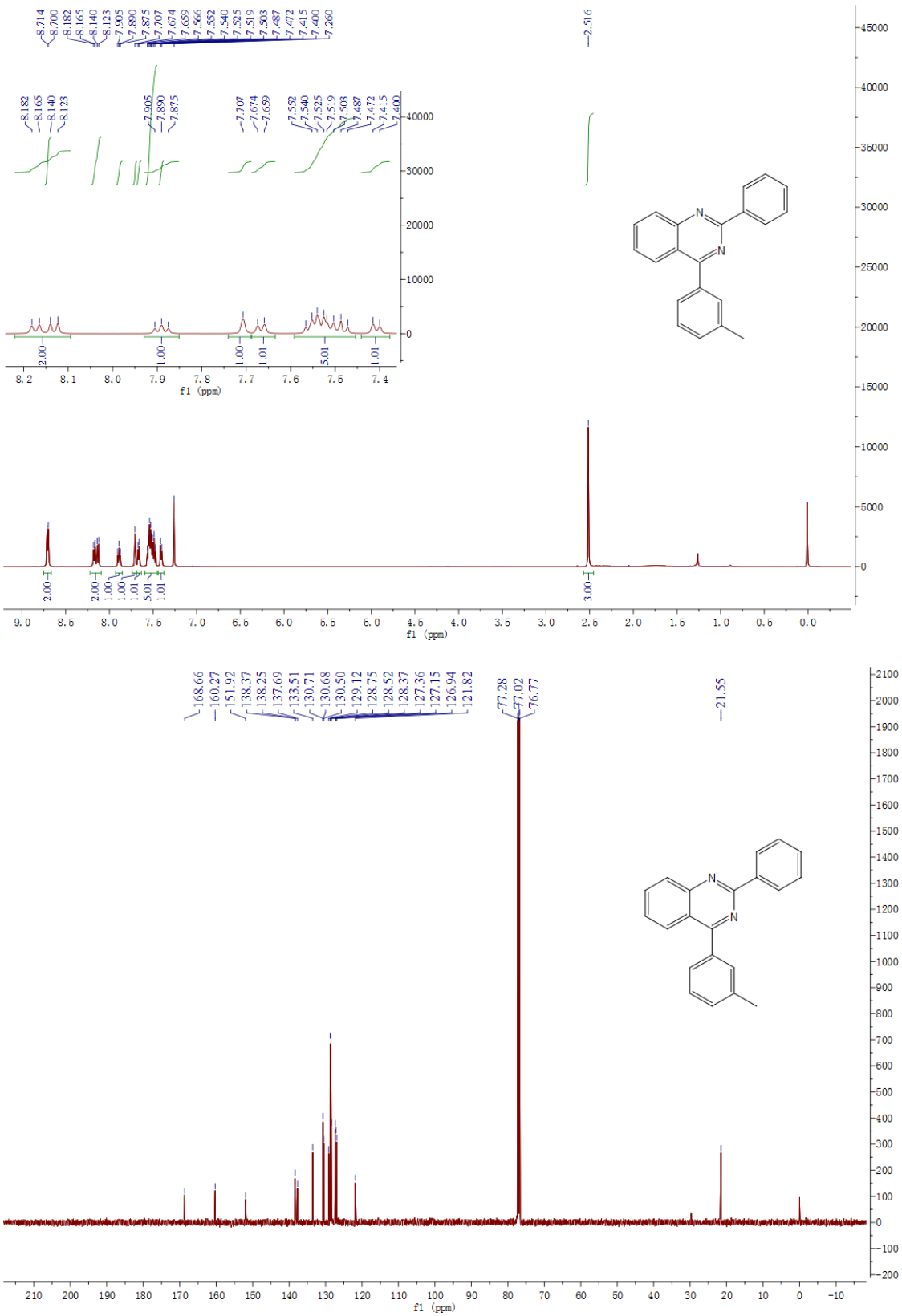


Figure S3. ^{1}H NMR of **3c** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3c** (125 MHz, $CDCl_3$)

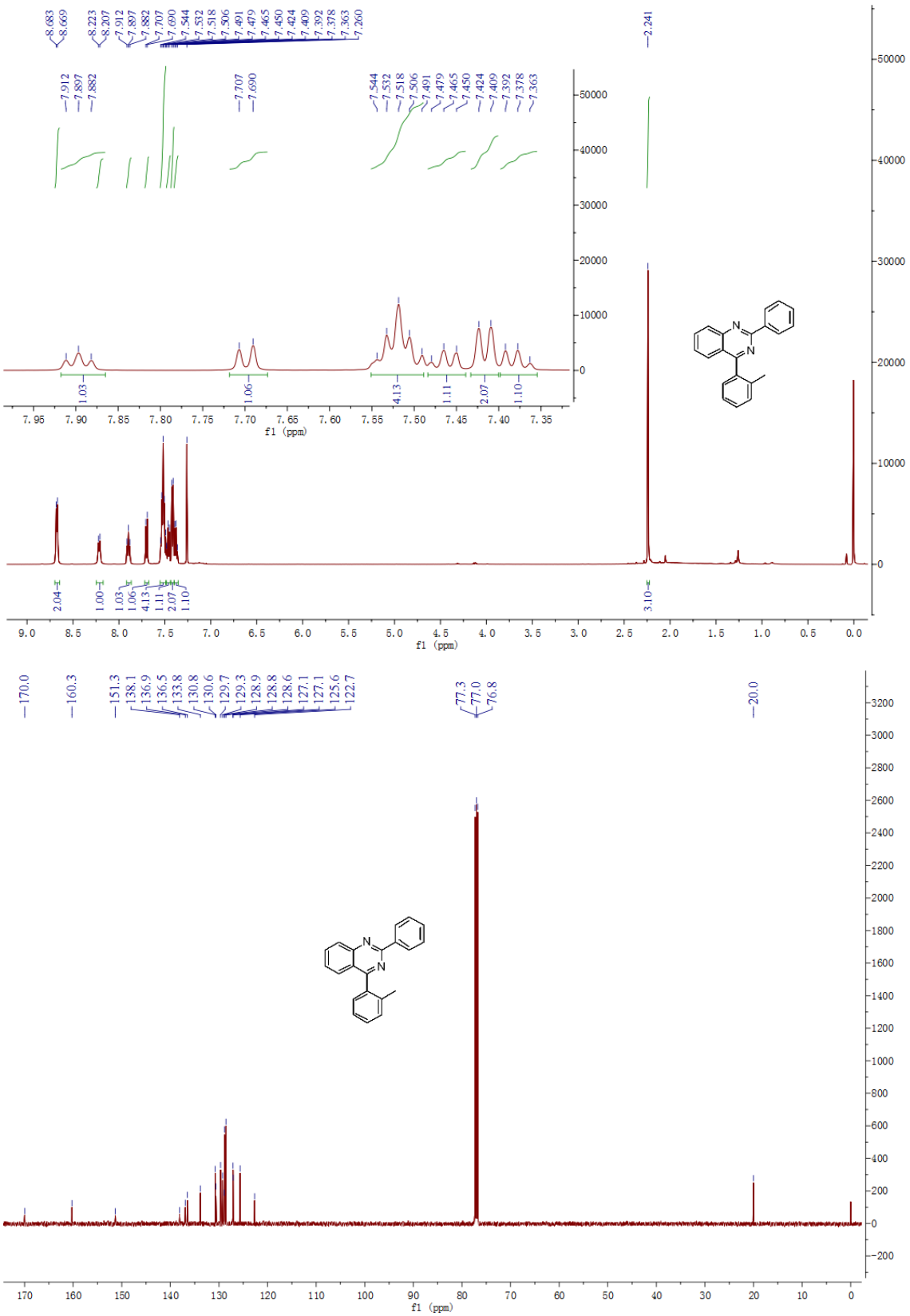


Figure S4. ^{1}H NMR of **3d** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3d** (125 MHz, $CDCl_3$)

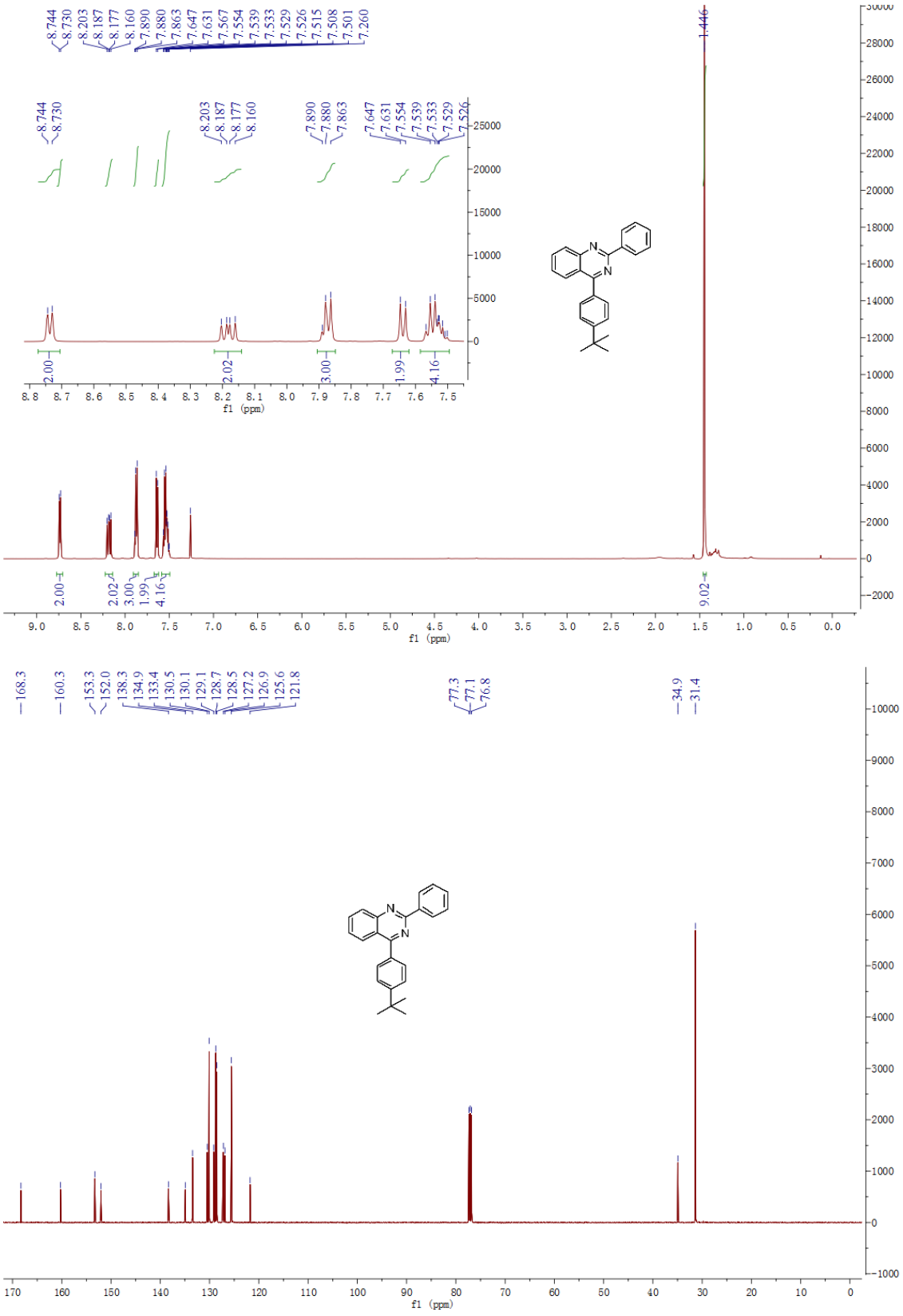


Figure S5. ^{1}H NMR of **3e** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3e** (125 MHz, $CDCl_3$)

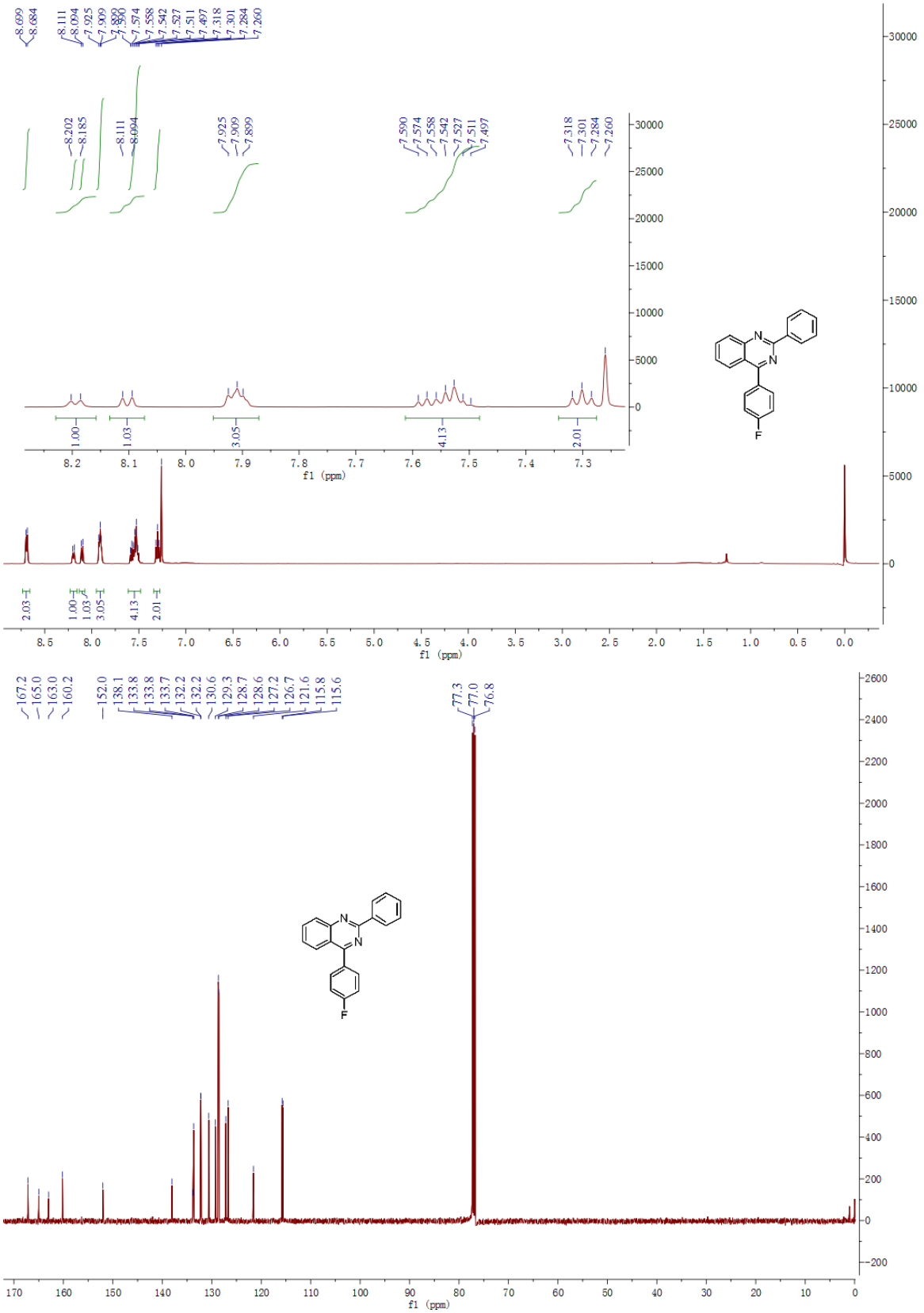


Figure S6. ^{1}H NMR of **3f** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3f** (125 MHz, $CDCl_3$)

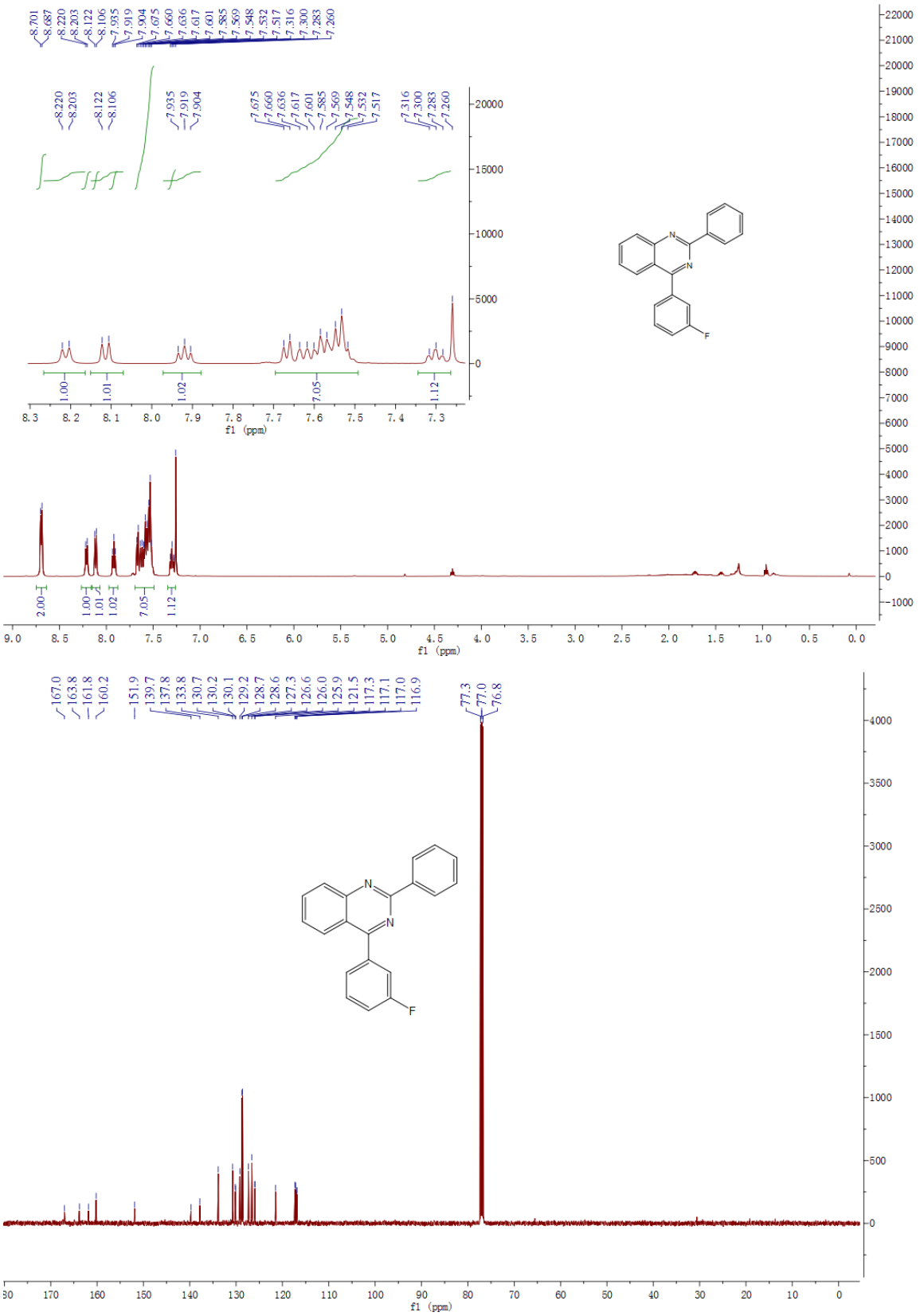


Figure S7. ^{1}H NMR of **3g** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3g** (125 MHz, $CDCl_3$)

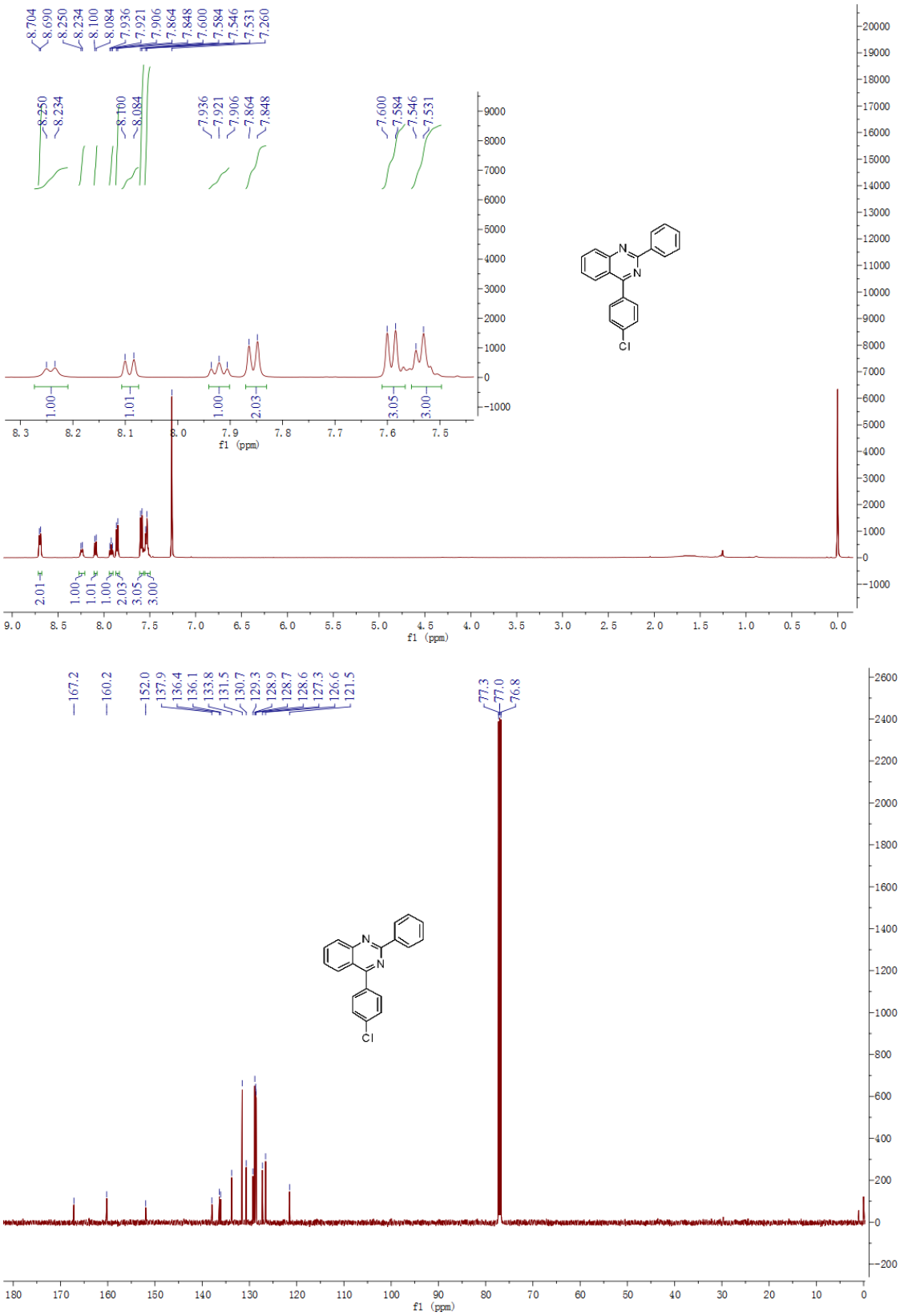


Figure S8. ^{1}H NMR of **3h** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3h** (125 MHz, $CDCl_3$)

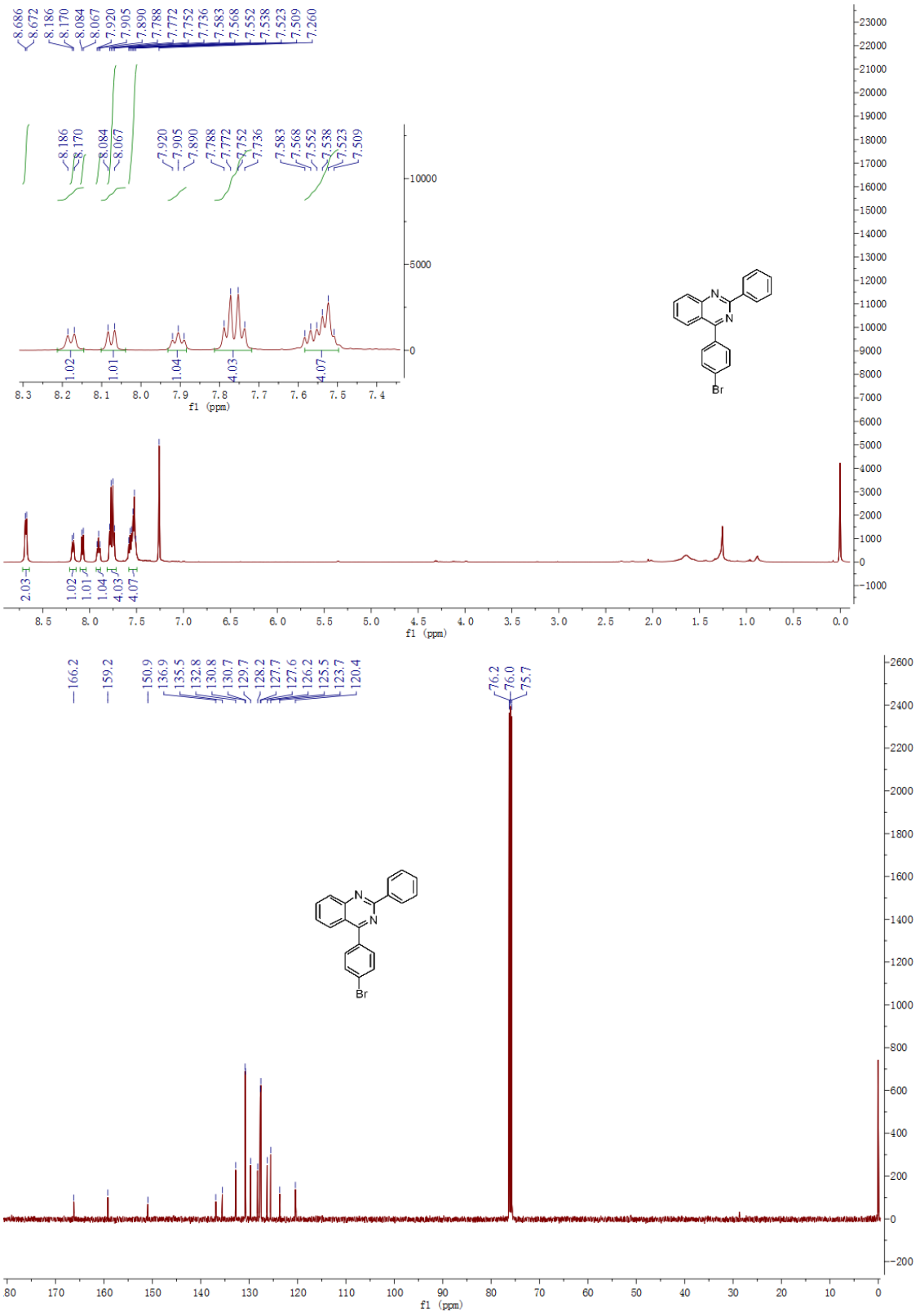


Figure S9. ^{1}H NMR of **3i** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3i** (125 MHz, $CDCl_3$)

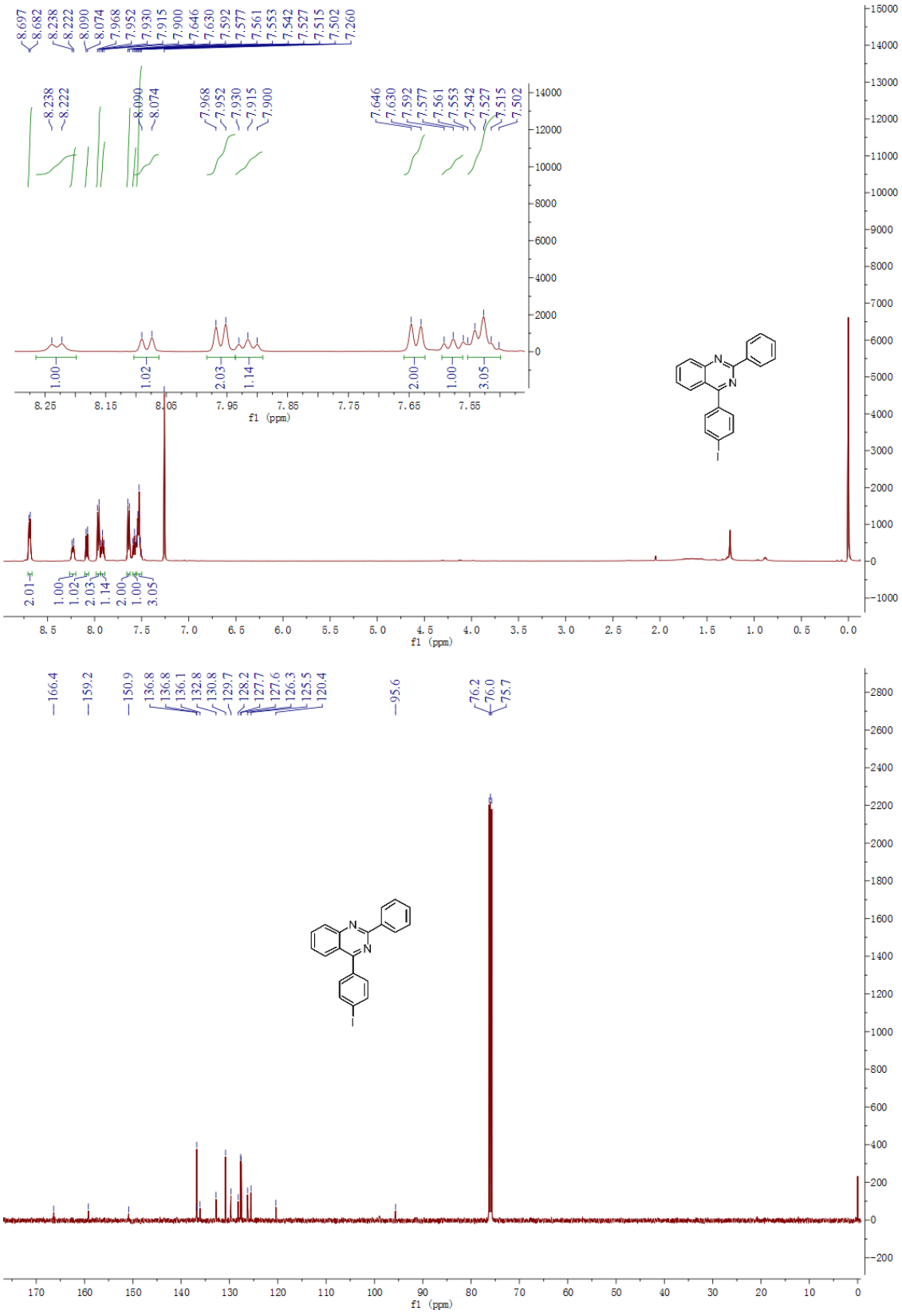


Figure S10. ^{1}H NMR of **3j** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3j** (125 MHz, $CDCl_3$)

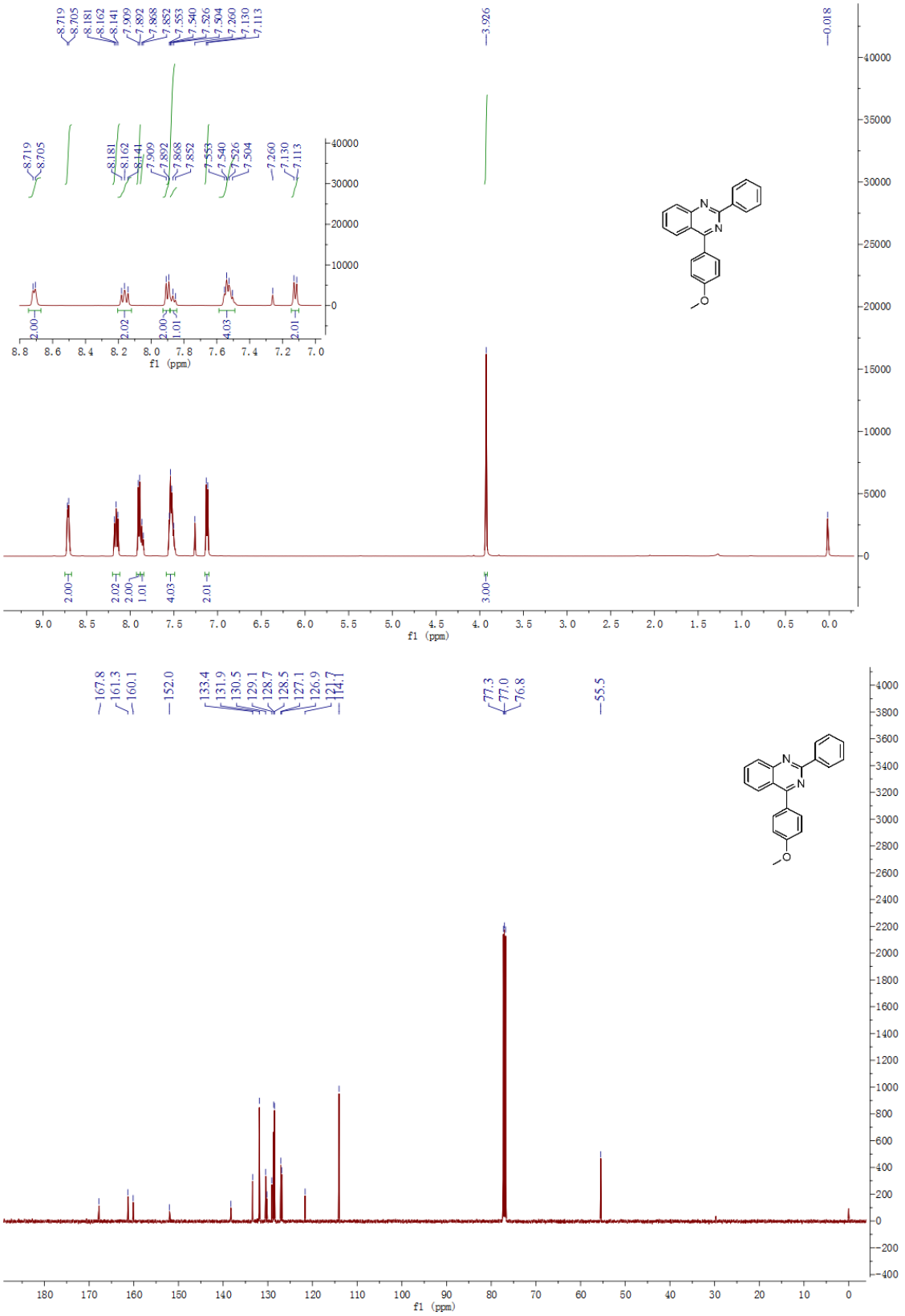


Figure S11. ^{1}H NMR of **3k** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3k** (125 MHz, $CDCl_3$)

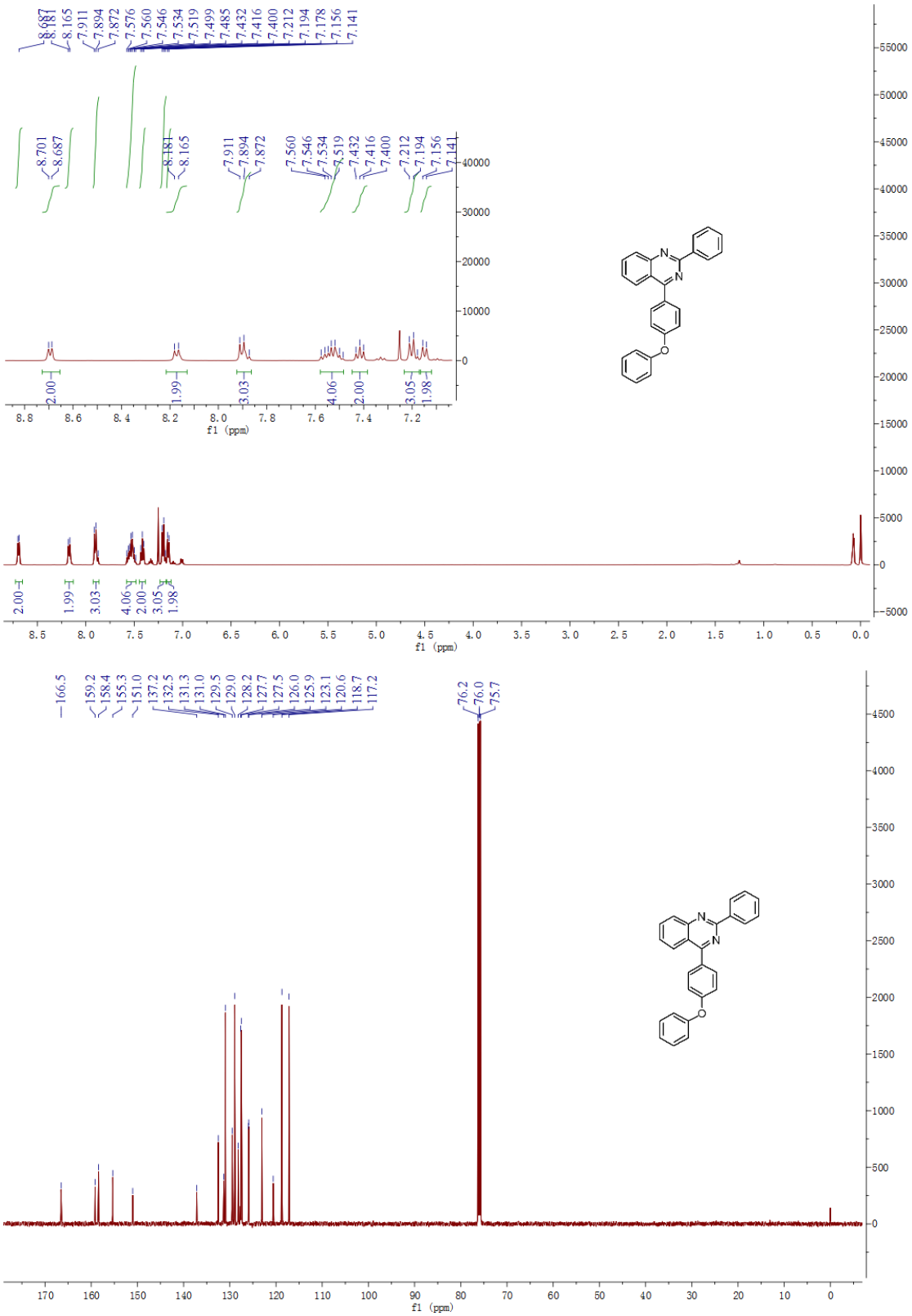


Figure S12. ^{1}H NMR of **3l** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3l** (125 MHz, $CDCl_3$)

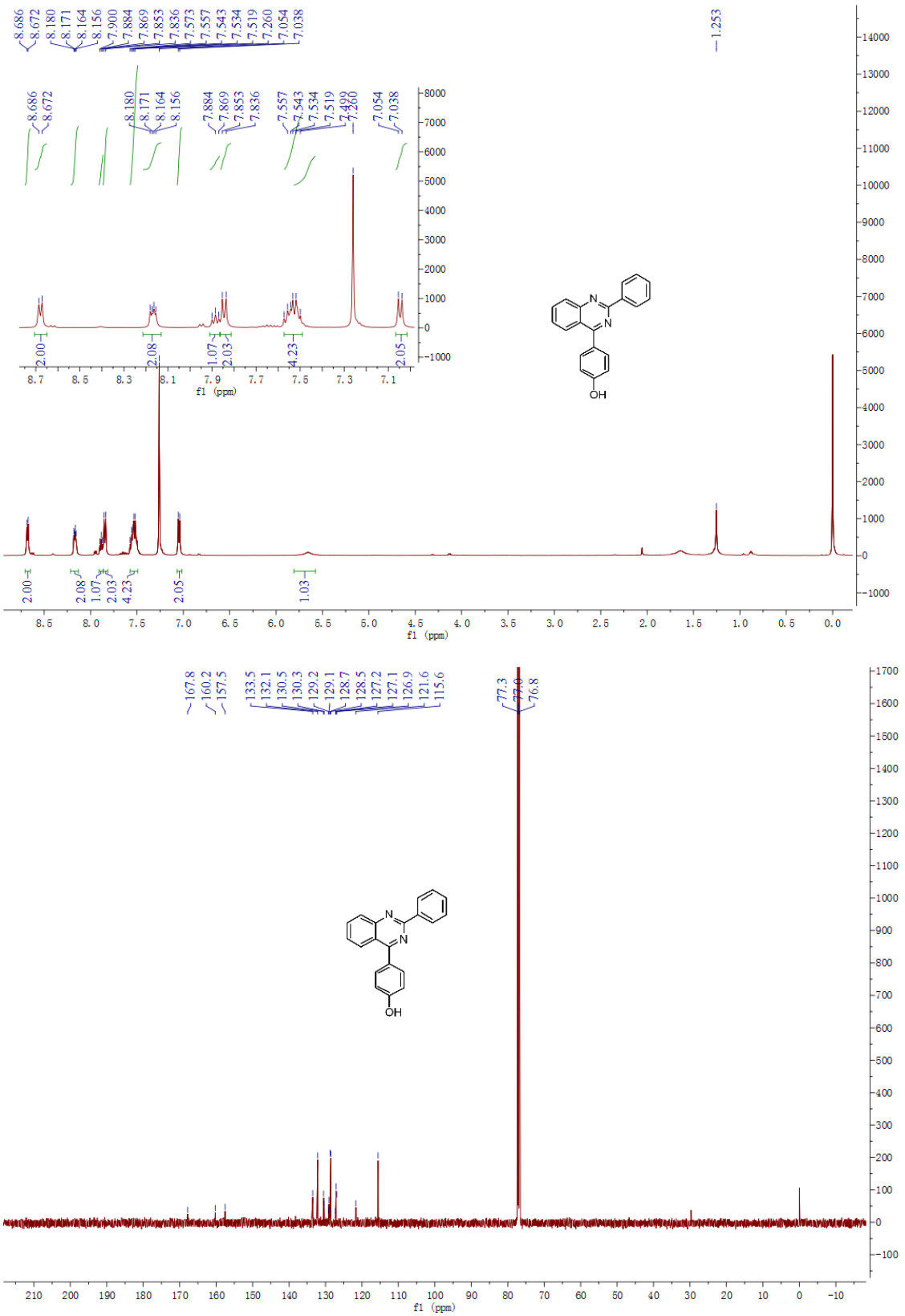


Figure S13. ^{1}H NMR of **3m** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3m** (125 MHz, $CDCl_3$)

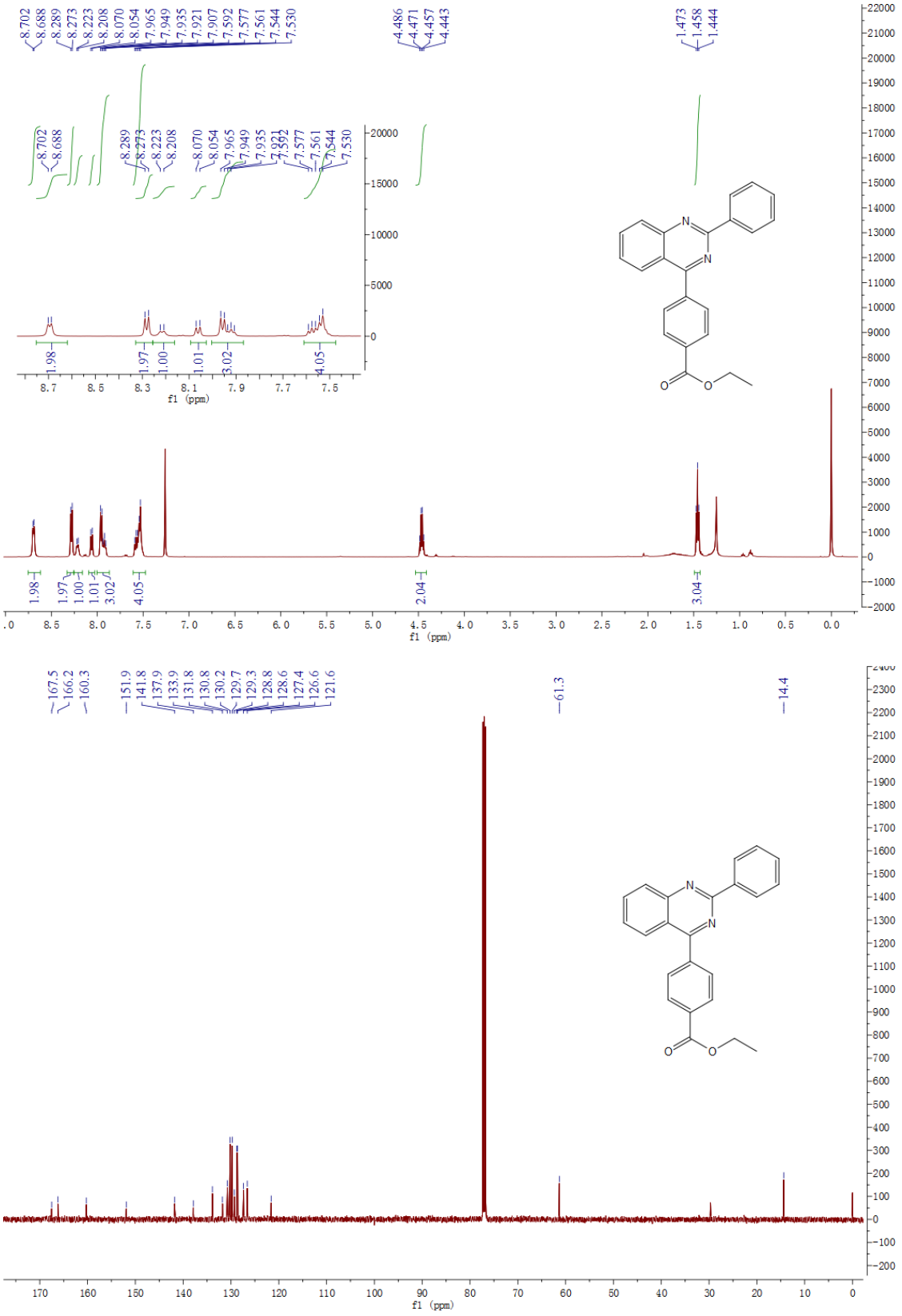


Figure S14. ^{1}H NMR of **3n** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3n** (125 MHz, $CDCl_3$)

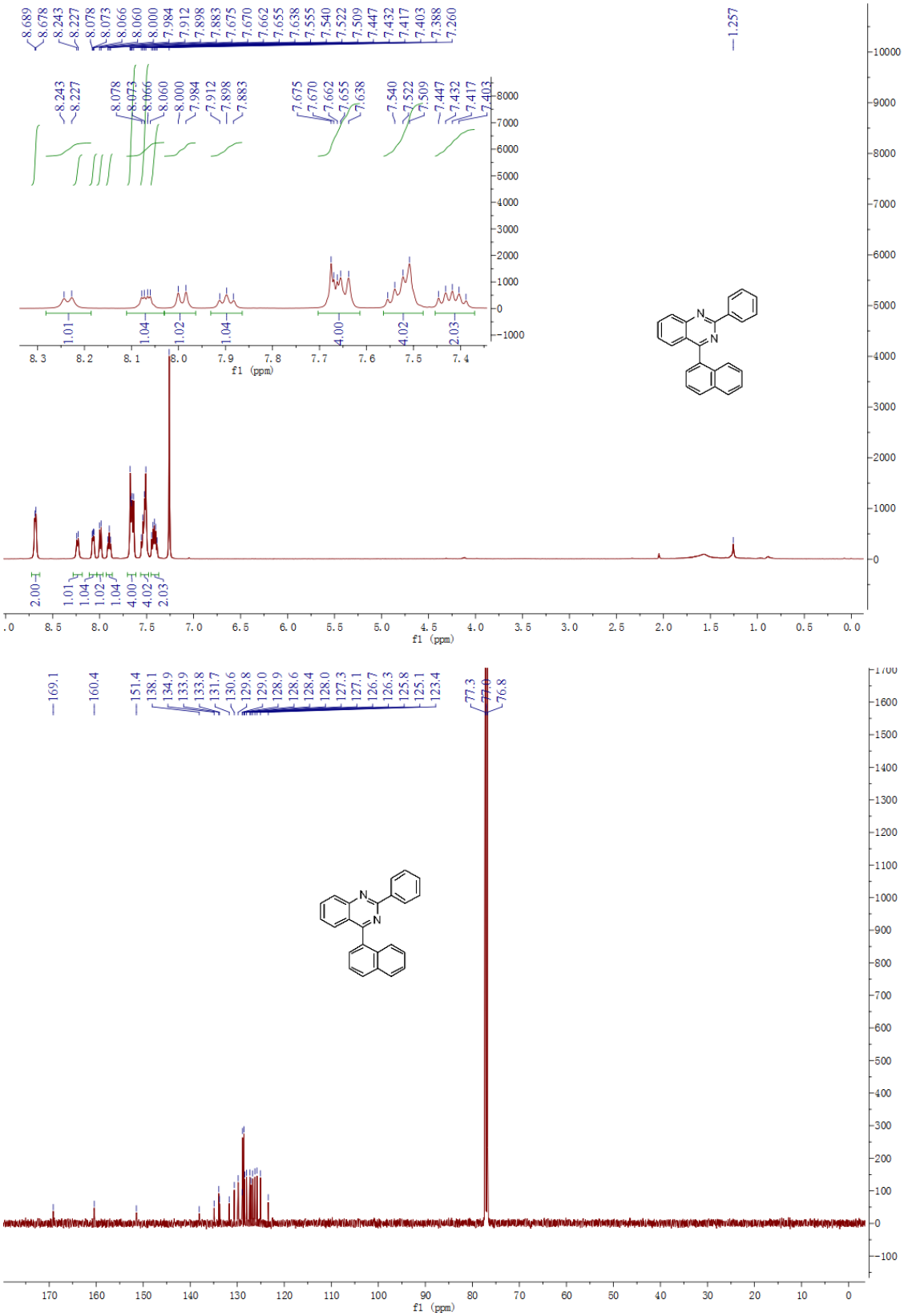


Figure S15. ^{1}H NMR of **3p** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3p** (125 MHz, $CDCl_3$)

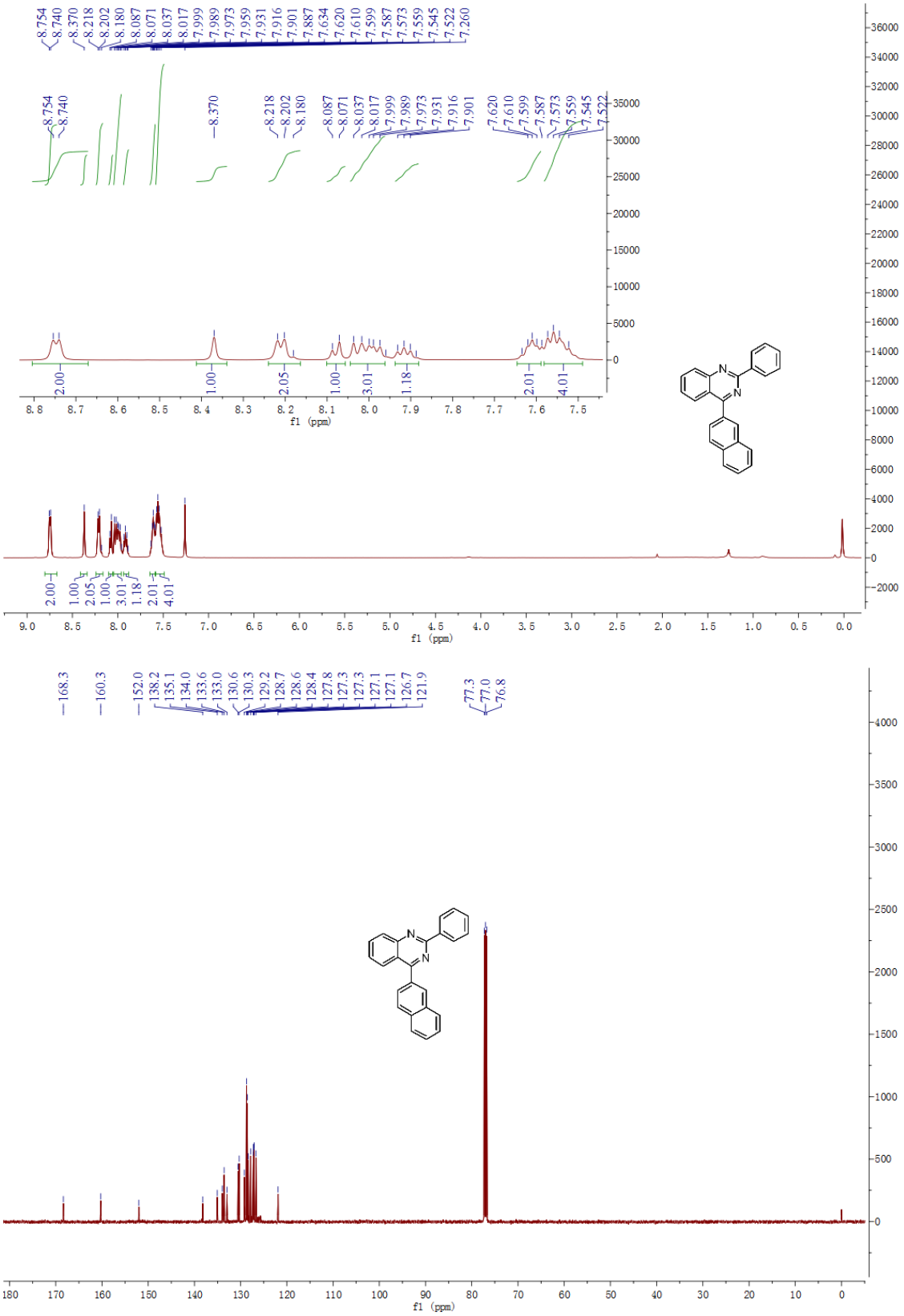


Figure S16. ^{1}H NMR of **3q** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3q** (125 MHz, $CDCl_3$)

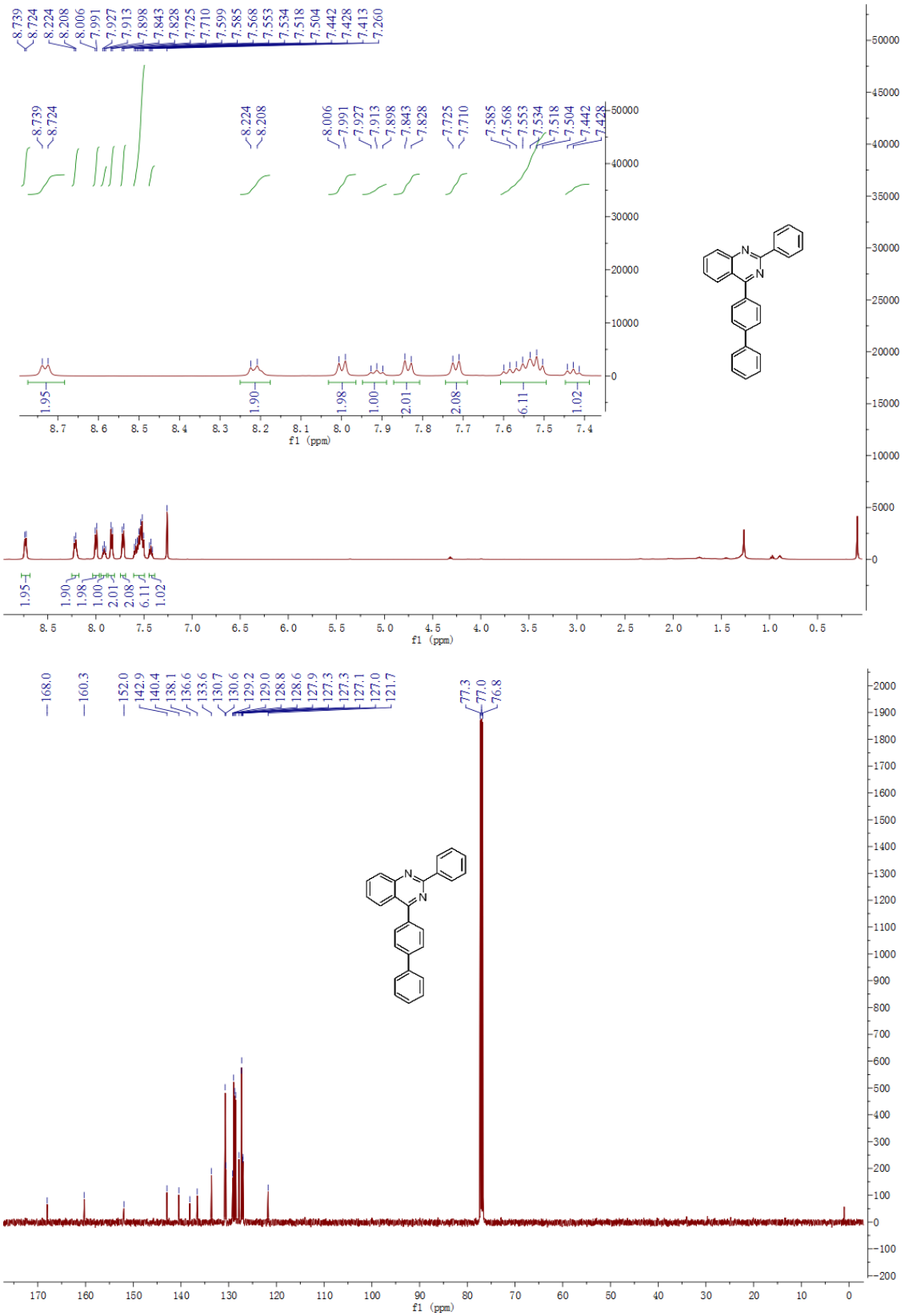


Figure S17. ^{1}H NMR of **3r** (500 MHz, $CDCl_3$) and ^{13}C NMR of **3r** (125 MHz, $CDCl_3$)

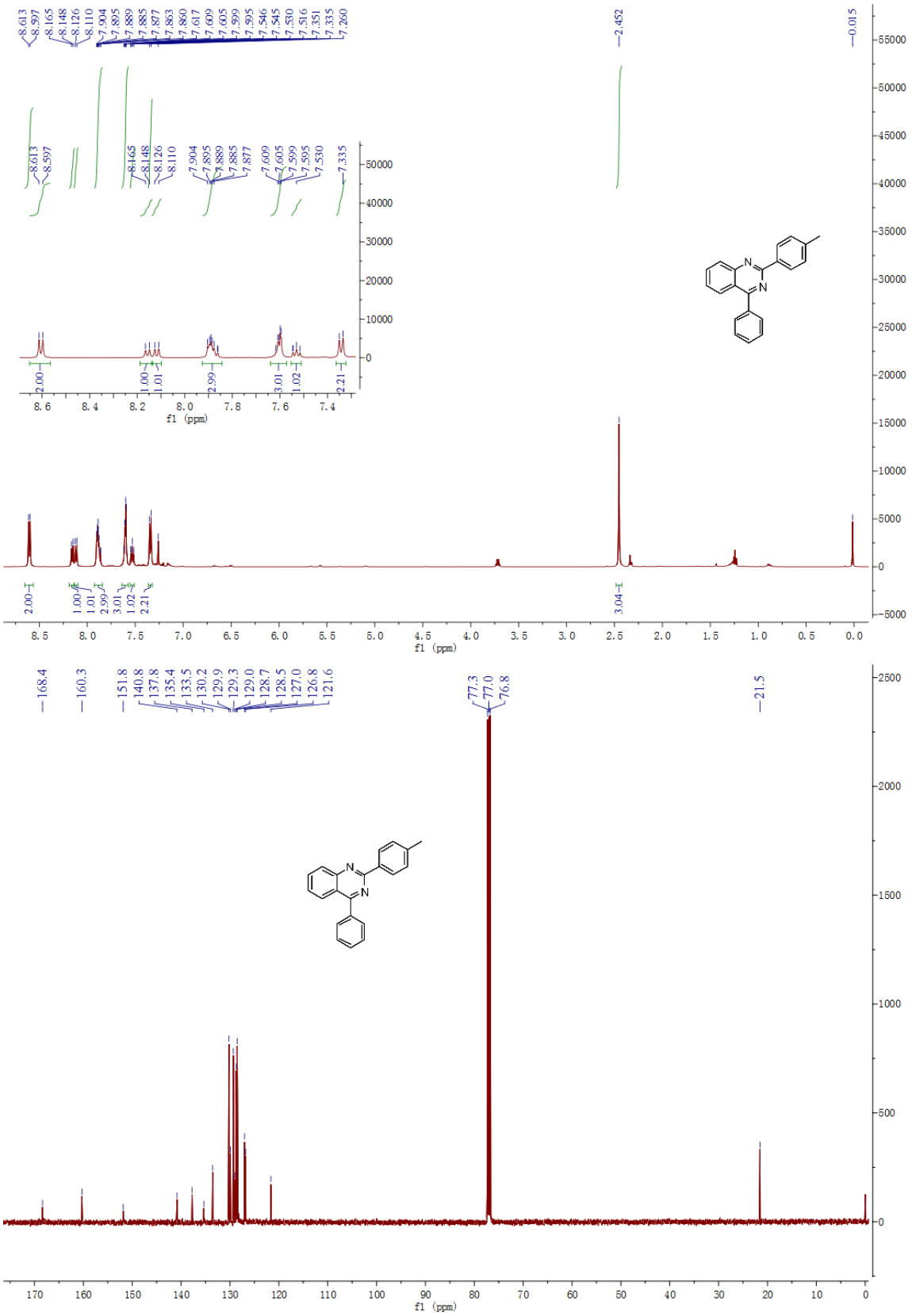


Figure S18. ^{1}H NMR of **4a** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4a** (125 MHz, $CDCl_3$)

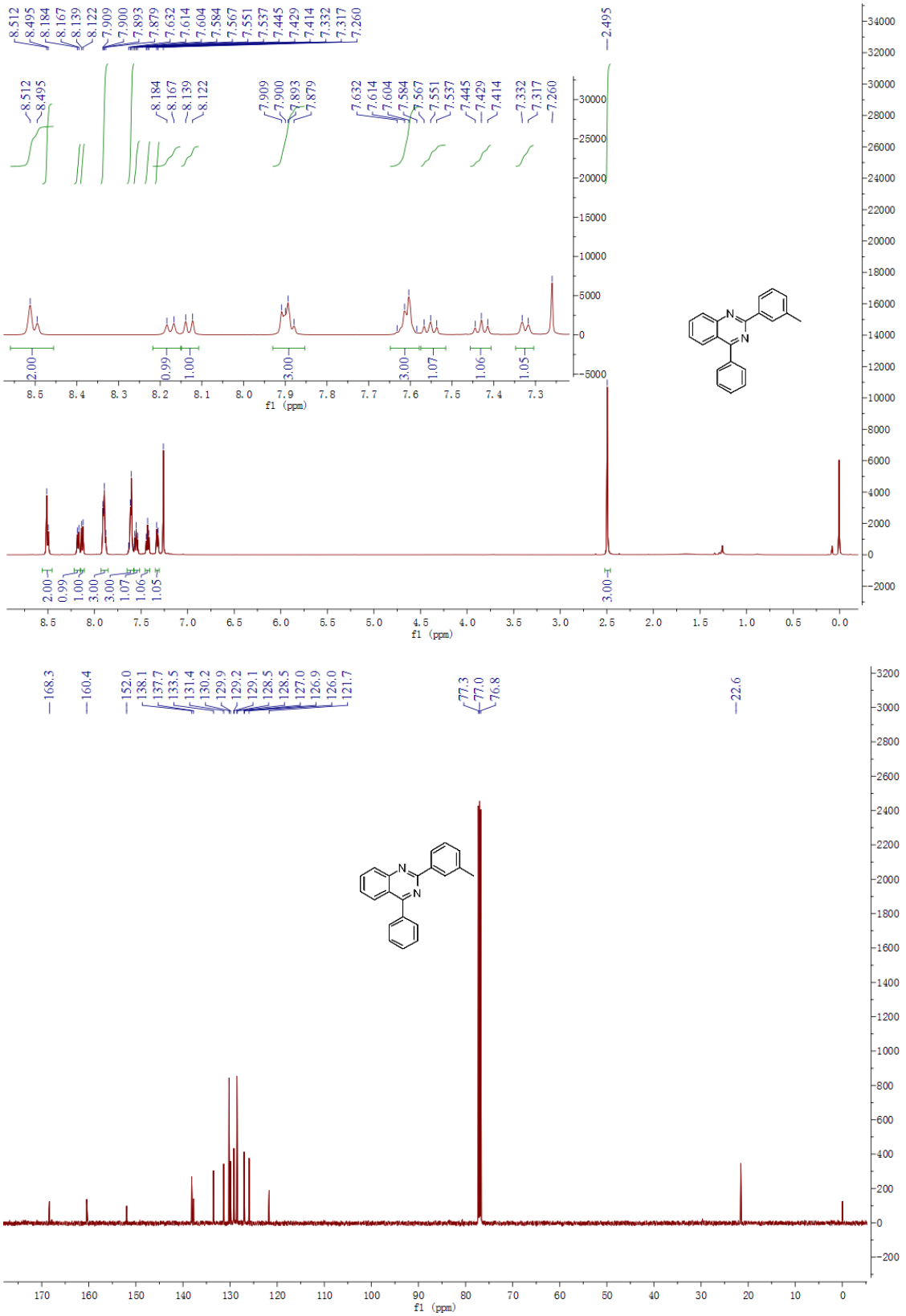


Figure S19. ^{1}H NMR of **4b** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4b** (125 MHz, $CDCl_3$)

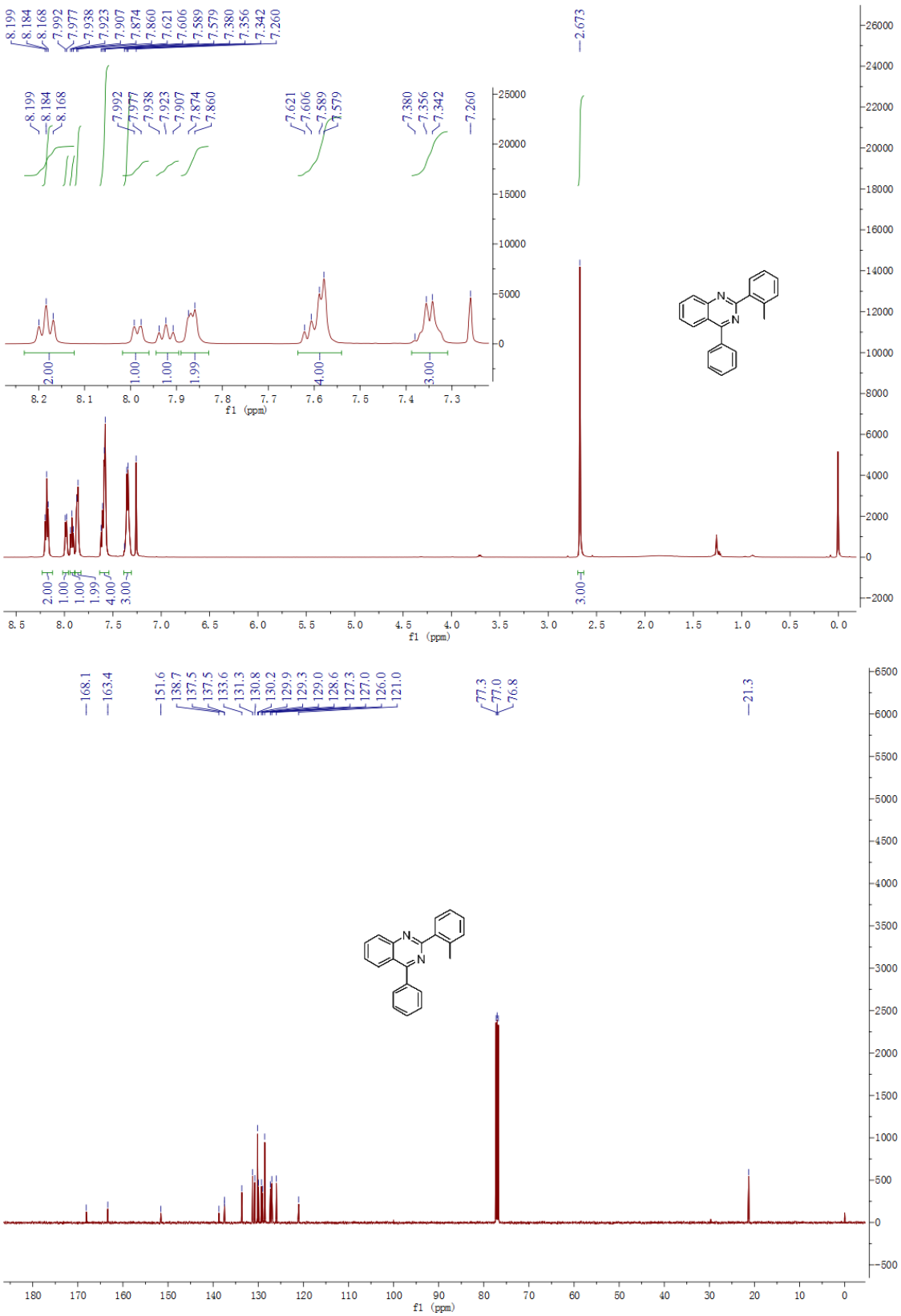


Figure S20. ^{1}H NMR of **4c** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4c** (125 MHz, $CDCl_3$)

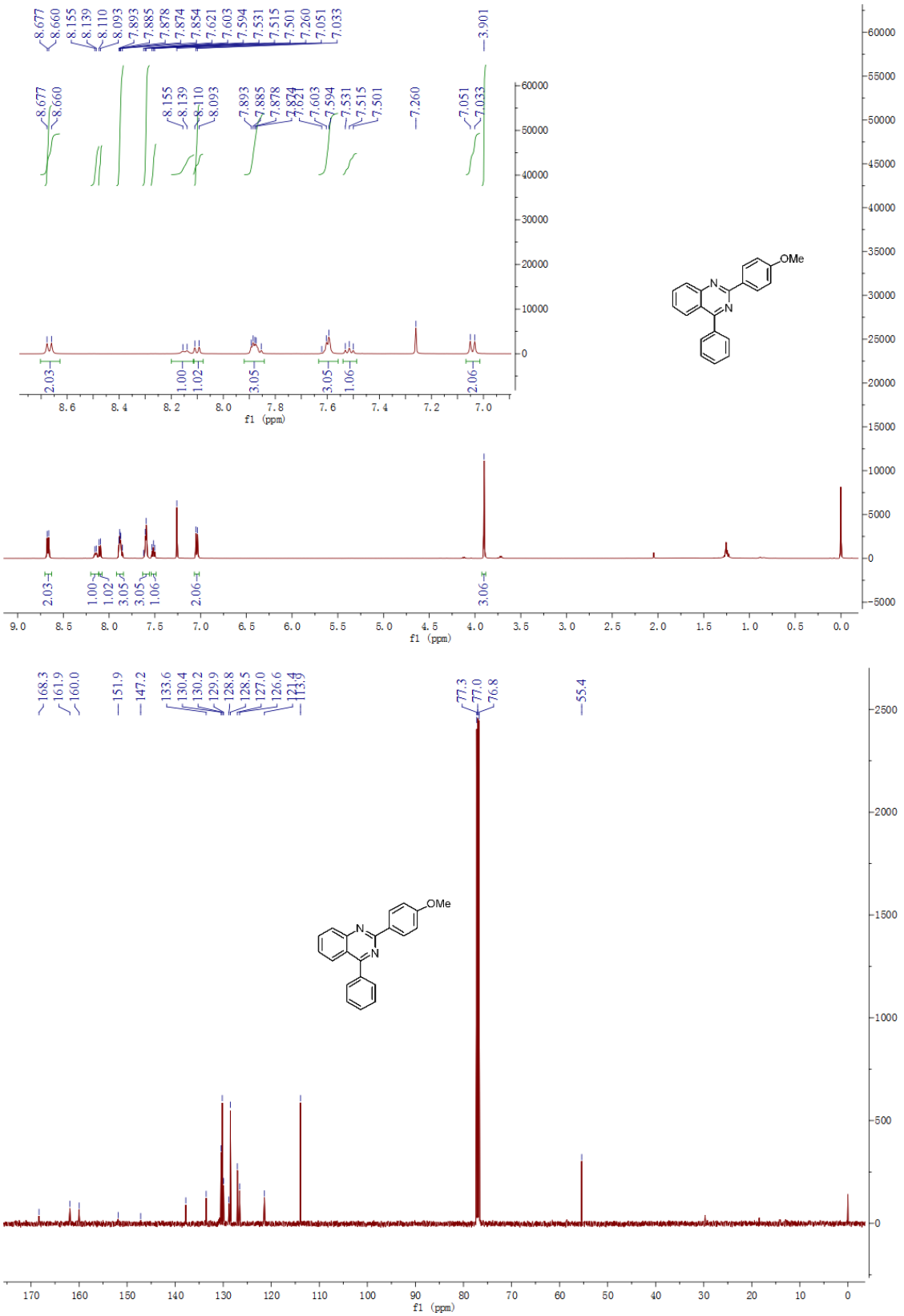


Figure S21. ^{1}H NMR of **4d** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4d** (125 MHz, $CDCl_3$)

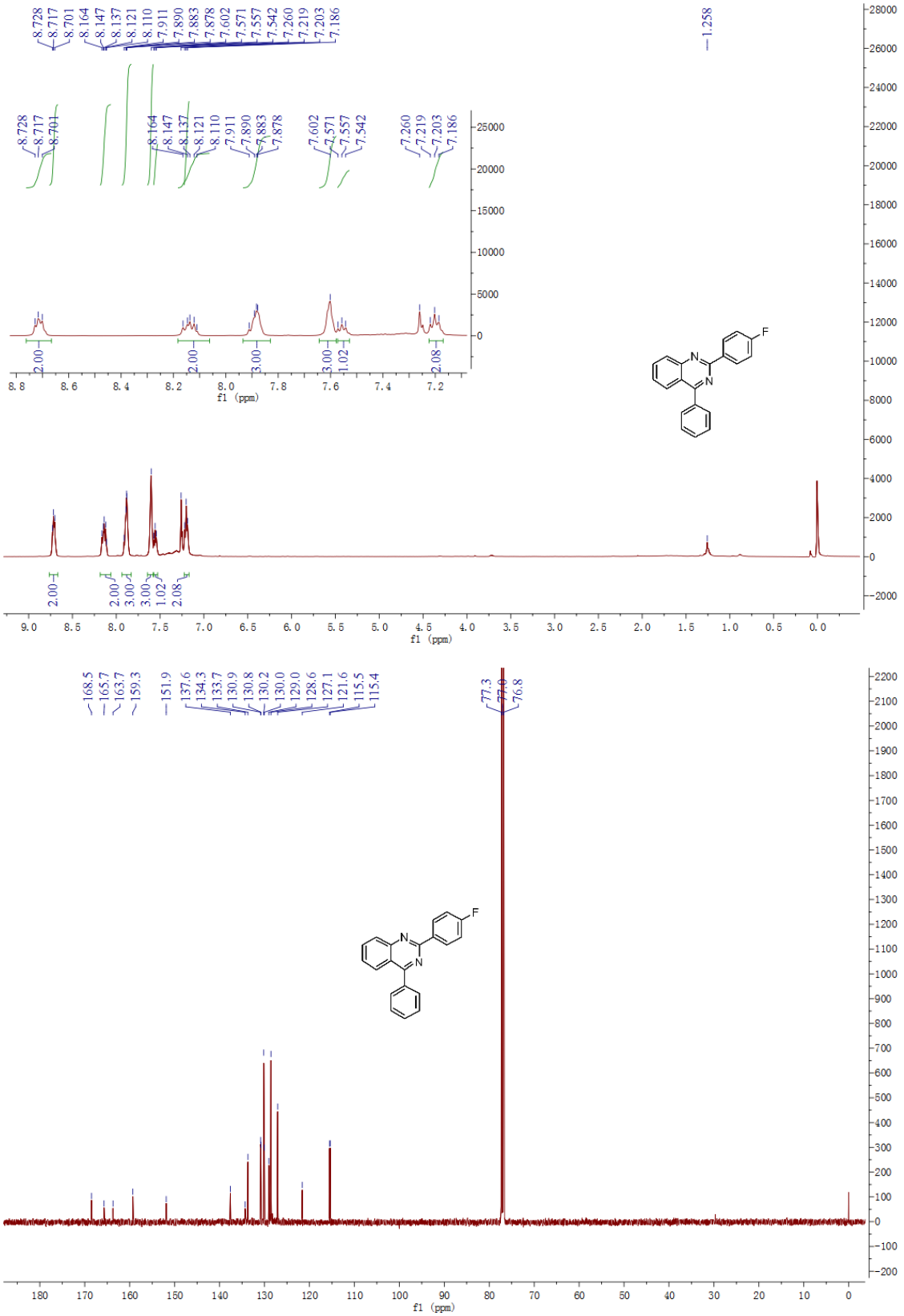


Figure S22. ^{1}H NMR of **4e** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4e** (125 MHz, $CDCl_3$)

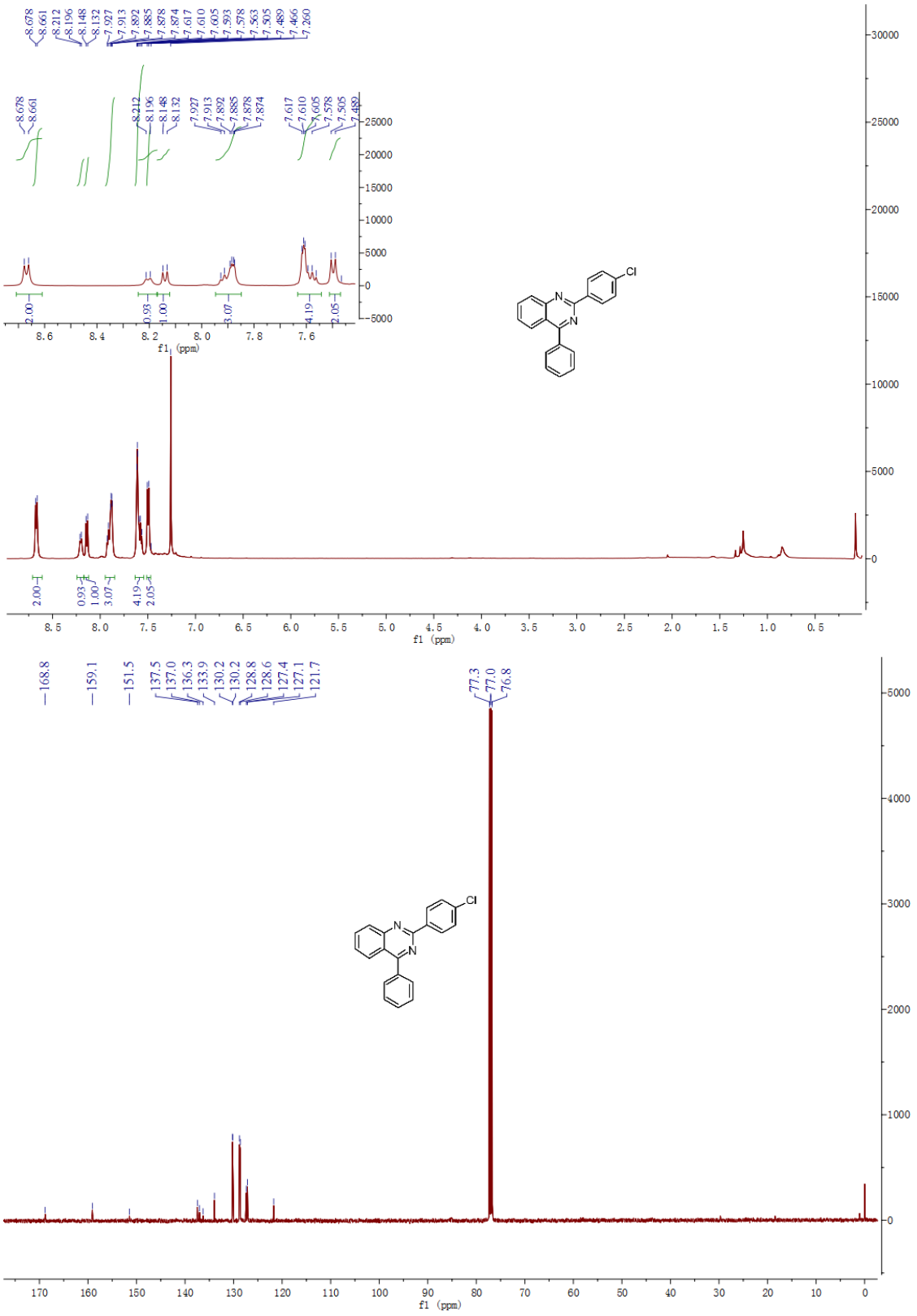


Figure S23. ^{1}H NMR of **4f** (500 MHz, , $CDCl_3$) and ^{13}C NMR of **4f** (125 MHz, , $CDCl_3$)

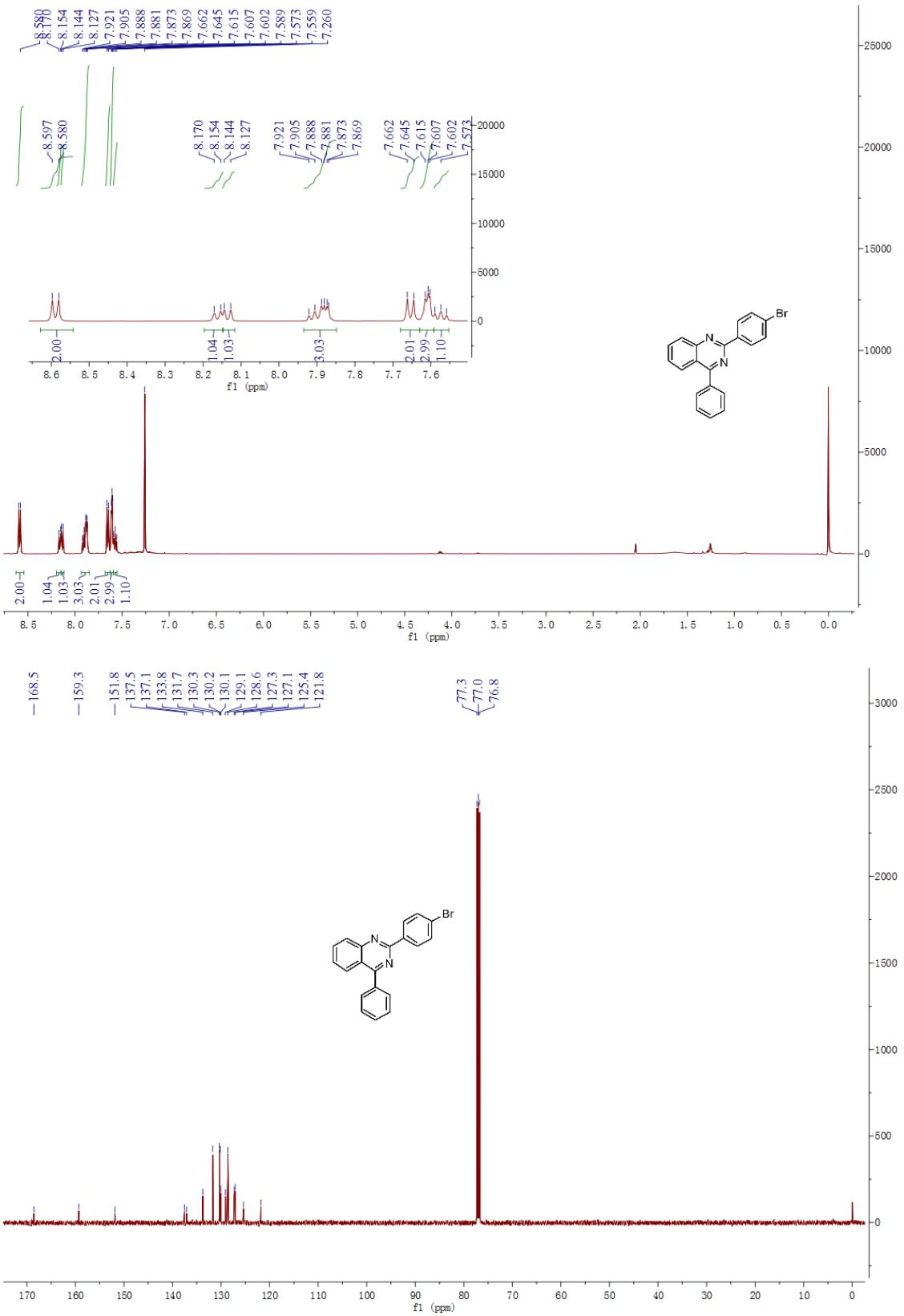


Figure S24. ^{1}H NMR of **4g** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4g** (125 MHz, $CDCl_3$)

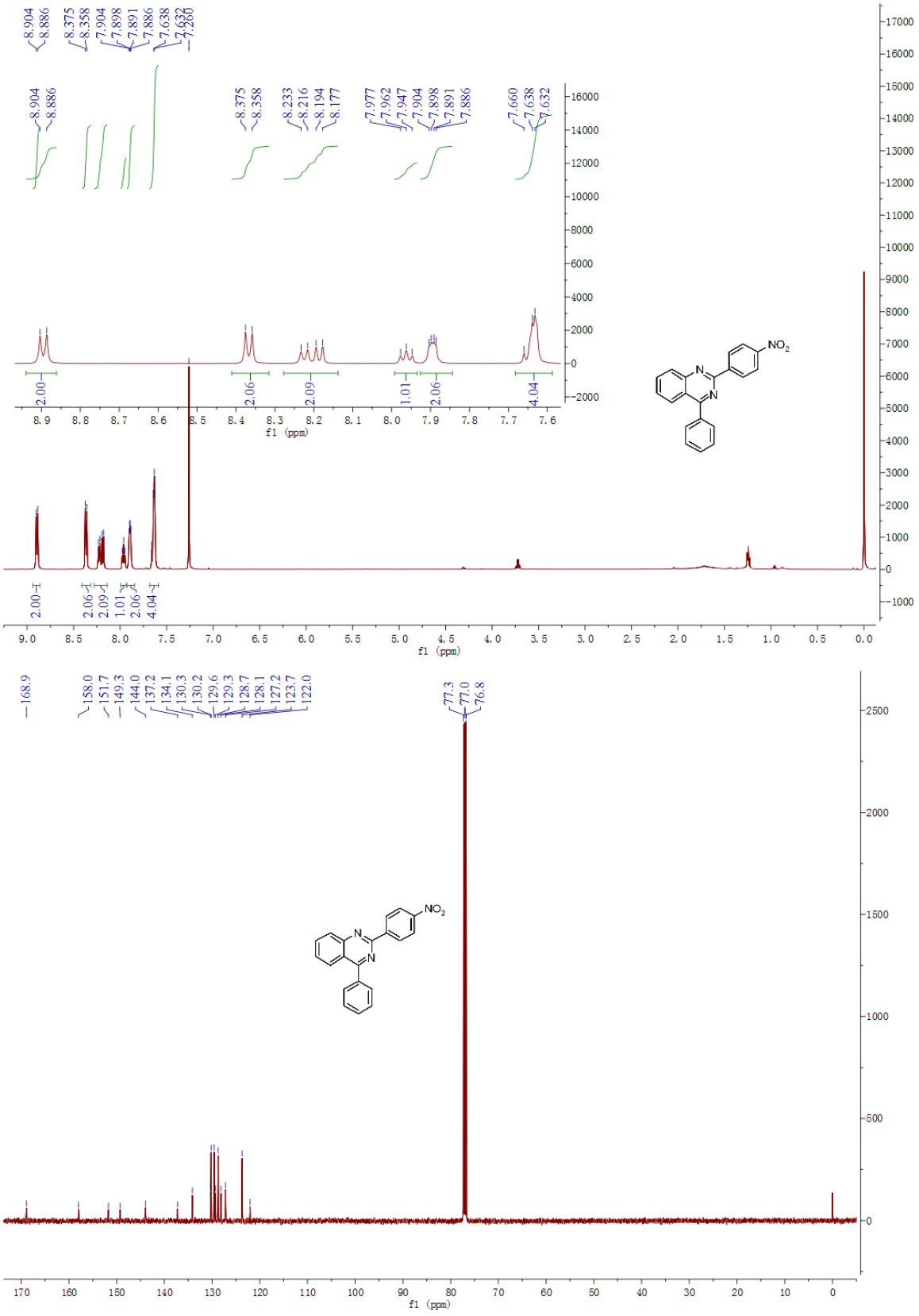


Figure S25. ^{1}H NMR of **4h** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4h** (125 MHz, $CDCl_3$)

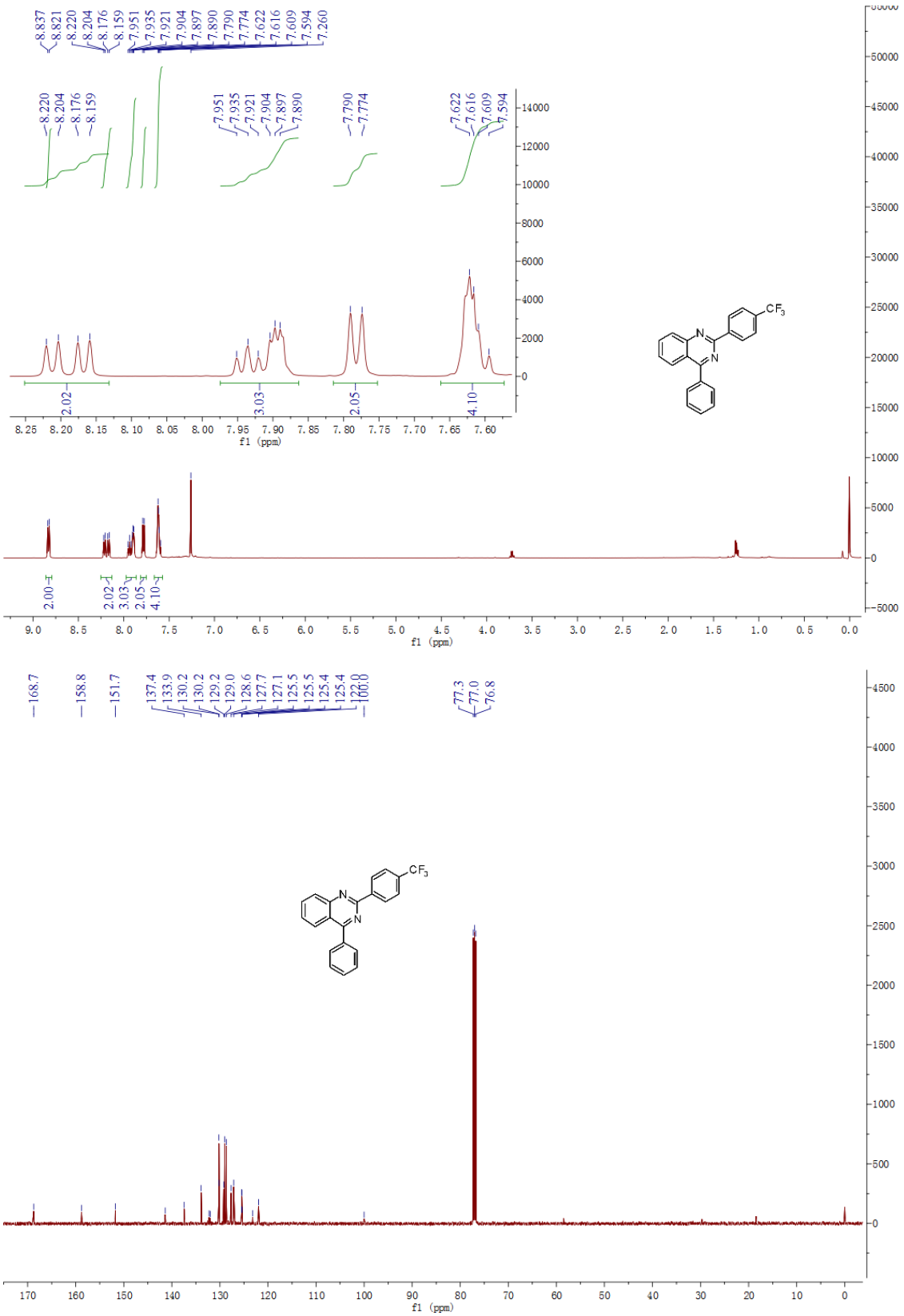


Figure S26. ^{1}H NMR of **4i** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4i** (125 MHz, $CDCl_3$)

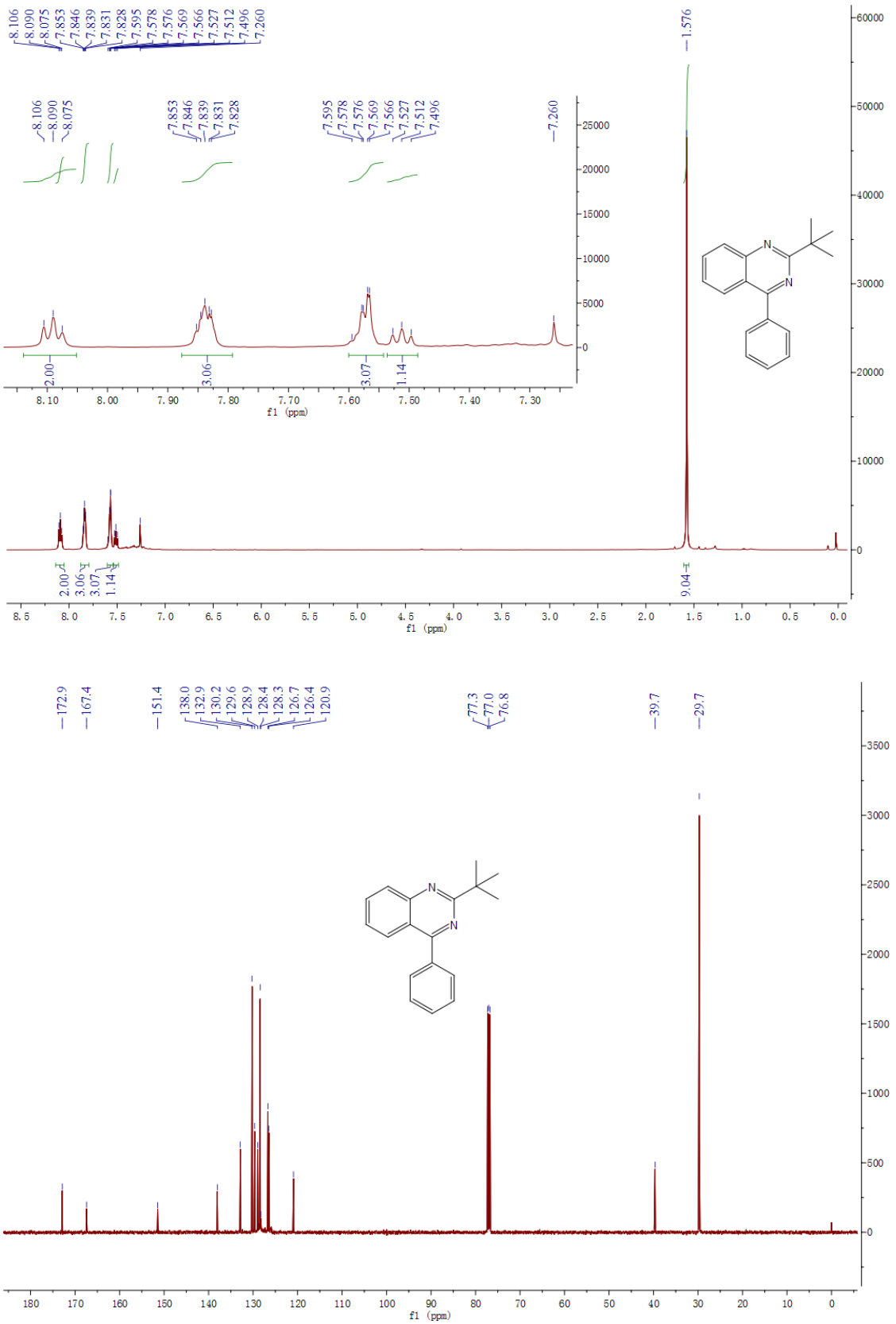


Figure S27. ^{1}H NMR of **4j** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4j** (125 MHz, $CDCl_3$)

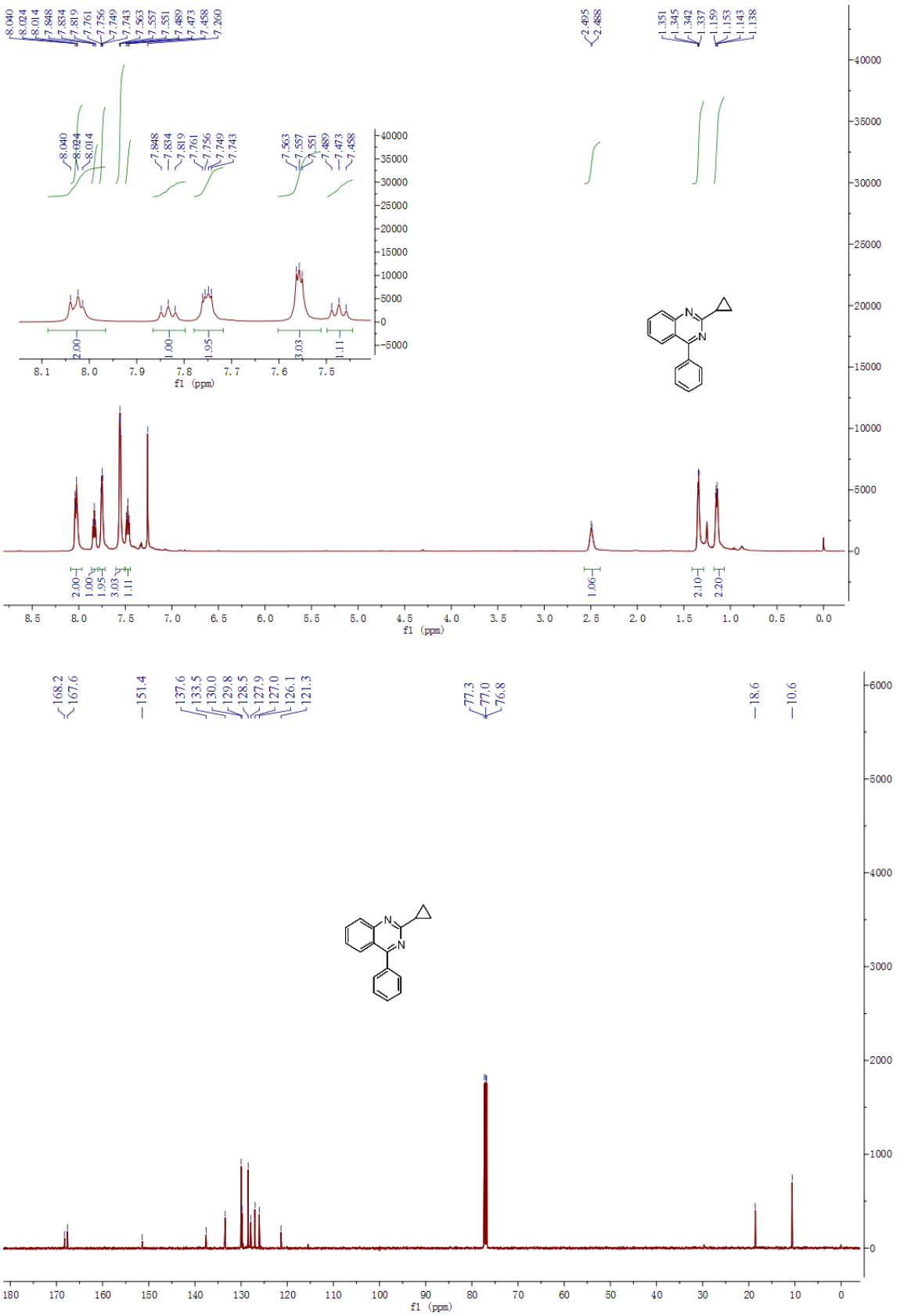


Figure S28. ^{1}H NMR of **4k** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4k** (125 MHz, $CDCl_3$)

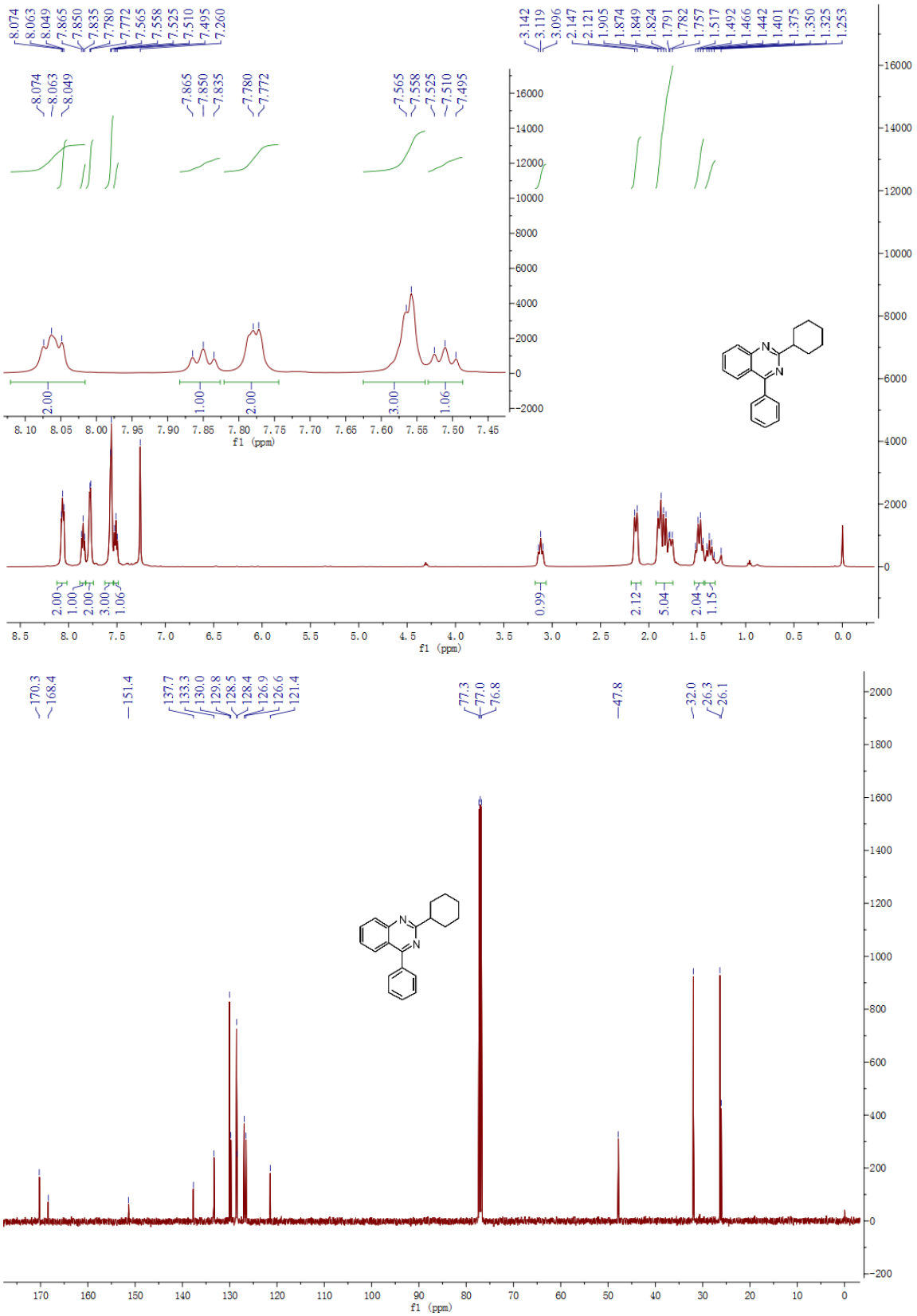


Figure S29. ^{1}H NMR of **4l** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4l** (125 MHz, $CDCl_3$)

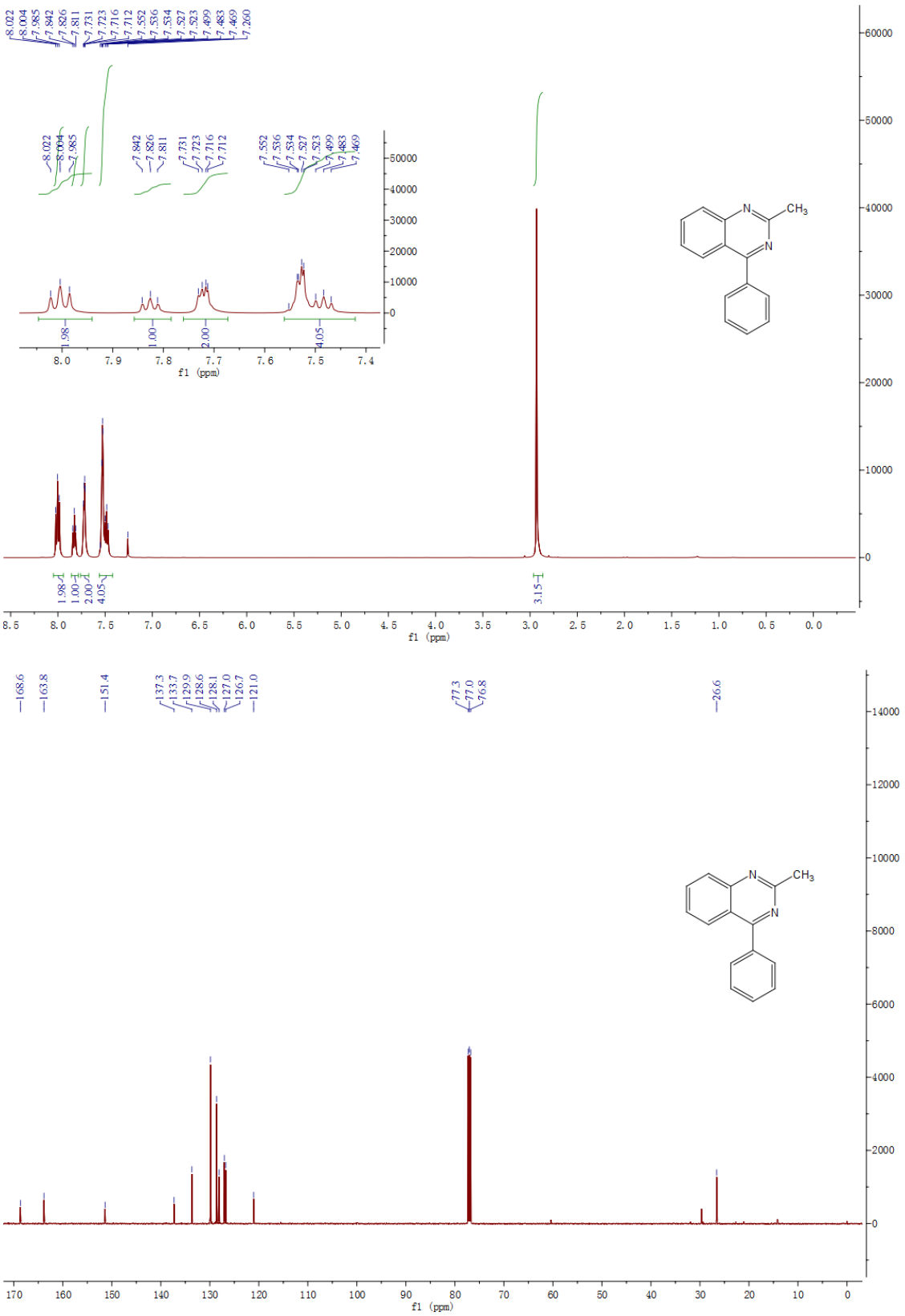


Figure S30. ^{1}H NMR of **4m** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4m** (125 MHz, $CDCl_3$)

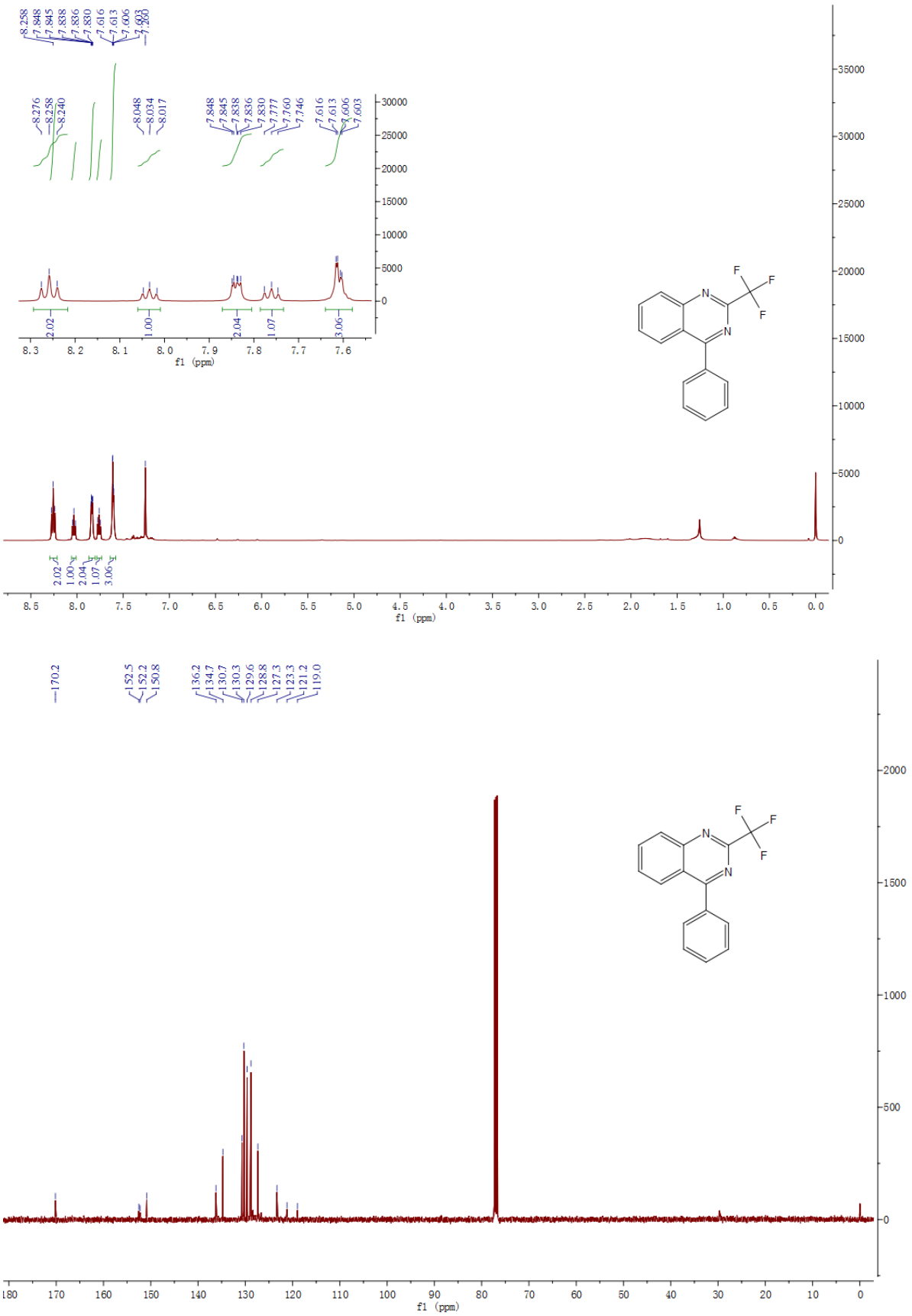


Figure S31. ^{1}H NMR of **4n** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4n** (125 MHz, $CDCl_3$)

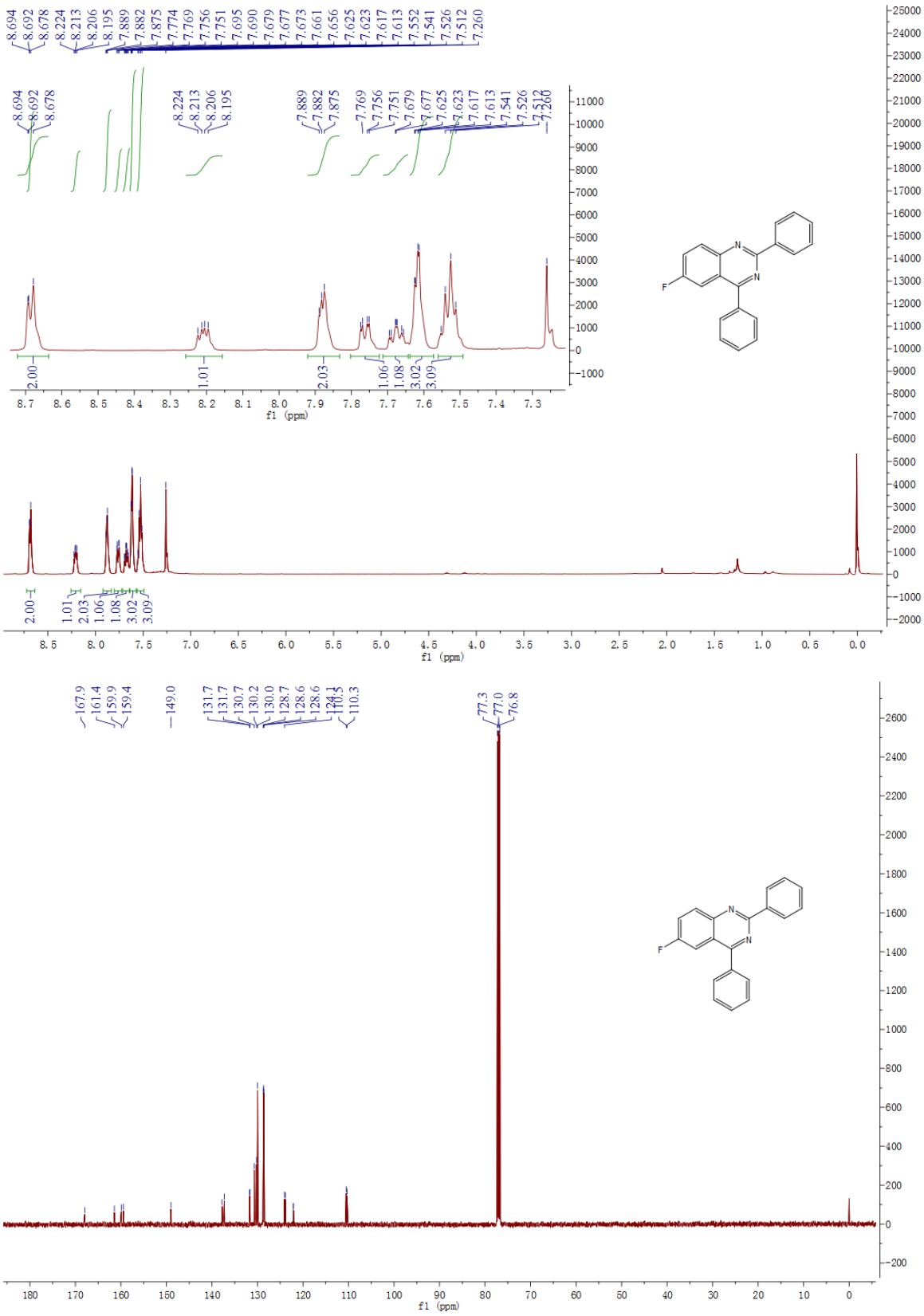


Figure S32. ^{1}H NMR of **4o** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4o** (125 MHz, $CDCl_3$)

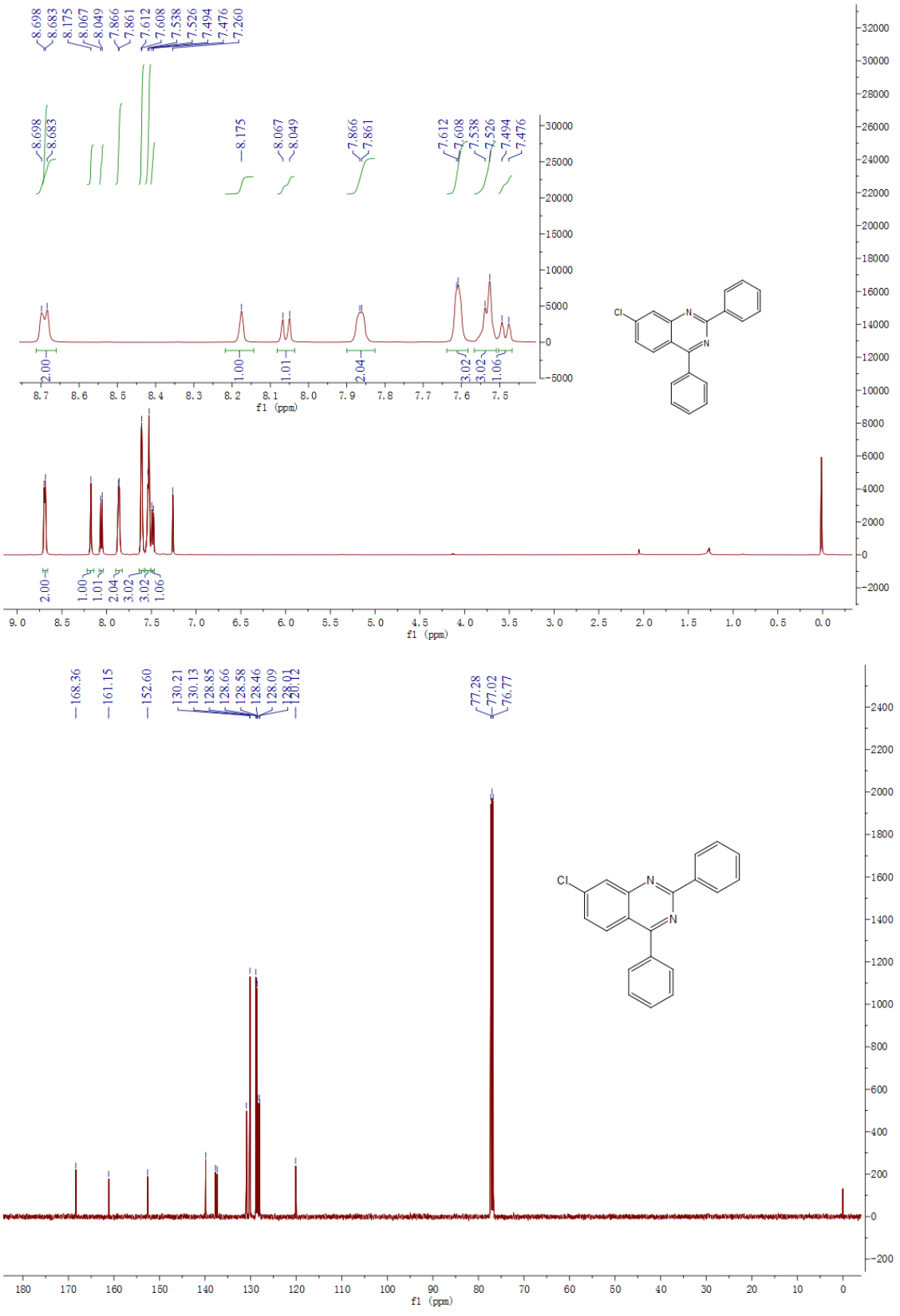


Figure S33. ^{1}H NMR of **4p** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4p** (125 MHz, $CDCl_3$)

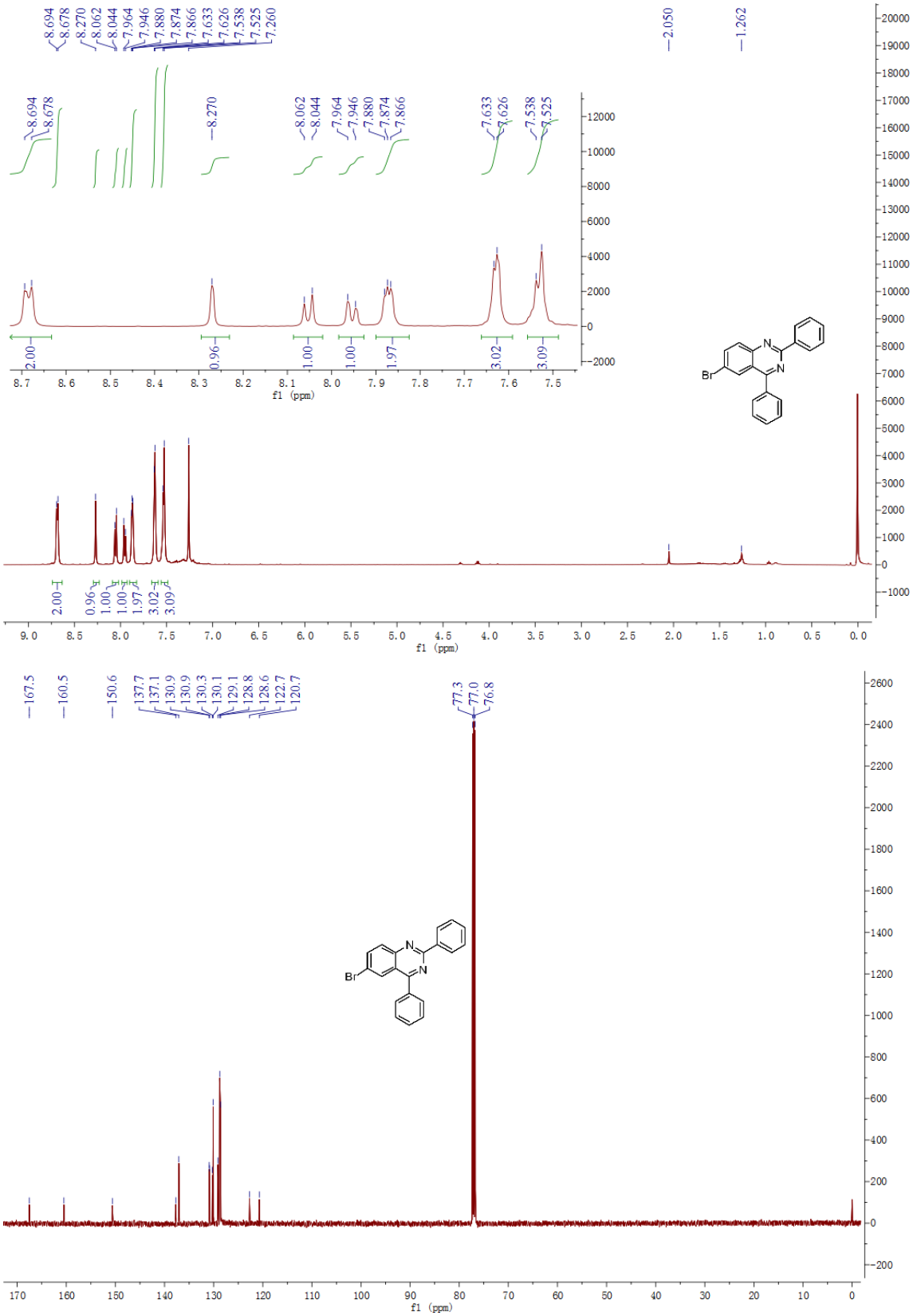


Figure S34. ^{1}H NMR of **4q** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4q** (125 MHz, $CDCl_3$)

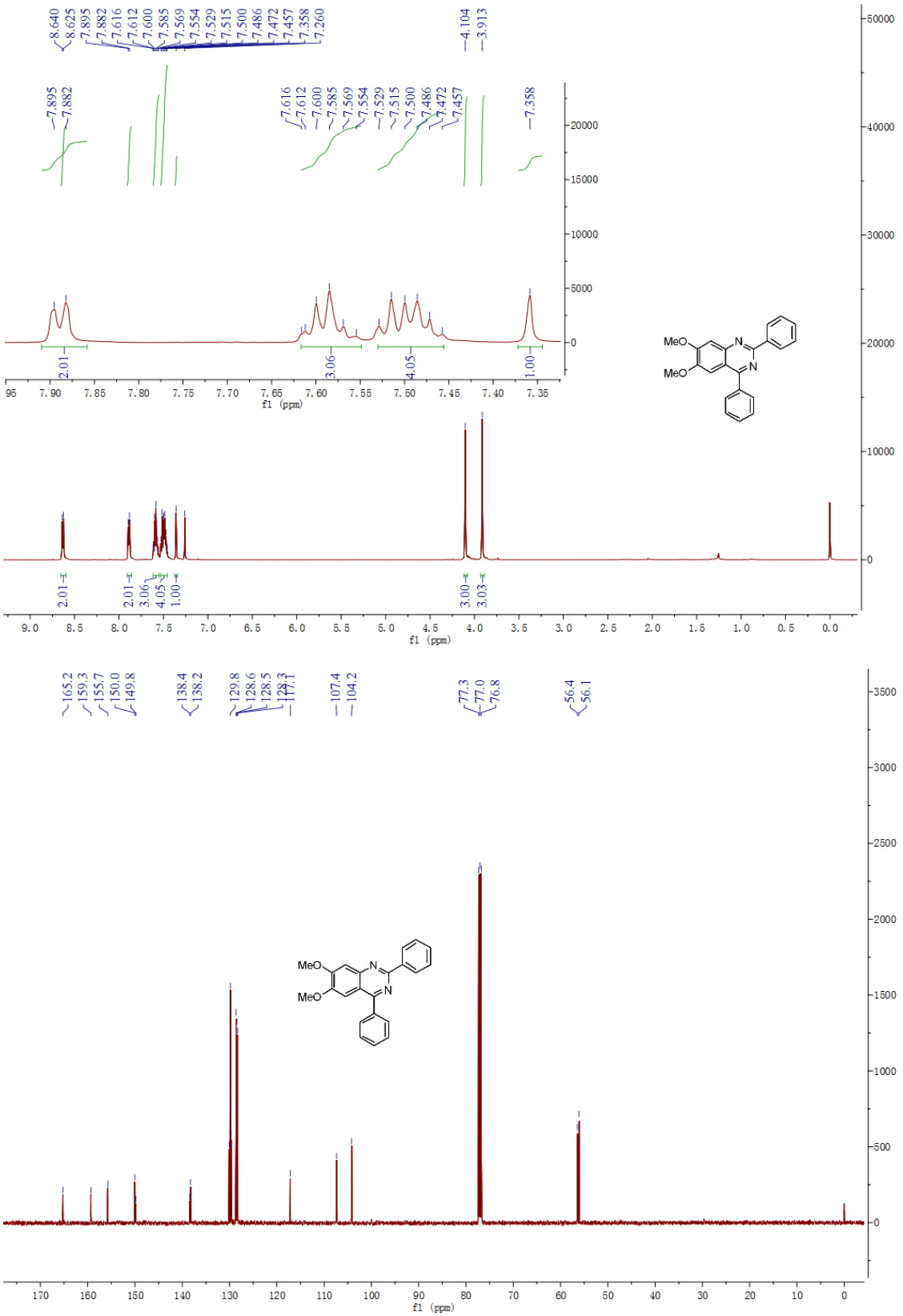


Figure S35. ^{1}H NMR of **4r** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4r** (125 MHz, $CDCl_3$)

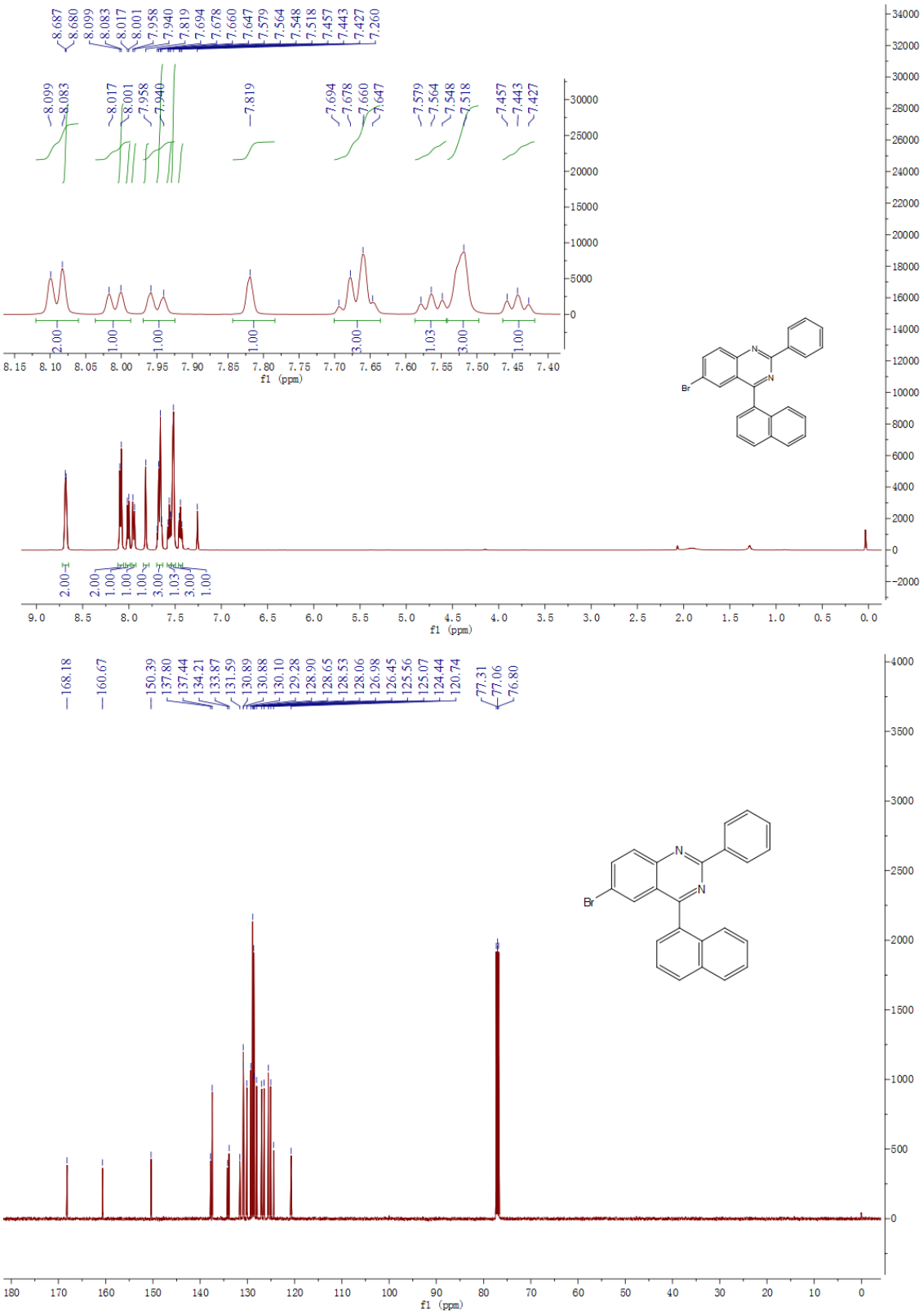


Figure S36. ^{1}H NMR of **4t** (500 MHz, $CDCl_3$) and ^{13}C NMR of **4t** (125 MHz, $CDCl_3$)